



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 07:45 AM EST

PDB ID : 6DG1
BMRB ID : 30469
Title : NMR structure of the second qRRM2 domain of human hnRNP H
Authors : Srinivasa, R.P.
Deposited on : 2018-05-16

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 : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

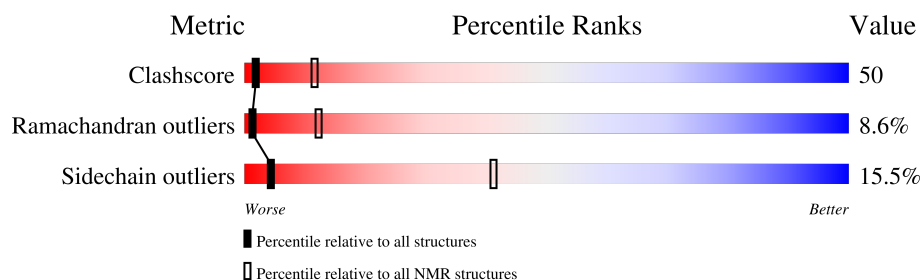
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 75%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	105	<div> <div></div> <div>26%</div> <div>52%</div> <div>11%</div> <div>10%</div> </div>

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 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:91-A:99, A:110-A:194 (94)	0.81	5

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

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

The models can be grouped into 2 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1657 atoms, of which 825 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called qRRM2 domain of Heterogeneous nuclear ribonucleoprotein H2.

Mol	Chain	Residues	Atoms						Trace
1	A	105	Total	C	H	N	O	S	0
			1657	526	825	150	154	2	

There are 5 discrepancies between the modelled and reference sequences:

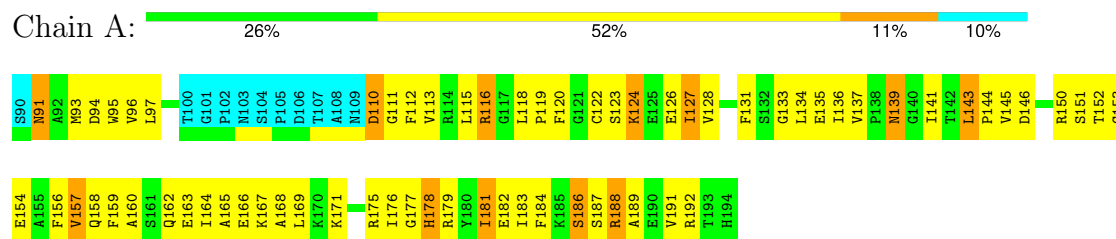
Chain	Residue	Modelled	Actual	Comment	Reference
A	90	SER	-	expression tag	UNP P55795
A	91	ASN	-	expression tag	UNP P55795
A	92	ALA	-	expression tag	UNP P55795
A	93	MET	-	expression tag	UNP P55795
A	141	ILE	MET	conflict	UNP P55795

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: qRRM2 domain of Heterogeneous nuclear ribonucleoprotein H2

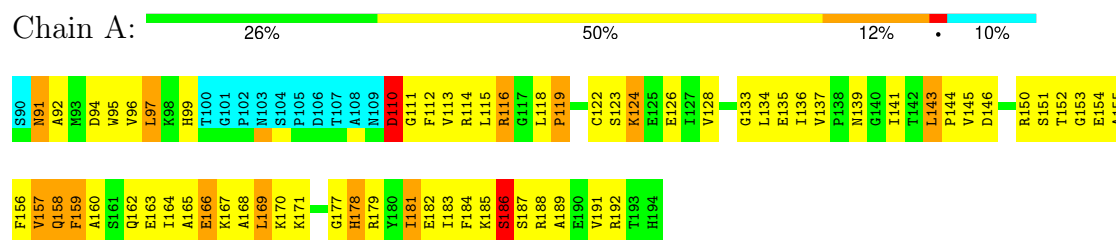


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

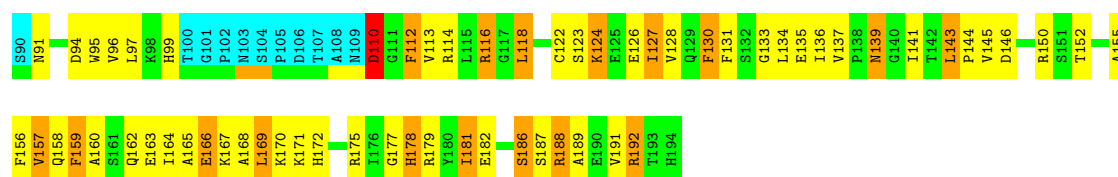
- Molecule 1: qRRM2 domain of Heterogeneous nuclear ribonucleoprotein H2



4.2.2 Score per residue for model 2

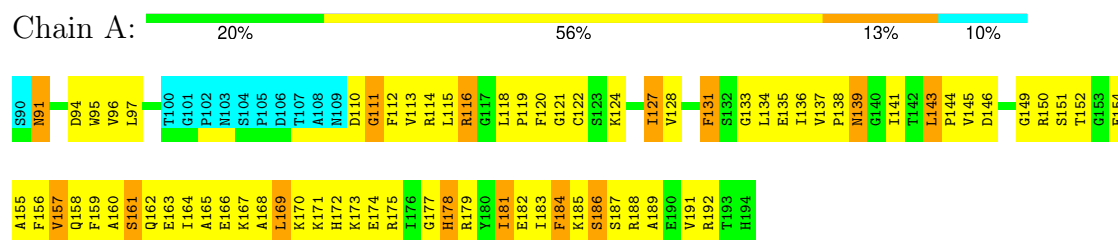
- Molecule 1: qRRM2 domain of Heterogeneous nuclear ribonucleoprotein H2





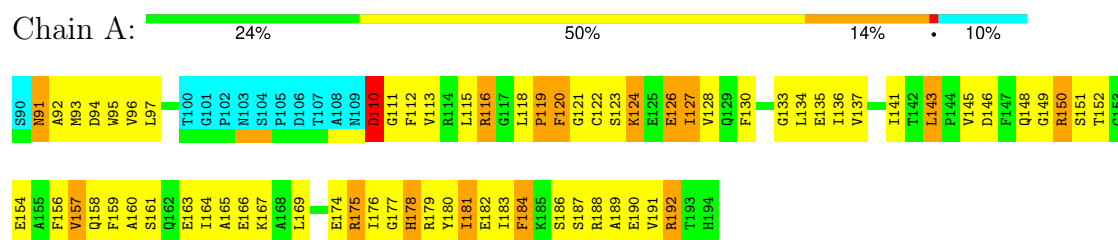
4.2.3 Score per residue for model 3

- Molecule 1: qRRM2 domain of Heterogeneous nuclear ribonucleoprotein H2



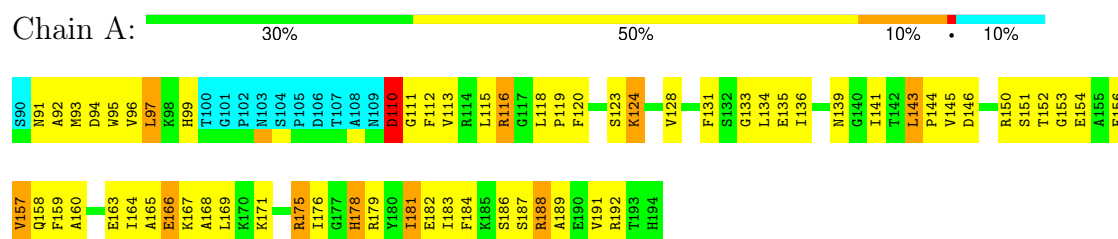
4.2.4 Score per residue for model 4

- Molecule 1: qRRM2 domain of Heterogeneous nuclear ribonucleoprotein H2



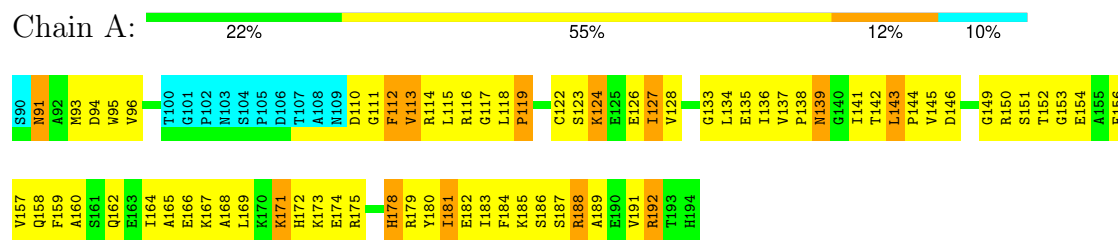
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: qRRM2 domain of Heterogeneous nuclear ribonucleoprotein H2



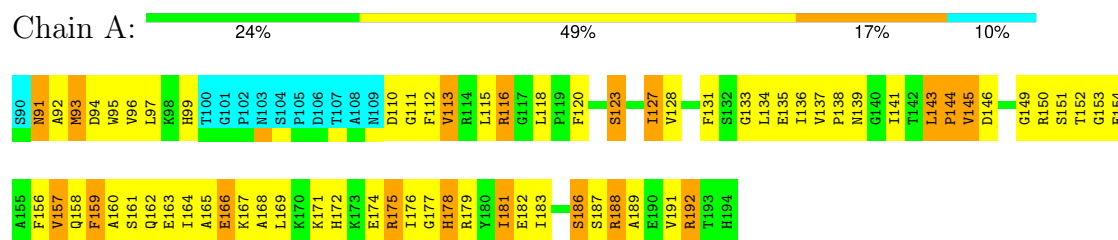
4.2.6 Score per residue for model 6

- Molecule 1: qRRM2 domain of Heterogeneous nuclear ribonucleoprotein H2



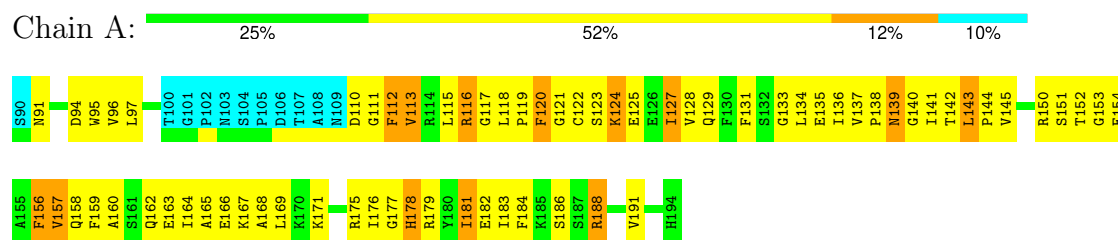
4.2.7 Score per residue for model 7

- Molecule 1: qRRM2 domain of Heterogeneous nuclear ribonucleoprotein H2



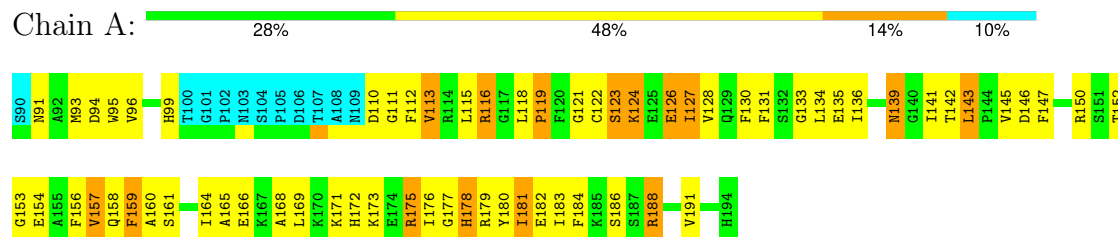
4.2.8 Score per residue for model 8

- Molecule 1: qRRM2 domain of Heterogeneous nuclear ribonucleoprotein H2



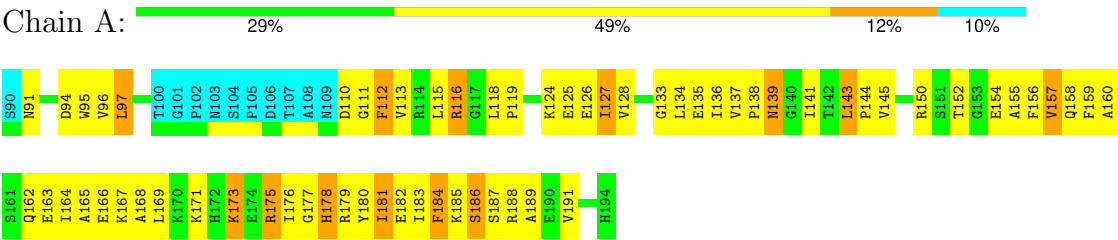
4.2.9 Score per residue for model 9

- Molecule 1: qRRM2 domain of Heterogeneous nuclear ribonucleoprotein H2



4.2.10 Score per residue for model 10

- Molecule 1: qRRM2 domain of Heterogeneous nuclear ribonucleoprotein H2



5 Refinement protocol and experimental data overview

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

Of the 800 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
ARIA	structure calculation	

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	1094
Number of shifts mapped to atoms	1094
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.70±0.02	0±0/776 (0.0± 0.0%)	0.80±0.02	0±0/1039 (0.0± 0.0%)
All	All	0.70	1/7760 (0.0%)	0.80	4/10390 (0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	166	GLU	CB-CG	-5.61	1.41	1.52	1	1

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	110	ASP	N-CA-CB	-6.42	99.05	110.60	1	4

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	759	761	757	76±7
All	All	7590	7610	7570	758

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 50.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:ILE:HA	1:A:156:PHE:O	0.94	1.62	6	10
1:A:128:VAL:HG11	1:A:138:PRO:HA	0.89	1.42	7	2
1:A:136:ILE:HG12	1:A:159:PHE:CE2	0.82	2.09	8	3
1:A:111:GLY:HA2	1:A:165:ALA:HB2	0.80	1.54	6	5
1:A:116:ARG:HD2	1:A:182:GLU:O	0.80	1.77	1	9
1:A:136:ILE:HG12	1:A:159:PHE:CE1	0.79	2.12	6	4
1:A:115:LEU:O	1:A:154:GLU:HA	0.79	1.77	6	8
1:A:133:GLY:C	1:A:134:LEU:HD12	0.75	2.00	3	8
1:A:159:PHE:CD2	1:A:165:ALA:HA	0.73	2.18	4	8
1:A:159:PHE:CD1	1:A:165:ALA:HA	0.73	2.17	8	2
1:A:94:ASP:HB3	1:A:133:GLY:O	0.73	1.83	8	10
1:A:113:VAL:HG11	1:A:159:PHE:CZ	0.72	2.18	6	2
1:A:113:VAL:C	1:A:186:SER:HB3	0.71	2.06	4	9
1:A:122:CYS:SG	1:A:181:ILE:HD11	0.71	2.26	3	3
1:A:174:GLU:O	1:A:181:ILE:HB	0.71	1.85	3	3
1:A:164:ILE:H	1:A:164:ILE:HD12	0.71	1.45	5	10
1:A:110:ASP:OD1	1:A:160:ALA:HA	0.70	1.86	1	4
1:A:134:LEU:HD21	1:A:167:LYS:HB2	0.68	1.64	6	6
1:A:110:ASP:OD2	1:A:158:GLN:HG3	0.67	1.90	7	1
1:A:175:ARG:HG3	1:A:179:ARG:C	0.67	2.10	4	1
1:A:113:VAL:O	1:A:157:VAL:HG23	0.65	1.92	4	9
1:A:163:GLU:O	1:A:166:GLU:HB2	0.65	1.91	8	6
1:A:143:LEU:HD22	1:A:145:VAL:HG11	0.65	1.69	5	8
1:A:123:SER:CB	1:A:143:LEU:HG	0.64	2.23	8	3
1:A:175:ARG:NE	1:A:179:ARG:HB2	0.64	2.06	9	2
1:A:116:ARG:HD2	1:A:154:GLU:CD	0.64	2.13	6	1
1:A:166:GLU:O	1:A:169:LEU:HB3	0.64	1.93	5	2
1:A:96:VAL:HG22	1:A:135:GLU:OE1	0.64	1.93	7	4
1:A:135:GLU:OE2	1:A:161:SER:HB3	0.64	1.93	3	1
1:A:116:ARG:NE	1:A:182:GLU:HB3	0.64	2.08	9	5
1:A:166:GLU:HA	1:A:169:LEU:HB3	0.63	1.70	8	6
1:A:119:PRO:HD2	1:A:122:CYS:SG	0.63	2.34	6	2
1:A:159:PHE:CD1	1:A:164:ILE:HG22	0.62	2.29	8	1
1:A:159:PHE:CD2	1:A:164:ILE:HG22	0.62	2.28	6	5
1:A:112:PHE:HA	1:A:186:SER:OG	0.62	1.93	6	4
1:A:113:VAL:HA	1:A:184:PHE:O	0.62	1.94	10	4
1:A:150:ARG:O	1:A:150:ARG:HG3	0.62	1.95	2	6
1:A:166:GLU:HA	1:A:169:LEU:HD22	0.62	1.72	3	1
1:A:119:PRO:HB3	1:A:176:ILE:O	0.61	1.94	4	1
1:A:128:VAL:HG12	1:A:136:ILE:HG22	0.61	1.71	7	1
1:A:175:ARG:HG2	1:A:179:ARG:O	0.61	1.96	2	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:GLU:CD	1:A:160:ALA:HB3	0.61	2.16	1	10
1:A:137:VAL:HG12	1:A:158:GLN:O	0.61	1.96	10	8
1:A:119:PRO:HB3	1:A:179:ARG:CB	0.61	2.26	1	1
1:A:156:PHE:HB3	1:A:191:VAL:HA	0.61	1.71	3	5
1:A:113:VAL:O	1:A:186:SER:HB3	0.61	1.95	6	7
1:A:143:LEU:HD22	1:A:145:VAL:CG1	0.60	2.27	9	5
1:A:166:GLU:OE2	1:A:169:LEU:HD13	0.60	1.95	2	2
1:A:124:LYS:O	1:A:128:VAL:HG23	0.60	1.97	6	8
1:A:113:VAL:N	1:A:186:SER:HB2	0.59	2.12	1	1
1:A:124:LYS:HA	1:A:141:ILE:HD12	0.59	1.73	9	3
1:A:111:GLY:CA	1:A:165:ALA:HB2	0.59	2.27	3	3
1:A:120:PHE:HA	1:A:151:SER:OG	0.59	1.97	5	3
1:A:164:ILE:HD12	1:A:164:ILE:N	0.59	2.11	5	10
1:A:110:ASP:HB2	1:A:188:ARG:HE	0.59	1.57	1	3
1:A:186:SER:HB2	1:A:191:VAL:HG21	0.59	1.73	3	3
1:A:175:ARG:HD2	1:A:178:HIS:H	0.58	1.58	10	4
1:A:136:ILE:HG12	1:A:159:PHE:CZ	0.58	2.33	4	7
1:A:110:ASP:HB2	1:A:188:ARG:NE	0.58	2.14	5	3
1:A:96:VAL:HG22	1:A:135:GLU:OE2	0.58	1.99	5	3
1:A:91:ASN:HB3	1:A:95:TRP:HA	0.57	1.75	8	10
1:A:112:PHE:HB2	1:A:186:SER:O	0.57	1.98	10	7
1:A:128:VAL:HG11	1:A:138:PRO:CA	0.57	2.24	7	1
1:A:164:ILE:H	1:A:164:ILE:CD1	0.57	2.12	6	10
1:A:177:GLY:O	1:A:178:HIS:HB2	0.57	2.00	10	8
1:A:119:PRO:HB3	1:A:175:ARG:CZ	0.57	2.30	10	3
1:A:99:HIS:HA	1:A:161:SER:OG	0.57	2.00	9	1
1:A:113:VAL:HG22	1:A:157:VAL:HB	0.57	1.75	7	4
1:A:92:ALA:H	1:A:96:VAL:HB	0.56	1.60	7	4
1:A:111:GLY:HA3	1:A:159:PHE:H	0.56	1.60	6	2
1:A:186:SER:CB	1:A:191:VAL:HG21	0.56	2.29	4	3
1:A:135:GLU:O	1:A:135:GLU:HG3	0.56	2.01	4	10
1:A:94:ASP:HB3	1:A:133:GLY:C	0.56	2.21	3	1
1:A:179:ARG:NE	1:A:179:ARG:HA	0.56	2.15	6	2
1:A:175:ARG:HD2	1:A:179:ARG:N	0.55	2.16	5	4
1:A:95:TRP:H	1:A:164:ILE:HD11	0.55	1.61	5	10
1:A:175:ARG:HD3	1:A:176:ILE:O	0.55	2.01	7	3
1:A:116:ARG:HG3	1:A:182:GLU:C	0.55	2.22	6	1
1:A:187:SER:O	1:A:191:VAL:HG23	0.55	2.01	7	3
1:A:146:ASP:H	1:A:150:ARG:HA	0.55	1.60	4	1
1:A:169:LEU:C	1:A:169:LEU:HD23	0.55	2.22	1	2
1:A:162:GLN:O	1:A:165:ALA:HB3	0.55	2.01	10	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:PHE:HA	1:A:151:SER:HB3	0.54	1.78	4	1
1:A:158:GLN:C	1:A:159:PHE:HD2	0.54	2.06	2	2
1:A:111:GLY:HA3	1:A:159:PHE:HB2	0.54	1.78	3	1
1:A:187:SER:HB3	1:A:190:GLU:OE2	0.54	2.02	4	1
1:A:141:ILE:HG23	1:A:157:VAL:HG13	0.54	1.79	1	8
1:A:115:LEU:HD12	1:A:122:CYS:O	0.54	2.03	9	2
1:A:114:ARG:HG3	1:A:155:ALA:O	0.54	2.02	3	2
1:A:138:PRO:O	1:A:139:ASN:HB2	0.54	2.01	8	3
1:A:113:VAL:HG23	1:A:183:ILE:HG21	0.54	1.80	8	1
1:A:120:PHE:HA	1:A:151:SER:CB	0.54	2.32	4	1
1:A:158:GLN:C	1:A:159:PHE:HD1	0.53	2.06	3	6
1:A:175:ARG:HG3	1:A:179:ARG:H	0.53	1.63	4	1
1:A:169:LEU:HD23	1:A:170:LYS:N	0.53	2.19	2	3
1:A:136:ILE:HG12	1:A:159:PHE:CD1	0.53	2.37	10	1
1:A:91:ASN:HA	1:A:96:VAL:N	0.53	2.19	6	8
1:A:135:GLU:H	1:A:164:ILE:CG2	0.53	2.17	3	8
1:A:134:LEU:HD11	1:A:167:LYS:HD2	0.53	1.80	5	1
1:A:142:THR:HB	1:A:156:PHE:CD2	0.53	2.38	8	1
1:A:142:THR:HB	1:A:156:PHE:CZ	0.53	2.39	6	2
1:A:95:TRP:HB3	1:A:163:GLU:HB3	0.52	1.81	3	4
1:A:112:PHE:HB2	1:A:186:SER:OG	0.52	2.05	2	1
1:A:121:GLY:HA2	1:A:143:LEU:CD2	0.52	2.34	9	3
1:A:175:ARG:HB2	1:A:179:ARG:O	0.52	2.04	6	2
1:A:175:ARG:CG	1:A:179:ARG:H	0.52	2.16	4	1
1:A:113:VAL:N	1:A:186:SER:HB3	0.52	2.19	10	2
1:A:186:SER:HB2	1:A:191:VAL:CG2	0.52	2.35	4	3
1:A:162:GLN:O	1:A:166:GLU:HG3	0.52	2.05	8	2
1:A:181:ILE:HG22	1:A:181:ILE:O	0.52	2.03	3	10
1:A:139:ASN:C	1:A:141:ILE:H	0.52	2.07	7	6
1:A:131:PHE:HB3	1:A:134:LEU:HD22	0.52	1.80	7	3
1:A:188:ARG:HA	1:A:191:VAL:HB	0.51	1.81	3	5
1:A:95:TRP:CD1	1:A:167:LYS:HE2	0.51	2.39	3	1
1:A:145:VAL:HG12	1:A:151:SER:HA	0.51	1.81	8	3
1:A:156:PHE:HB2	1:A:191:VAL:HA	0.51	1.83	6	5
1:A:133:GLY:O	1:A:134:LEU:HD12	0.51	2.05	4	4
1:A:186:SER:OG	1:A:191:VAL:HG21	0.51	2.06	1	2
1:A:175:ARG:HG3	1:A:179:ARG:O	0.51	2.06	9	3
1:A:172:HIS:CD2	1:A:182:GLU:HG3	0.51	2.41	2	1
1:A:168:ALA:HA	1:A:171:LYS:CG	0.51	2.35	8	1
1:A:159:PHE:CD1	1:A:159:PHE:N	0.51	2.77	9	7
1:A:116:ARG:CD	1:A:116:ARG:C	0.51	2.79	9	8

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:HIS:O	1:A:173:LYS:HB3	0.51	2.06	6	1
1:A:119:PRO:HB3	1:A:179:ARG:HB3	0.50	1.82	1	2
1:A:169:LEU:HD23	1:A:169:LEU:C	0.50	2.27	2	1
1:A:116:ARG:O	1:A:181:ILE:HA	0.50	2.06	7	1
1:A:168:ALA:HA	1:A:171:LYS:HG2	0.50	1.84	8	2
1:A:118:LEU:HG	1:A:153:GLY:O	0.50	2.06	7	2
1:A:131:PHE:HB2	1:A:134:LEU:O	0.50	2.06	3	1
1:A:121:GLY:O	1:A:126:GLU:HG3	0.50	2.05	4	1
1:A:136:ILE:HG12	1:A:159:PHE:CD2	0.50	2.40	7	2
1:A:183:ILE:HG22	1:A:184:PHE:N	0.50	2.21	8	7
1:A:174:GLU:C	1:A:181:ILE:HB	0.50	2.27	6	1
1:A:110:ASP:CB	1:A:188:ARG:HE	0.50	2.19	5	2
1:A:137:VAL:HG11	1:A:158:GLN:OE1	0.50	2.05	10	1
1:A:159:PHE:CE2	1:A:165:ALA:HA	0.50	2.41	10	1
1:A:158:GLN:HG2	1:A:192:ARG:NE	0.50	2.22	7	1
1:A:119:PRO:HG3	1:A:176:ILE:O	0.49	2.07	8	2
1:A:119:PRO:HG2	1:A:122:CYS:SG	0.49	2.47	4	1
1:A:112:PHE:HB3	1:A:186:SER:O	0.49	2.07	7	1
1:A:127:ILE:HG22	1:A:136:ILE:HG21	0.49	1.83	9	3
1:A:159:PHE:N	1:A:159:PHE:HD1	0.49	2.05	9	2
1:A:91:ASN:CB	1:A:95:TRP:HA	0.49	2.38	8	4
1:A:146:ASP:N	1:A:150:ARG:HG2	0.49	2.23	6	4
1:A:146:ASP:CB	1:A:150:ARG:HG2	0.49	2.38	1	3
1:A:191:VAL:O	1:A:192:ARG:HB2	0.49	2.08	5	2
1:A:123:SER:HB3	1:A:143:LEU:HG	0.49	1.83	5	4
1:A:175:ARG:HD2	1:A:179:ARG:HB2	0.49	1.85	6	1
1:A:188:ARG:NH2	1:A:192:ARG:HD2	0.48	2.22	4	2
1:A:137:VAL:HG13	1:A:140:GLY:HA3	0.48	1.84	8	1
1:A:143:LEU:HD12	1:A:143:LEU:N	0.48	2.24	1	8
1:A:168:ALA:O	1:A:171:LYS:HB2	0.48	2.07	2	5
1:A:143:LEU:H	1:A:143:LEU:HD12	0.48	1.68	9	5
1:A:173:LYS:HA	1:A:180:TYR:HA	0.48	1.85	6	2
1:A:159:PHE:N	1:A:159:PHE:CD2	0.48	2.82	2	1
1:A:127:ILE:CD1	1:A:127:ILE:N	0.48	2.76	7	4
1:A:172:HIS:O	1:A:173:LYS:HB2	0.48	2.09	9	2
1:A:116:ARG:HB3	1:A:182:GLU:O	0.48	2.08	10	2
1:A:95:TRP:CB	1:A:163:GLU:HB3	0.47	2.38	3	5
1:A:125:GLU:O	1:A:129:GLN:HG2	0.47	2.08	8	1
1:A:143:LEU:HD13	1:A:145:VAL:HG12	0.47	1.85	4	1
1:A:172:HIS:CE1	1:A:182:GLU:HG3	0.47	2.45	7	1
1:A:141:ILE:HG12	1:A:157:VAL:CG1	0.47	2.40	2	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:PHE:CE2	1:A:168:ALA:HB3	0.47	2.45	3	3
1:A:119:PRO:HD3	1:A:175:ARG:NE	0.47	2.24	4	1
1:A:188:ARG:NH1	1:A:188:ARG:HB3	0.47	2.25	5	1
1:A:93:MET:HG3	1:A:135:GLU:OE2	0.47	2.10	7	2
1:A:127:ILE:HA	1:A:131:PHE:CD1	0.47	2.45	8	1
1:A:112:PHE:CE2	1:A:185:LYS:HB2	0.47	2.45	10	1
1:A:141:ILE:CA	1:A:156:PHE:O	0.47	2.59	8	1
1:A:113:VAL:CG2	1:A:157:VAL:HB	0.47	2.39	10	2
1:A:93:MET:HG3	1:A:135:GLU:OE1	0.47	2.09	5	2
1:A:131:PHE:HB3	1:A:136:ILE:HD12	0.46	1.87	3	1
1:A:111:GLY:HA2	1:A:165:ALA:CB	0.46	2.39	9	2
1:A:187:SER:C	1:A:189:ALA:N	0.46	2.69	7	8
1:A:146:ASP:OD2	1:A:148:GLN:N	0.46	2.45	4	1
1:A:114:ARG:O	1:A:183:ILE:HG23	0.46	2.11	1	1
1:A:141:ILE:CG2	1:A:157:VAL:HG13	0.46	2.40	2	3
1:A:115:LEU:C	1:A:118:LEU:HD21	0.46	2.30	8	1
1:A:123:SER:O	1:A:127:ILE:HB	0.46	2.11	8	1
1:A:163:GLU:O	1:A:167:LYS:HG2	0.46	2.11	7	2
1:A:134:LEU:HD11	1:A:167:LYS:HB2	0.46	1.88	7	3
1:A:145:VAL:CG1	1:A:151:SER:HA	0.46	2.41	7	3
1:A:134:LEU:HD11	1:A:167:LYS:CD	0.46	2.41	5	1
1:A:168:ALA:O	1:A:183:ILE:HD12	0.46	2.11	7	1
1:A:144:PRO:HD2	1:A:154:GLU:O	0.45	2.11	7	1
1:A:146:ASP:H	1:A:150:ARG:CA	0.45	2.22	4	1
1:A:135:GLU:HG2	1:A:164:ILE:HG21	0.45	1.88	3	3
1:A:115:LEU:HD11	1:A:127:ILE:HG12	0.45	1.88	7	1
1:A:114:ARG:HB2	1:A:186:SER:OG	0.45	2.12	1	1
1:A:135:GLU:HG2	1:A:164:ILE:HG12	0.45	1.89	8	6
1:A:114:ARG:HD2	1:A:154:GLU:OE2	0.45	2.12	6	1
1:A:119:PRO:HD3	1:A:175:ARG:HG2	0.45	1.87	5	2
1:A:116:ARG:HD2	1:A:154:GLU:OE2	0.45	2.12	6	1
1:A:158:GLN:HB2	1:A:191:VAL:CG1	0.45	2.42	6	1
1:A:113:VAL:HG21	1:A:159:PHE:CE2	0.45	2.46	1	1
1:A:116:ARG:NH1	1:A:182:GLU:HG2	0.45	2.27	1	1
1:A:143:LEU:HA	1:A:155:ALA:CB	0.45	2.42	1	4
1:A:167:LYS:O	1:A:171:LYS:HG2	0.45	2.12	8	1
1:A:119:PRO:HB3	1:A:175:ARG:NH1	0.45	2.27	10	1
1:A:126:GLU:O	1:A:130:PHE:HB2	0.45	2.12	2	1
1:A:99:HIS:CE1	1:A:160:ALA:HB1	0.45	2.47	1	1
1:A:158:GLN:OE1	1:A:192:ARG:HG3	0.45	2.11	6	1
1:A:164:ILE:N	1:A:164:ILE:CD1	0.45	2.79	8	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:LEU:H	1:A:118:LEU:HD23	0.44	1.72	9	1
1:A:171:LYS:O	1:A:183:ILE:HG13	0.44	2.11	7	1
1:A:131:PHE:CB	1:A:136:ILE:HD12	0.44	2.43	3	1
1:A:126:GLU:HA	1:A:130:PHE:CD2	0.44	2.47	9	1
1:A:111:GLY:HA3	1:A:159:PHE:CB	0.44	2.43	10	1
1:A:175:ARG:HB2	1:A:179:ARG:H	0.44	1.73	6	1
1:A:111:GLY:HA3	1:A:159:PHE:O	0.44	2.12	7	1
1:A:127:ILE:O	1:A:136:ILE:HD13	0.44	2.12	8	1
1:A:166:GLU:HA	1:A:169:LEU:CB	0.44	2.43	4	2
1:A:143:LEU:HD12	1:A:143:LEU:H	0.44	1.71	7	1
1:A:131:PHE:CE2	1:A:171:LYS:HE2	0.44	2.48	9	1
1:A:112:PHE:CD2	1:A:185:LYS:HB2	0.44	2.48	10	1
1:A:114:ARG:HB2	1:A:186:SER:CB	0.44	2.43	2	1
1:A:135:GLU:O	1:A:135:GLU:CG	0.44	2.65	6	3
1:A:159:PHE:HE2	1:A:168:ALA:HB3	0.43	1.73	7	1
1:A:128:VAL:O	1:A:131:PHE:CG	0.43	2.72	3	1
1:A:96:VAL:HG13	1:A:161:SER:OG	0.43	2.13	4	1
1:A:114:ARG:HB2	1:A:186:SER:HB3	0.43	1.90	2	1
1:A:97:LEU:HD13	1:A:163:GLU:HG2	0.43	1.90	8	1
1:A:95:TRP:CD1	1:A:167:LYS:HG3	0.43	2.48	7	3
1:A:158:GLN:HB2	1:A:191:VAL:HG11	0.43	1.89	6	1
1:A:134:LEU:HD23	1:A:136:ILE:HD11	0.43	1.89	7	1
1:A:124:LYS:HG3	1:A:125:GLU:H	0.43	1.74	10	1
1:A:95:TRP:HD1	1:A:133:GLY:O	0.43	1.97	3	1
1:A:127:ILE:N	1:A:127:ILE:CD1	0.43	2.81	9	4
1:A:177:GLY:O	1:A:178:HIS:CB	0.43	2.66	9	2
1:A:159:PHE:CD2	1:A:159:PHE:N	0.43	2.87	8	1
1:A:156:PHE:CD1	1:A:156:PHE:C	0.43	2.92	8	1
1:A:110:ASP:HB3	1:A:188:ARG:HD3	0.43	1.89	7	1
1:A:135:GLU:OE1	1:A:160:ALA:HB3	0.43	2.13	2	2
1:A:95:TRP:O	1:A:163:GLU:HB2	0.42	2.14	5	1
1:A:115:LEU:HB2	1:A:155:ALA:HB3	0.42	1.89	1	1
1:A:116:ARG:HA	1:A:153:GLY:O	0.42	2.15	6	2
1:A:141:ILE:HG23	1:A:156:PHE:O	0.42	2.14	5	1
1:A:127:ILE:HD12	1:A:131:PHE:CE2	0.42	2.49	9	1
1:A:183:ILE:CG2	1:A:184:PHE:N	0.42	2.82	3	3
1:A:175:ARG:HG2	1:A:179:ARG:C	0.42	2.35	3	1
1:A:138:PRO:O	1:A:139:ASN:HB3	0.42	2.14	6	1
1:A:134:LEU:HD11	1:A:167:LYS:CB	0.42	2.45	10	1
1:A:187:SER:O	1:A:189:ALA:N	0.42	2.52	6	2
1:A:97:LEU:CD1	1:A:97:LEU:N	0.42	2.83	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:LEU:HA	1:A:155:ALA:HB2	0.42	1.92	1	1
1:A:171:LYS:HG3	1:A:174:GLU:OE1	0.42	2.15	7	1
1:A:134:LEU:CB	1:A:164:ILE:HG23	0.42	2.44	6	2
1:A:116:ARG:HG3	1:A:183:ILE:HA	0.42	1.90	6	1
1:A:117:GLY:N	1:A:153:GLY:O	0.41	2.53	8	2
1:A:118:LEU:O	1:A:118:LEU:HG	0.41	2.15	2	1
1:A:112:PHE:CD1	1:A:185:LYS:HB2	0.41	2.50	3	1
1:A:134:LEU:HD12	1:A:134:LEU:N	0.41	2.29	3	1
1:A:116:ARG:HG3	1:A:183:ILE:CA	0.41	2.45	6	1
1:A:122:CYS:SG	1:A:176:ILE:HD13	0.41	2.55	8	1
1:A:135:GLU:OE2	1:A:164:ILE:HD13	0.41	2.14	5	1
1:A:116:ARG:CG	1:A:182:GLU:O	0.41	2.69	6	1
1:A:146:ASP:HB3	1:A:150:ARG:HG2	0.41	1.92	9	1
1:A:119:PRO:HA	1:A:179:ARG:NH1	0.41	2.31	8	1
1:A:146:ASP:CG	1:A:147:PHE:N	0.41	2.73	9	1
1:A:115:LEU:CD2	1:A:157:VAL:HG21	0.41	2.45	8	1
1:A:137:VAL:CG1	1:A:140:GLY:HA3	0.41	2.46	8	1
1:A:97:LEU:N	1:A:97:LEU:CD1	0.41	2.83	1	1
1:A:113:VAL:HG11	1:A:159:PHE:CE2	0.41	2.51	8	1
1:A:119:PRO:CD	1:A:175:ARG:HG2	0.41	2.46	10	1
1:A:159:PHE:HD2	1:A:159:PHE:N	0.41	2.13	2	1
1:A:165:ALA:O	1:A:169:LEU:N	0.41	2.54	5	1
1:A:175:ARG:HG2	1:A:181:ILE:CG1	0.41	2.46	6	1
1:A:158:GLN:C	1:A:159:PHE:CD1	0.41	2.93	7	1
1:A:159:PHE:HE1	1:A:168:ALA:HB3	0.41	1.76	2	1
1:A:111:GLY:HA3	1:A:159:PHE:N	0.41	2.30	6	1
1:A:127:ILE:N	1:A:127:ILE:HD13	0.40	2.31	4	1
1:A:112:PHE:CE1	1:A:185:LYS:HB2	0.40	2.51	3	1
1:A:171:LYS:HB3	1:A:183:ILE:HD12	0.40	1.93	10	1
1:A:175:ARG:CD	1:A:178:HIS:H	0.40	2.28	10	1
1:A:123:SER:HB3	1:A:143:LEU:HD21	0.40	1.94	1	1
1:A:159:PHE:HD2	1:A:164:ILE:HG22	0.40	1.76	1	1
1:A:161:SER:O	1:A:164:ILE:HB	0.40	2.17	9	1
1:A:175:ARG:CZ	1:A:179:ARG:HB2	0.40	2.47	9	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	93/105 (89%)	60±3 (65±3%)	25±4 (26±4%)	8±2 (9±2%)	1	12
All	All	930/1050 (89%)	604 (65%)	246 (26%)	80 (9%)	1	12

All 20 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	178	HIS	10
1	A	139	ASN	8
1	A	144	PRO	8
1	A	124	LYS	7
1	A	91	ASN	5
1	A	188	ARG	5
1	A	192	ARG	5
1	A	111	GLY	4
1	A	119	PRO	4
1	A	123	SER	4
1	A	149	GLY	4
1	A	186	SER	3
1	A	120	PHE	3
1	A	153	GLY	2
1	A	185	LYS	2
1	A	180	TYR	2
1	A	150	ARG	1
1	A	145	VAL	1
1	A	97	LEU	1
1	A	173	LYS	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	80/89 (90%)	68±2 (84±2%)	12±2 (16±2%)	4	41
All	All	800/890 (90%)	676 (84%)	124 (16%)	4	41

All 28 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	143	LEU	10
1	A	152	THR	10
1	A	157	VAL	10
1	A	181	ILE	10
1	A	116	ARG	9
1	A	127	ILE	8
1	A	97	LEU	7
1	A	118	LEU	7
1	A	126	GLU	5
1	A	175	ARG	5
1	A	110	ASP	4
1	A	159	PHE	4
1	A	166	GLU	4
1	A	112	PHE	4
1	A	113	VAL	4
1	A	169	LEU	3
1	A	186	SER	3
1	A	184	PHE	3
1	A	151	SER	2
1	A	130	PHE	2
1	A	161	SER	2
1	A	93	MET	2
1	A	158	GLN	1
1	A	131	PHE	1
1	A	188	ARG	1
1	A	171	LYS	1
1	A	178	HIS	1
1	A	156	PHE	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 i

The completeness of assignment taking into account all chemical shift lists is 75% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `rrm2_shifts.list`

7.1.1 Bookkeeping i

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

Total number of shifts	1094
Number of shifts mapped to atoms	1094
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing i

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	104	2.35 ± 0.17	Should be checked
$^{13}\text{C}_\beta$	93	1.82 ± 0.18	Should be checked
$^{13}\text{C}'$	88	3.89 ± 0.15	Should be applied
^{15}N	97	0.39 ± 0.63	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments i

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 75%, i.e. 1005 atoms were assigned a chemical shift out of a possible 1332. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	452/472 (96%)	190/193 (98%)	173/188 (92%)	89/91 (98%)
Sidechain	553/727 (76%)	378/470 (80%)	175/223 (78%)	0/34 (0%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/133 (0%)	0/66 (0%)	0/58 (0%)	0/9 (0%)
Overall	1005/1332 (75%)	568/729 (78%)	348/469 (74%)	89/134 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 1094 atoms were assigned a chemical shift out of a possible 1442. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	499/524 (95%)	210/214 (98%)	192/210 (91%)	97/100 (97%)
Sidechain	595/785 (76%)	407/507 (80%)	188/242 (78%)	0/36 (0%)
Aromatic	0/133 (0%)	0/66 (0%)	0/58 (0%)	0/9 (0%)
Overall	1094/1442 (76%)	617/787 (78%)	380/510 (75%)	97/145 (67%)

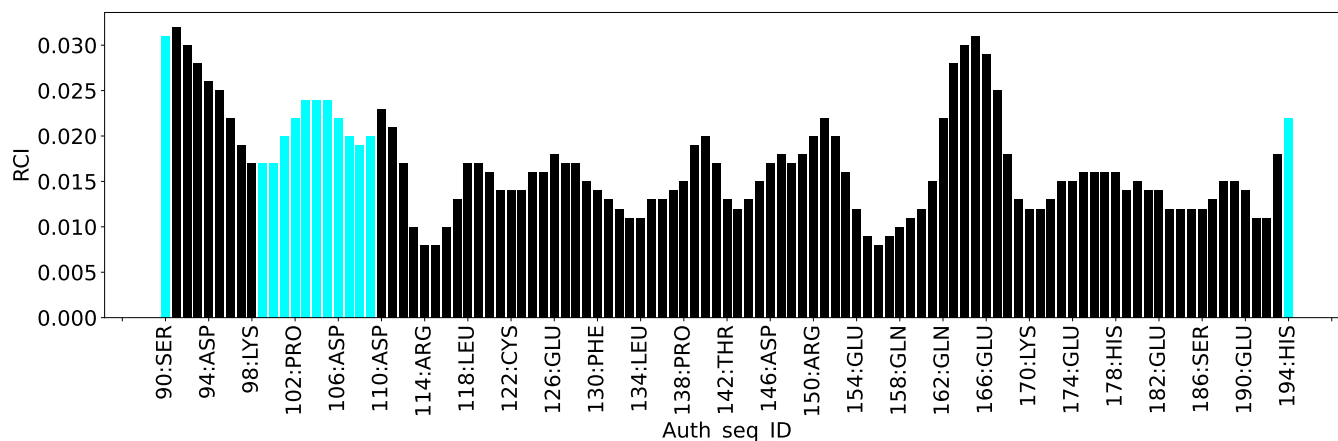
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain 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	12919
Intra-residue ($ i-j =0$)	7104
Sequential ($ i-j =1$)	3710
Medium range ($ i-j >1$ and $ i-j <5$)	919
Long range ($ i-j \geq 5$)	1129
Inter-chain	0
Hydrogen bond restraints	57
Disulfide bond restraints	0
Total dihedral-angle restraints	142
Number of unmapped restraints	0
Number of restraints per residue	124.4
Number of long range restraints per residue ¹	11.1

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)	242.3	0.2
0.2-0.5 (Medium)	324.1	0.5
>0.5 (Large)	204.4	9.68

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)	17.6	9.69
10.0-20.0 (Medium)	1.2	15.22
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

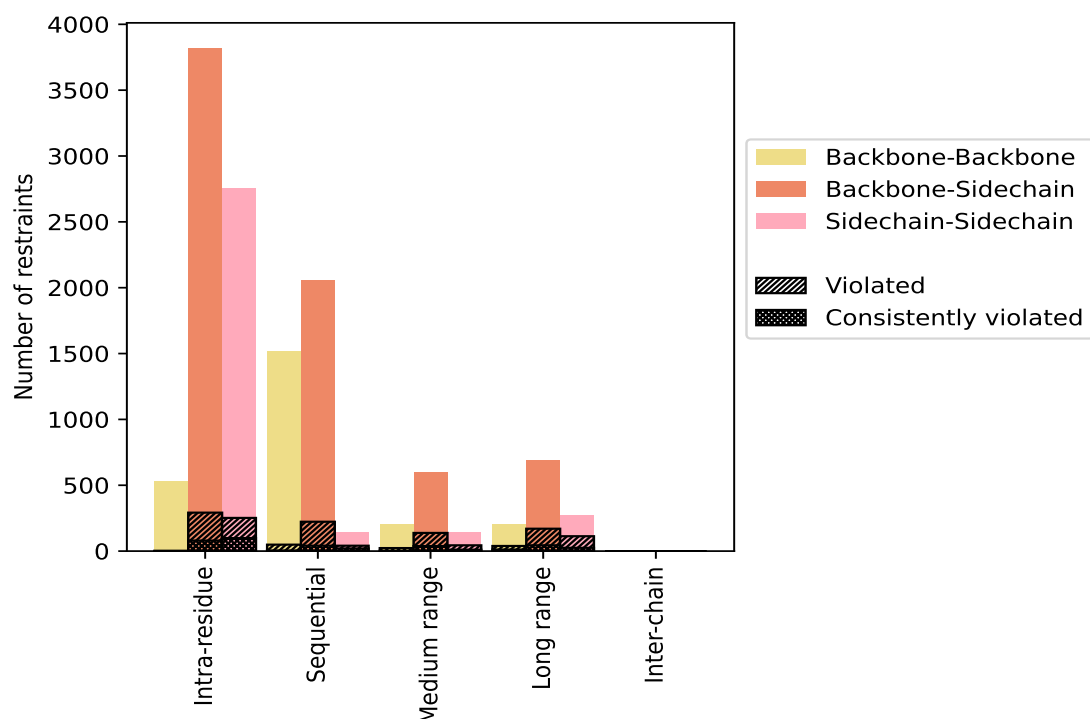
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	7104	55.0	546	7.7	4.2	180	2.5	1.4
Backbone-Backbone	529	4.1	2	0.4	0.0	1	0.2	0.0
Backbone-Sidechain	3820	29.6	292	7.6	2.3	80	2.1	0.6
Sidechain-Sidechain	2755	21.3	252	9.1	2.0	99	3.6	0.8
Sequential ($i-j =1$)	3710	28.7	313	8.4	2.4	66	1.8	0.5
Backbone-Backbone	1514	11.7	49	3.2	0.4	5	0.3	0.0
Backbone-Sidechain	2057	15.9	223	10.8	1.7	41	2.0	0.3
Sidechain-Sidechain	139	1.1	41	29.5	0.3	20	14.4	0.2
Medium range ($i-j >1$ & $i-j <5$)	919	7.1	194	21.1	1.5	47	5.1	0.4
Backbone-Backbone	206	1.6	23	11.2	0.2	3	1.5	0.0
Backbone-Sidechain	573	4.4	127	22.2	1.0	33	5.8	0.3
Sidechain-Sidechain	140	1.1	44	31.4	0.3	11	7.9	0.1
Long range ($i-j \geq 5$)	1129	8.7	305	27.0	2.4	79	7.0	0.6
Backbone-Backbone	200	1.5	39	19.5	0.3	12	6.0	0.1
Backbone-Sidechain	661	5.1	154	23.3	1.2	42	6.4	0.3
Sidechain-Sidechain	268	2.1	112	41.8	0.9	25	9.3	0.2
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	57	0.4	28	49.1	0.2	7	12.3	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	12919	100.0	1386	10.7	10.7	379	2.9	2.9
Backbone-Backbone	2449	19.0	113	4.6	0.9	21	0.9	0.2
Backbone-Sidechain	7167	55.5	823	11.5	6.4	203	2.8	1.6
Sidechain-Sidechain	3303	25.6	450	13.6	3.5	155	4.7	1.2

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

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



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

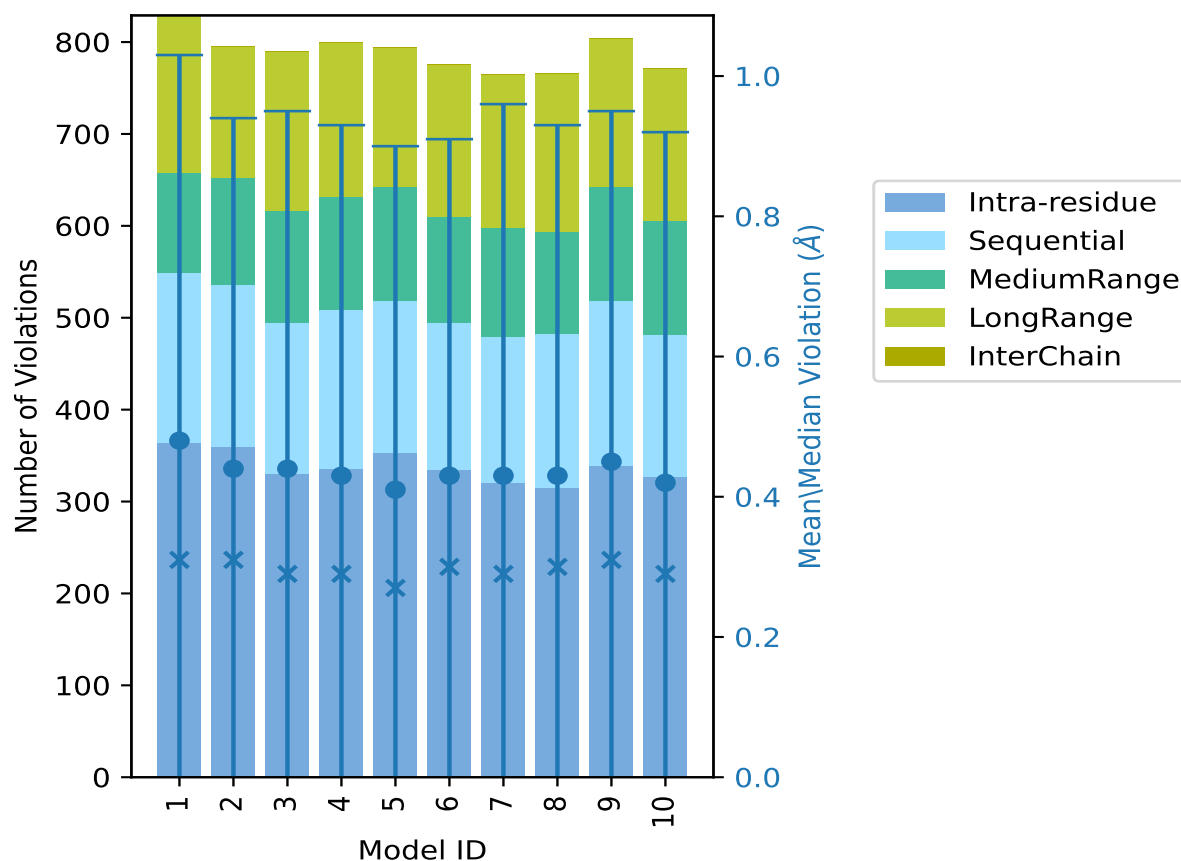
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	364	185	109	171	0	829	0.48	8.01	0.55	0.31
2	359	177	116	143	0	795	0.44	8.99	0.5	0.31
3	330	165	121	174	0	790	0.44	9.15	0.51	0.29
4	335	173	124	167	0	799	0.43	8.73	0.5	0.29
5	353	166	123	152	0	794	0.41	8.56	0.49	0.27
6	335	160	115	166	0	776	0.43	8.49	0.48	0.3
7	321	158	119	167	0	765	0.43	9.68	0.53	0.29
8	315	168	110	173	0	766	0.43	9.17	0.5	0.3
9	339	179	124	162	0	804	0.45	8.85	0.5	0.31
10	327	154	125	165	0	771	0.42	9.15	0.5	0.29

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 11504(IR:6558, SQ:3397, MR:725, LR:824, 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	%
113	72	39	67	0	291	1	10.0
48	20	13	25	0	106	2	20.0
30	26	24	23	0	103	3	30.0

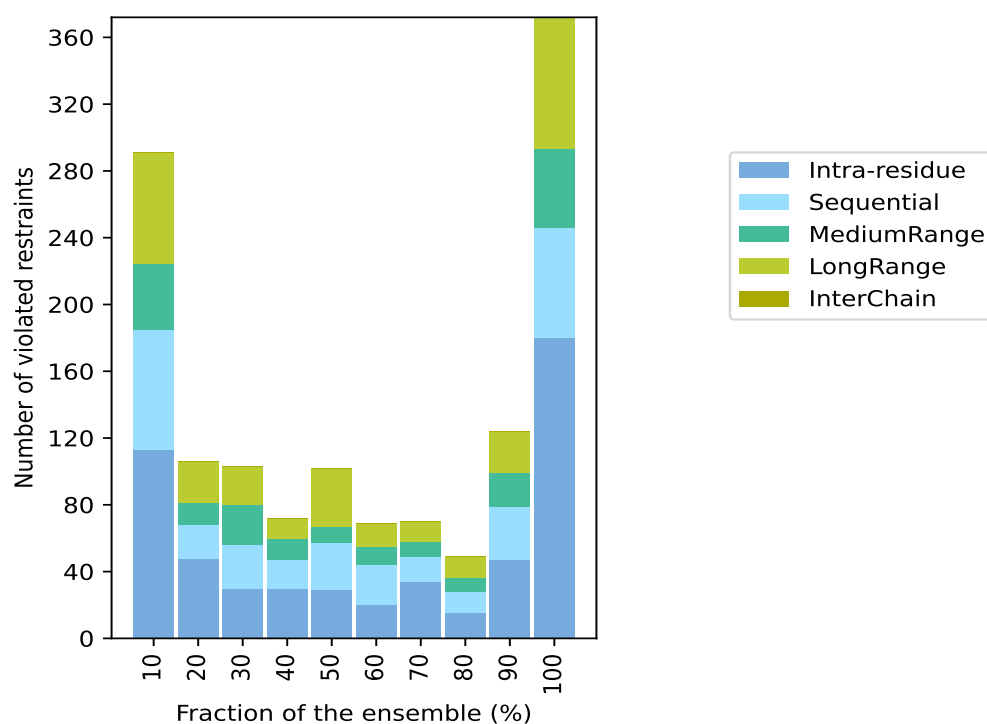
Continued on next page...

Continued from previous page...

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
30	17	13	12	0	72	4	40.0
29	28	10	35	0	102	5	50.0
20	24	11	14	0	69	6	60.0
34	15	9	12	0	70	7	70.0
15	13	8	13	0	49	8	80.0
47	32	20	25	0	124	9	90.0
180	66	47	79	0	372	10	100.0

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

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

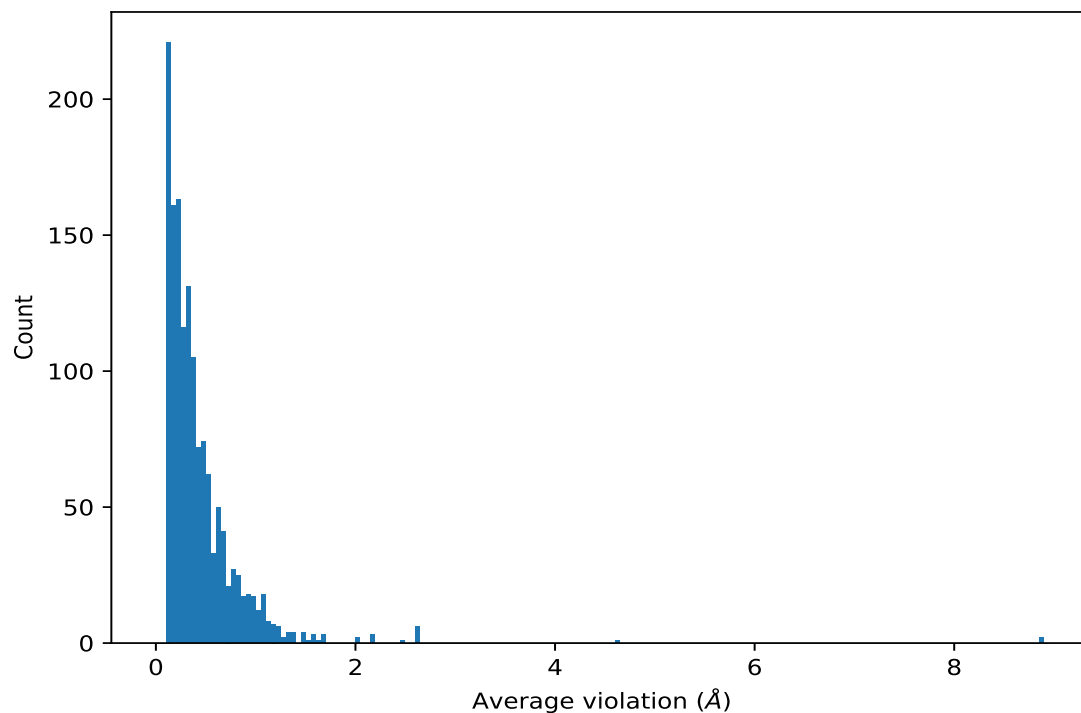


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2830)	1:164:A:ILE:HA	1:181:A:ILE:HD13	10	8.88	0.44	8.92
(1,2830)	1:164:A:ILE:HA	1:181:A:ILE:HD12	10	8.88	0.44	8.92
(4,53)	1:184:A:PHE:N	1:186:A:SER:O	10	4.64	0.08	4.61
(1,2774)	1:121:A:GLY:HA3	1:142:A:THR:HG23	10	2.64	0.16	2.65
(1,2774)	1:121:A:GLY:HA3	1:142:A:THR:HG21	10	2.64	0.16	2.65
(1,2774)	1:121:A:GLY:HA3	1:142:A:THR:HG22	10	2.64	0.16	2.65
(1,2165)	1:121:A:GLY:HA3	1:142:A:THR:HG23	10	2.63	0.16	2.64
(1,2165)	1:121:A:GLY:HA3	1:142:A:THR:HG21	10	2.63	0.16	2.64
(1,2165)	1:121:A:GLY:HA3	1:142:A:THR:HG22	10	2.63	0.16	2.64
(2,8122)	1:163:A:GLU:HA	1:164:A:ILE:HG12	10	2.48	0.05	2.49
(1,2222)	1:130:A:PHE:HA	1:136:A:ILE:HB	10	2.16	1.23	2.41
(1,2222)	1:113:A:VAL:HG12	1:109:A:ASN:HA	10	2.16	1.23	2.41
(1,2222)	1:113:A:VAL:HG13	1:109:A:ASN:HA	10	2.16	1.23	2.41
(2,8511)	1:157:A:VAL:HG23	1:190:A:GLU:H	10	2.03	0.14	2.06
(2,6788)	1:97:A:LEU:HG	1:98:A:LYS:H	10	2.03	0.1	2.0

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,479)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	10	1.69	0.13	1.64
(1,479)	1:159:A:PHE:HB2	1:164:A:ILE:HG12	10	1.69	0.13	1.64
(1,479)	1:159:A:PHE:HB2	1:136:A:ILE:HG23	10	1.69	0.13	1.64
(1,422)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	10	1.63	0.37	1.75
(2,4814)	1:157:A:VAL:HG23	1:190:A:GLU:H	10	1.59	0.14	1.61
(2,4908)	1:181:A:ILE:HG22	1:122:A:CYS:H	10	1.48	0.13	1.52
(2,130)	1:181:A:ILE:HG12	1:174:A:GLU:HB2	10	1.37	0.42	1.27
(2,104)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	10	1.35	0.67	1.24
(2,3295)	1:134:A:LEU:HB2	1:135:A:GLU:H	10	1.3	0.02	1.3
(2,6951)	1:134:A:LEU:HB2	1:135:A:GLU:H	10	1.23	0.02	1.23
(2,3008)	1:157:A:VAL:HG23	1:190:A:GLU:H	10	1.21	0.14	1.24
(2,5491)	1:191:A:VAL:HG13	1:189:A:ALA:HA	10	1.2	0.17	1.24
(2,7364)	1:191:A:VAL:HG13	1:189:A:ALA:HA	10	1.2	0.17	1.24
(2,8805)	1:134:A:LEU:HB2	1:135:A:GLU:H	10	1.18	0.02	1.18
(2,8568)	1:139:A:ASN:H	1:158:A:GLN:HB2	10	1.18	0.33	1.34
(1,1035)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	10	1.18	0.27	1.06
(1,1035)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	10	1.18	0.27	1.06
(1,1035)	1:139:A:ASN:HB2	1:137:A:VAL:HG22	10	1.18	0.27	1.06
(2,5095)	1:134:A:LEU:HB2	1:135:A:GLU:H	10	1.16	0.02	1.16
(2,6706)	1:139:A:ASN:H	1:158:A:GLN:HB2	10	1.15	0.33	1.31
(2,8503)	1:187:A:SER:H	1:184:A:PHE:HB2	10	1.11	0.73	1.45
(1,484)	1:141:A:ILE:HA	1:156:A:PHE:HB3	10	1.1	0.39	1.1
(1,484)	1:136:A:ILE:HA	1:159:A:PHE:HB2	10	1.1	0.39	1.1
(2,6638)	1:187:A:SER:H	1:184:A:PHE:HB2	10	1.07	0.73	1.41
(1,718)	1:154:A:GLU:HB3	1:154:A:GLU:H	10	1.07	0.11	1.12
(1,718)	1:118:A:LEU:HG	1:154:A:GLU:H	10	1.07	0.11	1.12
(1,423)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	10	1.06	0.29	1.16
(1,423)	1:139:A:ASN:HB2	1:137:A:VAL:HG22	10	1.06	0.29	1.16
(1,423)	1:156:A:PHE:HB3	1:157:A:VAL:HG23	10	1.06	0.29	1.16
(2,1883)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	10	1.01	0.12	1.05
(1,757)	1:179:A:ARG:HB3	1:119:A:PRO:HD2	10	1.01	0.09	1.04
(1,757)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	10	1.01	0.09	1.04
(1,757)	1:141:A:ILE:HG13	1:140:A:GLY:HA2	10	1.01	0.09	1.04
(1,2873)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	10	1.01	0.26	1.08
(1,2873)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	10	1.01	0.26	1.08
(1,221)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	10	1.0	0.2	0.98
(1,221)	1:116:A:ARG:HD2	1:181:A:ILE:HD12	10	1.0	0.2	0.98
(2,9054)	1:192:A:ARG:HG2	1:192:A:ARG:H	10	0.99	0.4	1.19
(2,7200)	1:192:A:ARG:HG2	1:192:A:ARG:H	10	0.99	0.4	1.18
(1,2499)	1:96:A:VAL:HG22	1:97:A:LEU:H	10	0.97	0.13	0.97
(1,2499)	1:181:A:ILE:HG21	1:181:A:ILE:H	10	0.97	0.13	0.97
(1,2671)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	10	0.96	0.11	1.0

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3995)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	10	0.96	0.04	0.98
(1,227)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	10	0.95	0.53	0.76
(1,227)	1:183:A:ILE:HG12	1:116:A:ARG:HD2	10	0.95	0.53	0.76
(2,3105)	1:181:A:ILE:HG22	1:122:A:CYS:H	10	0.95	0.13	0.99
(1,2065)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	10	0.94	0.11	0.98
(2,81)	1:192:A:ARG:HA	1:137:A:VAL:HG13	10	0.94	0.07	0.93
(2,81)	1:192:A:ARG:HA	1:137:A:VAL:HG12	10	0.94	0.07	0.93
(2,81)	1:192:A:ARG:HA	1:137:A:VAL:HG11	10	0.94	0.07	0.93
(1,125)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	10	0.93	0.03	0.94
(1,125)	1:141:A:ILE:HG13	1:140:A:GLY:HA2	10	0.93	0.03	0.94
(2,3687)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	10	0.92	0.11	0.96
(2,5483)	1:192:A:ARG:HA	1:137:A:VAL:HG13	10	0.91	0.07	0.9
(2,5483)	1:192:A:ARG:HA	1:137:A:VAL:HG12	10	0.91	0.07	0.9
(2,5483)	1:192:A:ARG:HA	1:137:A:VAL:HG11	10	0.91	0.07	0.9
(2,6619)	1:176:A:ILE:HG23	1:175:A:ARG:HB3	10	0.87	0.53	0.75
(2,6619)	1:176:A:ILE:HG21	1:175:A:ARG:HB3	10	0.87	0.53	0.75
(2,6619)	1:176:A:ILE:HG22	1:175:A:ARG:HB3	10	0.87	0.53	0.75
(1,2263)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	10	0.86	0.27	0.74
(1,2263)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	10	0.86	0.27	0.74
(1,2263)	1:139:A:ASN:HB2	1:137:A:VAL:HG22	10	0.86	0.27	0.74
(1,13)	1:181:A:ILE:HG12	1:175:A:ARG:HA	10	0.86	0.32	0.9
(2,1840)	1:191:A:VAL:HG11	1:186:A:SER:HA	10	0.85	0.04	0.85
(1,2488)	1:96:A:VAL:HG22	1:97:A:LEU:H	10	0.83	0.05	0.84
(1,2488)	1:137:A:VAL:HG23	1:140:A:GLY:H	10	0.83	0.05	0.84
(1,588)	1:164:A:ILE:HG13	1:165:A:ALA:H	10	0.83	0.04	0.84
(1,588)	1:165:A:ALA:H	1:134:A:LEU:HG	10	0.83	0.04	0.84
(2,7314)	1:191:A:VAL:HG13	1:193:A:THR:H	10	0.82	0.08	0.78
(2,7314)	1:191:A:VAL:HG12	1:193:A:THR:H	10	0.82	0.08	0.78
(2,1795)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	10	0.82	0.31	0.66
(2,3605)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	10	0.82	0.31	0.66
(1,233)	1:116:A:ARG:HD2	1:116:A:ARG:HA	10	0.81	0.22	0.88
(1,233)	1:116:A:ARG:HD3	1:116:A:ARG:HA	10	0.81	0.22	0.88
(1,2921)	1:176:A:ILE:HG23	1:175:A:ARG:HB2	10	0.81	0.14	0.82
(1,2921)	1:176:A:ILE:HG21	1:175:A:ARG:HB3	10	0.81	0.14	0.82
(1,2921)	1:176:A:ILE:HG23	1:175:A:ARG:HB3	10	0.81	0.14	0.82
(1,2921)	1:176:A:ILE:HG22	1:175:A:ARG:HB3	10	0.81	0.14	0.82
(1,4)	1:136:A:ILE:HD11	1:164:A:ILE:HA	10	0.81	0.08	0.82
(1,4)	1:136:A:ILE:HD13	1:164:A:ILE:HA	10	0.81	0.08	0.82
(2,6704)	1:139:A:ASN:H	1:141:A:ILE:HG22	10	0.78	0.03	0.78
(1,683)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	10	0.77	0.11	0.78
(1,683)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	10	0.77	0.11	0.78
(1,2352)	1:148:A:GLN:H	1:143:A:LEU:HD21	10	0.77	0.14	0.74

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2352)	1:148:A:GLN:H	1:143:A:LEU:HD22	10	0.77	0.14	0.74
(2,3060)	1:139:A:ASN:H	1:141:A:ILE:HG22	10	0.77	0.03	0.76
(2,7353)	1:192:A:ARG:HA	1:137:A:VAL:HG13	10	0.76	0.07	0.76
(2,7353)	1:192:A:ARG:HA	1:137:A:VAL:HG12	10	0.76	0.07	0.76
(2,7353)	1:192:A:ARG:HA	1:137:A:VAL:HG11	10	0.76	0.07	0.76
(2,2186)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	10	0.76	0.04	0.78
(2,7316)	1:191:A:VAL:HG11	1:186:A:SER:HA	10	0.76	0.04	0.76
(1,45)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	10	0.74	0.11	0.75
(1,45)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	10	0.74	0.11	0.75
(2,3649)	1:191:A:VAL:HG11	1:186:A:SER:HA	10	0.73	0.05	0.74
(1,1795)	1:122:A:CYS:H	1:127:A:ILE:HD13	10	0.72	0.1	0.7
(1,1795)	1:122:A:CYS:H	1:127:A:ILE:HD11	10	0.72	0.1	0.7
(2,4863)	1:139:A:ASN:H	1:141:A:ILE:HG22	10	0.72	0.03	0.72
(2,1909)	1:142:A:THR:HG23	1:141:A:ILE:HG21	10	0.71	0.12	0.75
(2,1909)	1:142:A:THR:HG21	1:141:A:ILE:HG21	10	0.71	0.12	0.75
(2,1909)	1:142:A:THR:HG22	1:141:A:ILE:HG21	10	0.71	0.12	0.75
(1,1057)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	10	0.71	0.36	0.64
(1,1057)	1:133:A:GLY:HA3	1:134:A:LEU:HG	10	0.71	0.36	0.64
(2,15)	1:189:A:ALA:HB2	1:186:A:SER:HA	10	0.7	0.09	0.7
(1,2968)	1:148:A:GLN:H	1:143:A:LEU:HD21	10	0.69	0.14	0.66
(1,2968)	1:148:A:GLN:H	1:143:A:LEU:HD22	10	0.69	0.14	0.66
(1,1288)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	10	0.69	0.11	0.7
(1,1288)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	10	0.69	0.11	0.7
(2,3717)	1:142:A:THR:HG23	1:141:A:ILE:HG21	10	0.68	0.12	0.72
(2,3717)	1:142:A:THR:HG21	1:141:A:ILE:HG21	10	0.68	0.12	0.72
(2,3717)	1:142:A:THR:HG22	1:141:A:ILE:HG21	10	0.68	0.12	0.72
(1,1083)	1:175:A:ARG:HB2	1:176:A:ILE:HD12	10	0.68	0.19	0.64
(1,1083)	1:175:A:ARG:HB3	1:176:A:ILE:HD12	10	0.68	0.19	0.64
(1,1083)	1:175:A:ARG:HB3	1:176:A:ILE:HD11	10	0.68	0.19	0.64
(1,473)	1:157:A:VAL:HG23	1:114:A:ARG:HB3	10	0.68	0.13	0.66
(1,473)	1:175:A:ARG:HB3	1:176:A:ILE:HD12	10	0.68	0.13	0.66
(1,473)	1:175:A:ARG:HB3	1:176:A:ILE:HD11	10	0.68	0.13	0.66
(2,8567)	1:139:A:ASN:H	1:141:A:ILE:HG22	10	0.67	0.03	0.66
(2,5931)	1:134:A:LEU:HG	1:134:A:LEU:HB2	10	0.66	0.01	0.66
(1,295)	1:164:A:ILE:HD11	1:165:A:ALA:HB1	10	0.66	0.23	0.58
(1,295)	1:164:A:ILE:HD12	1:166:A:GLU:HB2	10	0.66	0.23	0.58
(2,396)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	10	0.66	0.04	0.68
(1,1364)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	10	0.65	0.03	0.66
(1,1364)	1:141:A:ILE:HG13	1:140:A:GLY:HA2	10	0.65	0.03	0.66
(1,2399)	1:189:A:ALA:H	1:186:A:SER:HA	10	0.65	0.17	0.64
(2,2)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	10	0.65	0.31	0.48
(2,5400)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	10	0.65	0.31	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2970)	1:111:A:GLY:HA3	1:109:A:ASN:H	10	0.65	0.38	0.55
(1,397)	1:135:A:GLU:HA	1:136:A:ILE:HB	10	0.65	0.07	0.64
(2,2933)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	10	0.65	0.0	0.65
(1,2528)	1:162:A:GLN:HB2	1:163:A:GLU:HA	10	0.64	0.09	0.68
(1,2528)	1:166:A:GLU:HB3	1:167:A:LYS:HA	10	0.64	0.09	0.68
(2,6509)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	10	0.64	0.02	0.64
(2,120)	1:142:A:THR:HG23	1:141:A:ILE:HG21	10	0.63	0.12	0.67
(2,120)	1:142:A:THR:HG21	1:141:A:ILE:HG21	10	0.63	0.12	0.67
(2,120)	1:142:A:THR:HG22	1:141:A:ILE:HG21	10	0.63	0.12	0.67
(1,1696)	1:175:A:ARG:HB3	1:176:A:ILE:HD12	10	0.63	0.25	0.58
(1,1696)	1:175:A:ARG:HB3	1:176:A:ILE:HD11	10	0.63	0.25	0.58
(1,3066)	1:108:A:ALA:H	1:106:A:ASP:HB3	10	0.62	0.12	0.59
(2,51)	1:191:A:VAL:HG11	1:186:A:SER:HA	10	0.62	0.05	0.62
(1,365)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	10	0.62	0.05	0.62
(1,365)	1:143:A:LEU:HG	1:143:A:LEU:HD23	10	0.62	0.05	0.62
(1,541)	1:181:A:ILE:H	1:172:A:HIS:HA	10	0.61	0.18	0.67
(1,541)	1:159:A:PHE:HA	1:135:A:GLU:H	10	0.61	0.18	0.67
(2,4741)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	10	0.61	0.01	0.61
(1,191)	1:98:A:LYS:HA	1:100:A:THR:HG23	10	0.61	0.24	0.62
(1,191)	1:98:A:LYS:HA	1:100:A:THR:HG22	10	0.61	0.24	0.62
(1,191)	1:93:A:MET:HA	1:92:A:ALA:HB2	10	0.61	0.24	0.62
(2,2950)	1:162:A:GLN:HG2	1:165:A:ALA:H	10	0.6	0.17	0.59
(2,55)	1:191:A:VAL:HG11	1:190:A:GLU:H	10	0.6	0.08	0.6
(2,55)	1:191:A:VAL:HG13	1:190:A:GLU:H	10	0.6	0.08	0.6
(2,55)	1:191:A:VAL:HG12	1:190:A:GLU:H	10	0.6	0.08	0.6
(1,983)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	10	0.6	0.05	0.6
(1,983)	1:143:A:LEU:HG	1:143:A:LEU:HD23	10	0.6	0.05	0.6
(1,522)	1:169:A:LEU:H	1:169:A:LEU:HG	10	0.58	0.09	0.62
(1,522)	1:100:A:THR:HG22	1:98:A:LYS:H	10	0.58	0.09	0.62
(1,522)	1:100:A:THR:HG23	1:98:A:LYS:H	10	0.58	0.09	0.62
(1,2994)	1:150:A:ARG:H	1:143:A:LEU:HD21	10	0.58	0.07	0.59
(1,2994)	1:150:A:ARG:H	1:143:A:LEU:HD22	10	0.58	0.07	0.59
(1,1670)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	10	0.58	0.36	0.52
(1,1670)	1:133:A:GLY:HA3	1:134:A:LEU:HG	10	0.58	0.36	0.52
(1,1596)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	10	0.57	0.05	0.57
(1,1596)	1:143:A:LEU:HG	1:143:A:LEU:HD23	10	0.57	0.05	0.57
(2,5446)	1:191:A:VAL:HG11	1:186:A:SER:HA	10	0.57	0.05	0.57
(2,8382)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	10	0.57	0.02	0.57
(2,1283)	1:105:A:PRO:HB3	1:106:A:ASP:H	10	0.57	0.17	0.58
(2,816)	1:161:A:SER:HB2	1:162:A:GLN:H	10	0.56	0.22	0.57
(2,6569)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	10	0.55	0.0	0.55
(2,1560)	1:150:A:ARG:HG3	1:150:A:ARG:H	10	0.55	0.16	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1429)	1:98:A:LYS:HA	1:100:A:THR:HG23	10	0.54	0.24	0.55
(1,1429)	1:98:A:LYS:HA	1:100:A:THR:HG22	10	0.54	0.24	0.55
(1,1429)	1:93:A:MET:HA	1:92:A:ALA:HB2	10	0.54	0.24	0.55
(2,5807)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	10	0.54	0.04	0.56
(1,2379)	1:150:A:ARG:H	1:143:A:LEU:HD21	10	0.54	0.07	0.55
(1,2379)	1:150:A:ARG:H	1:143:A:LEU:HD22	10	0.54	0.07	0.55
(2,8439)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	10	0.49	0.01	0.49
(2,9034)	1:187:A:SER:HB3	1:188:A:ARG:H	10	0.49	0.18	0.57
(1,33)	1:137:A:VAL:HG22	1:139:A:ASN:H	10	0.48	0.06	0.46
(2,3383)	1:154:A:GLU:HB3	1:154:A:GLU:H	10	0.48	0.02	0.49
(1,837)	1:92:A:ALA:HA	1:93:A:MET:H	10	0.48	0.01	0.48
(1,837)	1:108:A:ALA:HA	1:109:A:ASN:H	10	0.48	0.01	0.48
(1,2211)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	10	0.47	0.03	0.48
(1,376)	1:174:A:GLU:HB2	1:181:A:ILE:HD13	10	0.47	0.54	0.32
(1,3013)	1:189:A:ALA:H	1:186:A:SER:HA	10	0.47	0.17	0.46
(2,129)	1:155:A:ALA:HB2	1:154:A:GLU:H	10	0.47	0.05	0.48
(2,1807)	1:113:A:VAL:HG12	1:113:A:VAL:HB	10	0.47	0.07	0.44
(2,1807)	1:113:A:VAL:HG13	1:113:A:VAL:HB	10	0.47	0.07	0.44
(2,1807)	1:113:A:VAL:HG11	1:113:A:VAL:HB	10	0.47	0.07	0.44
(1,2821)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	10	0.47	0.03	0.48
(1,614)	1:108:A:ALA:H	1:106:A:ASP:HB3	10	0.46	0.12	0.43
(1,1338)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.46	0.0	0.46
(1,1338)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.46	0.0	0.46
(1,1338)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.46	0.0	0.46
(1,732)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.46	0.0	0.46
(1,732)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.46	0.0	0.46
(1,732)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.46	0.0	0.46
(2,6609)	1:95:A:TRP:HA	1:164:A:ILE:HG13	10	0.46	0.04	0.45
(2,3986)	1:119:A:PRO:HB2	1:119:A:PRO:HA	10	0.46	0.03	0.45
(2,4477)	1:166:A:GLU:HG2	1:166:A:GLU:H	10	0.46	0.38	0.2
(1,1961)	1:179:A:ARG:HB3	1:119:A:PRO:HD2	10	0.45	0.1	0.48
(1,1961)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	10	0.45	0.1	0.48
(1,1961)	1:141:A:ILE:HG13	1:140:A:GLY:HA2	10	0.45	0.1	0.48
(1,2210)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	10	0.45	0.05	0.45
(1,2210)	1:143:A:LEU:HG	1:143:A:LEU:HD23	10	0.45	0.05	0.45
(1,95)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.45	0.0	0.45
(1,95)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.45	0.0	0.45
(1,95)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.45	0.0	0.45
(2,2666)	1:166:A:GLU:HG2	1:166:A:GLU:H	10	0.45	0.38	0.2
(3,537)	1:118:A:LEU:HA	1:183:A:ILE:HG12	10	0.45	0.37	0.38
(1,97)	1:105:A:PRO:HB2	1:105:A:PRO:HA	10	0.45	0.02	0.45
(1,97)	1:119:A:PRO:HB2	1:119:A:PRO:HA	10	0.45	0.02	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,7042)	1:154:A:GLU:H	1:154:A:GLU:HB3	10	0.45	0.03	0.46
(1,12)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	10	0.45	0.02	0.45
(1,12)	1:164:A:ILE:HD11	1:164:A:ILE:HB	10	0.45	0.02	0.45
(1,19)	1:96:A:VAL:HG21	1:96:A:VAL:HB	10	0.44	0.08	0.42
(1,19)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.44	0.08	0.42
(2,5499)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	10	0.44	0.17	0.43
(1,2820)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	10	0.44	0.05	0.44
(1,2820)	1:143:A:LEU:HG	1:143:A:LEU:HD23	10	0.44	0.05	0.44
(1,1446)	1:92:A:ALA:HA	1:93:A:MET:H	10	0.44	0.01	0.44
(1,1446)	1:108:A:ALA:HA	1:109:A:ASN:H	10	0.44	0.01	0.44
(1,2493)	1:96:A:VAL:HG21	1:96:A:VAL:HB	10	0.44	0.01	0.44
(1,2493)	1:96:A:VAL:HG23	1:96:A:VAL:HB	10	0.44	0.01	0.44
(1,657)	1:96:A:VAL:HG21	1:96:A:VAL:HB	10	0.44	0.08	0.42
(1,657)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.44	0.08	0.42
(1,395)	1:135:A:GLU:HB3	1:135:A:GLU:HA	10	0.44	0.01	0.43
(2,4997)	1:110:A:ASP:HB3	1:110:A:ASP:H	10	0.44	0.28	0.4
(2,47)	1:191:A:VAL:HG13	1:192:A:ARG:HA	10	0.43	0.06	0.42
(2,47)	1:191:A:VAL:HG12	1:192:A:ARG:HA	10	0.43	0.06	0.42
(1,648)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	10	0.43	0.02	0.44
(1,648)	1:164:A:ILE:HD11	1:164:A:ILE:HB	10	0.43	0.02	0.44
(1,783)	1:130:A:PHE:HB3	1:132:A:SER:H	10	0.43	0.04	0.43
(1,1262)	1:96:A:VAL:HG21	1:96:A:VAL:HB	10	0.43	0.08	0.4
(1,1262)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.43	0.08	0.4
(2,5525)	1:142:A:THR:HG23	1:141:A:ILE:HG21	10	0.43	0.12	0.46
(2,5525)	1:142:A:THR:HG21	1:141:A:ILE:HG21	10	0.43	0.12	0.46
(2,5525)	1:142:A:THR:HG22	1:141:A:ILE:HG21	10	0.43	0.12	0.46
(1,691)	1:166:A:GLU:HB3	1:168:A:ALA:H	10	0.42	0.14	0.38
(1,691)	1:166:A:GLU:HB2	1:168:A:ALA:H	10	0.42	0.14	0.38
(1,2738)	1:143:A:LEU:HG	1:141:A:ILE:HG21	10	0.42	0.16	0.39
(2,2177)	1:119:A:PRO:HB2	1:119:A:PRO:HA	10	0.41	0.03	0.4
(2,6587)	1:93:A:MET:HB2	1:164:A:ILE:HG12	10	0.41	0.04	0.4
(1,40)	1:134:A:LEU:HD13	1:136:A:ILE:HB	10	0.41	0.02	0.41
(1,678)	1:134:A:LEU:HD13	1:136:A:ILE:HB	10	0.41	0.02	0.41
(1,1284)	1:134:A:LEU:HD13	1:136:A:ILE:HB	10	0.41	0.02	0.41
(1,1903)	1:134:A:LEU:HD13	1:136:A:ILE:HB	10	0.41	0.02	0.41
(1,2510)	1:134:A:LEU:HD13	1:136:A:ILE:HB	10	0.41	0.02	0.41
(2,3095)	1:159:A:PHE:H	1:110:A:ASP:HA	10	0.41	0.08	0.42
(2,1575)	1:154:A:GLU:HB3	1:154:A:GLU:H	10	0.41	0.03	0.42
(2,3616)	1:113:A:VAL:HG12	1:113:A:VAL:HB	10	0.41	0.07	0.38
(2,3616)	1:113:A:VAL:HG13	1:113:A:VAL:HB	10	0.41	0.07	0.38
(2,3616)	1:113:A:VAL:HG11	1:113:A:VAL:HB	10	0.41	0.07	0.38
(1,662)	1:127:A:ILE:HG21	1:127:A:ILE:HB	10	0.41	0.07	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,662)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.41	0.07	0.38
(1,988)	1:190:A:GLU:HG3	1:186:A:SER:HA	10	0.4	0.09	0.44
(1,988)	1:190:A:GLU:HG2	1:186:A:SER:HA	10	0.4	0.09	0.44
(1,1266)	1:127:A:ILE:HG21	1:127:A:ILE:HB	10	0.4	0.07	0.38
(1,1266)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.4	0.07	0.38
(1,1266)	1:96:A:VAL:HG23	1:93:A:MET:HG3	10	0.4	0.07	0.38
(1,1524)	1:93:A:MET:HB2	1:135:A:GLU:HB3	10	0.4	0.07	0.4
(1,1524)	1:93:A:MET:HB2	1:93:A:MET:HG2	10	0.4	0.07	0.4
(1,205)	1:142:A:THR:HA	1:142:A:THR:HB	10	0.4	0.01	0.4
(1,54)	1:166:A:GLU:HB3	1:168:A:ALA:H	10	0.4	0.14	0.36
(1,54)	1:166:A:GLU:HB2	1:168:A:ALA:H	10	0.4	0.14	0.36
(1,809)	1:169:A:LEU:HB2	1:169:A:LEU:HA	10	0.4	0.07	0.42
(1,809)	1:154:A:GLU:HG2	1:154:A:GLU:HA	10	0.4	0.07	0.42
(2,418)	1:124:A:LYS:HA	1:124:A:LYS:HB2	10	0.4	0.22	0.3
(1,2238)	1:152:A:THR:HA	1:117:A:GLY:H	10	0.39	0.08	0.43
(1,2238)	1:173:A:LYS:HA	1:172:A:HIS:H	10	0.39	0.08	0.43
(1,2846)	1:152:A:THR:HA	1:117:A:GLY:H	10	0.39	0.08	0.43
(1,2846)	1:173:A:LYS:HA	1:172:A:HIS:H	10	0.39	0.08	0.43
(2,2466)	1:144:A:PRO:HB2	1:144:A:PRO:HA	10	0.39	0.03	0.38
(2,1781)	1:164:A:ILE:HG13	1:167:A:LYS:H	10	0.39	0.04	0.38
(1,1949)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.39	0.0	0.39
(1,1949)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.39	0.0	0.39
(1,1949)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.39	0.0	0.39
(1,845)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	10	0.39	0.1	0.39
(1,845)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	10	0.39	0.1	0.39
(1,845)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	10	0.39	0.1	0.39
(2,2117)	1:115:A:LEU:HA	1:115:A:LEU:HB2	10	0.39	0.0	0.39
(1,1597)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	10	0.38	0.03	0.39
(1,366)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	10	0.38	0.04	0.39
(1,984)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	10	0.38	0.03	0.39
(2,7678)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	10	0.38	0.04	0.4
(2,106)	1:93:A:MET:HB2	1:93:A:MET:HG2	10	0.38	0.1	0.36
(1,2515)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	10	0.38	0.11	0.39
(1,2515)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	10	0.38	0.11	0.39
(2,1256)	1:139:A:ASN:H	1:141:A:ILE:HG22	10	0.38	0.03	0.38
(2,3647)	1:191:A:VAL:HG13	1:193:A:THR:H	10	0.38	0.08	0.34
(2,3647)	1:191:A:VAL:HG12	1:193:A:THR:H	10	0.38	0.08	0.34
(1,25)	1:176:A:ILE:HG22	1:176:A:ILE:HG12	10	0.38	0.03	0.38
(1,25)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.38	0.03	0.38
(1,25)	1:176:A:ILE:HG21	1:176:A:ILE:HG12	10	0.38	0.03	0.38
(2,3054)	1:167:A:LYS:HB3	1:168:A:ALA:H	10	0.37	0.1	0.4
(2,5183)	1:154:A:GLU:HB3	1:154:A:GLU:H	10	0.37	0.02	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4872)	1:157:A:VAL:HG21	1:158:A:GLN:H	10	0.37	0.02	0.38
(2,5798)	1:119:A:PRO:HB2	1:119:A:PRO:HA	10	0.37	0.03	0.36
(1,1950)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.37	0.0	0.37
(1,1950)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.37	0.0	0.37
(1,1950)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.37	0.0	0.37
(1,2554)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.37	0.0	0.37
(1,2554)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.37	0.0	0.37
(1,2554)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.37	0.0	0.37
(1,3081)	1:118:A:LEU:H	1:118:A:LEU:HD12	10	0.37	0.14	0.42
(1,3081)	1:118:A:LEU:H	1:118:A:LEU:HD11	10	0.37	0.14	0.42
(2,5808)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	10	0.37	0.01	0.37
(2,6845)	1:110:A:ASP:HB3	1:110:A:ASP:H	10	0.37	0.28	0.34
(1,447)	1:154:A:GLU:HG2	1:118:A:LEU:HD23	10	0.36	0.12	0.35
(1,377)	1:123:A:SER:HB3	1:181:A:ILE:HD11	10	0.36	0.15	0.32
(2,8577)	1:157:A:VAL:HG21	1:158:A:GLN:H	10	0.36	0.02	0.37
(2,6715)	1:157:A:VAL:HG21	1:158:A:GLN:H	10	0.36	0.02	0.37
(1,2585)	1:179:A:ARG:HB3	1:119:A:PRO:HD2	10	0.36	0.1	0.41
(1,2585)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	10	0.36	0.1	0.41
(1,1451)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	10	0.36	0.1	0.36
(1,1451)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	10	0.36	0.1	0.36
(1,1451)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	10	0.36	0.1	0.36
(1,1919)	1:162:A:GLN:HB2	1:163:A:GLU:HA	10	0.35	0.09	0.39
(1,1919)	1:166:A:GLU:HB3	1:167:A:LYS:HA	10	0.35	0.09	0.39
(2,4276)	1:144:A:PRO:HB2	1:144:A:PRO:HA	10	0.35	0.03	0.34
(1,914)	1:93:A:MET:HB2	1:135:A:GLU:HB3	10	0.35	0.07	0.36
(1,914)	1:93:A:MET:HB2	1:93:A:MET:HG2	10	0.35	0.07	0.36
(1,1417)	1:169:A:LEU:HB2	1:169:A:LEU:HA	10	0.35	0.07	0.38
(1,1417)	1:154:A:GLU:HG2	1:154:A:GLU:HA	10	0.35	0.07	0.38
(1,1173)	1:189:A:ALA:H	1:186:A:SER:HA	10	0.35	0.17	0.34
(1,2555)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.35	0.0	0.35
(1,2555)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.35	0.0	0.35
(1,2555)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.35	0.0	0.35
(1,1976)	1:179:A:ARG:HB3	1:119:A:PRO:HD2	10	0.34	0.1	0.4
(1,1976)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	10	0.34	0.1	0.4
(2,3068)	1:157:A:VAL:HG21	1:158:A:GLN:H	10	0.34	0.02	0.35
(2,7669)	1:119:A:PRO:HB2	1:119:A:PRO:HA	10	0.34	0.03	0.34
(1,153)	1:130:A:PHE:HB3	1:132:A:SER:H	10	0.34	0.04	0.34
(1,105)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.34	0.0	0.34
(1,105)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.34	0.0	0.34
(1,105)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.34	0.0	0.34
(1,927)	1:164:A:ILE:HA	1:91:A:ASN:HB3	10	0.34	0.11	0.34
(1,927)	1:164:A:ILE:HA	1:91:A:ASN:HB2	10	0.34	0.11	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3926)	1:115:A:LEU:HA	1:115:A:LEU:HB2	10	0.34	0.0	0.34
(1,2403)	1:96:A:VAL:HB	1:97:A:LEU:H	10	0.34	0.09	0.36
(1,2403)	1:97:A:LEU:H	1:163:A:GLU:HB2	10	0.34	0.09	0.36
(2,3707)	1:188:A:ARG:HB2	1:187:A:SER:H	10	0.34	0.03	0.34
(2,3726)	1:155:A:ALA:HB2	1:154:A:GLU:H	10	0.34	0.05	0.34
(2,7408)	1:155:A:ALA:HB2	1:154:A:GLU:H	10	0.34	0.05	0.34
(1,1348)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.34	0.01	0.34
(1,1348)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.34	0.01	0.34
(1,1348)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.34	0.01	0.34
(1,2477)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	10	0.34	0.02	0.34
(1,2477)	1:164:A:ILE:HD11	1:164:A:ILE:HB	10	0.34	0.02	0.34
(2,3607)	1:164:A:ILE:HD13	1:91:A:ASN:HA	10	0.33	0.12	0.35
(1,681)	1:134:A:LEU:HD13	1:133:A:GLY:H	10	0.33	0.06	0.32
(1,742)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.33	0.0	0.33
(1,742)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.33	0.0	0.33
(1,742)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.33	0.0	0.33
(1,1864)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	10	0.33	0.02	0.34
(1,1864)	1:164:A:ILE:HD11	1:164:A:ILE:HB	10	0.33	0.02	0.34
(2,7273)	1:164:A:ILE:HD13	1:135:A:GLU:H	10	0.33	0.08	0.3
(1,1297)	1:166:A:GLU:HB3	1:168:A:ALA:H	10	0.33	0.14	0.29
(1,1297)	1:166:A:GLU:HB2	1:168:A:ALA:H	10	0.33	0.14	0.29
(1,1826)	1:185:A:LYS:H	1:186:A:SER:HB3	10	0.32	0.48	0.17
(1,1826)	1:184:A:PHE:H	1:186:A:SER:HB3	10	0.32	0.48	0.17
(2,63)	1:95:A:TRP:HB2	1:96:A:VAL:HG21	10	0.32	0.11	0.31
(4,11)	1:118:A:LEU:H	1:152:A:THR:O	10	0.32	0.09	0.34
(1,320)	1:97:A:LEU:HG	1:97:A:LEU:HD13	10	0.32	0.03	0.32
(1,320)	1:169:A:LEU:HB2	1:169:A:LEU:HD11	10	0.32	0.03	0.32
(2,2051)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	10	0.32	0.14	0.38
(1,178)	1:169:A:LEU:HB2	1:169:A:LEU:HA	10	0.32	0.07	0.34
(1,178)	1:154:A:GLU:HG2	1:154:A:GLU:HA	10	0.32	0.07	0.34
(1,1410)	1:156:A:PHE:HA	1:141:A:ILE:HA	10	0.32	0.03	0.32
(2,5404)	1:164:A:ILE:HD13	1:135:A:GLU:H	10	0.31	0.07	0.29
(1,1881)	1:127:A:ILE:HG21	1:127:A:ILE:HB	10	0.31	0.07	0.29
(1,1881)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.31	0.07	0.29
(1,1881)	1:96:A:VAL:HG23	1:93:A:MET:HG3	10	0.31	0.07	0.29
(1,803)	1:156:A:PHE:HA	1:141:A:ILE:HA	10	0.31	0.03	0.31
(2,264)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	10	0.31	0.14	0.37
(2,3435)	1:164:A:ILE:H	1:164:A:ILE:HG21	10	0.31	0.03	0.31
(2,5235)	1:164:A:ILE:H	1:164:A:ILE:HG21	10	0.3	0.03	0.31
(2,1901)	1:188:A:ARG:HB2	1:187:A:SER:H	10	0.3	0.03	0.31
(2,7825)	1:135:A:GLU:HA	1:135:A:GLU:HG2	10	0.3	0.01	0.3
(1,1623)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.3	0.01	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1877)	1:96:A:VAL:HG21	1:96:A:VAL:HB	10	0.29	0.08	0.26
(1,1877)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.29	0.08	0.26
(1,39)	1:134:A:LEU:HD11	1:134:A:LEU:HG	10	0.29	0.02	0.29
(1,99)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	10	0.29	0.02	0.29
(2,5952)	1:135:A:GLU:HA	1:135:A:GLU:HG2	10	0.29	0.01	0.29
(1,1012)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.29	0.01	0.29
(2,1918)	1:155:A:ALA:HB2	1:154:A:GLU:H	10	0.29	0.05	0.29
(2,4733)	1:192:A:ARG:HB2	1:192:A:ARG:H	10	0.28	0.04	0.28
(1,2207)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	10	0.28	0.02	0.29
(1,2495)	1:127:A:ILE:HG21	1:127:A:ILE:HB	10	0.28	0.07	0.26
(1,2495)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.28	0.07	0.26
(4,40)	1:168:A:ALA:H	1:164:A:ILE:O	10	0.28	0.03	0.28
(1,1520)	1:141:A:ILE:HG21	1:143:A:LEU:HG	10	0.28	0.16	0.24
(4,24)	1:146:A:ASP:OD2	1:148:A:GLN:N	10	0.27	0.01	0.28
(4,25)	1:148:A:GLN:N	1:146:A:ASP:OD2	10	0.27	0.01	0.28
(2,6100)	1:144:A:PRO:HB2	1:144:A:PRO:HA	10	0.27	0.03	0.26
(2,7973)	1:144:A:PRO:HB2	1:144:A:PRO:HA	10	0.27	0.03	0.26
(1,222)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	10	0.27	0.02	0.27
(1,222)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	10	0.27	0.02	0.27
(2,4772)	1:155:A:ALA:HA	1:155:A:ALA:HB3	10	0.27	0.02	0.27
(2,1861)	1:154:A:GLU:HG2	1:118:A:LEU:H	10	0.26	0.04	0.26
(1,2140)	1:93:A:MET:HB2	1:135:A:GLU:HB3	10	0.26	0.07	0.27
(1,2140)	1:93:A:MET:HB2	1:93:A:MET:HG2	10	0.26	0.07	0.27
(1,2377)	1:146:A:ASP:H	1:143:A:LEU:HD21	10	0.26	0.03	0.26
(1,731)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.26	0.01	0.26
(1,2817)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	10	0.26	0.02	0.26
(2,6461)	1:182:A:GLU:HB2	1:182:A:GLU:HG3	10	0.26	0.02	0.26
(2,2965)	1:155:A:ALA:HA	1:155:A:ALA:HB3	10	0.26	0.02	0.26
(1,1337)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.26	0.01	0.26
(2,6185)	1:155:A:ALA:HA	1:155:A:ALA:HB1	10	0.25	0.0	0.25
(1,1959)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.25	0.0	0.25
(1,1959)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.25	0.0	0.25
(1,1959)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.25	0.0	0.25
(2,2925)	1:192:A:ARG:HB2	1:192:A:ARG:H	10	0.25	0.04	0.24
(2,3682)	1:134:A:LEU:HA	1:136:A:ILE:H	10	0.25	0.02	0.26
(1,868)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	10	0.25	0.06	0.24
(1,868)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	10	0.25	0.06	0.24
(1,869)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	10	0.25	0.06	0.24
(1,869)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	10	0.25	0.06	0.24
(1,869)	1:114:A:ARG:HD3	1:114:A:ARG:HB3	10	0.25	0.06	0.24
(2,5473)	1:109:A:ASN:HA	1:108:A:ALA:HB1	10	0.25	0.06	0.24
(2,521)	1:134:A:LEU:HD11	1:134:A:LEU:HA	10	0.24	0.08	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,871)	1:166:A:GLU:HG3	1:166:A:GLU:HA	10	0.24	0.04	0.24
(2,1923)	1:135:A:GLU:HA	1:164:A:ILE:HA	10	0.24	0.02	0.24
(2,7344)	1:109:A:ASN:HA	1:108:A:ALA:HB1	10	0.24	0.06	0.24
(2,5327)	1:190:A:GLU:HB3	1:190:A:GLU:H	10	0.24	0.03	0.22
(1,2992)	1:146:A:ASP:H	1:143:A:LEU:HD21	10	0.24	0.03	0.24
(1,939)	1:97:A:LEU:HG	1:97:A:LEU:HD13	10	0.24	0.03	0.24
(1,939)	1:169:A:LEU:HB2	1:169:A:LEU:HD11	10	0.24	0.03	0.24
(1,2958)	1:189:A:ALA:HB2	1:190:A:GLU:H	10	0.24	0.02	0.24
(1,958)	1:96:A:VAL:HG21	1:96:A:VAL:HB	10	0.23	0.01	0.23
(1,958)	1:96:A:VAL:HG23	1:96:A:VAL:HB	10	0.23	0.01	0.23
(4,50)	1:183:A:ILE:H	1:181:A:ILE:O	10	0.23	0.2	0.16
(2,3716)	1:188:A:ARG:HG2	1:189:A:ALA:H	10	0.23	0.02	0.24
(2,387)	1:119:A:PRO:HB2	1:119:A:PRO:HA	10	0.23	0.03	0.22
(1,2566)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.23	0.0	0.23
(1,2566)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.23	0.0	0.23
(1,2566)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.23	0.0	0.23
(1,247)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	10	0.22	0.06	0.22
(1,247)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	10	0.22	0.06	0.22
(1,1286)	1:134:A:LEU:HD13	1:133:A:GLY:H	10	0.22	0.06	0.22
(1,223)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	10	0.22	0.01	0.22
(1,223)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	10	0.22	0.01	0.22
(1,1478)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	10	0.22	0.03	0.22
(1,1478)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	10	0.22	0.03	0.22
(1,1478)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	10	0.22	0.03	0.22
(2,5821)	1:122:A:CYS:HA	1:121:A:GLY:H	10	0.22	0.05	0.22
(1,32)	1:141:A:ILE:HG21	1:141:A:ILE:HB	10	0.22	0.02	0.22
(1,32)	1:181:A:ILE:HG21	1:181:A:ILE:HB	10	0.22	0.02	0.22
(1,1270)	1:141:A:ILE:HG21	1:141:A:ILE:HB	10	0.22	0.02	0.22
(1,1270)	1:181:A:ILE:HG21	1:181:A:ILE:HB	10	0.22	0.02	0.22
(2,5444)	1:191:A:VAL:HG13	1:193:A:THR:H	10	0.22	0.08	0.18
(2,5444)	1:191:A:VAL:HG12	1:193:A:THR:H	10	0.22	0.08	0.18
(1,1477)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	10	0.22	0.03	0.22
(1,1477)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	10	0.22	0.03	0.22
(1,1477)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	10	0.22	0.03	0.22
(1,248)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	10	0.21	0.06	0.21
(1,248)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	10	0.21	0.06	0.21
(1,2847)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.21	0.01	0.21
(2,8895)	1:154:A:GLU:H	1:154:A:GLU:HB3	10	0.21	0.02	0.22
(3,618)	1:152:A:THR:HB	1:117:A:GLY:H	10	0.21	0.03	0.22
(2,7096)	1:164:A:ILE:H	1:164:A:ILE:HG21	10	0.21	0.03	0.22
(2,1838)	1:191:A:VAL:HG13	1:193:A:THR:H	10	0.21	0.08	0.17
(2,1838)	1:191:A:VAL:HG12	1:193:A:THR:H	10	0.21	0.08	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4650)	1:183:A:ILE:HG21	1:184:A:PHE:HA	10	0.21	0.03	0.22
(1,226)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	10	0.21	0.01	0.21
(1,226)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	10	0.21	0.01	0.21
(2,8781)	1:127:A:ILE:H	1:127:A:ILE:HG13	10	0.21	0.04	0.21
(2,80)	1:156:A:PHE:HA	1:141:A:ILE:HA	10	0.21	0.03	0.2
(1,1571)	1:96:A:VAL:HG21	1:96:A:VAL:HB	10	0.2	0.01	0.2
(1,1571)	1:96:A:VAL:HG23	1:96:A:VAL:HB	10	0.2	0.01	0.2
(2,5519)	1:150:A:ARG:HB2	1:150:A:ARG:HA	10	0.2	0.02	0.21
(2,8697)	1:110:A:ASP:HA	1:110:A:ASP:H	10	0.2	0.07	0.21
(1,2239)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.2	0.01	0.2
(1,304)	1:150:A:ARG:HB2	1:150:A:ARG:HA	10	0.2	0.02	0.2
(1,668)	1:141:A:ILE:HG21	1:141:A:ILE:HB	10	0.2	0.02	0.2
(1,668)	1:181:A:ILE:HG21	1:181:A:ILE:HB	10	0.2	0.02	0.2
(2,126)	1:115:A:LEU:HA	1:115:A:LEU:HD21	10	0.2	0.02	0.2
(2,3731)	1:135:A:GLU:HA	1:164:A:ILE:HA	10	0.2	0.02	0.2
(1,1948)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.2	0.01	0.2
(2,16)	1:113:A:VAL:HG12	1:113:A:VAL:HB	10	0.2	0.07	0.17
(2,16)	1:113:A:VAL:HG13	1:113:A:VAL:HB	10	0.2	0.07	0.17
(2,16)	1:113:A:VAL:HG11	1:113:A:VAL:HB	10	0.2	0.07	0.17
(2,5537)	1:155:A:ALA:HB2	1:154:A:GLU:H	10	0.2	0.05	0.2
(2,7679)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	10	0.2	0.01	0.2
(2,7193)	1:190:A:GLU:HB3	1:190:A:GLU:H	10	0.2	0.03	0.18
(2,6784)	1:97:A:LEU:HB2	1:98:A:LYS:H	10	0.19	0.01	0.19
(2,677)	1:144:A:PRO:HB2	1:144:A:PRO:HA	10	0.19	0.03	0.18
(2,18)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	10	0.19	0.03	0.18
(2,1021)	1:181:A:ILE:HG12	1:181:A:ILE:HD13	10	0.19	0.01	0.2
(2,5866)	1:127:A:ILE:HG23	1:127:A:ILE:HG12	10	0.19	0.08	0.16
(2,829)	1:163:A:GLU:HB2	1:163:A:GLU:HG2	10	0.19	0.04	0.19
(1,1552)	1:97:A:LEU:HG	1:97:A:LEU:HD13	10	0.19	0.02	0.2
(1,1552)	1:97:A:LEU:HG	1:97:A:LEU:HD11	10	0.19	0.02	0.2
(2,4496)	1:169:A:LEU:HD22	1:169:A:LEU:HA	10	0.19	0.07	0.16
(1,1148)	1:146:A:ASP:H	1:143:A:LEU:HD21	10	0.18	0.03	0.2
(2,1207)	1:172:A:HIS:H	1:171:A:LYS:H	10	0.18	0.04	0.19
(2,8405)	1:191:A:VAL:HG22	1:191:A:VAL:HB	10	0.18	0.03	0.18
(2,8578)	1:143:A:LEU:H	1:141:A:ILE:HB	10	0.18	0.04	0.19
(2,3532)	1:190:A:GLU:HB3	1:190:A:GLU:H	10	0.18	0.03	0.16
(2,1853)	1:95:A:TRP:HB3	1:91:A:ASN:HB3	10	0.18	0.02	0.17
(2,2969)	1:116:A:ARG:HG2	1:154:A:GLU:HG2	10	0.18	0.09	0.15
(1,2553)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.18	0.01	0.18
(1,94)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.17	0.01	0.17
(1,106)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.17	0.0	0.17
(1,106)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.17	0.0	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,106)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.17	0.0	0.17
(2,1168)	1:155:A:ALA:HA	1:155:A:ALA:HB3	10	0.17	0.02	0.18
(2,7413)	1:181:A:ILE:HD12	1:183:A:ILE:H	10	0.17	0.04	0.18
(1,1349)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.17	0.0	0.17
(1,1349)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.17	0.0	0.17
(1,1349)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.17	0.0	0.17
(1,1537)	1:150:A:ARG:HB2	1:150:A:ARG:HA	10	0.17	0.02	0.17
(1,1260)	1:183:A:ILE:HG21	1:184:A:PHE:HA	10	0.17	0.04	0.18
(1,743)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.17	0.0	0.17
(1,743)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.17	0.0	0.17
(1,743)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.17	0.0	0.17
(1,1363)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.17	0.01	0.17
(1,1363)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.17	0.01	0.17
(1,1363)	1:144:A:PRO:HB2	1:144:A:PRO:HB3	10	0.17	0.01	0.17
(2,2459)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	10	0.17	0.02	0.18
(2,3091)	1:181:A:ILE:H	1:116:A:ARG:H	10	0.17	0.01	0.17
(2,6533)	1:191:A:VAL:HG22	1:191:A:VAL:HB	10	0.17	0.03	0.16
(2,2660)	1:166:A:GLU:HG3	1:166:A:GLU:HA	10	0.16	0.04	0.17
(2,3606)	1:164:A:ILE:HD12	1:164:A:ILE:HA	10	0.16	0.02	0.16
(2,4433)	1:163:A:GLU:HB3	1:164:A:ILE:H	10	0.16	0.03	0.16
(1,756)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.16	0.01	0.16
(1,756)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.16	0.01	0.16
(1,756)	1:144:A:PRO:HB2	1:144:A:PRO:HB3	10	0.16	0.01	0.16
(1,1350)	1:144:A:PRO:HB3	1:144:A:PRO:HA	10	0.16	0.01	0.16
(2,6519)	1:189:A:ALA:HB1	1:190:A:GLU:H	10	0.15	0.01	0.15
(2,6599)	1:155:A:ALA:HA	1:155:A:ALA:HB3	10	0.15	0.02	0.15
(1,124)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	10	0.15	0.01	0.15
(1,124)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	10	0.15	0.01	0.15
(1,124)	1:144:A:PRO:HB2	1:144:A:PRO:HB3	10	0.15	0.01	0.15
(2,1796)	1:164:A:ILE:HD12	1:164:A:ILE:HA	10	0.15	0.01	0.15
(1,84)	1:115:A:LEU:HG	1:115:A:LEU:HB2	10	0.15	0.02	0.14
(1,858)	1:159:A:PHE:HB2	1:159:A:PHE:HA	10	0.15	0.01	0.15
(2,7388)	1:150:A:ARG:HB2	1:150:A:ARG:HA	10	0.15	0.02	0.15
(1,15)	1:160:A:ALA:HB1	1:160:A:ALA:HA	10	0.15	0.0	0.15
(1,31)	1:181:A:ILE:HG21	1:181:A:ILE:HB	10	0.15	0.01	0.15
(4,1)	1:113:A:VAL:H	1:157:A:VAL:O	10	0.15	0.03	0.14
(1,1341)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.14	0.01	0.14
(2,1849)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	10	0.14	0.01	0.14
(1,1466)	1:159:A:PHE:HB2	1:159:A:PHE:HA	10	0.14	0.01	0.14
(2,4269)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	10	0.14	0.02	0.15
(2,5741)	1:115:A:LEU:HA	1:115:A:LEU:HB2	10	0.14	0.0	0.14
(1,744)	1:144:A:PRO:HB3	1:144:A:PRO:HA	10	0.13	0.01	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1329)	1:115:A:LEU:HG	1:115:A:LEU:HB2	10	0.13	0.01	0.12
(1,734)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.13	0.01	0.13
(1,107)	1:126:A:GLU:HB3	1:126:A:GLU:HA	10	0.13	0.02	0.12
(1,107)	1:144:A:PRO:HB3	1:144:A:PRO:HA	10	0.13	0.02	0.12
(1,1362)	1:144:A:PRO:HB3	1:144:A:PRO:HA	10	0.13	0.01	0.13
(1,993)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	10	0.13	0.01	0.13
(2,3657)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	10	0.12	0.01	0.12
(2,1892)	1:92:A:ALA:HA	1:92:A:ALA:HB1	10	0.12	0.0	0.12
(2,2585)	1:159:A:PHE:HA	1:158:A:GLN:HA	10	0.12	0.0	0.12
(1,1346)	1:144:A:PRO:HB3	1:144:A:PRO:HA	10	0.12	0.01	0.12
(2,4133)	1:135:A:GLU:HG3	1:135:A:GLU:HA	10	0.11	0.01	0.11
(2,883)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	9	1.45	0.29	1.65
(2,500)	1:130:A:PHE:HB2	1:131:A:PHE:H	9	1.13	0.26	1.27
(1,132)	1:166:A:GLU:HG3	1:168:A:ALA:H	9	1.03	0.15	0.97
(2,1161)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	9	1.01	0.06	1.02
(2,2287)	1:130:A:PHE:HB2	1:131:A:PHE:H	9	0.98	0.25	1.12
(2,837)	1:163:A:GLU:HG3	1:163:A:GLU:H	9	0.96	0.1	0.98
(2,3538)	1:192:A:ARG:HG2	1:192:A:ARG:H	9	0.96	0.3	1.07
(2,4098)	1:130:A:PHE:HB2	1:131:A:PHE:H	9	0.95	0.26	1.09
(1,329)	1:166:A:GLU:HG3	1:168:A:ALA:H	9	0.9	0.15	0.85
(2,4764)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	9	0.89	0.06	0.9
(1,838)	1:115:A:LEU:HA	1:114:A:ARG:HG3	9	0.87	0.39	0.99
(1,1447)	1:115:A:LEU:HA	1:114:A:ARG:HG3	9	0.87	0.39	0.99
(2,1844)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	9	0.85	0.6	1.09
(2,95)	1:159:A:PHE:HB2	1:135:A:GLU:H	9	0.82	0.41	0.76
(2,2957)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	9	0.81	0.07	0.82
(1,1188)	1:165:A:ALA:H	1:110:A:ASP:HB3	9	0.76	0.43	0.56
(1,1188)	1:165:A:ALA:H	1:112:A:PHE:HB3	9	0.76	0.43	0.56
(1,2666)	1:115:A:LEU:HA	1:114:A:ARG:HG3	9	0.74	0.39	0.86
(2,7788)	1:130:A:PHE:HB2	1:131:A:PHE:H	9	0.68	0.25	0.82
(2,5915)	1:130:A:PHE:HB2	1:131:A:PHE:H	9	0.67	0.26	0.81
(2,5840)	1:126:A:GLU:HG3	1:127:A:ILE:H	9	0.65	0.5	0.58
(1,2415)	1:165:A:ALA:H	1:110:A:ASP:HB3	9	0.64	0.43	0.45
(1,2415)	1:165:A:ALA:H	1:112:A:PHE:HB3	9	0.64	0.43	0.45
(1,160)	1:102:A:PRO:HG2	1:101:A:GLY:HA3	9	0.63	0.12	0.66
(2,22)	1:113:A:VAL:HG13	1:112:A:PHE:H	9	0.63	0.96	0.34
(2,22)	1:113:A:VAL:HG12	1:112:A:PHE:H	9	0.63	0.96	0.34
(1,1106)	1:161:A:SER:H	1:110:A:ASP:HB3	9	0.63	0.53	0.33
(1,570)	1:150:A:ARG:HG2	1:151:A:SER:H	9	0.6	0.05	0.61
(1,570)	1:150:A:ARG:HB3	1:151:A:SER:H	9	0.6	0.05	0.61
(2,1638)	1:166:A:GLU:HB3	1:166:A:GLU:H	9	0.59	0.15	0.67
(1,1788)	1:132:A:SER:H	1:136:A:ILE:HB	9	0.59	0.19	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1069)	1:168:A:ALA:HB3	1:167:A:LYS:H	9	0.59	0.14	0.54
(1,1069)	1:168:A:ALA:HB2	1:167:A:LYS:H	9	0.59	0.14	0.54
(1,1069)	1:168:A:ALA:HB1	1:167:A:LYS:H	9	0.59	0.14	0.54
(2,1647)	1:171:A:LYS:H	1:170:A:LYS:HB2	9	0.58	0.41	0.86
(2,4777)	1:111:A:GLY:HA3	1:109:A:ASN:H	9	0.58	0.36	0.44
(1,1681)	1:168:A:ALA:HB3	1:167:A:LYS:H	9	0.54	0.14	0.49
(1,1681)	1:168:A:ALA:HB2	1:167:A:LYS:H	9	0.54	0.14	0.49
(1,1681)	1:168:A:ALA:HB1	1:167:A:LYS:H	9	0.54	0.14	0.49
(2,5243)	1:166:A:GLU:HB3	1:166:A:GLU:H	9	0.53	0.15	0.6
(1,459)	1:168:A:ALA:HB3	1:167:A:LYS:H	9	0.53	0.14	0.48
(1,459)	1:168:A:ALA:HB2	1:167:A:LYS:H	9	0.53	0.14	0.48
(1,459)	1:168:A:ALA:HB1	1:167:A:LYS:H	9	0.53	0.14	0.48
(2,54)	1:191:A:VAL:HG13	1:137:A:VAL:HG13	9	0.52	0.24	0.53
(2,54)	1:191:A:VAL:HG13	1:137:A:VAL:HG12	9	0.52	0.24	0.53
(2,54)	1:191:A:VAL:HG12	1:137:A:VAL:HG11	9	0.52	0.24	0.53
(2,54)	1:191:A:VAL:HG13	1:137:A:VAL:HG11	9	0.52	0.24	0.53
(2,5451)	1:191:A:VAL:HG13	1:137:A:VAL:HG13	9	0.52	0.24	0.53
(2,5451)	1:191:A:VAL:HG13	1:137:A:VAL:HG12	9	0.52	0.24	0.53
(2,5451)	1:191:A:VAL:HG12	1:137:A:VAL:HG11	9	0.52	0.24	0.53
(2,5451)	1:191:A:VAL:HG13	1:137:A:VAL:HG11	9	0.52	0.24	0.53
(2,7320)	1:191:A:VAL:HG13	1:137:A:VAL:HG13	9	0.52	0.24	0.53
(2,7320)	1:191:A:VAL:HG13	1:137:A:VAL:HG12	9	0.52	0.24	0.53
(2,7320)	1:191:A:VAL:HG12	1:137:A:VAL:HG11	9	0.52	0.24	0.53
(2,7320)	1:191:A:VAL:HG13	1:137:A:VAL:HG11	9	0.52	0.24	0.53
(1,846)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.52	0.25	0.72
(1,846)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	9	0.52	0.25	0.72
(2,7269)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	9	0.52	0.29	0.32
(1,1798)	1:165:A:ALA:H	1:110:A:ASP:HB3	9	0.51	0.43	0.31
(1,1798)	1:165:A:ALA:H	1:112:A:PHE:HB3	9	0.51	0.43	0.31
(1,46)	1:167:A:LYS:HG2	1:134:A:LEU:HD11	9	0.51	0.07	0.52
(1,46)	1:167:A:LYS:HG2	1:134:A:LEU:HD12	9	0.51	0.07	0.52
(1,1452)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.5	0.25	0.7
(1,1452)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	9	0.5	0.25	0.7
(1,820)	1:98:A:LYS:HA	1:100:A:THR:HG23	9	0.5	0.2	0.53
(1,820)	1:98:A:LYS:HA	1:100:A:THR:HG22	9	0.5	0.2	0.53
(1,820)	1:93:A:MET:HA	1:92:A:ALA:HB2	9	0.5	0.2	0.53
(1,2674)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.5	0.25	0.7
(1,2674)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	9	0.5	0.25	0.7
(1,2298)	1:168:A:ALA:HB3	1:167:A:LYS:H	9	0.49	0.14	0.45
(1,2298)	1:168:A:ALA:HB2	1:167:A:LYS:H	9	0.49	0.14	0.45
(1,2298)	1:168:A:ALA:HB1	1:167:A:LYS:H	9	0.49	0.14	0.45
(1,224)	1:116:A:ARG:HD2	1:116:A:ARG:HA	9	0.48	0.04	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,224)	1:116:A:ARG:HD3	1:116:A:ARG:HA	9	0.48	0.04	0.48
(1,2068)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.48	0.25	0.68
(1,2068)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	9	0.48	0.25	0.68
(2,8131)	1:163:A:GLU:HG3	1:163:A:GLU:H	9	0.47	0.1	0.49
(2,3443)	1:166:A:GLU:HB3	1:166:A:GLU:H	9	0.47	0.15	0.54
(1,3030)	1:165:A:ALA:H	1:110:A:ASP:HB3	9	0.46	0.43	0.27
(1,3030)	1:165:A:ALA:H	1:112:A:PHE:HB3	9	0.46	0.43	0.27
(4,7)	1:116:A:ARG:H	1:182:A:GLU:O	9	0.46	0.15	0.45
(2,8959)	1:166:A:GLU:HB3	1:166:A:GLU:H	9	0.45	0.16	0.53
(2,2657)	1:166:A:GLU:HB2	1:166:A:GLU:HA	9	0.38	0.05	0.37
(2,7230)	1:150:A:ARG:HG2	1:151:A:SER:H	9	0.38	0.2	0.35
(1,2910)	1:168:A:ALA:HB3	1:167:A:LYS:H	9	0.38	0.14	0.33
(1,2910)	1:168:A:ALA:HB2	1:167:A:LYS:H	9	0.38	0.14	0.33
(1,2910)	1:168:A:ALA:HB1	1:167:A:LYS:H	9	0.38	0.14	0.33
(2,7104)	1:166:A:GLU:HB3	1:166:A:GLU:H	9	0.37	0.15	0.44
(2,3906)	1:111:A:GLY:HA3	1:112:A:PHE:H	9	0.36	0.06	0.34
(2,868)	1:166:A:GLU:HB2	1:166:A:GLU:HA	9	0.35	0.05	0.35
(2,307)	1:111:A:GLY:HA3	1:112:A:PHE:H	9	0.35	0.06	0.34
(1,848)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.34	0.07	0.33
(1,848)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	9	0.34	0.07	0.33
(1,3003)	1:108:A:ALA:H	1:109:A:ASN:HA	9	0.34	0.21	0.31
(2,6592)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	9	0.33	0.07	0.34
(2,5829)	1:124:A:LYS:HA	1:124:A:LYS:HB2	9	0.32	0.22	0.22
(1,411)	1:164:A:ILE:HD13	1:135:A:GLU:HA	9	0.32	0.04	0.32
(1,411)	1:164:A:ILE:HD13	1:93:A:MET:HA	9	0.32	0.04	0.32
(2,100)	1:181:A:ILE:HG21	1:174:A:GLU:HA	9	0.31	0.11	0.3
(1,1178)	1:132:A:SER:H	1:136:A:ILE:HB	9	0.31	0.18	0.21
(2,2202)	1:122:A:CYS:HA	1:122:A:CYS:HB2	9	0.31	0.01	0.31
(2,5498)	1:116:A:ARG:HD2	1:116:A:ARG:HA	9	0.31	0.04	0.3
(1,1455)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.31	0.07	0.3
(1,1455)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	9	0.31	0.07	0.3
(1,2405)	1:132:A:SER:H	1:136:A:ILE:HB	9	0.3	0.19	0.2
(1,910)	1:97:A:LEU:HD11	1:163:A:GLU:HB3	9	0.3	0.14	0.26
(1,910)	1:97:A:LEU:HD12	1:163:A:GLU:HB3	9	0.3	0.14	0.26
(1,910)	1:141:A:ILE:HG21	1:143:A:LEU:HG	9	0.3	0.14	0.26
(1,1175)	1:106:A:ASP:H	1:105:A:PRO:HD2	9	0.29	0.09	0.27
(1,1175)	1:106:A:ASP:H	1:105:A:PRO:HD3	9	0.29	0.09	0.27
(1,2675)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.29	0.07	0.29
(1,2675)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	9	0.29	0.07	0.29
(2,4792)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	9	0.29	0.04	0.31
(1,764)	1:166:A:GLU:HG3	1:168:A:ALA:H	9	0.29	0.15	0.23
(2,1806)	1:160:A:ALA:HB2	1:162:A:GLN:H	9	0.29	0.05	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,6699)	1:168:A:ALA:H	1:167:A:LYS:HB3	9	0.28	0.08	0.3
(2,1797)	1:164:A:ILE:HD13	1:91:A:ASN:HA	9	0.28	0.1	0.32
(1,995)	1:123:A:SER:HB3	1:181:A:ILE:HD11	9	0.28	0.13	0.25
(1,1784)	1:189:A:ALA:H	1:186:A:SER:HA	9	0.28	0.16	0.31
(2,7105)	1:166:A:GLU:HB3	1:167:A:LYS:H	9	0.28	0.13	0.26
(2,3050)	1:159:A:PHE:HA	1:135:A:GLU:H	9	0.28	0.09	0.23
(2,6751)	1:151:A:SER:H	1:151:A:SER:HB2	9	0.27	0.04	0.28
(2,7290)	1:96:A:VAL:HG22	1:97:A:LEU:H	9	0.27	0.08	0.31
(2,4012)	1:122:A:CYS:HA	1:122:A:CYS:HB2	9	0.27	0.01	0.27
(2,7569)	1:107:A:THR:HA	1:107:A:THR:HG22	9	0.26	0.01	0.27
(2,1639)	1:166:A:GLU:HB3	1:167:A:LYS:H	9	0.26	0.13	0.24
(2,3728)	1:123:A:SER:HB3	1:181:A:ILE:HD11	9	0.26	0.13	0.22
(2,8608)	1:151:A:SER:H	1:151:A:SER:HB2	9	0.25	0.04	0.26
(2,595)	1:139:A:ASN:HA	1:140:A:GLY:HA3	9	0.24	0.04	0.26
(2,4430)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	9	0.24	0.01	0.24
(1,2069)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.24	0.06	0.23
(1,2069)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	9	0.24	0.06	0.23
(2,7322)	1:191:A:VAL:HG11	1:190:A:GLU:H	9	0.24	0.07	0.25
(2,7322)	1:191:A:VAL:HG13	1:190:A:GLU:H	9	0.24	0.07	0.25
(2,7322)	1:191:A:VAL:HG12	1:190:A:GLU:H	9	0.24	0.07	0.25
(1,2076)	1:159:A:PHE:HB2	1:166:A:GLU:H	9	0.23	0.07	0.23
(1,2076)	1:150:A:ARG:HD3	1:149:A:GLY:H	9	0.23	0.07	0.23
(2,4468)	1:166:A:GLU:HB2	1:166:A:GLU:HA	9	0.23	0.05	0.22
(2,76)	1:107:A:THR:HB	1:110:A:ASP:HA	9	0.23	0.05	0.25
(2,7379)	1:126:A:GLU:HA	1:136:A:ILE:HB	9	0.23	0.05	0.21
(1,1027)	1:164:A:ILE:HD13	1:135:A:GLU:HA	9	0.22	0.04	0.22
(1,1027)	1:164:A:ILE:HD13	1:93:A:MET:HA	9	0.22	0.04	0.22
(2,1169)	1:115:A:LEU:HD23	1:114:A:ARG:HA	9	0.22	0.03	0.22
(2,4898)	1:159:A:PHE:H	1:110:A:ASP:HA	9	0.22	0.05	0.22
(2,1106)	1:191:A:VAL:HG11	1:191:A:VAL:HA	9	0.22	0.09	0.18
(2,880)	1:167:A:LYS:HB2	1:167:A:LYS:HA	9	0.22	0.01	0.22
(2,2097)	1:111:A:GLY:HA3	1:112:A:PHE:H	9	0.22	0.06	0.2
(2,5328)	1:190:A:GLU:HB3	1:191:A:VAL:H	9	0.21	0.05	0.23
(2,9104)	1:122:A:CYS:H	1:151:A:SER:HB2	9	0.21	0.04	0.2
(2,6558)	1:192:A:ARG:HD2	1:192:A:ARG:HB2	9	0.2	0.13	0.14
(1,1315)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	9	0.2	0.02	0.2
(2,2578)	1:157:A:VAL:HG21	1:157:A:VAL:HA	9	0.2	0.03	0.19
(2,3608)	1:164:A:ILE:HD11	1:161:A:SER:H	9	0.19	0.03	0.19
(1,1956)	1:96:A:VAL:HB	1:96:A:VAL:HA	9	0.18	0.01	0.19
(1,1956)	1:181:A:ILE:HB	1:181:A:ILE:HA	9	0.18	0.01	0.19
(1,1759)	1:146:A:ASP:H	1:143:A:LEU:HD21	9	0.17	0.03	0.17
(2,3668)	1:154:A:GLU:HG2	1:118:A:LEU:H	9	0.16	0.03	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4481)	1:167:A:LYS:HB2	1:167:A:LYS:HA	9	0.16	0.01	0.16
(2,1067)	1:187:A:SER:HB2	1:187:A:SER:HA	9	0.15	0.02	0.15
(2,2619)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	9	0.15	0.01	0.15
(2,2670)	1:167:A:LYS:HB2	1:167:A:LYS:HA	9	0.15	0.01	0.15
(2,4390)	1:157:A:VAL:HG21	1:157:A:VAL:HA	9	0.15	0.03	0.14
(1,2777)	1:97:A:LEU:HG	1:97:A:LEU:HD13	9	0.15	0.02	0.15
(1,2777)	1:97:A:LEU:HG	1:97:A:LEU:HD11	9	0.15	0.02	0.15
(1,2003)	1:130:A:PHE:HB3	1:132:A:SER:H	9	0.14	0.03	0.14
(2,8566)	1:139:A:ASN:H	1:141:A:ILE:HD12	9	0.14	0.02	0.14
(2,2180)	1:119:A:PRO:HA	1:119:A:PRO:HG3	9	0.13	0.02	0.13
(2,6036)	1:141:A:ILE:HG13	1:141:A:ILE:H	9	0.13	0.01	0.13
(2,7270)	1:164:A:ILE:HD12	1:164:A:ILE:HA	9	0.13	0.01	0.13
(1,667)	1:181:A:ILE:HG21	1:181:A:ILE:HB	9	0.13	0.01	0.12
(1,1624)	1:144:A:PRO:HB3	1:144:A:PRO:HA	9	0.12	0.0	0.12
(2,3697)	1:92:A:ALA:HA	1:92:A:ALA:HB1	9	0.11	0.0	0.11
(1,841)	1:111:A:GLY:HA3	1:188:A:ARG:HG3	8	1.12	0.63	1.35
(1,841)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	8	1.12	0.63	1.35
(2,5335)	1:192:A:ARG:HG2	1:192:A:ARG:H	8	0.93	0.02	0.94
(2,1730)	1:192:A:ARG:HG2	1:192:A:ARG:H	8	0.88	0.02	0.88
(1,2772)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	8	0.79	0.81	0.42
(2,1777)	1:166:A:GLU:H	1:169:A:LEU:HB2	8	0.77	0.73	0.26
(1,456)	1:165:A:ALA:HA	1:113:A:VAL:HG23	8	0.65	0.29	0.7
(1,456)	1:165:A:ALA:HA	1:113:A:VAL:HG21	8	0.65	0.29	0.7
(1,456)	1:94:A:ASP:HA	1:164:A:ILE:HD13	8	0.65	0.29	0.7
(2,85)	1:187:A:SER:HB3	1:189:A:ALA:H	8	0.63	0.22	0.64
(2,4)	1:164:A:ILE:HD11	1:161:A:SER:HB3	8	0.61	0.06	0.63
(2,4670)	1:187:A:SER:HB3	1:188:A:ARG:H	8	0.5	0.06	0.51
(1,643)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	8	0.39	0.04	0.38
(1,643)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	8	0.39	0.04	0.38
(2,932)	1:174:A:GLU:HG3	1:175:A:ARG:H	8	0.39	0.06	0.38
(1,1992)	1:158:A:GLN:HG2	1:161:A:SER:H	8	0.39	0.12	0.4
(1,1992)	1:158:A:GLN:HG3	1:161:A:SER:H	8	0.39	0.12	0.4
(2,2984)	1:188:A:ARG:HD2	1:108:A:ALA:H	8	0.37	0.16	0.38
(1,2432)	1:145:A:VAL:HA	1:151:A:SER:H	8	0.36	0.12	0.34
(1,1251)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	8	0.32	0.04	0.3
(1,1251)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	8	0.32	0.04	0.3
(1,3050)	1:145:A:VAL:HA	1:151:A:SER:H	8	0.32	0.12	0.31
(2,1069)	1:187:A:SER:HB3	1:188:A:ARG:H	8	0.31	0.06	0.32
(1,1563)	1:166:A:GLU:HG3	1:168:A:ALA:H	8	0.3	0.15	0.24
(2,7377)	1:181:A:ILE:HG21	1:174:A:GLU:HA	8	0.27	0.11	0.27
(1,8)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	8	0.26	0.04	0.24
(1,8)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	8	0.26	0.04	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1850)	1:118:A:LEU:H	1:118:A:LEU:HD12	8	0.26	0.03	0.26
(4,30)	1:157:A:VAL:H	1:113:A:VAL:O	8	0.24	0.06	0.26
(2,5)	1:164:A:ILE:HD13	1:91:A:ASN:HA	8	0.24	0.09	0.26
(1,2739)	1:143:A:LEU:HG	1:141:A:ILE:HG21	8	0.24	0.16	0.2
(1,297)	1:164:A:ILE:HD13	1:93:A:MET:HG3	8	0.23	0.14	0.17
(2,8461)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	8	0.23	0.05	0.23
(1,288)	1:141:A:ILE:HG21	1:143:A:LEU:HG	8	0.23	0.16	0.18
(1,2133)	1:97:A:LEU:HD12	1:163:A:GLU:HB3	8	0.22	0.13	0.18
(1,2133)	1:143:A:LEU:HG	1:141:A:ILE:HG21	8	0.22	0.13	0.18
(1,2133)	1:97:A:LEU:HD11	1:163:A:GLU:HB3	8	0.22	0.13	0.18
(2,8779)	1:127:A:ILE:H	1:127:A:ILE:HG12	8	0.2	0.03	0.2
(2,27)	1:181:A:ILE:HG21	1:174:A:GLU:H	8	0.2	0.05	0.2
(2,139)	1:102:A:PRO:HA	1:103:A:ASN:H	8	0.18	0.03	0.19
(2,5721)	1:111:A:GLY:HA3	1:112:A:PHE:H	8	0.18	0.05	0.18
(1,1859)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	8	0.17	0.04	0.16
(1,1859)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	8	0.17	0.04	0.16
(2,4869)	1:108:A:ALA:H	1:188:A:ARG:HG2	8	0.17	0.04	0.16
(2,2172)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	8	0.16	0.01	0.16
(1,1269)	1:137:A:VAL:HG22	1:140:A:GLY:H	8	0.16	0.03	0.15
(4,48)	1:183:A:ILE:H	1:171:A:LYS:O	8	0.16	0.05	0.15
(2,8951)	1:164:A:ILE:H	1:164:A:ILE:HG21	8	0.16	0.02	0.16
(4,10)	1:117:A:GLY:N	1:153:A:GLY:O	8	0.16	0.02	0.16
(2,1729)	1:191:A:VAL:HG13	1:191:A:VAL:H	8	0.15	0.05	0.14
(2,1729)	1:191:A:VAL:HG12	1:191:A:VAL:H	8	0.15	0.05	0.14
(1,2472)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	8	0.15	0.04	0.12
(1,2472)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	8	0.15	0.04	0.12
(3,499)	1:139:A:ASN:H	1:128:A:VAL:HA	8	0.15	0.02	0.14
(3,625)	1:139:A:ASN:H	1:128:A:VAL:HA	8	0.15	0.02	0.14
(2,6233)	1:161:A:SER:HB2	1:161:A:SER:HA	8	0.14	0.01	0.14
(2,8120)	1:163:A:GLU:HB3	1:163:A:GLU:HA	8	0.14	0.02	0.14
(2,1630)	1:164:A:ILE:H	1:164:A:ILE:HG21	8	0.14	0.02	0.13
(2,8105)	1:160:A:ALA:HB3	1:161:A:SER:H	8	0.14	0.02	0.14
(2,7721)	1:127:A:ILE:HD12	1:127:A:ILE:HB	8	0.13	0.04	0.11
(2,352)	1:115:A:LEU:HA	1:115:A:LEU:HD21	8	0.12	0.01	0.12
(2,5526)	1:97:A:LEU:HD13	1:97:A:LEU:HA	8	0.12	0.01	0.12
(2,3981)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	8	0.12	0.01	0.12
(2,8106)	1:161:A:SER:HB2	1:161:A:SER:HA	8	0.11	0.01	0.11
(2,3635)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	7	1.28	0.68	1.63
(1,854)	1:179:A:ARG:HD2	1:179:A:ARG:HA	7	0.9	0.6	0.76
(1,854)	1:156:A:PHE:HB3	1:142:A:THR:HB	7	0.9	0.6	0.76
(1,2316)	1:156:A:PHE:HB2	1:141:A:ILE:HG23	7	0.79	0.4	0.97
(1,2316)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	7	0.79	0.4	0.97

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,232)	1:100:A:THR:HA	1:99:A:HIS:HB2	7	0.78	0.07	0.78
(1,2928)	1:156:A:PHE:HB2	1:141:A:ILE:HG23	7	0.76	0.4	0.94
(1,2928)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	7	0.76	0.4	0.94
(2,2019)	1:100:A:THR:HA	1:99:A:HIS:HB2	7	0.69	0.07	0.7
(2,4516)	1:171:A:LYS:HB3	1:171:A:LYS:H	7	0.61	0.07	0.62
(2,2705)	1:171:A:LYS:HB3	1:171:A:LYS:H	7	0.61	0.07	0.62
(1,368)	1:169:A:LEU:HD21	1:167:A:LYS:H	7	0.51	0.05	0.51
(1,251)	1:188:A:ARG:HD3	1:191:A:VAL:HG22	7	0.49	0.19	0.49
(1,251)	1:112:A:PHE:HB2	1:191:A:VAL:HG22	7	0.49	0.19	0.49
(2,5466)	1:166:A:GLU:HG2	1:166:A:GLU:H	7	0.48	0.4	0.23
(2,915)	1:171:A:LYS:HB3	1:171:A:LYS:H	7	0.46	0.07	0.47
(2,6345)	1:171:A:LYS:HB3	1:171:A:LYS:H	7	0.44	0.07	0.45
(1,2596)	1:163:A:GLU:HG3	1:163:A:GLU:HA	7	0.41	0.03	0.4
(2,1243)	1:127:A:ILE:H	1:115:A:LEU:HD22	7	0.39	0.15	0.48
(2,8217)	1:171:A:LYS:HB3	1:171:A:LYS:H	7	0.39	0.07	0.4
(2,1574)	1:155:A:ALA:H	1:154:A:GLU:HB2	7	0.39	0.06	0.39
(1,1706)	1:174:A:GLU:HA	1:181:A:ILE:H	7	0.37	0.14	0.39
(1,1706)	1:141:A:ILE:HA	1:140:A:GLY:H	7	0.37	0.14	0.39
(2,3679)	1:187:A:SER:HB3	1:189:A:ALA:H	7	0.37	0.16	0.32
(1,159)	1:95:A:TRP:HA	1:96:A:VAL:H	7	0.33	0.02	0.33
(1,159)	1:159:A:PHE:HA	1:137:A:VAL:H	7	0.33	0.02	0.33
(2,1815)	1:176:A:ILE:HG22	1:120:A:PHE:H	7	0.31	0.05	0.33
(2,1815)	1:176:A:ILE:HG21	1:120:A:PHE:H	7	0.31	0.05	0.33
(2,1815)	1:176:A:ILE:HG23	1:120:A:PHE:H	7	0.31	0.05	0.33
(2,1873)	1:187:A:SER:HB3	1:189:A:ALA:H	7	0.31	0.16	0.26
(2,3470)	1:175:A:ARG:HB3	1:176:A:ILE:H	7	0.3	0.25	0.22
(1,1868)	1:113:A:VAL:HG12	1:113:A:VAL:HB	7	0.29	0.09	0.25
(1,1868)	1:183:A:ILE:HG22	1:113:A:VAL:HB	7	0.29	0.09	0.25
(1,1868)	1:113:A:VAL:HG13	1:113:A:VAL:HB	7	0.29	0.09	0.25
(1,1868)	1:113:A:VAL:HG11	1:113:A:VAL:HB	7	0.29	0.09	0.25
(1,2974)	1:100:A:THR:HG23	1:98:A:LYS:H	7	0.29	0.08	0.29
(1,2974)	1:100:A:THR:HG22	1:98:A:LYS:H	7	0.29	0.08	0.29
(2,7514)	1:100:A:THR:HA	1:99:A:HIS:HB2	7	0.27	0.07	0.28
(1,2483)	1:113:A:VAL:HG12	1:113:A:VAL:HB	7	0.25	0.09	0.21
(1,2483)	1:183:A:ILE:HG22	1:113:A:VAL:HB	7	0.25	0.09	0.21
(1,2483)	1:113:A:VAL:HG13	1:113:A:VAL:HB	7	0.25	0.09	0.21
(1,2483)	1:113:A:VAL:HG11	1:113:A:VAL:HB	7	0.25	0.09	0.21
(1,1486)	1:143:A:LEU:HA	1:143:A:LEU:HB2	7	0.24	0.07	0.27
(1,1486)	1:169:A:LEU:HB2	1:166:A:GLU:HA	7	0.24	0.07	0.27
(2,4436)	1:163:A:GLU:HG3	1:163:A:GLU:H	7	0.23	0.04	0.23
(2,5402)	1:164:A:ILE:HD13	1:91:A:ASN:HA	7	0.22	0.08	0.23
(2,225)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	7	0.22	0.02	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2625)	1:163:A:GLU:HG3	1:163:A:GLU:H	7	0.22	0.04	0.22
(1,1342)	1:119:A:PRO:HB2	1:177:A:GLY:HA3	7	0.21	0.04	0.23
(1,1342)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	7	0.21	0.04	0.23
(2,5643)	1:100:A:THR:HA	1:99:A:HIS:HB2	7	0.2	0.07	0.21
(1,2635)	1:169:A:LEU:HB2	1:169:A:LEU:HA	7	0.19	0.03	0.19
(2,25)	1:96:A:VAL:HG22	1:161:A:SER:H	7	0.19	0.07	0.18
(1,2030)	1:169:A:LEU:HB2	1:169:A:LEU:HA	7	0.18	0.03	0.18
(1,2746)	1:93:A:MET:HB2	1:93:A:MET:HG2	7	0.18	0.04	0.17
(1,2746)	1:93:A:MET:HB2	1:135:A:GLU:HB3	7	0.18	0.04	0.17
(2,7180)	1:187:A:SER:HB3	1:188:A:ARG:H	7	0.18	0.03	0.19
(2,720)	1:148:A:GLN:HB2	1:148:A:GLN:HG2	7	0.18	0.0	0.18
(2,7394)	1:142:A:THR:HG23	1:141:A:ILE:HG21	7	0.17	0.05	0.16
(2,7394)	1:142:A:THR:HG21	1:141:A:ILE:HG21	7	0.17	0.05	0.16
(2,7394)	1:142:A:THR:HG22	1:141:A:ILE:HG21	7	0.17	0.05	0.16
(1,684)	1:167:A:LYS:HG2	1:134:A:LEU:HD11	7	0.17	0.05	0.16
(1,684)	1:167:A:LYS:HG2	1:134:A:LEU:HD12	7	0.17	0.05	0.16
(1,1700)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	7	0.16	0.02	0.17
(1,1700)	1:114:A:ARG:HG3	1:114:A:ARG:HD2	7	0.16	0.02	0.17
(1,1700)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	7	0.16	0.02	0.17
(2,2510)	1:148:A:GLN:HB2	1:148:A:GLN:HG2	7	0.16	0.0	0.16
(2,2012)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	7	0.16	0.02	0.17
(1,1087)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	7	0.16	0.02	0.16
(1,1087)	1:114:A:ARG:HG3	1:114:A:ARG:HD2	7	0.16	0.02	0.16
(1,1087)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	7	0.16	0.02	0.16
(2,2861)	1:187:A:SER:HB3	1:188:A:ARG:H	7	0.15	0.03	0.16
(1,1638)	1:164:A:ILE:HD13	1:135:A:GLU:HA	7	0.15	0.03	0.17
(1,1638)	1:164:A:ILE:HD13	1:93:A:MET:HA	7	0.15	0.03	0.17
(2,996)	1:181:A:ILE:HD12	1:181:A:ILE:HB	7	0.15	0.03	0.16
(2,3066)	1:108:A:ALA:H	1:188:A:ARG:HG2	7	0.15	0.03	0.13
(2,3104)	1:151:A:SER:H	1:151:A:SER:HB2	7	0.15	0.02	0.14
(2,4907)	1:151:A:SER:H	1:151:A:SER:HB2	7	0.14	0.02	0.14
(2,2841)	1:183:A:ILE:HG21	1:184:A:PHE:HA	7	0.14	0.02	0.14
(2,4657)	1:183:A:ILE:HA	1:183:A:ILE:HD11	7	0.14	0.03	0.14
(4,36)	1:160:A:ALA:H	1:135:A:GLU:O	7	0.14	0.04	0.12
(2,8352)	1:183:A:ILE:HG21	1:184:A:PHE:HA	7	0.14	0.02	0.14
(2,1231)	1:169:A:LEU:H	1:169:A:LEU:HG	7	0.13	0.01	0.13
(2,6)	1:164:A:ILE:HD11	1:161:A:SER:H	7	0.13	0.03	0.12
(1,1272)	1:181:A:ILE:HG21	1:181:A:ILE:HB	7	0.13	0.01	0.13
(1,2563)	1:96:A:VAL:HB	1:96:A:VAL:HA	7	0.13	0.01	0.13
(1,2563)	1:181:A:ILE:HB	1:181:A:ILE:HA	7	0.13	0.01	0.13
(2,6226)	1:157:A:VAL:HG22	1:158:A:GLN:H	7	0.13	0.02	0.13
(3,6)	1:188:A:ARG:HG2	1:190:A:GLU:H	7	0.12	0.01	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,150)	1:188:A:ARG:HG2	1:190:A:GLU:H	7	0.12	0.01	0.12
(3,281)	1:188:A:ARG:HG2	1:190:A:GLU:H	7	0.12	0.01	0.12
(2,121)	1:97:A:LEU:HD13	1:97:A:LEU:HA	7	0.12	0.01	0.12
(2,1133)	1:192:A:ARG:HB2	1:193:A:THR:HA	7	0.12	0.01	0.12
(2,2031)	1:101:A:GLY:HA3	1:101:A:GLY:H	7	0.12	0.01	0.13
(1,1607)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	7	0.11	0.01	0.11
(2,551)	1:136:A:ILE:HG12	1:136:A:ILE:HG22	7	0.11	0.01	0.11
(2,6205)	1:157:A:VAL:HG22	1:157:A:VAL:HG11	7	0.11	0.01	0.11
(1,1960)	1:144:A:PRO:HB3	1:144:A:PRO:HA	7	0.11	0.0	0.11
(2,7300)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	6	1.39	0.54	1.57
(2,5432)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	6	1.37	0.54	1.55
(2,3000)	1:187:A:SER:H	1:184:A:PHE:HB2	6	1.3	0.17	1.39
(2,4805)	1:187:A:SER:H	1:184:A:PHE:HB2	6	1.24	0.17	1.34
(2,1200)	1:187:A:SER:H	1:184:A:PHE:HB2	6	1.1	0.17	1.19
(2,3652)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	6	1.08	0.43	1.2
(2,6313)	1:167:A:LYS:HG2	1:167:A:LYS:HE3	6	0.88	0.04	0.87
(1,2926)	1:179:A:ARG:HD2	1:179:A:ARG:HA	6	0.85	0.55	0.94
(1,2926)	1:156:A:PHE:HB3	1:142:A:THR:HB	6	0.85	0.55	0.94
(1,2060)	1:115:A:LEU:HA	1:114:A:ARG:HG3	6	0.83	0.18	0.77
(1,2314)	1:179:A:ARG:HD2	1:179:A:ARG:HA	6	0.81	0.55	0.9
(1,2314)	1:156:A:PHE:HB3	1:142:A:THR:HB	6	0.81	0.55	0.9
(1,2058)	1:115:A:LEU:HA	1:114:A:ARG:HG3	6	0.79	0.18	0.74
(2,9)	1:181:A:ILE:HG12	1:175:A:ARG:HD2	6	0.77	0.64	0.43
(2,3622)	1:113:A:VAL:HG13	1:112:A:PHE:H	6	0.74	1.1	0.26
(2,3622)	1:113:A:VAL:HG12	1:112:A:PHE:H	6	0.74	1.1	0.26
(2,1813)	1:113:A:VAL:HG13	1:112:A:PHE:H	6	0.69	1.11	0.2
(2,1813)	1:113:A:VAL:HG12	1:112:A:PHE:H	6	0.69	1.11	0.2
(1,2702)	1:169:A:LEU:HB2	1:166:A:GLU:HA	6	0.65	0.52	0.63
(1,2702)	1:143:A:LEU:HG	1:143:A:LEU:HA	6	0.65	0.52	0.63
(2,6165)	1:150:A:ARG:HG3	1:150:A:ARG:HD3	6	0.63	0.01	0.63
(2,2530)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	6	0.6	0.01	0.6
(2,8017)	1:148:A:GLN:HB2	1:149:A:GLY:H	6	0.58	0.19	0.66
(2,8038)	1:150:A:ARG:HG3	1:150:A:ARG:HD3	6	0.57	0.01	0.56
(2,4341)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	6	0.55	0.01	0.54
(1,1462)	1:175:A:ARG:HD2	1:178:A:HIS:HA	6	0.47	0.11	0.48
(1,1462)	1:116:A:ARG:HD2	1:116:A:ARG:HA	6	0.47	0.11	0.48
(2,4321)	1:148:A:GLN:HB2	1:149:A:GLY:H	6	0.47	0.19	0.54
(2,2511)	1:148:A:GLN:HB2	1:149:A:GLY:H	6	0.44	0.19	0.52
(1,1067)	1:165:A:ALA:HA	1:113:A:VAL:HG23	6	0.43	0.15	0.42
(1,1067)	1:94:A:ASP:HA	1:164:A:ILE:HD13	6	0.43	0.15	0.42
(2,2663)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	6	0.4	0.21	0.38
(2,3196)	1:110:A:ASP:HB3	1:110:A:ASP:H	6	0.39	0.28	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,8035)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	6	0.39	0.01	0.38
(2,874)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	6	0.38	0.21	0.37
(2,9082)	1:150:A:ARG:HG2	1:151:A:SER:H	6	0.37	0.17	0.32
(1,2932)	1:174:A:GLU:HA	1:181:A:ILE:H	6	0.36	0.1	0.38
(1,2932)	1:141:A:ILE:HA	1:140:A:GLY:H	6	0.36	0.1	0.38
(2,8701)	1:110:A:ASP:HB3	1:110:A:ASP:H	6	0.35	0.28	0.19
(2,4474)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	6	0.35	0.21	0.34
(2,6162)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	6	0.35	0.01	0.35
(1,2319)	1:174:A:GLU:HA	1:181:A:ILE:H	6	0.31	0.1	0.34
(1,2319)	1:141:A:ILE:HA	1:140:A:GLY:H	6	0.31	0.1	0.34
(1,1091)	1:174:A:GLU:HA	1:181:A:ILE:H	6	0.3	0.09	0.3
(1,1091)	1:141:A:ILE:HA	1:140:A:GLY:H	6	0.3	0.09	0.3
(1,1091)	1:137:A:VAL:HA	1:140:A:GLY:H	6	0.3	0.09	0.3
(1,1658)	1:143:A:LEU:HD23	1:123:A:SER:HA	6	0.3	0.12	0.32
(2,1327)	1:96:A:VAL:HG13	1:97:A:LEU:H	6	0.27	0.02	0.26
(2,3444)	1:166:A:GLU:HB3	1:167:A:LYS:H	6	0.27	0.11	0.28
(2,1613)	1:162:A:GLN:HB2	1:163:A:GLU:H	6	0.27	0.31	0.13
(2,5244)	1:166:A:GLU:HB3	1:167:A:LYS:H	6	0.25	0.11	0.26
(2,7356)	1:175:A:ARG:HA	1:179:A:ARG:H	6	0.24	0.03	0.24
(2,2090)	1:110:A:ASP:HB2	1:110:A:ASP:HA	6	0.23	0.1	0.19
(2,3676)	1:175:A:ARG:HA	1:179:A:ARG:H	6	0.23	0.03	0.22
(2,8182)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	6	0.23	0.03	0.23
(2,4934)	1:96:A:VAL:HG13	1:97:A:LEU:H	6	0.22	0.02	0.21
(1,504)	1:166:A:GLU:H	1:169:A:LEU:HD13	6	0.21	0.11	0.15
(2,8560)	1:168:A:ALA:H	1:167:A:LYS:HB3	6	0.2	0.05	0.2
(1,641)	1:141:A:ILE:HD13	1:125:A:GLU:H	6	0.19	0.03	0.18
(1,641)	1:141:A:ILE:HD12	1:125:A:GLU:H	6	0.19	0.03	0.18
(1,985)	1:169:A:LEU:HD21	1:167:A:LYS:H	6	0.19	0.05	0.18
(2,8688)	1:107:A:THR:HB	1:107:A:THR:H	6	0.18	0.02	0.18
(1,1014)	1:135:A:GLU:HA	1:136:A:ILE:HB	6	0.17	0.05	0.17
(1,1598)	1:169:A:LEU:HD21	1:167:A:LYS:H	6	0.17	0.05	0.16
(2,8414)	1:191:A:VAL:HG13	1:192:A:ARG:HA	6	0.15	0.04	0.14
(2,7693)	1:122:A:CYS:HA	1:121:A:GLY:H	6	0.14	0.03	0.15
(2,5355)	1:158:A:GLN:H	1:141:A:ILE:HB	6	0.14	0.03	0.13
(2,790)	1:157:A:VAL:HG21	1:157:A:VAL:HA	6	0.14	0.02	0.14
(2,3821)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	6	0.14	0.01	0.14
(2,2987)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	6	0.14	0.01	0.14
(2,7498)	1:96:A:VAL:HG22	1:97:A:LEU:H	6	0.14	0.02	0.14
(2,5542)	1:181:A:ILE:HD12	1:183:A:ILE:H	6	0.13	0.02	0.13
(2,7433)	1:92:A:ALA:HB3	1:93:A:MET:H	6	0.13	0.02	0.13
(4,32)	1:158:A:GLN:H	1:140:A:GLY:O	6	0.13	0.01	0.13
(1,1046)	1:115:A:LEU:HD23	1:114:A:ARG:HA	6	0.12	0.02	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3017)	1:96:A:VAL:HB	1:97:A:LEU:H	6	0.12	0.01	0.12
(2,175)	1:96:A:VAL:HG13	1:96:A:VAL:HA	6	0.12	0.01	0.12
(2,2154)	1:116:A:ARG:HB2	1:117:A:GLY:H	6	0.12	0.01	0.12
(2,2333)	1:137:A:VAL:HA	1:136:A:ILE:HA	6	0.12	0.01	0.12
(1,1365)	1:150:A:ARG:HB2	1:150:A:ARG:HA	6	0.11	0.01	0.12
(2,2334)	1:136:A:ILE:HG12	1:136:A:ILE:HB	6	0.11	0.01	0.12
(2,4894)	1:181:A:ILE:H	1:116:A:ARG:H	6	0.11	0.0	0.11
(2,1825)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	5	1.47	0.1	1.44
(2,5448)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	5	1.12	0.21	1.25
(2,35)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	5	1.09	0.1	1.05
(1,906)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	5	1.07	0.24	1.08
(1,906)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	5	1.07	0.24	1.08
(1,1516)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	5	1.07	0.24	1.08
(1,1516)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	5	1.07	0.24	1.08
(1,2130)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	5	1.07	0.24	1.08
(1,2130)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	5	1.07	0.24	1.08
(1,2735)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	5	1.07	0.24	1.08
(1,2735)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	5	1.07	0.24	1.08
(1,232)	1:110:A:ASP:HB2	1:107:A:THR:HG22	5	1.05	0.06	1.01
(2,7318)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	5	1.05	0.21	1.17
(2,226)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	5	1.01	0.27	1.21
(2,1185)	1:156:A:PHE:HB2	1:191:A:VAL:H	5	1.0	0.06	1.02
(2,2013)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	5	0.98	0.27	1.18
(2,3822)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	5	0.96	0.27	1.16
(2,4030)	1:126:A:GLU:HG3	1:127:A:ILE:H	5	0.95	0.25	1.03
(2,2219)	1:126:A:GLU:HG3	1:127:A:ILE:H	5	0.94	0.25	1.02
(2,9020)	1:185:A:LYS:H	1:185:A:LYS:HB2	5	0.81	0.02	0.82
(2,5637)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	5	0.81	0.28	1.01
(2,7508)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	5	0.79	0.27	0.99
(1,367)	1:110:A:ASP:HB2	1:107:A:THR:HG22	5	0.75	0.07	0.72
(2,7166)	1:185:A:LYS:H	1:185:A:LYS:HB2	5	0.75	0.02	0.76
(1,1093)	1:136:A:ILE:HA	1:159:A:PHE:HB2	5	0.71	0.06	0.7
(1,1708)	1:136:A:ILE:HA	1:159:A:PHE:HB2	5	0.71	0.06	0.7
(2,5305)	1:185:A:LYS:H	1:185:A:LYS:HB2	5	0.7	0.02	0.7
(2,3508)	1:185:A:LYS:H	1:185:A:LYS:HB2	5	0.67	0.02	0.67
(2,69)	1:166:A:GLU:HG2	1:166:A:GLU:H	5	0.62	0.38	0.88
(2,5252)	1:171:A:LYS:H	1:170:A:LYS:HB2	5	0.61	0.05	0.64
(2,431)	1:126:A:GLU:HG3	1:127:A:ILE:H	5	0.61	0.25	0.69
(2,1699)	1:185:A:LYS:H	1:185:A:LYS:HB2	5	0.61	0.02	0.62
(2,53)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	5	0.61	0.21	0.73
(1,2320)	1:136:A:ILE:HA	1:159:A:PHE:HB2	5	0.58	0.06	0.57
(2,7113)	1:171:A:LYS:H	1:170:A:LYS:HB2	5	0.56	0.05	0.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,6942)	1:132:A:SER:HB2	1:133:A:GLY:H	5	0.55	0.11	0.62
(2,1236)	1:130:A:PHE:H	1:136:A:ILE:HG22	5	0.53	0.23	0.66
(2,8282)	1:179:A:ARG:HG3	1:179:A:ARG:HB3	5	0.53	0.19	0.62
(1,2933)	1:136:A:ILE:HA	1:159:A:PHE:HB2	5	0.53	0.06	0.52
(2,3452)	1:171:A:LYS:H	1:170:A:LYS:HB2	5	0.52	0.05	0.55
(2,8464)	1:123:A:SER:HB3	1:126:A:GLU:HB2	5	0.5	0.42	0.28
(2,3691)	1:156:A:PHE:HB2	1:191:A:VAL:H	5	0.5	0.06	0.51
(2,1664)	1:175:A:ARG:HG2	1:176:A:ILE:H	5	0.5	0.45	0.3
(1,935)	1:110:A:ASP:HB3	1:188:A:ARG:HG2	5	0.48	0.18	0.44
(1,935)	1:112:A:PHE:HB3	1:188:A:ARG:HG2	5	0.48	0.18	0.44
(2,3286)	1:132:A:SER:HB2	1:133:A:GLY:H	5	0.47	0.11	0.53
(1,413)	1:162:A:GLN:HG3	1:110:A:ASP:HA	5	0.46	0.23	0.41
(1,2324)	1:188:A:ARG:HA	1:186:A:SER:HA	5	0.45	0.18	0.32
(2,1887)	1:156:A:PHE:HB2	1:191:A:VAL:H	5	0.44	0.06	0.46
(1,102)	1:96:A:VAL:HB	1:96:A:VAL:HA	5	0.41	0.01	0.42
(1,102)	1:181:A:ILE:HB	1:181:A:ILE:HA	5	0.41	0.01	0.42
(2,1396)	1:112:A:PHE:H	1:111:A:GLY:H	5	0.4	0.23	0.32
(2,5086)	1:132:A:SER:HB2	1:133:A:GLY:H	5	0.39	0.11	0.45
(2,1404)	1:114:A:ARG:H	1:113:A:VAL:HG12	5	0.37	0.09	0.4
(2,1404)	1:114:A:ARG:H	1:113:A:VAL:HG13	5	0.37	0.09	0.4
(1,417)	1:107:A:THR:HB	1:110:A:ASP:HB3	5	0.35	0.06	0.38
(2,7280)	1:160:A:ALA:HB3	1:159:A:PHE:HB2	5	0.34	0.09	0.37
(1,1345)	1:96:A:VAL:HB	1:96:A:VAL:HA	5	0.33	0.01	0.34
(1,1345)	1:181:A:ILE:HB	1:181:A:ILE:HA	5	0.33	0.01	0.34
(2,748)	1:151:A:SER:HB3	1:152:A:THR:H	5	0.33	0.1	0.31
(2,8796)	1:132:A:SER:HB2	1:133:A:GLY:H	5	0.33	0.11	0.39
(2,8724)	1:114:A:ARG:HG3	1:115:A:LEU:H	5	0.32	0.14	0.33
(1,1770)	1:108:A:ALA:H	1:109:A:ASN:HA	5	0.32	0.15	0.41
(2,6858)	1:114:A:ARG:H	1:113:A:VAL:HG12	5	0.31	0.09	0.35
(2,6858)	1:114:A:ARG:H	1:113:A:VAL:HG13	5	0.31	0.09	0.35
(1,2706)	1:143:A:LEU:HA	1:122:A:CYS:HB2	5	0.31	0.11	0.27
(1,2706)	1:166:A:GLU:HA	1:159:A:PHE:HB2	5	0.31	0.11	0.27
(1,2706)	1:174:A:GLU:HA	1:175:A:ARG:HD2	5	0.31	0.11	0.27
(2,5009)	1:114:A:ARG:H	1:113:A:VAL:HG12	5	0.3	0.1	0.34
(2,5009)	1:114:A:ARG:H	1:113:A:VAL:HG13	5	0.3	0.1	0.34
(1,1918)	1:163:A:GLU:HB2	1:164:A:ILE:HG12	5	0.29	0.06	0.27
(1,1918)	1:163:A:GLU:HB2	1:96:A:VAL:HG13	5	0.29	0.06	0.27
(1,2908)	1:94:A:ASP:HA	1:164:A:ILE:HD13	5	0.29	0.13	0.26
(1,2908)	1:165:A:ALA:HA	1:113:A:VAL:HG23	5	0.29	0.13	0.26
(2,7360)	1:187:A:SER:HB3	1:189:A:ALA:H	5	0.29	0.13	0.23
(2,5413)	1:160:A:ALA:HB3	1:159:A:PHE:HB2	5	0.28	0.09	0.31
(2,1867)	1:161:A:SER:HA	1:106:A:ASP:HB3	5	0.28	0.17	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2101)	1:143:A:LEU:HA	1:122:A:CYS:HB2	5	0.26	0.11	0.22
(1,2101)	1:166:A:GLU:HA	1:159:A:PHE:HB2	5	0.26	0.11	0.22
(1,2101)	1:174:A:GLU:HA	1:175:A:ARG:HD2	5	0.26	0.11	0.22
(1,458)	1:136:A:ILE:HG13	1:159:A:PHE:HA	5	0.25	0.05	0.24
(2,6740)	1:97:A:LEU:H	1:92:A:ALA:H	5	0.24	0.05	0.23
(1,1259)	1:113:A:VAL:HG11	1:168:A:ALA:HB2	5	0.24	0.07	0.23
(1,1259)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	5	0.24	0.07	0.23
(1,2527)	1:163:A:GLU:HB2	1:164:A:ILE:HG12	5	0.24	0.06	0.21
(1,2527)	1:163:A:GLU:HB2	1:96:A:VAL:HG13	5	0.24	0.06	0.21
(1,653)	1:113:A:VAL:HG11	1:168:A:ALA:HB2	5	0.23	0.07	0.23
(1,653)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	5	0.23	0.07	0.23
(2,7372)	1:156:A:PHE:HB2	1:191:A:VAL:H	5	0.23	0.06	0.25
(1,1908)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	5	0.21	0.04	0.2
(1,1908)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	5	0.21	0.04	0.2
(2,4579)	1:179:A:ARG:HG2	1:179:A:ARG:HB3	5	0.2	0.0	0.2
(2,6714)	1:108:A:ALA:H	1:189:A:ALA:H	5	0.2	0.06	0.17
(2,6733)	1:150:A:ARG:HB2	1:147:A:PHE:H	5	0.19	0.05	0.22
(2,2210)	1:126:A:GLU:HB2	1:126:A:GLU:HA	5	0.19	0.01	0.19
(2,7271)	1:164:A:ILE:HD13	1:91:A:ASN:HA	5	0.18	0.06	0.15
(1,1442)	1:144:A:PRO:HD2	1:118:A:LEU:HD11	5	0.17	0.02	0.18
(2,111)	1:188:A:ARG:HB2	1:189:A:ALA:H	5	0.17	0.03	0.18
(1,1289)	1:167:A:LYS:HG2	1:134:A:LEU:HD11	5	0.15	0.04	0.14
(1,1289)	1:167:A:LYS:HG2	1:134:A:LEU:HD12	5	0.15	0.04	0.14
(2,5676)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	5	0.14	0.03	0.13
(2,3793)	1:97:A:LEU:HD12	1:97:A:LEU:H	5	0.14	0.03	0.12
(2,1870)	1:175:A:ARG:HA	1:179:A:ARG:H	5	0.14	0.03	0.14
(1,2315)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	5	0.13	0.01	0.14
(1,2315)	1:114:A:ARG:HG3	1:114:A:ARG:HD2	5	0.13	0.01	0.14
(1,2315)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	5	0.13	0.01	0.14
(1,1432)	1:141:A:ILE:HA	1:140:A:GLY:H	5	0.13	0.02	0.13
(1,1432)	1:137:A:VAL:HA	1:140:A:GLY:H	5	0.13	0.02	0.13
(2,125)	1:115:A:LEU:HD23	1:115:A:LEU:H	5	0.13	0.02	0.14
(4,4)	1:114:A:ARG:N	1:184:A:PHE:O	5	0.13	0.03	0.12
(2,1553)	1:150:A:ARG:H	1:149:A:GLY:H	5	0.13	0.01	0.13
(2,1071)	1:188:A:ARG:HG3	1:188:A:ARG:HA	5	0.13	0.0	0.13
(1,2376)	1:145:A:VAL:HB	1:146:A:ASP:H	5	0.12	0.01	0.12
(1,2927)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	5	0.12	0.01	0.13
(1,2927)	1:114:A:ARG:HG3	1:114:A:ARG:HD2	5	0.12	0.01	0.13
(1,2927)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	5	0.12	0.01	0.13
(2,3735)	1:102:A:PRO:HA	1:103:A:ASN:H	5	0.12	0.02	0.11
(2,6728)	1:93:A:MET:H	1:91:A:ASN:HA	5	0.12	0.01	0.12
(1,2113)	1:96:A:VAL:HA	1:97:A:LEU:HA	5	0.11	0.01	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,7358)	1:141:A:ILE:HA	1:140:A:GLY:H	5	0.11	0.01	0.11
(2,6776)	1:96:A:VAL:H	1:95:A:TRP:H	5	0.11	0.01	0.11
(2,4437)	1:164:A:ILE:HD12	1:164:A:ILE:HA	5	0.11	0.01	0.11
(2,6796)	1:98:A:LYS:HG3	1:98:A:LYS:H	5	0.11	0.01	0.11
(2,405)	1:120:A:PHE:HA	1:120:A:PHE:HB3	5	0.11	0.0	0.11
(1,1463)	1:159:A:PHE:HB2	1:159:A:PHE:HA	5	0.11	0.0	0.11
(2,5422)	1:96:A:VAL:HG22	1:96:A:VAL:HA	5	0.11	0.0	0.11
(2,6063)	1:141:A:ILE:HD13	1:141:A:ILE:HG12	5	0.11	0.0	0.11
(2,8125)	1:163:A:GLU:HG2	1:163:A:GLU:HB3	5	0.11	0.0	0.11
(2,4420)	1:162:A:GLN:HB2	1:162:A:GLN:HG2	5	0.1	0.0	0.1
(2,8576)	1:108:A:ALA:H	1:102:A:PRO:HG3	4	0.94	0.44	1.17
(2,976)	1:179:A:ARG:HD2	1:179:A:ARG:HB3	4	0.9	0.34	0.92
(2,99)	1:188:A:ARG:HD3	1:191:A:VAL:HG22	4	0.74	0.4	0.69
(2,8175)	1:166:A:GLU:HG2	1:166:A:GLU:H	4	0.72	0.31	0.86
(2,272)	1:105:A:PRO:HD3	1:104:A:SER:HB3	4	0.69	0.27	0.7
(2,6604)	1:111:A:GLY:HA3	1:109:A:ASN:H	4	0.6	0.16	0.68
(1,2296)	1:165:A:ALA:HA	1:113:A:VAL:HG21	4	0.6	0.28	0.62
(1,2296)	1:165:A:ALA:HA	1:113:A:VAL:HG23	4	0.6	0.28	0.62
(2,1173)	1:111:A:GLY:HA3	1:109:A:ASN:H	4	0.56	0.16	0.64
(2,6409)	1:179:A:ARG:HG3	1:179:A:ARG:HB3	4	0.54	0.01	0.54
(2,17)	1:113:A:VAL:HG11	1:113:A:VAL:H	4	0.53	0.73	0.12
(2,17)	1:113:A:VAL:HG12	1:113:A:VAL:H	4	0.53	0.73	0.12
(2,91)	1:155:A:ALA:HA	1:144:A:PRO:HD2	4	0.52	0.68	0.12
(2,2981)	1:158:A:GLN:HG3	1:112:A:PHE:HA	4	0.51	0.13	0.48
(2,7410)	1:98:A:LYS:HB3	1:100:A:THR:HG23	4	0.51	0.1	0.5
(2,7410)	1:98:A:LYS:HB3	1:100:A:THR:HG22	4	0.51	0.1	0.5
(3,102)	1:158:A:GLN:HG3	1:112:A:PHE:HA	4	0.45	0.13	0.42
(2,2659)	1:166:A:GLU:HG2	1:166:A:GLU:HA	4	0.39	0.04	0.4
(2,4470)	1:166:A:GLU:HG2	1:166:A:GLU:HA	4	0.39	0.04	0.4
(2,721)	1:148:A:GLN:HB2	1:149:A:GLY:H	4	0.38	0.07	0.37
(2,4788)	1:158:A:GLN:HG3	1:112:A:PHE:HA	4	0.36	0.13	0.32
(2,6144)	1:148:A:GLN:HB2	1:149:A:GLY:H	4	0.35	0.07	0.34
(2,7608)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	4	0.34	0.01	0.34
(2,6616)	1:158:A:GLN:HG3	1:112:A:PHE:HA	4	0.33	0.13	0.3
(2,3218)	1:114:A:ARG:HG3	1:115:A:LEU:H	4	0.33	0.11	0.36
(2,1749)	1:175:A:ARG:H	1:178:A:HIS:HA	4	0.33	0.06	0.35
(2,8032)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	4	0.32	0.29	0.16
(2,5539)	1:98:A:LYS:HB3	1:100:A:THR:HG23	4	0.32	0.1	0.3
(2,5539)	1:98:A:LYS:HB3	1:100:A:THR:HG22	4	0.32	0.1	0.3
(1,3020)	1:132:A:SER:H	1:136:A:ILE:HB	4	0.31	0.08	0.32
(2,3208)	1:114:A:ARG:H	1:113:A:VAL:HG12	4	0.3	0.04	0.31
(2,3208)	1:114:A:ARG:H	1:113:A:VAL:HG13	4	0.3	0.04	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,316)	1:98:A:LYS:HB3	1:100:A:THR:HG23	4	0.3	0.09	0.28
(1,316)	1:98:A:LYS:HB3	1:100:A:THR:HG22	4	0.3	0.09	0.28
(1,937)	1:98:A:LYS:HB3	1:100:A:THR:HG23	4	0.28	0.1	0.26
(1,937)	1:98:A:LYS:HB3	1:100:A:THR:HG22	4	0.28	0.1	0.26
(1,1370)	1:166:A:GLU:HG3	1:169:A:LEU:HD13	4	0.27	0.12	0.28
(2,2992)	1:161:A:SER:H	1:159:A:PHE:HB2	4	0.27	0.1	0.26
(2,4797)	1:161:A:SER:H	1:159:A:PHE:HB2	4	0.26	0.1	0.25
(2,8714)	1:114:A:ARG:H	1:113:A:VAL:HG12	4	0.25	0.04	0.25
(2,8714)	1:114:A:ARG:H	1:113:A:VAL:HG13	4	0.25	0.04	0.25
(1,2773)	1:98:A:LYS:HB3	1:100:A:THR:HG23	4	0.24	0.1	0.22
(1,2773)	1:98:A:LYS:HB3	1:100:A:THR:HG22	4	0.24	0.1	0.22
(1,722)	1:148:A:GLN:HB3	1:147:A:PHE:H	4	0.22	0.1	0.18
(2,1600)	1:159:A:PHE:H	1:158:A:GLN:HG3	4	0.22	0.08	0.2
(1,2526)	1:166:A:GLU:HB3	1:168:A:ALA:H	4	0.21	0.05	0.24
(1,2526)	1:166:A:GLU:HB2	1:168:A:ALA:H	4	0.21	0.05	0.24
(1,2072)	1:175:A:ARG:HD2	1:178:A:HIS:HA	4	0.21	0.07	0.18
(2,3903)	1:110:A:ASP:HB3	1:110:A:ASP:HA	4	0.19	0.01	0.18
(1,1339)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	4	0.18	0.01	0.18
(1,1869)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	4	0.18	0.05	0.17
(1,1869)	1:113:A:VAL:HG11	1:168:A:ALA:HB2	4	0.18	0.05	0.17
(2,3568)	1:188:A:ARG:HG2	1:188:A:ARG:H	4	0.18	0.04	0.19
(2,8968)	1:171:A:LYS:H	1:170:A:LYS:HB2	4	0.18	0.03	0.19
(2,1852)	1:95:A:TRP:HB2	1:96:A:VAL:HG21	4	0.18	0.03	0.19
(2,3695)	1:181:A:ILE:HG21	1:174:A:GLU:HA	4	0.17	0.07	0.14
(4,34)	1:159:A:PHE:H	1:111:A:GLY:O	4	0.17	0.03	0.18
(2,5502)	1:156:A:PHE:HB2	1:191:A:VAL:H	4	0.16	0.04	0.16
(1,2097)	1:169:A:LEU:HB2	1:166:A:GLU:HA	4	0.16	0.02	0.16
(1,2097)	1:143:A:LEU:HA	1:143:A:LEU:HB2	4	0.16	0.02	0.16
(1,1625)	1:135:A:GLU:HA	1:136:A:ILE:HB	4	0.15	0.03	0.14
(2,3182)	1:107:A:THR:HA	1:108:A:ALA:H	4	0.14	0.04	0.14
(4,41)	1:168:A:ALA:N	1:164:A:ILE:O	4	0.14	0.03	0.14
(1,735)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	4	0.14	0.01	0.14
(2,1186)	1:188:A:ARG:HG2	1:188:A:ARG:HD2	4	0.14	0.02	0.14
(2,2985)	1:188:A:ARG:HG2	1:188:A:ARG:HD2	4	0.14	0.02	0.14
(2,8412)	1:191:A:VAL:HG13	1:191:A:VAL:HB	4	0.14	0.01	0.14
(1,41)	1:134:A:LEU:HD11	1:134:A:LEU:HA	4	0.13	0.03	0.12
(2,2520)	1:150:A:ARG:HG2	1:150:A:ARG:HA	4	0.13	0.01	0.12
(2,2848)	1:183:A:ILE:HA	1:183:A:ILE:HD11	4	0.13	0.01	0.13
(2,4330)	1:150:A:ARG:HG2	1:150:A:ARG:HA	4	0.12	0.01	0.12
(1,1647)	1:111:A:GLY:HA3	1:112:A:PHE:H	4	0.12	0.01	0.12
(2,2790)	1:181:A:ILE:HG22	1:181:A:ILE:HG12	4	0.12	0.01	0.12
(2,4785)	1:185:A:LYS:HB3	1:185:A:LYS:H	4	0.12	0.02	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2863)	1:164:A:ILE:HD13	1:135:A:GLU:HA	4	0.12	0.01	0.12
(1,2863)	1:164:A:ILE:HD13	1:93:A:MET:HA	4	0.12	0.01	0.12
(2,7385)	1:188:A:ARG:HB2	1:187:A:SER:H	4	0.12	0.01	0.12
(2,3963)	1:116:A:ARG:HB2	1:117:A:GLY:H	4	0.11	0.01	0.11
(2,4660)	1:183:A:ILE:HG22	1:183:A:ILE:HD13	4	0.11	0.01	0.12
(1,758)	1:150:A:ARG:HB2	1:150:A:ARG:HA	4	0.11	0.01	0.12
(2,390)	1:119:A:PRO:HA	1:119:A:PRO:HG3	4	0.11	0.0	0.11
(2,6216)	1:157:A:VAL:HG23	1:157:A:VAL:HG12	4	0.11	0.01	0.12
(2,6710)	1:142:A:THR:H	1:155:A:ALA:HA	4	0.11	0.01	0.12
(2,4020)	1:126:A:GLU:HB2	1:126:A:GLU:HA	4	0.11	0.0	0.11
(2,1962)	1:96:A:VAL:HG13	1:96:A:VAL:HA	4	0.11	0.01	0.11
(1,2167)	1:97:A:LEU:HG	1:97:A:LEU:HD13	4	0.11	0.0	0.11
(1,2167)	1:97:A:LEU:HG	1:97:A:LEU:HD11	4	0.11	0.0	0.11
(2,526)	1:134:A:LEU:HD21	1:134:A:LEU:HA	4	0.1	0.0	0.1
(2,3584)	1:166:A:GLU:H	1:169:A:LEU:HB2	3	1.51	0.02	1.52
(2,7247)	1:166:A:GLU:H	1:169:A:LEU:HB2	3	1.45	0.01	1.46
(2,5377)	1:166:A:GLU:H	1:169:A:LEU:HB2	3	1.34	0.02	1.35
(2,9101)	1:166:A:GLU:H	1:169:A:LEU:HB2	3	1.32	0.02	1.33
(2,428)	1:126:A:GLU:HB2	1:127:A:ILE:H	3	1.27	0.08	1.28
(1,2872)	1:131:A:PHE:HB2	1:136:A:ILE:HB	3	1.21	0.27	1.24
(2,3669)	1:169:A:LEU:HB2	1:166:A:GLU:HA	3	0.98	0.22	1.05
(2,7340)	1:169:A:LEU:HB2	1:166:A:GLU:HA	3	0.76	0.22	0.83
(2,1862)	1:169:A:LEU:HB2	1:166:A:GLU:HA	3	0.65	0.22	0.72
(2,408)	1:120:A:PHE:HB3	1:120:A:PHE:H	3	0.65	0.38	0.91
(2,5471)	1:169:A:LEU:HB2	1:166:A:GLU:HA	3	0.6	0.22	0.67
(2,3056)	1:168:A:ALA:H	1:169:A:LEU:HB2	3	0.48	0.08	0.44
(1,1418)	1:169:A:LEU:HA	1:169:A:LEU:HD11	3	0.47	0.09	0.45
(2,6701)	1:168:A:ALA:H	1:169:A:LEU:HB2	3	0.45	0.08	0.41
(2,8472)	1:111:A:GLY:HA3	1:109:A:ASN:H	3	0.45	0.04	0.47
(1,1034)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	3	0.44	0.21	0.58
(2,8562)	1:168:A:ALA:H	1:169:A:LEU:HB2	3	0.42	0.08	0.38
(2,4859)	1:168:A:ALA:H	1:169:A:LEU:HB2	3	0.41	0.08	0.37
(2,8172)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	3	0.41	0.02	0.42
(2,7701)	1:124:A:LYS:HA	1:124:A:LYS:HB2	3	0.4	0.0	0.4
(1,140)	1:190:A:GLU:HG2	1:190:A:GLU:HA	3	0.4	0.27	0.32
(1,140)	1:163:A:GLU:HG3	1:163:A:GLU:HA	3	0.4	0.27	0.32
(2,3042)	1:130:A:PHE:H	1:136:A:ILE:HG22	3	0.39	0.06	0.36
(1,3)	1:127:A:ILE:HD11	1:126:A:GLU:HB2	3	0.36	0.21	0.26
(1,1548)	1:112:A:PHE:HB3	1:188:A:ARG:HG2	3	0.36	0.14	0.33
(1,1548)	1:110:A:ASP:HB3	1:188:A:ARG:HG2	3	0.36	0.14	0.33
(2,6300)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	3	0.35	0.02	0.37
(2,2710)	1:173:A:LYS:HG2	1:173:A:LYS:HA	3	0.34	0.17	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1159)	1:108:A:ALA:H	1:109:A:ASN:HA	3	0.34	0.02	0.35
(1,625)	1:97:A:LEU:H	1:99:A:HIS:HA	3	0.34	0.13	0.3
(2,424)	1:126:A:GLU:HG2	1:126:A:GLU:HB2	3	0.34	0.04	0.33
(2,738)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	3	0.33	0.32	0.12
(2,1667)	1:176:A:ILE:H	1:176:A:ILE:HD11	3	0.33	0.07	0.37
(2,1667)	1:176:A:ILE:H	1:176:A:ILE:HD12	3	0.33	0.07	0.37
(2,903)	1:169:A:LEU:HB2	1:169:A:LEU:HD13	3	0.32	0.05	0.33
(2,1292)	1:111:A:GLY:HA3	1:159:A:PHE:H	3	0.32	0.12	0.35
(1,2031)	1:169:A:LEU:HA	1:169:A:LEU:HD11	3	0.32	0.09	0.29
(2,3096)	1:111:A:GLY:HA3	1:159:A:PHE:H	3	0.3	0.12	0.33
(2,4899)	1:111:A:GLY:HA3	1:159:A:PHE:H	3	0.29	0.12	0.32
(2,6629)	1:161:A:SER:H	1:159:A:PHE:HB2	3	0.28	0.08	0.24
(1,1530)	1:165:A:ALA:HB3	1:113:A:VAL:HG23	3	0.28	0.02	0.28
(1,1530)	1:164:A:ILE:HD13	1:93:A:MET:HG3	3	0.28	0.02	0.28
(1,2588)	1:166:A:GLU:HG3	1:168:A:ALA:H	3	0.27	0.04	0.26
(1,2636)	1:169:A:LEU:HA	1:169:A:LEU:HD11	3	0.26	0.09	0.24
(1,3006)	1:117:A:GLY:H	1:118:A:LEU:HD12	3	0.26	0.14	0.2
(2,5487)	1:187:A:SER:HB3	1:189:A:ALA:H	3	0.26	0.1	0.31
(2,8960)	1:166:A:GLU:HB3	1:167:A:LYS:H	3	0.25	0.01	0.26
(1,1550)	1:98:A:LYS:HB3	1:100:A:THR:HG23	3	0.25	0.08	0.21
(1,1981)	1:166:A:GLU:HG3	1:168:A:ALA:H	3	0.25	0.04	0.23
(1,810)	1:169:A:LEU:HA	1:169:A:LEU:HD11	3	0.24	0.09	0.22
(1,1234)	1:97:A:LEU:H	1:99:A:HIS:HA	3	0.24	0.13	0.2
(1,179)	1:169:A:LEU:HA	1:169:A:LEU:HD11	3	0.23	0.09	0.21
(1,2388)	1:108:A:ALA:H	1:109:A:ASN:HA	3	0.23	0.02	0.24
(1,1704)	1:169:A:LEU:HB2	1:166:A:GLU:HA	3	0.23	0.09	0.26
(1,1704)	1:166:A:GLU:HB2	1:166:A:GLU:HA	3	0.23	0.09	0.26
(1,2134)	1:143:A:LEU:HG	1:141:A:ILE:HG21	3	0.23	0.14	0.15
(1,2134)	1:97:A:LEU:HD12	1:163:A:GLU:HB3	3	0.23	0.14	0.15
(1,606)	1:185:A:LYS:HB3	1:185:A:LYS:H	3	0.22	0.02	0.22
(1,606)	1:114:A:ARG:HG3	1:115:A:LEU:H	3	0.22	0.02	0.22
(1,1917)	1:166:A:GLU:HB3	1:168:A:ALA:H	3	0.22	0.05	0.21
(1,1917)	1:163:A:GLU:HB2	1:96:A:VAL:H	3	0.22	0.05	0.21
(1,1917)	1:166:A:GLU:HB2	1:168:A:ALA:H	3	0.22	0.05	0.21
(2,4586)	1:179:A:ARG:HG3	1:179:A:ARG:HD2	3	0.22	0.01	0.21
(2,3179)	1:106:A:ASP:H	1:105:A:PRO:HD2	3	0.21	0.09	0.21
(1,545)	1:168:A:ALA:H	1:169:A:LEU:HB2	3	0.2	0.08	0.16
(2,2776)	1:179:A:ARG:HG3	1:179:A:ARG:HD2	3	0.2	0.01	0.2
(1,482)	1:141:A:ILE:HA	1:140:A:GLY:H	3	0.19	0.06	0.22
(1,482)	1:174:A:GLU:HA	1:181:A:ILE:H	3	0.19	0.06	0.22
(2,6621)	1:166:A:GLU:HA	1:169:A:LEU:HD11	3	0.19	0.05	0.16
(1,598)	1:116:A:ARG:H	1:181:A:ILE:HD12	3	0.18	0.08	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,43)	1:134:A:LEU:HD13	1:133:A:GLY:H	3	0.18	0.05	0.17
(2,1562)	1:150:A:ARG:H	1:151:A:SER:H	3	0.18	0.09	0.14
(1,919)	1:165:A:ALA:HB3	1:113:A:VAL:HG23	3	0.18	0.02	0.18
(1,919)	1:164:A:ILE:HD13	1:93:A:MET:HG3	3	0.18	0.02	0.18
(1,1805)	1:158:A:GLN:H	1:141:A:ILE:HG23	3	0.16	0.03	0.16
(2,7399)	1:166:A:GLU:HG2	1:168:A:ALA:H	3	0.15	0.03	0.14
(2,3615)	1:160:A:ALA:HB2	1:162:A:GLN:H	3	0.14	0.01	0.14
(2,8563)	1:168:A:ALA:H	1:95:A:TRP:HB2	3	0.14	0.02	0.13
(2,4318)	1:148:A:GLN:HA	1:149:A:GLY:H	3	0.13	0.01	0.14
(1,165)	1:109:A:ASN:HA	1:108:A:ALA:HB3	3	0.13	0.02	0.12
(1,592)	1:97:A:LEU:HB2	1:97:A:LEU:H	3	0.13	0.01	0.13
(1,647)	1:164:A:ILE:HD12	1:95:A:TRP:HA	3	0.13	0.01	0.14
(1,647)	1:164:A:ILE:HD13	1:95:A:TRP:HA	3	0.13	0.01	0.14
(1,1255)	1:164:A:ILE:HD12	1:95:A:TRP:HA	3	0.13	0.01	0.14
(1,1255)	1:164:A:ILE:HD13	1:95:A:TRP:HA	3	0.13	0.01	0.14
(2,4963)	1:101:A:GLY:H	1:100:A:THR:H	3	0.13	0.0	0.13
(1,2694)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	3	0.13	0.01	0.13
(1,2694)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	3	0.13	0.01	0.13
(1,2694)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	3	0.13	0.01	0.13
(1,195)	1:141:A:ILE:HA	1:140:A:GLY:H	3	0.12	0.0	0.12
(1,834)	1:144:A:PRO:HD2	1:118:A:LEU:HD11	3	0.12	0.01	0.13
(1,2087)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	3	0.12	0.01	0.12
(1,2087)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	3	0.12	0.01	0.12
(1,2087)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	3	0.12	0.01	0.12
(2,36)	1:191:A:VAL:HG23	1:191:A:VAL:H	3	0.12	0.01	0.13
(2,5424)	1:96:A:VAL:HG22	1:97:A:LEU:H	3	0.12	0.01	0.12
(2,6633)	1:101:A:GLY:H	1:110:A:ASP:HA	3	0.12	0.0	0.12
(2,2622)	1:163:A:GLU:HB3	1:164:A:ILE:H	3	0.12	0.02	0.12
(2,5382)	1:164:A:ILE:HG13	1:167:A:LYS:H	3	0.12	0.02	0.11
(4,15)	1:129:A:GLN:H	1:125:A:GLU:O	3	0.12	0.01	0.11
(2,2927)	1:192:A:ARG:HB2	1:193:A:THR:HA	3	0.12	0.01	0.11
(2,4471)	1:166:A:GLU:HG3	1:166:A:GLU:HA	3	0.12	0.02	0.11
(2,5103)	1:135:A:GLU:HB3	1:135:A:GLU:H	3	0.12	0.02	0.11
(2,7246)	1:166:A:GLU:H	1:95:A:TRP:HB2	3	0.12	0.01	0.11
(2,8166)	1:166:A:GLU:HB2	1:166:A:GLU:HA	3	0.12	0.0	0.12
(2,8637)	1:96:A:VAL:HG13	1:97:A:LEU:H	3	0.12	0.01	0.12
(1,1640)	1:162:A:GLN:HB2	1:162:A:GLN:HG3	3	0.11	0.0	0.11
(1,1640)	1:162:A:GLN:HB3	1:162:A:GLN:HG2	3	0.11	0.0	0.11
(2,5376)	1:166:A:GLU:H	1:95:A:TRP:HB2	3	0.11	0.01	0.11
(3,104)	1:101:A:GLY:H	1:110:A:ASP:HA	3	0.11	0.0	0.11
(3,145)	1:136:A:ILE:HD13	1:164:A:ILE:HA	3	0.11	0.0	0.11
(3,276)	1:136:A:ILE:HD13	1:164:A:ILE:HA	3	0.11	0.0	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,620)	1:101:A:GLY:H	1:110:A:ASP:HA	3	0.11	0.0	0.11
(2,5552)	1:91:A:ASN:HB2	1:92:A:ALA:HA	3	0.11	0.0	0.11
(2,8334)	1:182:A:GLU:HB2	1:182:A:GLU:HG3	3	0.11	0.0	0.11
(2,6415)	1:179:A:ARG:HG3	1:179:A:ARG:HD2	3	0.11	0.01	0.11
(2,3661)	1:95:A:TRP:HB3	1:91:A:ASN:HB3	3	0.11	0.0	0.11
(2,6293)	1:166:A:GLU:HB2	1:166:A:GLU:HA	3	0.11	0.0	0.11
(2,8099)	1:157:A:VAL:HG22	1:158:A:GLN:H	3	0.11	0.01	0.1
(2,8632)	1:96:A:VAL:H	1:95:A:TRP:H	3	0.11	0.0	0.11
(1,20)	1:96:A:VAL:HG22	1:96:A:VAL:HA	3	0.1	0.0	0.1
(2,7288)	1:96:A:VAL:HG22	1:96:A:VAL:HA	3	0.1	0.0	0.1
(2,5418)	1:113:A:VAL:HG13	1:112:A:PHE:H	2	1.58	1.44	1.58
(2,5418)	1:113:A:VAL:HG12	1:112:A:PHE:H	2	1.58	1.44	1.58
(2,1073)	1:188:A:ARG:HA	1:188:A:ARG:HD3	2	0.94	0.03	0.94
(2,3685)	1:155:A:ALA:HA	1:144:A:PRO:HD2	2	0.89	0.78	0.89
(2,4007)	1:120:A:PHE:HB3	1:120:A:PHE:H	2	0.84	0.01	0.84
(2,2198)	1:120:A:PHE:HB3	1:120:A:PHE:H	2	0.82	0.01	0.82
(3,101)	1:126:A:GLU:HB2	1:123:A:SER:HB3	2	0.75	0.29	0.75
(2,5818)	1:120:A:PHE:HB3	1:120:A:PHE:H	2	0.72	0.01	0.72
(2,2498)	1:147:A:PHE:HB3	1:147:A:PHE:HA	2	0.64	0.01	0.64
(2,4308)	1:147:A:PHE:HB3	1:147:A:PHE:HA	2	0.63	0.0	0.63
(2,4768)	1:126:A:GLU:HB2	1:123:A:SER:HB3	2	0.62	0.3	0.62
(2,426)	1:126:A:GLU:HG3	1:126:A:GLU:HB2	2	0.56	0.01	0.56
(2,2924)	1:192:A:ARG:HD3	1:192:A:ARG:HB2	2	0.55	0.1	0.55
(2,4732)	1:192:A:ARG:HD3	1:192:A:ARG:HB2	2	0.55	0.1	0.55
(2,7690)	1:120:A:PHE:HB3	1:120:A:PHE:H	2	0.55	0.01	0.55
(2,6131)	1:147:A:PHE:HB3	1:147:A:PHE:HA	2	0.52	0.01	0.52
(1,1645)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	2	0.52	0.01	0.52
(2,1130)	1:192:A:ARG:HD3	1:192:A:ARG:HB2	2	0.52	0.1	0.52
(2,3611)	1:181:A:ILE:HG12	1:175:A:ARG:HD2	2	0.51	0.37	0.51
(2,5684)	1:105:A:PRO:HD3	1:104:A:SER:HB3	2	0.5	0.02	0.5
(2,8004)	1:147:A:PHE:HB3	1:147:A:PHE:HA	2	0.5	0.0	0.5
(2,6596)	1:123:A:SER:HB3	1:126:A:GLU:HB2	2	0.5	0.3	0.5
(2,6559)	1:192:A:ARG:HD3	1:192:A:ARG:HB2	2	0.48	0.09	0.48
(2,2961)	1:126:A:GLU:HB2	1:123:A:SER:HB3	2	0.48	0.29	0.48
(1,364)	1:96:A:VAL:HG12	1:93:A:MET:HG2	2	0.46	0.02	0.46
(2,1757)	1:173:A:LYS:HB2	1:172:A:HIS:H	2	0.45	0.05	0.45
(1,133)	1:166:A:GLU:HG3	1:169:A:LEU:HD13	2	0.45	0.13	0.45
(2,920)	1:173:A:LYS:HG2	1:173:A:LYS:HA	2	0.43	0.04	0.43
(2,4521)	1:173:A:LYS:HG2	1:173:A:LYS:HA	2	0.4	0.04	0.4
(1,444)	1:144:A:PRO:HD2	1:118:A:LEU:HD22	2	0.32	0.03	0.32
(1,982)	1:96:A:VAL:HG12	1:93:A:MET:HG2	2	0.32	0.03	0.32
(1,1668)	1:144:A:PRO:HD2	1:118:A:LEU:HD22	2	0.32	0.03	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2285)	1:144:A:PRO:HD2	1:118:A:LEU:HD22	2	0.32	0.03	0.32
(1,2898)	1:144:A:PRO:HD2	1:118:A:LEU:HD22	2	0.32	0.03	0.32
(1,739)	1:181:A:ILE:HB	1:181:A:ILE:HA	2	0.3	0.0	0.3
(2,8430)	1:192:A:ARG:HD2	1:192:A:ARG:HB2	2	0.3	0.01	0.3
(2,6350)	1:173:A:LYS:HG2	1:173:A:LYS:HA	2	0.29	0.04	0.29
(2,6627)	1:111:A:GLY:H	1:188:A:ARG:HG2	2	0.29	0.01	0.29
(2,8431)	1:192:A:ARG:HD3	1:192:A:ARG:HB2	2	0.28	0.1	0.28
(4,23)	1:144:A:PRO:O	1:152:A:THR:OG1	2	0.26	0.03	0.26
(1,343)	1:120:A:PHE:HA	1:120:A:PHE:HB2	2	0.25	0.0	0.25
(1,343)	1:159:A:PHE:HB2	1:159:A:PHE:HA	2	0.25	0.0	0.25
(1,618)	1:166:A:GLU:H	1:169:A:LEU:HD13	2	0.25	0.03	0.25
(2,8222)	1:173:A:LYS:HG2	1:173:A:LYS:HA	2	0.24	0.04	0.24
(2,239)	1:100:A:THR:HG22	1:100:A:THR:HB	2	0.24	0.0	0.24
(2,925)	1:173:A:LYS:HG2	1:174:A:GLU:H	2	0.23	0.11	0.23
(2,3868)	1:105:A:PRO:HD3	1:104:A:SER:HB3	2	0.22	0.02	0.22
(1,1841)	1:134:A:LEU:HD12	1:167:A:LYS:H	2	0.22	0.07	0.22
(1,2576)	1:141:A:ILE:HG12	1:158:A:GLN:H	2	0.2	0.03	0.2
(2,2954)	1:110:A:ASP:HB2	1:107:A:THR:HB	2	0.2	0.06	0.2
(2,7713)	1:126:A:GLU:HG3	1:127:A:ILE:H	2	0.2	0.06	0.2
(2,1215)	1:110:A:ASP:H	1:188:A:ARG:HG2	2	0.2	0.01	0.2
(2,3581)	1:108:A:ALA:H	1:188:A:ARG:HG3	2	0.2	0.06	0.2
(1,1327)	1:148:A:GLN:HB3	1:147:A:PHE:H	2	0.2	0.08	0.2
(2,1921)	1:143:A:LEU:HG	1:123:A:SER:HA	2	0.18	0.05	0.18
(2,2997)	1:145:A:VAL:H	1:155:A:ALA:HA	2	0.18	0.04	0.18
(1,1304)	1:166:A:GLU:HB2	1:169:A:LEU:HD13	2	0.18	0.02	0.18
(2,74)	1:169:A:LEU:HB2	1:166:A:GLU:HA	2	0.18	0.08	0.18
(4,8)	1:116:A:ARG:N	1:182:A:GLU:O	2	0.18	0.07	0.18
(2,1374)	1:106:A:ASP:H	1:105:A:PRO:HD2	2	0.17	0.05	0.17
(3,627)	1:108:A:ALA:H	1:189:A:ALA:H	2	0.17	0.01	0.17
(1,1090)	1:166:A:GLU:HB2	1:166:A:GLU:HA	2	0.16	0.02	0.16
(1,645)	1:164:A:ILE:HD13	1:91:A:ASN:HB2	2	0.16	0.04	0.16
(1,645)	1:164:A:ILE:HD13	1:91:A:ASN:HB3	2	0.16	0.04	0.16
(2,6258)	1:163:A:GLU:HG3	1:163:A:GLU:H	2	0.16	0.01	0.16
(2,1171)	1:190:A:GLU:HB2	1:187:A:SER:H	2	0.15	0.01	0.15
(1,2181)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	2	0.15	0.03	0.15
(1,3018)	1:97:A:LEU:H	1:99:A:HIS:H	2	0.15	0.0	0.15
(1,10)	1:164:A:ILE:HD13	1:91:A:ASN:HB2	2	0.14	0.03	0.14
(1,10)	1:164:A:ILE:HD13	1:91:A:ASN:HB3	2	0.14	0.03	0.14
(1,1253)	1:164:A:ILE:HD13	1:91:A:ASN:HB2	2	0.14	0.03	0.14
(1,1253)	1:164:A:ILE:HD13	1:91:A:ASN:HB3	2	0.14	0.03	0.14
(2,1068)	1:187:A:SER:HB3	1:187:A:SER:HA	2	0.14	0.01	0.14
(2,2607)	1:162:A:GLN:HG3	1:162:A:GLN:HA	2	0.14	0.02	0.14

Continued on next page...

Continued from previous page...

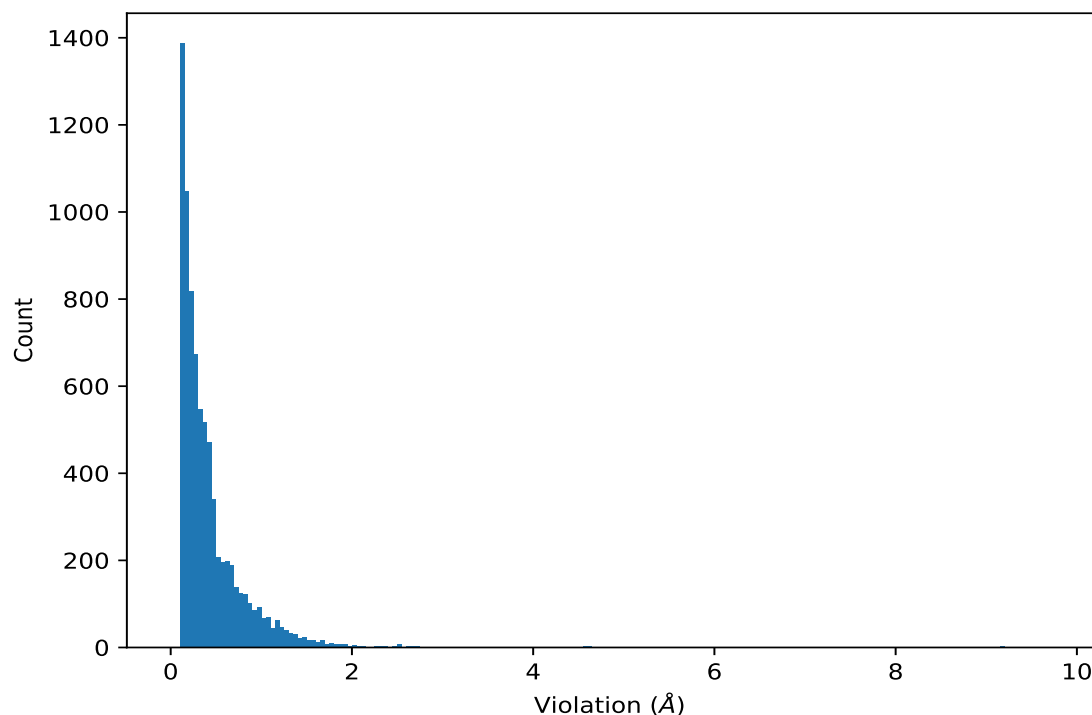
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2860)	1:187:A:SER:HB3	1:187:A:SER:HA	2	0.14	0.01	0.14
(2,5278)	1:179:A:ARG:HG3	1:179:A:ARG:H	2	0.14	0.02	0.14
(2,6321)	1:169:A:LEU:HD22	1:169:A:LEU:HA	2	0.14	0.01	0.14
(1,1196)	1:158:A:GLN:H	1:141:A:ILE:HG23	2	0.13	0.02	0.13
(2,348)	1:115:A:LEU:HB3	1:115:A:LEU:HD13	2	0.13	0.0	0.13
(2,4037)	1:127:A:ILE:HD12	1:127:A:ILE:HB	2	0.13	0.0	0.13
(2,4761)	1:107:A:THR:HB	1:110:A:ASP:HB3	2	0.13	0.0	0.13
(2,5249)	1:167:A:LYS:HG2	1:168:A:ALA:H	2	0.13	0.0	0.13
(1,1873)	1:96:A:VAL:HG21	1:96:A:VAL:HB	2	0.12	0.01	0.12
(2,1180)	1:188:A:ARG:HB2	1:188:A:ARG:HG2	2	0.12	0.01	0.12
(2,5364)	1:188:A:ARG:HG2	1:188:A:ARG:H	2	0.12	0.01	0.12
(2,6298)	1:166:A:GLU:HA	1:167:A:LYS:H	2	0.12	0.02	0.12
(1,152)	1:130:A:PHE:HB2	1:131:A:PHE:H	2	0.12	0.01	0.12
(1,1701)	1:188:A:ARG:HG2	1:188:A:ARG:HD2	2	0.12	0.0	0.12
(1,1876)	1:127:A:ILE:HG21	1:127:A:ILE:HB	2	0.12	0.0	0.12
(1,2355)	1:143:A:LEU:HG	1:122:A:CYS:H	2	0.12	0.01	0.12
(2,1685)	1:183:A:ILE:H	1:182:A:GLU:HG3	2	0.12	0.0	0.12
(2,3533)	1:190:A:GLU:HB3	1:191:A:VAL:H	2	0.12	0.01	0.12
(2,3559)	1:158:A:GLN:H	1:141:A:ILE:HB	2	0.12	0.01	0.12
(2,1798)	1:164:A:ILE:HD11	1:161:A:SER:H	2	0.12	0.02	0.12
(2,3019)	1:110:A:ASP:H	1:188:A:ARG:HG2	2	0.12	0.02	0.12
(2,4891)	1:105:A:PRO:HA	1:106:A:ASP:H	2	0.12	0.02	0.12
(1,2487)	1:96:A:VAL:HG21	1:96:A:VAL:HB	2	0.12	0.0	0.12
(2,3768)	1:96:A:VAL:HG11	1:96:A:VAL:H	2	0.12	0.0	0.12
(1,654)	1:183:A:ILE:HG21	1:184:A:PHE:HA	2	0.11	0.01	0.11
(2,899)	1:169:A:LEU:HD22	1:169:A:LEU:HD12	2	0.11	0.01	0.11
(2,1583)	1:156:A:PHE:HB2	1:157:A:VAL:H	2	0.11	0.01	0.11
(2,4791)	1:188:A:ARG:HD2	1:108:A:ALA:H	2	0.11	0.01	0.11
(4,2)	1:113:A:VAL:N	1:157:A:VAL:O	2	0.11	0.01	0.11
(1,126)	1:150:A:ARG:HB2	1:150:A:ARG:HA	2	0.11	0.0	0.11
(1,549)	1:108:A:ALA:H	1:109:A:ASN:HA	2	0.11	0.0	0.11
(1,1814)	1:97:A:LEU:HB2	1:97:A:LEU:H	2	0.11	0.0	0.11
(2,2615)	1:163:A:GLU:HB3	1:163:A:GLU:HA	2	0.11	0.0	0.11
(2,2626)	1:164:A:ILE:HD12	1:164:A:ILE:HA	2	0.11	0.0	0.11
(2,4600)	1:181:A:ILE:HG22	1:181:A:ILE:HG12	2	0.11	0.0	0.11
(2,5534)	1:115:A:LEU:HD23	1:115:A:LEU:H	2	0.11	0.0	0.11
(2,5848)	1:127:A:ILE:HD12	1:127:A:ILE:HB	2	0.11	0.0	0.11
(2,6232)	1:160:A:ALA:HB3	1:161:A:SER:H	2	0.11	0.0	0.11
(2,8216)	1:171:A:LYS:HB3	1:171:A:LYS:HA	2	0.11	0.0	0.11
(4,12)	1:118:A:LEU:N	1:152:A:THR:O	2	0.11	0.0	0.11
(2,2226)	1:127:A:ILE:HD12	1:127:A:ILE:HB	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations [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)
(1,2830)	1:164:A:ILE:HA	1:181:A:ILE:HD12	7	9.68
(1,2830)	1:164:A:ILE:HA	1:181:A:ILE:HD13	8	9.17
(1,2830)	1:164:A:ILE:HA	1:181:A:ILE:HD13	3	9.15
(1,2830)	1:164:A:ILE:HA	1:181:A:ILE:HD13	10	9.15
(1,2830)	1:164:A:ILE:HA	1:181:A:ILE:HD13	2	8.99
(1,2830)	1:164:A:ILE:HA	1:181:A:ILE:HD13	9	8.85
(1,2830)	1:164:A:ILE:HA	1:181:A:ILE:HD13	4	8.73
(1,2830)	1:164:A:ILE:HA	1:181:A:ILE:HD13	5	8.56
(1,2830)	1:164:A:ILE:HA	1:181:A:ILE:HD13	6	8.49
(1,2830)	1:164:A:ILE:HA	1:181:A:ILE:HD13	1	8.01

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,53)	1:184:A:PHE:N	1:186:A:SER:O	6	4.81
(4,53)	1:184:A:PHE:N	1:186:A:SER:O	3	4.74
(4,53)	1:184:A:PHE:N	1:186:A:SER:O	10	4.68
(4,53)	1:184:A:PHE:N	1:186:A:SER:O	8	4.63
(4,53)	1:184:A:PHE:N	1:186:A:SER:O	9	4.62
(4,53)	1:184:A:PHE:N	1:186:A:SER:O	2	4.6
(4,53)	1:184:A:PHE:N	1:186:A:SER:O	5	4.6
(4,53)	1:184:A:PHE:N	1:186:A:SER:O	1	4.58
(4,53)	1:184:A:PHE:N	1:186:A:SER:O	4	4.58
(4,53)	1:184:A:PHE:N	1:186:A:SER:O	7	4.55
(1,2222)	1:130:A:PHE:HA	1:136:A:ILE:HB	7	3.72
(1,2222)	1:130:A:PHE:HA	1:136:A:ILE:HB	5	3.39
(2,22)	1:113:A:VAL:HG13	1:112:A:PHE:H	1	3.33
(1,2222)	1:130:A:PHE:HA	1:136:A:ILE:HB	1	3.32
(1,2222)	1:130:A:PHE:HA	1:136:A:ILE:HB	4	3.23
(2,3622)	1:113:A:VAL:HG13	1:112:A:PHE:H	1	3.21
(2,1813)	1:113:A:VAL:HG13	1:112:A:PHE:H	1	3.16
(1,2222)	1:130:A:PHE:HA	1:136:A:ILE:HB	2	3.06
(2,5418)	1:113:A:VAL:HG13	1:112:A:PHE:H	1	3.02
(1,2774)	1:121:A:GLY:HA3	1:142:A:THR:HG21	2	2.99
(1,2165)	1:121:A:GLY:HA3	1:142:A:THR:HG21	2	2.98
(2,7285)	1:113:A:VAL:HG13	1:112:A:PHE:H	1	2.88
(1,2774)	1:121:A:GLY:HA3	1:142:A:THR:HG22	10	2.74
(1,2165)	1:121:A:GLY:HA3	1:142:A:THR:HG22	10	2.73
(1,2774)	1:121:A:GLY:HA3	1:142:A:THR:HG22	3	2.7
(1,2165)	1:121:A:GLY:HA3	1:142:A:THR:HG22	3	2.7
(1,2774)	1:121:A:GLY:HA3	1:142:A:THR:HG22	5	2.69
(1,2165)	1:121:A:GLY:HA3	1:142:A:THR:HG22	5	2.69
(1,2774)	1:121:A:GLY:HA3	1:142:A:THR:HG23	1	2.68
(1,2165)	1:121:A:GLY:HA3	1:142:A:THR:HG23	1	2.68
(1,2774)	1:121:A:GLY:HA3	1:142:A:THR:HG22	9	2.62
(1,2165)	1:121:A:GLY:HA3	1:142:A:THR:HG22	9	2.61
(2,130)	1:181:A:ILE:HG12	1:174:A:GLU:HB2	7	2.6
(1,2774)	1:121:A:GLY:HA3	1:142:A:THR:HG21	8	2.58
(1,2165)	1:121:A:GLY:HA3	1:142:A:THR:HG21	8	2.57
(2,8122)	1:163:A:GLU:HA	1:164:A:ILE:HG12	4	2.52
(1,2774)	1:121:A:GLY:HA3	1:142:A:THR:HG22	7	2.52
(2,8122)	1:163:A:GLU:HA	1:164:A:ILE:HG12	1	2.51
(2,8122)	1:163:A:GLU:HA	1:164:A:ILE:HG12	3	2.51
(2,8122)	1:163:A:GLU:HA	1:164:A:ILE:HG12	7	2.51
(1,2774)	1:121:A:GLY:HA3	1:142:A:THR:HG21	4	2.51
(1,2165)	1:121:A:GLY:HA3	1:142:A:THR:HG22	7	2.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2165)	1:121:A:GLY:HA3	1:142:A:THR:HG21	4	2.5
(2,8122)	1:163:A:GLU:HA	1:164:A:ILE:HG12	9	2.49
(2,8122)	1:163:A:GLU:HA	1:164:A:ILE:HG12	10	2.49
(2,8122)	1:163:A:GLU:HA	1:164:A:ILE:HG12	2	2.48
(2,8122)	1:163:A:GLU:HA	1:164:A:ILE:HG12	5	2.48
(2,8122)	1:163:A:GLU:HA	1:164:A:ILE:HG12	6	2.42
(2,6619)	1:176:A:ILE:HG23	1:175:A:ARG:HB3	1	2.39
(2,104)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	8	2.37
(2,8122)	1:163:A:GLU:HA	1:164:A:ILE:HG12	8	2.35
(1,2774)	1:121:A:GLY:HA3	1:142:A:THR:HG21	6	2.34
(1,2165)	1:121:A:GLY:HA3	1:142:A:THR:HG21	6	2.34
(2,104)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	9	2.33
(2,6788)	1:97:A:LEU:HG	1:98:A:LYS:H	9	2.27
(1,2772)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	9	2.27
(2,8511)	1:157:A:VAL:HG23	1:190:A:GLU:H	5	2.25
(2,8511)	1:157:A:VAL:HG23	1:190:A:GLU:H	1	2.18
(2,8511)	1:157:A:VAL:HG23	1:190:A:GLU:H	10	2.14
(2,6788)	1:97:A:LEU:HG	1:98:A:LYS:H	8	2.13
(2,8511)	1:157:A:VAL:HG23	1:190:A:GLU:H	6	2.1
(2,8511)	1:157:A:VAL:HG23	1:190:A:GLU:H	3	2.09
(1,2772)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	8	2.09
(1,376)	1:174:A:GLU:HB2	1:181:A:ILE:HD13	7	2.09
(2,6788)	1:97:A:LEU:HG	1:98:A:LYS:H	6	2.05
(2,8511)	1:157:A:VAL:HG23	1:190:A:GLU:H	9	2.03
(2,6788)	1:97:A:LEU:HG	1:98:A:LYS:H	7	2.01
(2,6788)	1:97:A:LEU:HG	1:98:A:LYS:H	2	2.0
(2,6788)	1:97:A:LEU:HG	1:98:A:LYS:H	5	2.0
(2,6788)	1:97:A:LEU:HG	1:98:A:LYS:H	10	2.0
(2,6788)	1:97:A:LEU:HG	1:98:A:LYS:H	3	1.99
(2,9)	1:181:A:ILE:HG12	1:175:A:ARG:HD2	3	1.99
(2,8511)	1:157:A:VAL:HG23	1:190:A:GLU:H	2	1.98
(2,6788)	1:97:A:LEU:HG	1:98:A:LYS:H	1	1.95
(1,841)	1:111:A:GLY:HA3	1:188:A:ARG:HG3	3	1.94
(1,422)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	10	1.94
(2,8511)	1:157:A:VAL:HG23	1:190:A:GLU:H	4	1.93
(2,104)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	3	1.93
(2,6788)	1:97:A:LEU:HG	1:98:A:LYS:H	4	1.92
(1,422)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	3	1.91
(1,422)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	1	1.9
(2,3635)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	5	1.89
(1,479)	1:159:A:PHE:HB2	1:136:A:ILE:HG23	7	1.89
(1,227)	1:183:A:ILE:HG12	1:116:A:ARG:HD2	8	1.89

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,8511)	1:157:A:VAL:HG23	1:190:A:GLU:H	7	1.88
(1,422)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	4	1.88
(1,479)	1:159:A:PHE:HB2	1:164:A:ILE:HG12	2	1.87
(1,1188)	1:165:A:ALA:H	1:112:A:PHE:HB3	7	1.86
(1,227)	1:183:A:ILE:HG12	1:116:A:ARG:HD2	9	1.85
(2,8503)	1:187:A:SER:H	1:184:A:PHE:HB2	6	1.84
(2,8503)	1:187:A:SER:H	1:184:A:PHE:HB2	1	1.83
(1,1106)	1:161:A:SER:H	1:110:A:ASP:HB3	7	1.83
(1,422)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	5	1.83
(2,8503)	1:187:A:SER:H	1:184:A:PHE:HB2	2	1.81
(2,7300)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	5	1.81
(2,4814)	1:157:A:VAL:HG23	1:190:A:GLU:H	5	1.81
(2,6638)	1:187:A:SER:H	1:184:A:PHE:HB2	6	1.8
(1,479)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	8	1.8
(2,6638)	1:187:A:SER:H	1:184:A:PHE:HB2	1	1.79
(2,5432)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	5	1.79
(2,17)	1:113:A:VAL:HG11	1:113:A:VAL:H	1	1.79
(1,479)	1:159:A:PHE:HB2	1:164:A:ILE:HG12	9	1.78
(2,8503)	1:187:A:SER:H	1:184:A:PHE:HB2	10	1.77
(2,6638)	1:187:A:SER:H	1:184:A:PHE:HB2	2	1.77
(1,1826)	1:185:A:LYS:H	1:186:A:SER:HB3	1	1.77
(1,2222)	1:113:A:VAL:HG12	1:109:A:ASN:HA	3	1.76
(2,8511)	1:157:A:VAL:HG23	1:190:A:GLU:H	8	1.75
(1,2415)	1:165:A:ALA:H	1:112:A:PHE:HB3	7	1.75
(2,4814)	1:157:A:VAL:HG23	1:190:A:GLU:H	1	1.74
(2,6638)	1:187:A:SER:H	1:184:A:PHE:HB2	10	1.73
(2,3635)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	1	1.73
(2,1777)	1:166:A:GLU:H	1:169:A:LEU:HB2	1	1.73
(2,1777)	1:166:A:GLU:H	1:169:A:LEU:HB2	2	1.73
(1,841)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	6	1.73
(2,3571)	1:184:A:PHE:H	1:186:A:SER:HB3	1	1.72
(2,4814)	1:157:A:VAL:HG23	1:190:A:GLU:H	10	1.7
(2,91)	1:155:A:ALA:HA	1:144:A:PRO:HD2	9	1.7
(2,1777)	1:166:A:GLU:H	1:169:A:LEU:HB2	3	1.69
(2,1765)	1:184:A:PHE:H	1:186:A:SER:HB3	1	1.69
(2,883)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	10	1.69
(1,854)	1:156:A:PHE:HB3	1:142:A:THR:HB	4	1.68
(2,3685)	1:155:A:ALA:HA	1:144:A:PRO:HD2	9	1.67
(2,3635)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	10	1.67
(2,104)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	10	1.67
(1,422)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	6	1.67
(2,883)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	2	1.66

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7300)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	1	1.65
(2,4908)	1:181:A:ILE:HG22	1:122:A:CYS:H	9	1.65
(2,4814)	1:157:A:VAL:HG23	1:190:A:GLU:H	6	1.65
(2,1825)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	5	1.65
(2,883)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	4	1.65
(2,883)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	6	1.65
(2,883)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	8	1.65
(2,4814)	1:157:A:VAL:HG23	1:190:A:GLU:H	3	1.64
(1,479)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	3	1.64
(1,479)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	4	1.64
(1,422)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	9	1.64
(2,3635)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	3	1.63
(2,3635)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	4	1.63
(2,3617)	1:113:A:VAL:HG11	1:113:A:VAL:H	1	1.63
(1,479)	1:159:A:PHE:HB2	1:164:A:ILE:HG12	6	1.63
(2,5432)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	1	1.62
(2,4908)	1:181:A:ILE:HG22	1:122:A:CYS:H	5	1.62
(2,104)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	6	1.62
(1,1798)	1:165:A:ALA:H	1:112:A:PHE:HB3	7	1.61
(1,479)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	1	1.6
(2,7300)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	10	1.59
(2,4908)	1:181:A:ILE:HG22	1:122:A:CYS:H	7	1.59
(1,1035)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	1	1.59
(2,4814)	1:157:A:VAL:HG23	1:190:A:GLU:H	9	1.58
(2,1844)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	3	1.58
(2,883)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	3	1.58
(1,479)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	5	1.58
(2,5432)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	10	1.57
(2,3093)	1:114:A:ARG:H	1:186:A:SER:HB3	1	1.57
(2,1808)	1:113:A:VAL:HG11	1:113:A:VAL:H	1	1.57
(1,3030)	1:165:A:ALA:H	1:112:A:PHE:HB3	7	1.57
(1,484)	1:136:A:ILE:HA	1:159:A:PHE:HB2	2	1.56
(2,8568)	1:139:A:ASN:H	1:158:A:GLN:HB2	10	1.55
(2,7300)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	3	1.55
(2,7300)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	4	1.55
(2,1881)	1:155:A:ALA:HA	1:144:A:PRO:HD2	9	1.55
(1,423)	1:156:A:PHE:HB3	1:157:A:VAL:HG23	6	1.55
(3,537)	1:118:A:LEU:HA	1:183:A:ILE:HG12	7	1.54
(2,4814)	1:157:A:VAL:HG23	1:190:A:GLU:H	2	1.54
(1,484)	1:136:A:ILE:HA	1:159:A:PHE:HB2	7	1.54
(2,5432)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	4	1.53
(2,4908)	1:181:A:ILE:HG22	1:122:A:CYS:H	1	1.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3584)	1:166:A:GLU:H	1:169:A:LEU:HB2	1	1.53
(2,1844)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	4	1.53
(1,2872)	1:131:A:PHE:HB2	1:136:A:ILE:HB	1	1.53
(1,854)	1:179:A:ARG:HD2	1:179:A:ARG:HA	1	1.53
(2,6706)	1:139:A:ASN:H	1:158:A:GLN:HB2	10	1.52
(2,5432)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	3	1.52
(2,4908)	1:181:A:ILE:HG22	1:122:A:CYS:H	4	1.52
(2,4908)	1:181:A:ILE:HG22	1:122:A:CYS:H	6	1.52
(2,3584)	1:166:A:GLU:H	1:169:A:LEU:HB2	2	1.52
(2,7366)	1:155:A:ALA:HA	1:144:A:PRO:HD2	9	1.51
(1,2926)	1:156:A:PHE:HB3	1:142:A:THR:HB	4	1.51
(1,1035)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	7	1.51
(2,7281)	1:113:A:VAL:HG11	1:113:A:VAL:H	1	1.49
(2,4814)	1:157:A:VAL:HG23	1:190:A:GLU:H	4	1.49
(2,3584)	1:166:A:GLU:H	1:169:A:LEU:HB2	3	1.49
(2,1844)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	10	1.49
(2,1825)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	1	1.49
(1,841)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	10	1.48
(1,484)	1:136:A:ILE:HA	1:159:A:PHE:HB2	9	1.48
(2,8503)	1:187:A:SER:H	1:184:A:PHE:HB2	4	1.47
(2,3652)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	3	1.47
(1,479)	1:159:A:PHE:HB2	1:164:A:ILE:HG12	10	1.47
(2,7247)	1:166:A:GLU:H	1:169:A:LEU:HB2	1	1.46
(2,7247)	1:166:A:GLU:H	1:169:A:LEU:HB2	2	1.46
(2,5493)	1:155:A:ALA:HA	1:144:A:PRO:HD2	9	1.46
(1,2314)	1:156:A:PHE:HB3	1:142:A:THR:HB	4	1.46
(1,1035)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	2	1.46
(1,1035)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	4	1.46
(1,854)	1:179:A:ARG:HD2	1:179:A:ARG:HA	3	1.46
(1,484)	1:136:A:ILE:HA	1:159:A:PHE:HB2	8	1.46
(2,8568)	1:139:A:ASN:H	1:158:A:GLN:HB2	3	1.45
(2,4908)	1:181:A:ILE:HG22	1:122:A:CYS:H	2	1.45
(1,1447)	1:115:A:LEU:HA	1:114:A:ARG:HG3	4	1.45
(1,838)	1:115:A:LEU:HA	1:114:A:ARG:HG3	4	1.45
(1,422)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	2	1.45
(2,8568)	1:139:A:ASN:H	1:158:A:GLN:HB2	8	1.44
(2,4814)	1:157:A:VAL:HG23	1:190:A:GLU:H	7	1.44
(2,3000)	1:187:A:SER:H	1:184:A:PHE:HB2	1	1.44
(2,3000)	1:187:A:SER:H	1:184:A:PHE:HB2	6	1.44
(2,1825)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	10	1.44
(2,8503)	1:187:A:SER:H	1:184:A:PHE:HB2	3	1.43
(2,7247)	1:166:A:GLU:H	1:169:A:LEU:HB2	3	1.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6638)	1:187:A:SER:H	1:184:A:PHE:HB2	4	1.43
(2,5414)	1:113:A:VAL:HG11	1:113:A:VAL:H	1	1.43
(2,3008)	1:157:A:VAL:HG23	1:190:A:GLU:H	5	1.43
(2,6706)	1:139:A:ASN:H	1:158:A:GLN:HB2	3	1.42
(2,4908)	1:181:A:ILE:HG22	1:122:A:CYS:H	3	1.42
(2,7364)	1:191:A:VAL:HG13	1:189:A:ALA:HA	7	1.41
(2,6706)	1:139:A:ASN:H	1:158:A:GLN:HB2	8	1.41
(2,5491)	1:191:A:VAL:HG13	1:189:A:ALA:HA	7	1.41
(2,3652)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	4	1.41
(2,3000)	1:187:A:SER:H	1:184:A:PHE:HB2	2	1.41
(1,484)	1:136:A:ILE:HA	1:159:A:PHE:HB2	6	1.41
(1,422)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	7	1.41
(2,8568)	1:139:A:ASN:H	1:158:A:GLN:HB2	9	1.4
(1,227)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	7	1.4
(2,6638)	1:187:A:SER:H	1:184:A:PHE:HB2	3	1.39
(2,4805)	1:187:A:SER:H	1:184:A:PHE:HB2	6	1.39
(2,1825)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	3	1.39
(2,1825)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	4	1.39
(2,1664)	1:175:A:ARG:HG2	1:176:A:ILE:H	1	1.39
(2,7364)	1:191:A:VAL:HG13	1:189:A:ALA:HA	9	1.38
(2,5491)	1:191:A:VAL:HG13	1:189:A:ALA:HA	9	1.38
(2,4805)	1:187:A:SER:H	1:184:A:PHE:HB2	1	1.38
(2,3652)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	10	1.38
(1,13)	1:181:A:ILE:HG12	1:175:A:ARG:HA	3	1.38
(2,6706)	1:139:A:ASN:H	1:158:A:GLN:HB2	9	1.37
(2,3000)	1:187:A:SER:H	1:184:A:PHE:HB2	10	1.37
(1,841)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	8	1.37
(2,5377)	1:166:A:GLU:H	1:169:A:LEU:HB2	1	1.36
(2,3008)	1:157:A:VAL:HG23	1:190:A:GLU:H	1	1.36
(2,428)	1:126:A:GLU:HB2	1:127:A:ILE:H	7	1.36
(1,2735)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	8	1.36
(1,2130)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	8	1.36
(1,1516)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	8	1.36
(1,906)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	8	1.36
(2,8568)	1:139:A:ASN:H	1:158:A:GLN:HB2	2	1.35
(2,7364)	1:191:A:VAL:HG13	1:189:A:ALA:HA	6	1.35
(2,7364)	1:191:A:VAL:HG13	1:189:A:ALA:HA	8	1.35
(2,5491)	1:191:A:VAL:HG13	1:189:A:ALA:HA	6	1.35
(2,5491)	1:191:A:VAL:HG13	1:189:A:ALA:HA	8	1.35
(2,5377)	1:166:A:GLU:H	1:169:A:LEU:HB2	2	1.35
(2,4805)	1:187:A:SER:H	1:184:A:PHE:HB2	2	1.35
(2,95)	1:159:A:PHE:HB2	1:135:A:GLU:H	1	1.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,95)	1:159:A:PHE:HB2	1:135:A:GLU:H	4	1.35
(1,2926)	1:179:A:ARG:HD2	1:179:A:ARG:HA	1	1.35
(2,5448)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	3	1.34
(1,2873)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	1	1.34
(2,9101)	1:166:A:GLU:H	1:169:A:LEU:HB2	1	1.33
(2,9101)	1:166:A:GLU:H	1:169:A:LEU:HB2	2	1.33
(2,500)	1:130:A:PHE:HB2	1:131:A:PHE:H	3	1.33
(2,130)	1:181:A:ILE:HG12	1:174:A:GLU:HB2	2	1.33
(1,841)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	9	1.33
(2,8568)	1:139:A:ASN:H	1:158:A:GLN:HB2	6	1.32
(2,6706)	1:139:A:ASN:H	1:158:A:GLN:HB2	2	1.32
(2,5377)	1:166:A:GLU:H	1:169:A:LEU:HB2	3	1.32
(2,4805)	1:187:A:SER:H	1:184:A:PHE:HB2	10	1.32
(2,3008)	1:157:A:VAL:HG23	1:190:A:GLU:H	10	1.32
(2,1165)	1:123:A:SER:HB3	1:143:A:LEU:HD23	8	1.32
(1,2735)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	9	1.32
(1,2666)	1:115:A:LEU:HA	1:114:A:ARG:HG3	4	1.32
(1,2130)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	9	1.32
(1,1516)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	9	1.32
(1,906)	1:169:A:LEU:HB2	1:111:A:GLY:HA3	9	1.32
(2,7364)	1:191:A:VAL:HG13	1:189:A:ALA:HA	2	1.31
(2,5491)	1:191:A:VAL:HG13	1:189:A:ALA:HA	2	1.31
(2,4908)	1:181:A:ILE:HG22	1:122:A:CYS:H	10	1.31
(2,3295)	1:134:A:LEU:HB2	1:135:A:GLU:H	1	1.31
(2,3295)	1:134:A:LEU:HB2	1:135:A:GLU:H	2	1.31
(2,3295)	1:134:A:LEU:HB2	1:135:A:GLU:H	4	1.31
(2,3295)	1:134:A:LEU:HB2	1:135:A:GLU:H	7	1.31
(2,500)	1:130:A:PHE:HB2	1:131:A:PHE:H	6	1.31
(2,95)	1:159:A:PHE:HB2	1:135:A:GLU:H	5	1.31
(1,2314)	1:179:A:ARG:HD2	1:179:A:ARG:HA	1	1.31
(2,5840)	1:126:A:GLU:HG3	1:127:A:ILE:H	7	1.3
(2,4814)	1:157:A:VAL:HG23	1:190:A:GLU:H	8	1.3
(2,3295)	1:134:A:LEU:HB2	1:135:A:GLU:H	8	1.3
(2,3295)	1:134:A:LEU:HB2	1:135:A:GLU:H	9	1.3
(2,2960)	1:123:A:SER:HB3	1:122:A:CYS:H	8	1.3
(2,9101)	1:166:A:GLU:H	1:169:A:LEU:HB2	3	1.29
(2,6706)	1:139:A:ASN:H	1:158:A:GLN:HB2	6	1.29
(2,3295)	1:134:A:LEU:HB2	1:135:A:GLU:H	6	1.29
(2,3295)	1:134:A:LEU:HB2	1:135:A:GLU:H	10	1.29
(2,500)	1:130:A:PHE:HB2	1:131:A:PHE:H	7	1.29
(1,2926)	1:179:A:ARG:HD2	1:179:A:ARG:HA	3	1.29
(1,132)	1:166:A:GLU:HG3	1:168:A:ALA:H	5	1.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5448)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	4	1.28
(2,3727)	1:181:A:ILE:HG12	1:174:A:GLU:HB2	7	1.28
(2,3605)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	5	1.28
(2,3295)	1:134:A:LEU:HB2	1:135:A:GLU:H	5	1.28
(2,1795)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	5	1.28
(2,428)	1:126:A:GLU:HB2	1:127:A:ILE:H	5	1.28
(2,130)	1:181:A:ILE:HG12	1:174:A:GLU:HB2	1	1.28
(2,130)	1:181:A:ILE:HG12	1:174:A:GLU:HB2	8	1.28
(2,130)	1:181:A:ILE:HG12	1:174:A:GLU:HB2	10	1.28
(1,423)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	1	1.28
(2,3008)	1:157:A:VAL:HG23	1:190:A:GLU:H	3	1.27
(2,3008)	1:157:A:VAL:HG23	1:190:A:GLU:H	6	1.27
(2,500)	1:130:A:PHE:HB2	1:131:A:PHE:H	8	1.27
(2,500)	1:130:A:PHE:HB2	1:131:A:PHE:H	10	1.27
(2,226)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	2	1.27
(2,35)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	5	1.27
(1,2263)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	1	1.27
(2,7318)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	3	1.26
(2,3605)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	1	1.26
(2,3295)	1:134:A:LEU:HB2	1:135:A:GLU:H	3	1.26
(2,1795)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	1	1.26
(2,130)	1:181:A:ILE:HG12	1:174:A:GLU:HB2	6	1.26
(1,2873)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	7	1.26
(2,8464)	1:123:A:SER:HB3	1:126:A:GLU:HB2	7	1.25
(2,6951)	1:134:A:LEU:HB2	1:135:A:GLU:H	1	1.25
(2,6951)	1:134:A:LEU:HB2	1:135:A:GLU:H	4	1.25
(2,5448)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	10	1.25
(2,1200)	1:187:A:SER:H	1:184:A:PHE:HB2	6	1.25
(2,976)	1:179:A:ARG:HD2	1:179:A:ARG:HB3	6	1.25
(2,500)	1:130:A:PHE:HB2	1:131:A:PHE:H	5	1.25
(2,9)	1:181:A:ILE:HG12	1:175:A:ARG:HD2	1	1.25
(1,2873)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	8	1.25
(1,2314)	1:179:A:ARG:HD2	1:179:A:ARG:HA	3	1.25
(1,221)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	3	1.25
(2,6951)	1:134:A:LEU:HB2	1:135:A:GLU:H	2	1.24
(2,6951)	1:134:A:LEU:HB2	1:135:A:GLU:H	7	1.24
(2,2013)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	2	1.24
(2,1200)	1:187:A:SER:H	1:184:A:PHE:HB2	1	1.24
(2,976)	1:179:A:ARG:HD2	1:179:A:ARG:HB3	5	1.24
(2,130)	1:181:A:ILE:HG12	1:174:A:GLU:HB2	9	1.24
(2,99)	1:188:A:ARG:HD3	1:191:A:VAL:HG22	8	1.24
(1,2872)	1:131:A:PHE:HB2	1:136:A:ILE:HB	2	1.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,838)	1:115:A:LEU:HA	1:114:A:ARG:HG3	9	1.24
(2,8576)	1:108:A:ALA:H	1:102:A:PRO:HG3	5	1.23
(2,6951)	1:134:A:LEU:HB2	1:135:A:GLU:H	8	1.23
(2,6951)	1:134:A:LEU:HB2	1:135:A:GLU:H	9	1.23
(2,1183)	1:190:A:GLU:HG3	1:186:A:SER:HA	4	1.23
(1,2702)	1:143:A:LEU:HG	1:143:A:LEU:HA	3	1.23
(1,1447)	1:115:A:LEU:HA	1:114:A:ARG:HG3	9	1.23
(1,221)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	1	1.23
(2,9054)	1:192:A:ARG:HG2	1:192:A:ARG:H	5	1.22
(2,6951)	1:134:A:LEU:HB2	1:135:A:GLU:H	6	1.22
(2,6951)	1:134:A:LEU:HB2	1:135:A:GLU:H	10	1.22
(2,4908)	1:181:A:ILE:HG22	1:122:A:CYS:H	8	1.22
(2,3822)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	2	1.22
(2,226)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	9	1.22
(1,2316)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	8	1.22
(1,221)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	2	1.22
(2,9054)	1:192:A:ARG:HG2	1:192:A:ARG:H	2	1.21
(2,9054)	1:192:A:ARG:HG2	1:192:A:ARG:H	4	1.21
(2,9054)	1:192:A:ARG:HG2	1:192:A:ARG:H	9	1.21
(2,7318)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	4	1.21
(2,7200)	1:192:A:ARG:HG2	1:192:A:ARG:H	2	1.21
(2,7200)	1:192:A:ARG:HG2	1:192:A:ARG:H	5	1.21
(2,7200)	1:192:A:ARG:HG2	1:192:A:ARG:H	9	1.21
(2,6951)	1:134:A:LEU:HB2	1:135:A:GLU:H	5	1.21
(2,3669)	1:169:A:LEU:HB2	1:166:A:GLU:HA	3	1.21
(2,3008)	1:157:A:VAL:HG23	1:190:A:GLU:H	9	1.21
(2,1200)	1:187:A:SER:H	1:184:A:PHE:HB2	2	1.21
(2,226)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	6	1.21
(1,2873)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	2	1.21
(1,2873)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	4	1.21
(1,423)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	7	1.21
(1,132)	1:166:A:GLU:HG3	1:168:A:ALA:H	7	1.21
(2,9054)	1:192:A:ARG:HG2	1:192:A:ARG:H	8	1.2
(2,8805)	1:134:A:LEU:HB2	1:135:A:GLU:H	1	1.2
(2,8805)	1:134:A:LEU:HB2	1:135:A:GLU:H	2	1.2
(2,8805)	1:134:A:LEU:HB2	1:135:A:GLU:H	4	1.2
(2,8805)	1:134:A:LEU:HB2	1:135:A:GLU:H	7	1.2
(2,7200)	1:192:A:ARG:HG2	1:192:A:ARG:H	4	1.2
(2,2970)	1:111:A:GLY:HA3	1:109:A:ASN:H	3	1.2
(2,8805)	1:134:A:LEU:HB2	1:135:A:GLU:H	8	1.19
(2,8576)	1:108:A:ALA:H	1:102:A:PRO:HG3	7	1.19
(2,7200)	1:192:A:ARG:HG2	1:192:A:ARG:H	8	1.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6951)	1:134:A:LEU:HB2	1:135:A:GLU:H	3	1.19
(2,6741)	1:114:A:ARG:H	1:186:A:SER:HB3	1	1.19
(2,5840)	1:126:A:GLU:HG3	1:127:A:ILE:H	8	1.19
(2,4030)	1:126:A:GLU:HG3	1:127:A:ILE:H	7	1.19
(2,2970)	1:111:A:GLY:HA3	1:109:A:ASN:H	10	1.19
(2,2013)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	9	1.19
(2,1919)	1:181:A:ILE:HG12	1:174:A:GLU:HB2	7	1.19
(1,2928)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	8	1.19
(1,2263)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	7	1.19
(1,132)	1:166:A:GLU:HG3	1:168:A:ALA:H	2	1.19
(1,13)	1:181:A:ILE:HG12	1:175:A:ARG:HA	4	1.19
(2,9054)	1:192:A:ARG:HG2	1:192:A:ARG:H	1	1.18
(2,8805)	1:134:A:LEU:HB2	1:135:A:GLU:H	9	1.18
(2,8805)	1:134:A:LEU:HB2	1:135:A:GLU:H	10	1.18
(2,5095)	1:134:A:LEU:HB2	1:135:A:GLU:H	1	1.18
(2,5095)	1:134:A:LEU:HB2	1:135:A:GLU:H	4	1.18
(2,2287)	1:130:A:PHE:HB2	1:131:A:PHE:H	3	1.18
(2,2219)	1:126:A:GLU:HG3	1:127:A:ILE:H	7	1.18
(2,2013)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	6	1.18
(2,1200)	1:187:A:SER:H	1:184:A:PHE:HB2	10	1.18
(2,130)	1:181:A:ILE:HG12	1:174:A:GLU:HB2	5	1.18
(2,8805)	1:134:A:LEU:HB2	1:135:A:GLU:H	5	1.17
(2,8805)	1:134:A:LEU:HB2	1:135:A:GLU:H	6	1.17
(2,7364)	1:191:A:VAL:HG13	1:189:A:ALA:HA	5	1.17
(2,7318)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	10	1.17
(2,7200)	1:192:A:ARG:HG2	1:192:A:ARG:H	1	1.17
(2,5491)	1:191:A:VAL:HG13	1:189:A:ALA:HA	5	1.17
(2,5095)	1:134:A:LEU:HB2	1:135:A:GLU:H	2	1.17
(2,5095)	1:134:A:LEU:HB2	1:135:A:GLU:H	7	1.17
(2,3822)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	9	1.17
(2,3605)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	4	1.17
(2,1795)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	4	1.17
(2,1164)	1:123:A:SER:HB3	1:122:A:CYS:H	8	1.17
(2,428)	1:126:A:GLU:HB2	1:127:A:ILE:H	2	1.17
(1,2702)	1:143:A:LEU:HG	1:143:A:LEU:HA	2	1.17
(1,1057)	1:133:A:GLY:HA3	1:134:A:LEU:HG	2	1.17
(1,423)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	9	1.17
(1,329)	1:166:A:GLU:HG3	1:168:A:ALA:H	5	1.17
(1,221)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	8	1.17
(2,9054)	1:192:A:ARG:HG2	1:192:A:ARG:H	7	1.16
(2,7200)	1:192:A:ARG:HG2	1:192:A:ARG:H	7	1.16
(2,5268)	1:175:A:ARG:HG2	1:176:A:ILE:H	1	1.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5095)	1:134:A:LEU:HB2	1:135:A:GLU:H	8	1.16
(2,5095)	1:134:A:LEU:HB2	1:135:A:GLU:H	9	1.16
(2,5095)	1:134:A:LEU:HB2	1:135:A:GLU:H	10	1.16
(2,4997)	1:110:A:ASP:HB3	1:110:A:ASP:H	9	1.16
(2,3822)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	6	1.16
(2,3008)	1:157:A:VAL:HG23	1:190:A:GLU:H	2	1.16
(2,2287)	1:130:A:PHE:HB2	1:131:A:PHE:H	6	1.16
(1,2060)	1:115:A:LEU:HA	1:114:A:ARG:HG3	4	1.16
(1,1696)	1:175:A:ARG:HB3	1:176:A:ILE:HD12	1	1.16
(1,423)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	2	1.16
(1,423)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	4	1.16
(2,9054)	1:192:A:ARG:HG2	1:192:A:ARG:H	10	1.15
(2,8805)	1:134:A:LEU:HB2	1:135:A:GLU:H	3	1.15
(2,8576)	1:108:A:ALA:H	1:102:A:PRO:HG3	1	1.15
(2,5095)	1:134:A:LEU:HB2	1:135:A:GLU:H	6	1.15
(2,4896)	1:114:A:ARG:H	1:186:A:SER:HB3	1	1.15
(2,4098)	1:130:A:PHE:HB2	1:131:A:PHE:H	3	1.15
(2,7200)	1:192:A:ARG:HG2	1:192:A:ARG:H	10	1.14
(2,5840)	1:126:A:GLU:HG3	1:127:A:ILE:H	1	1.14
(2,5095)	1:134:A:LEU:HB2	1:135:A:GLU:H	5	1.14
(2,2287)	1:130:A:PHE:HB2	1:131:A:PHE:H	7	1.14
(2,1844)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	5	1.14
(1,2499)	1:181:A:ILE:HG21	1:181:A:ILE:H	2	1.14
(1,2263)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	2	1.14
(1,2263)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	4	1.14
(1,1447)	1:115:A:LEU:HA	1:114:A:ARG:HG3	8	1.14
(1,838)	1:115:A:LEU:HA	1:114:A:ARG:HG3	8	1.14
(1,718)	1:154:A:GLU:HB3	1:154:A:GLU:H	2	1.14
(1,718)	1:154:A:GLU:HB3	1:154:A:GLU:H	10	1.14
(1,232)	1:110:A:ASP:HB2	1:107:A:THR:HG22	7	1.14
(2,5095)	1:134:A:LEU:HB2	1:135:A:GLU:H	3	1.13
(2,4098)	1:130:A:PHE:HB2	1:131:A:PHE:H	6	1.13
(2,130)	1:181:A:ILE:HG12	1:174:A:GLU:HB2	3	1.13
(1,718)	1:154:A:GLU:HB3	1:154:A:GLU:H	3	1.13
(1,718)	1:154:A:GLU:HB3	1:154:A:GLU:H	4	1.13
(1,718)	1:154:A:GLU:HB3	1:154:A:GLU:H	5	1.13
(1,423)	1:156:A:PHE:HB3	1:157:A:VAL:HG21	5	1.13
(2,5400)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	5	1.12
(2,3105)	1:181:A:ILE:HG22	1:122:A:CYS:H	9	1.12
(2,2287)	1:130:A:PHE:HB2	1:131:A:PHE:H	8	1.12
(2,2287)	1:130:A:PHE:HB2	1:131:A:PHE:H	10	1.12
(2,2)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	5	1.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,718)	1:154:A:GLU:HB3	1:154:A:GLU:H	9	1.12
(2,4098)	1:130:A:PHE:HB2	1:131:A:PHE:H	7	1.11
(2,3008)	1:157:A:VAL:HG23	1:190:A:GLU:H	4	1.11
(2,2970)	1:111:A:GLY:HA3	1:109:A:ASN:H	6	1.11
(2,2287)	1:130:A:PHE:HB2	1:131:A:PHE:H	5	1.11
(2,130)	1:181:A:ILE:HG12	1:174:A:GLU:HB2	4	1.11
(2,35)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	1	1.11
(1,2058)	1:115:A:LEU:HA	1:114:A:ARG:HG3	4	1.11
(1,1106)	1:161:A:SER:H	1:110:A:ASP:HB3	3	1.11
(1,295)	1:164:A:ILE:HD11	1:165:A:ALA:HB1	1	1.11
(1,232)	1:110:A:ASP:HB2	1:107:A:THR:HG22	2	1.11
(2,5840)	1:126:A:GLU:HG3	1:127:A:ILE:H	9	1.1
(2,5400)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	1	1.1
(2,4477)	1:166:A:GLU:HG2	1:166:A:GLU:H	4	1.1
(2,2)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	1	1.1
(1,2702)	1:169:A:LEU:HB2	1:166:A:GLU:HA	1	1.1
(1,2666)	1:115:A:LEU:HA	1:114:A:ARG:HG3	9	1.1
(1,2499)	1:181:A:ILE:HG21	1:181:A:ILE:H	8	1.1
(1,1057)	1:133:A:GLY:HA3	1:134:A:LEU:HG	7	1.1
(1,1035)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	5	1.1
(2,8568)	1:139:A:ASN:H	1:158:A:GLN:HB2	4	1.09
(2,6845)	1:110:A:ASP:HB3	1:110:A:ASP:H	9	1.09
(2,5538)	1:181:A:ILE:HG12	1:174:A:GLU:HB2	7	1.09
(2,4098)	1:130:A:PHE:HB2	1:131:A:PHE:H	8	1.09
(2,4098)	1:130:A:PHE:HB2	1:131:A:PHE:H	10	1.09
(2,3538)	1:192:A:ARG:HG2	1:192:A:ARG:H	5	1.09
(2,3538)	1:192:A:ARG:HG2	1:192:A:ARG:H	9	1.09
(2,3105)	1:181:A:ILE:HG22	1:122:A:CYS:H	5	1.09
(2,2666)	1:166:A:GLU:HG2	1:166:A:GLU:H	4	1.09
(2,1844)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	1	1.09
(2,1161)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	1	1.09
(2,500)	1:130:A:PHE:HB2	1:131:A:PHE:H	1	1.09
(1,757)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	10	1.09
(1,718)	1:154:A:GLU:HB3	1:154:A:GLU:H	1	1.09
(1,329)	1:166:A:GLU:HG3	1:168:A:ALA:H	7	1.09
(1,17)	1:113:A:VAL:HG11	1:186:A:SER:HB3	1	1.09
(2,6617)	1:190:A:GLU:HG3	1:186:A:SER:HA	4	1.08
(2,4030)	1:126:A:GLU:HG3	1:127:A:ILE:H	8	1.08
(2,3538)	1:192:A:ARG:HG2	1:192:A:ARG:H	2	1.08
(2,3538)	1:192:A:ARG:HG2	1:192:A:ARG:H	4	1.08
(2,1883)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	4	1.08
(2,1883)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	7	1.08

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1185)	1:156:A:PHE:HB2	1:191:A:VAL:H	1	1.08
(2,1161)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	9	1.08
(1,2735)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	3	1.08
(1,2130)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	3	1.08
(1,1516)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	3	1.08
(1,1057)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	1	1.08
(1,906)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	3	1.08
(1,757)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	4	1.08
(1,757)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	5	1.08
(1,757)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	7	1.08
(3,623)	1:185:A:LYS:H	1:186:A:SER:HB3	1	1.07
(3,497)	1:185:A:LYS:H	1:186:A:SER:HB3	1	1.07
(3,372)	1:185:A:LYS:H	1:186:A:SER:HB3	1	1.07
(3,242)	1:185:A:LYS:H	1:186:A:SER:HB3	1	1.07
(3,107)	1:185:A:LYS:H	1:186:A:SER:HB3	1	1.07
(2,7364)	1:191:A:VAL:HG13	1:189:A:ALA:HA	3	1.07
(2,5637)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	2	1.07
(2,5491)	1:191:A:VAL:HG13	1:189:A:ALA:HA	3	1.07
(2,4777)	1:111:A:GLY:HA3	1:109:A:ASN:H	3	1.07
(2,4098)	1:130:A:PHE:HB2	1:131:A:PHE:H	5	1.07
(2,3538)	1:192:A:ARG:HG2	1:192:A:ARG:H	8	1.07
(2,3000)	1:187:A:SER:H	1:184:A:PHE:HB2	4	1.07
(2,2219)	1:126:A:GLU:HG3	1:127:A:ILE:H	8	1.07
(2,1883)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	3	1.07
(2,1883)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	10	1.07
(2,837)	1:163:A:GLU:HG3	1:163:A:GLU:H	7	1.07
(2,6706)	1:139:A:ASN:H	1:158:A:GLN:HB2	4	1.06
(2,4777)	1:111:A:GLY:HA3	1:109:A:ASN:H	10	1.06
(2,3105)	1:181:A:ILE:HG22	1:122:A:CYS:H	7	1.06
(2,3008)	1:157:A:VAL:HG23	1:190:A:GLU:H	7	1.06
(2,1883)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	1	1.06
(2,1161)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	2	1.06
(2,883)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	9	1.06
(2,837)	1:163:A:GLU:HG3	1:163:A:GLU:H	4	1.06
(1,1057)	1:133:A:GLY:HA3	1:134:A:LEU:HG	4	1.06
(1,718)	1:154:A:GLU:HB3	1:154:A:GLU:H	6	1.06
(1,329)	1:166:A:GLU:HG3	1:168:A:ALA:H	2	1.06
(2,7508)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	2	1.05
(2,3669)	1:169:A:LEU:HB2	1:166:A:GLU:HA	2	1.05
(2,3538)	1:192:A:ARG:HG2	1:192:A:ARG:H	1	1.05
(2,1424)	1:116:A:ARG:HG2	1:117:A:GLY:H	6	1.05
(2,81)	1:192:A:ARG:HA	1:137:A:VAL:HG12	4	1.05

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,35)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	10	1.05
(1,2499)	1:181:A:ILE:HG21	1:181:A:ILE:H	3	1.05
(1,1670)	1:133:A:GLY:HA3	1:134:A:LEU:HG	2	1.05
(1,757)	1:141:A:ILE:HG13	1:140:A:GLY:HA2	9	1.05
(1,221)	1:116:A:ARG:HD2	1:181:A:ILE:HD12	4	1.05
(3,101)	1:126:A:GLU:HB2	1:123:A:SER:HB3	7	1.04
(2,3000)	1:187:A:SER:H	1:184:A:PHE:HB2	3	1.04
(2,1883)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	2	1.04
(2,1883)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	5	1.04
(2,883)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	7	1.04
(1,2316)	1:156:A:PHE:HB2	1:141:A:ILE:HG23	7	1.04
(2,7364)	1:191:A:VAL:HG13	1:189:A:ALA:HA	1	1.03
(2,5491)	1:191:A:VAL:HG13	1:189:A:ALA:HA	1	1.03
(2,4477)	1:166:A:GLU:HG2	1:166:A:GLU:H	9	1.03
(2,4030)	1:126:A:GLU:HG3	1:127:A:ILE:H	1	1.03
(2,3538)	1:192:A:ARG:HG2	1:192:A:ARG:H	7	1.03
(2,2891)	1:190:A:GLU:HG2	1:190:A:GLU:H	4	1.03
(2,2666)	1:166:A:GLU:HG2	1:166:A:GLU:H	9	1.03
(2,1185)	1:156:A:PHE:HB2	1:191:A:VAL:H	4	1.03
(2,883)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	1	1.03
(1,2671)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	4	1.03
(1,2671)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	7	1.03
(1,2499)	1:96:A:VAL:HG22	1:97:A:LEU:H	7	1.03
(2,5637)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	9	1.02
(2,5483)	1:192:A:ARG:HA	1:137:A:VAL:HG12	4	1.02
(2,4805)	1:187:A:SER:H	1:184:A:PHE:HB2	4	1.02
(2,3652)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	5	1.02
(2,3538)	1:192:A:ARG:HG2	1:192:A:ARG:H	10	1.02
(2,2219)	1:126:A:GLU:HG3	1:127:A:ILE:H	1	1.02
(2,1185)	1:156:A:PHE:HB2	1:191:A:VAL:H	10	1.02
(2,1161)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	3	1.02
(2,1161)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	5	1.02
(1,2671)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	3	1.02
(1,2671)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	10	1.02
(1,757)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	2	1.02
(1,757)	1:141:A:ILE:HG13	1:140:A:GLY:HA2	6	1.02
(1,456)	1:165:A:ALA:HA	1:113:A:VAL:HG23	9	1.02
(2,7364)	1:191:A:VAL:HG13	1:189:A:ALA:HA	10	1.01
(2,5637)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	6	1.01
(2,5491)	1:191:A:VAL:HG13	1:189:A:ALA:HA	10	1.01
(2,5400)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	4	1.01
(2,3995)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	2	1.01

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,837)	1:163:A:GLU:HG3	1:163:A:GLU:H	3	1.01
(2,837)	1:163:A:GLU:HG3	1:163:A:GLU:H	9	1.01
(2,99)	1:188:A:ARG:HD3	1:191:A:VAL:HG22	9	1.01
(2,81)	1:192:A:ARG:HA	1:137:A:VAL:HG11	6	1.01
(2,81)	1:192:A:ARG:HA	1:137:A:VAL:HG12	10	1.01
(2,35)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	3	1.01
(2,35)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	4	1.01
(2,2)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	4	1.01
(1,2928)	1:156:A:PHE:HB2	1:141:A:ILE:HG23	7	1.01
(1,2671)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	1	1.01
(1,2666)	1:115:A:LEU:HA	1:114:A:ARG:HG3	8	1.01
(1,2316)	1:156:A:PHE:HB2	1:141:A:ILE:HG23	2	1.01
(1,2065)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	4	1.01
(1,2065)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	7	1.01
(1,1035)	1:139:A:ASN:HB2	1:137:A:VAL:HG22	10	1.01
(1,232)	1:110:A:ASP:HB2	1:107:A:THR:HG22	1	1.01
(2,7508)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	9	1.0
(2,5466)	1:166:A:GLU:HG2	1:166:A:GLU:H	4	1.0
(2,3995)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	1	1.0
(2,3995)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	3	1.0
(2,3105)	1:181:A:ILE:HG22	1:122:A:CYS:H	1	1.0
(2,1883)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	9	1.0
(2,816)	1:161:A:SER:HB2	1:162:A:GLN:H	7	1.0
(1,2065)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	3	1.0
(1,2065)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	10	1.0
(1,1447)	1:115:A:LEU:HA	1:114:A:ARG:HG3	2	1.0
(1,1106)	1:161:A:SER:H	1:110:A:ASP:HB3	6	1.0
(1,838)	1:115:A:LEU:HA	1:114:A:ARG:HG3	2	1.0
(1,757)	1:179:A:ARG:HB3	1:119:A:PRO:HD2	1	1.0
(1,232)	1:110:A:ASP:HB2	1:107:A:THR:HG22	4	1.0
(2,7508)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	6	0.99
(2,5483)	1:192:A:ARG:HA	1:137:A:VAL:HG11	6	0.99
(2,4777)	1:111:A:GLY:HA3	1:109:A:ASN:H	6	0.99
(2,4545)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	1	0.99
(2,4030)	1:126:A:GLU:HG3	1:127:A:ILE:H	9	0.99
(2,3995)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	6	0.99
(2,3687)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	4	0.99
(2,3687)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	7	0.99
(2,3105)	1:181:A:ILE:HG22	1:122:A:CYS:H	4	0.99
(2,3105)	1:181:A:ILE:HG22	1:122:A:CYS:H	6	0.99
(2,1883)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	8	0.99
(2,1647)	1:171:A:LYS:H	1:170:A:LYS:HB2	6	0.99

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1161)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	10	0.99
(2,69)	1:166:A:GLU:HG2	1:166:A:GLU:H	4	0.99
(1,2921)	1:176:A:ILE:HG21	1:175:A:ARG:HB3	3	0.99
(1,2671)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	2	0.99
(1,2671)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	5	0.99
(1,2352)	1:148:A:GLN:H	1:143:A:LEU:HD22	5	0.99
(1,2065)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	1	0.99
(1,1447)	1:115:A:LEU:HA	1:114:A:ARG:HG3	5	0.99
(1,838)	1:115:A:LEU:HA	1:114:A:ARG:HG3	5	0.99
(1,132)	1:166:A:GLU:HG3	1:168:A:ALA:H	4	0.99
(1,13)	1:181:A:ILE:HG12	1:175:A:ARG:HA	10	0.99
(2,7340)	1:169:A:LEU:HB2	1:166:A:GLU:HA	3	0.98
(2,5483)	1:192:A:ARG:HA	1:137:A:VAL:HG12	10	0.98
(2,4805)	1:187:A:SER:H	1:184:A:PHE:HB2	3	0.98
(2,4477)	1:166:A:GLU:HG2	1:166:A:GLU:H	6	0.98
(2,3995)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	8	0.98
(2,3687)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	3	0.98
(2,3687)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	10	0.98
(2,3652)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	1	0.98
(2,3196)	1:110:A:ASP:HB3	1:110:A:ASP:H	9	0.98
(2,2666)	1:166:A:GLU:HG2	1:166:A:GLU:H	6	0.98
(2,2219)	1:126:A:GLU:HG3	1:127:A:ILE:H	9	0.98
(2,1795)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	3	0.98
(2,1647)	1:171:A:LYS:H	1:170:A:LYS:HB2	3	0.98
(2,1647)	1:171:A:LYS:H	1:170:A:LYS:HB2	8	0.98
(2,837)	1:163:A:GLU:HG3	1:163:A:GLU:H	5	0.98
(2,272)	1:105:A:PRO:HD3	1:104:A:SER:HB3	5	0.98
(1,2928)	1:156:A:PHE:HB2	1:141:A:ILE:HG23	2	0.98
(1,2921)	1:176:A:ILE:HG21	1:175:A:ARG:HB3	8	0.98
(1,2499)	1:181:A:ILE:HG21	1:181:A:ILE:H	9	0.98
(1,2399)	1:189:A:ALA:H	1:186:A:SER:HA	9	0.98
(1,232)	1:110:A:ASP:HB2	1:107:A:THR:HG22	5	0.98
(2,6313)	1:167:A:LYS:HG2	1:167:A:LYS:HE3	3	0.97
(2,4764)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	1	0.97
(2,3995)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	9	0.97
(2,3687)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	1	0.97
(2,3605)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	3	0.97
(2,1613)	1:162:A:GLN:HB2	1:163:A:GLU:H	6	0.97
(2,1073)	1:188:A:ARG:HA	1:188:A:ARG:HD3	9	0.97
(2,81)	1:192:A:ARG:HA	1:137:A:VAL:HG11	3	0.97
(1,2316)	1:156:A:PHE:HB2	1:141:A:ILE:HG23	9	0.97
(1,2065)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	2	0.97

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2065)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	5	0.97
(1,1670)	1:133:A:GLY:HA3	1:134:A:LEU:HG	7	0.97
(1,1083)	1:175:A:ARG:HB3	1:176:A:ILE:HD12	2	0.97
(1,233)	1:116:A:ARG:HD2	1:116:A:ARG:HA	1	0.97
(1,132)	1:166:A:GLU:HG3	1:168:A:ALA:H	6	0.97
(1,13)	1:181:A:ILE:HG12	1:175:A:ARG:HA	9	0.97
(2,8175)	1:166:A:GLU:HG2	1:166:A:GLU:H	4	0.96
(2,5335)	1:192:A:ARG:HG2	1:192:A:ARG:H	5	0.96
(2,4764)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	9	0.96
(2,1185)	1:156:A:PHE:HB2	1:191:A:VAL:H	3	0.96
(2,837)	1:163:A:GLU:HG3	1:163:A:GLU:H	1	0.96
(1,2671)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	9	0.96
(1,2499)	1:96:A:VAL:HG22	1:97:A:LEU:H	1	0.96
(1,125)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	10	0.96
(2,8568)	1:139:A:ASN:H	1:158:A:GLN:HB2	1	0.95
(2,7314)	1:191:A:VAL:HG13	1:193:A:THR:H	5	0.95
(2,5335)	1:192:A:ARG:HG2	1:192:A:ARG:H	2	0.95
(2,5335)	1:192:A:ARG:HG2	1:192:A:ARG:H	9	0.95
(2,4764)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	2	0.95
(2,3687)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	2	0.95
(2,3687)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	5	0.95
(2,2734)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	1	0.95
(2,2287)	1:130:A:PHE:HB2	1:131:A:PHE:H	1	0.95
(2,1161)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	6	0.95
(2,1161)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	8	0.95
(2,837)	1:163:A:GLU:HG3	1:163:A:GLU:H	2	0.95
(2,272)	1:105:A:PRO:HD3	1:104:A:SER:HB3	4	0.95
(2,81)	1:192:A:ARG:HA	1:137:A:VAL:HG13	1	0.95
(1,2671)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	8	0.95
(1,2499)	1:181:A:ILE:HG21	1:181:A:ILE:H	5	0.95
(1,2352)	1:148:A:GLN:H	1:143:A:LEU:HD21	8	0.95
(1,1670)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	1	0.95
(1,1083)	1:175:A:ARG:HB3	1:176:A:ILE:HD12	3	0.95
(1,456)	1:94:A:ASP:HA	1:164:A:ILE:HD13	6	0.95
(1,125)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	1	0.95
(1,125)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	4	0.95
(1,125)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	5	0.95
(1,125)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	7	0.95
(2,8701)	1:110:A:ASP:HB3	1:110:A:ASP:H	9	0.94
(2,7269)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	5	0.94
(2,5483)	1:192:A:ARG:HA	1:137:A:VAL:HG11	3	0.94
(2,5335)	1:192:A:ARG:HG2	1:192:A:ARG:H	4	0.94

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5335)	1:192:A:ARG:HG2	1:192:A:ARG:H	8	0.94
(2,3995)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	7	0.94
(2,85)	1:187:A:SER:HB3	1:189:A:ALA:H	9	0.94
(1,2928)	1:156:A:PHE:HB2	1:141:A:ILE:HG23	9	0.94
(1,2921)	1:176:A:ILE:HG21	1:175:A:ARG:HB3	6	0.94
(1,2873)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	10	0.94
(1,2316)	1:156:A:PHE:HB2	1:141:A:ILE:HG23	6	0.94
(1,2065)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	9	0.94
(1,2060)	1:115:A:LEU:HA	1:114:A:ARG:HG3	9	0.94
(1,1035)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	6	0.94
(1,132)	1:166:A:GLU:HG3	1:168:A:ALA:H	9	0.94
(2,7364)	1:191:A:VAL:HG13	1:189:A:ALA:HA	4	0.93
(2,5491)	1:191:A:VAL:HG13	1:189:A:ALA:HA	4	0.93
(2,5466)	1:166:A:GLU:HG2	1:166:A:GLU:H	9	0.93
(2,3995)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	5	0.93
(2,3008)	1:157:A:VAL:HG23	1:190:A:GLU:H	8	0.93
(2,1840)	1:191:A:VAL:HG11	1:186:A:SER:HA	4	0.93
(2,408)	1:120:A:PHE:HB3	1:120:A:PHE:H	10	0.93
(2,232)	1:100:A:THR:HA	1:99:A:HIS:HB2	9	0.93
(1,2921)	1:176:A:ILE:HG21	1:175:A:ARG:HB3	2	0.93
(1,2296)	1:165:A:ALA:HA	1:113:A:VAL:HG21	6	0.93
(1,2065)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	8	0.93
(1,1670)	1:133:A:GLY:HA3	1:134:A:LEU:HG	4	0.93
(1,1188)	1:165:A:ALA:H	1:110:A:ASP:HB3	3	0.93
(1,1035)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	9	0.93
(1,473)	1:157:A:VAL:HG23	1:114:A:ARG:HB3	9	0.93
(1,295)	1:164:A:ILE:HD12	1:166:A:GLU:HB2	4	0.93
(2,7320)	1:191:A:VAL:HG12	1:137:A:VAL:HG11	3	0.92
(2,7314)	1:191:A:VAL:HG13	1:193:A:THR:H	4	0.92
(2,7269)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	1	0.92
(2,6706)	1:139:A:ASN:H	1:158:A:GLN:HB2	1	0.92
(2,5483)	1:192:A:ARG:HA	1:137:A:VAL:HG13	1	0.92
(2,5451)	1:191:A:VAL:HG12	1:137:A:VAL:HG11	3	0.92
(2,5335)	1:192:A:ARG:HG2	1:192:A:ARG:H	1	0.92
(2,4768)	1:126:A:GLU:HB2	1:123:A:SER:HB3	7	0.92
(2,3687)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	9	0.92
(2,3105)	1:181:A:ILE:HG22	1:122:A:CYS:H	2	0.92
(2,1647)	1:171:A:LYS:H	1:170:A:LYS:HB2	4	0.92
(2,69)	1:166:A:GLU:HG2	1:166:A:GLU:H	9	0.92
(2,54)	1:191:A:VAL:HG12	1:137:A:VAL:HG11	3	0.92
(1,3066)	1:108:A:ALA:H	1:106:A:ASP:HB3	9	0.92
(1,2352)	1:148:A:GLN:H	1:143:A:LEU:HD21	9	0.92

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1447)	1:115:A:LEU:HA	1:114:A:ARG:HG3	3	0.92
(1,838)	1:115:A:LEU:HA	1:114:A:ARG:HG3	3	0.92
(1,683)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	2	0.92
(1,132)	1:166:A:GLU:HG3	1:168:A:ALA:H	8	0.92
(1,125)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	8	0.92
(2,7314)	1:191:A:VAL:HG13	1:193:A:THR:H	1	0.91
(2,4098)	1:130:A:PHE:HB2	1:131:A:PHE:H	1	0.91
(2,3995)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	10	0.91
(2,3687)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	8	0.91
(2,3470)	1:175:A:ARG:HB3	1:176:A:ILE:H	1	0.91
(2,1185)	1:156:A:PHE:HB2	1:191:A:VAL:H	5	0.91
(2,408)	1:120:A:PHE:HB3	1:120:A:PHE:H	2	0.91
(2,81)	1:192:A:ARG:HA	1:137:A:VAL:HG12	2	0.91
(2,81)	1:192:A:ARG:HA	1:137:A:VAL:HG13	7	0.91
(1,2968)	1:148:A:GLN:H	1:143:A:LEU:HD22	5	0.91
(1,2928)	1:156:A:PHE:HB2	1:141:A:ILE:HG23	6	0.91
(1,2499)	1:181:A:ILE:HG21	1:181:A:ILE:H	4	0.91
(1,2222)	1:113:A:VAL:HG12	1:109:A:ASN:HA	10	0.91
(1,1188)	1:165:A:ALA:H	1:110:A:ASP:HB3	6	0.91
(1,1035)	1:139:A:ASN:HB2	1:137:A:VAL:HG22	8	0.91
(1,233)	1:116:A:ARG:HD2	1:116:A:ARG:HA	3	0.91
(1,125)	1:141:A:ILE:HG13	1:140:A:GLY:HA2	9	0.91
(1,4)	1:136:A:ILE:HD13	1:164:A:ILE:HA	6	0.91
(2,5335)	1:192:A:ARG:HG2	1:192:A:ARG:H	7	0.9
(2,4764)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	3	0.9
(2,4764)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	5	0.9
(2,2957)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	1	0.9
(2,2950)	1:162:A:GLN:HG2	1:165:A:ALA:H	5	0.9
(2,1730)	1:192:A:ARG:HG2	1:192:A:ARG:H	2	0.9
(2,1730)	1:192:A:ARG:HG2	1:192:A:ARG:H	5	0.9
(2,1730)	1:192:A:ARG:HG2	1:192:A:ARG:H	9	0.9
(2,1073)	1:188:A:ARG:HA	1:188:A:ARG:HD3	8	0.9
(2,85)	1:187:A:SER:HB3	1:189:A:ALA:H	8	0.9
(1,2058)	1:115:A:LEU:HA	1:114:A:ARG:HG3	9	0.9
(1,1083)	1:175:A:ARG:HB3	1:176:A:ILE:HD11	9	0.9
(1,251)	1:188:A:ARG:HD3	1:191:A:VAL:HG22	7	0.9
(1,221)	1:116:A:ARG:HD2	1:181:A:ILE:HD12	10	0.9
(1,125)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	3	0.9
(1,13)	1:181:A:ILE:HG12	1:175:A:ARG:HA	5	0.9
(2,8175)	1:166:A:GLU:HG2	1:166:A:GLU:H	9	0.89
(2,6313)	1:167:A:LYS:HG2	1:167:A:LYS:HE3	8	0.89
(2,5483)	1:192:A:ARG:HA	1:137:A:VAL:HG13	7	0.89

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5466)	1:166:A:GLU:HG2	1:166:A:GLU:H	6	0.89
(2,5448)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	5	0.89
(2,5335)	1:192:A:ARG:HG2	1:192:A:ARG:H	10	0.89
(2,3105)	1:181:A:ILE:HG22	1:122:A:CYS:H	3	0.89
(2,2957)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	9	0.89
(2,1730)	1:192:A:ARG:HG2	1:192:A:ARG:H	4	0.89
(2,1161)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	7	0.89
(1,2499)	1:181:A:ILE:HG21	1:181:A:ILE:H	10	0.89
(1,2488)	1:137:A:VAL:HG23	1:140:A:GLY:H	10	0.89
(1,1788)	1:132:A:SER:H	1:136:A:ILE:HB	9	0.89
(1,1035)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	3	0.89
(1,233)	1:116:A:ARG:HD2	1:116:A:ARG:HA	9	0.89
(1,233)	1:116:A:ARG:HD2	1:116:A:ARG:HA	10	0.89
(1,125)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	2	0.89
(1,125)	1:141:A:ILE:HG13	1:140:A:GLY:HA2	6	0.89
(1,45)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	2	0.89
(1,13)	1:181:A:ILE:HG12	1:175:A:ARG:HA	6	0.89
(2,7788)	1:130:A:PHE:HB2	1:131:A:PHE:H	3	0.88
(2,7353)	1:192:A:ARG:HA	1:137:A:VAL:HG12	4	0.88
(2,7314)	1:191:A:VAL:HG13	1:193:A:THR:H	2	0.88
(2,6626)	1:111:A:GLY:H	1:162:A:GLN:HB3	6	0.88
(2,6619)	1:176:A:ILE:HG21	1:175:A:ARG:HB3	3	0.88
(2,6313)	1:167:A:LYS:HG2	1:167:A:LYS:HE3	6	0.88
(2,5483)	1:192:A:ARG:HA	1:137:A:VAL:HG12	2	0.88
(2,3995)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	4	0.88
(2,3611)	1:181:A:ILE:HG12	1:175:A:ARG:HD2	3	0.88
(2,3471)	1:175:A:ARG:HG2	1:176:A:ILE:H	1	0.88
(2,1862)	1:169:A:LEU:HB2	1:166:A:GLU:HA	3	0.88
(2,1840)	1:191:A:VAL:HG11	1:186:A:SER:HA	1	0.88
(2,1840)	1:191:A:VAL:HG11	1:186:A:SER:HA	2	0.88
(2,1730)	1:192:A:ARG:HG2	1:192:A:ARG:H	8	0.88
(2,1200)	1:187:A:SER:H	1:184:A:PHE:HB2	4	0.88
(2,69)	1:166:A:GLU:HG2	1:166:A:GLU:H	6	0.88
(1,1795)	1:122:A:CYS:H	1:127:A:ILE:HD11	7	0.88
(1,1795)	1:122:A:CYS:H	1:127:A:ILE:HD11	8	0.88
(1,1057)	1:133:A:GLY:HA3	1:134:A:LEU:HG	5	0.88
(1,718)	1:118:A:LEU:HG	1:154:A:GLU:H	8	0.88
(1,588)	1:164:A:ILE:HG13	1:165:A:ALA:H	8	0.88
(1,233)	1:116:A:ARG:HD2	1:116:A:ARG:HA	7	0.88
(1,191)	1:93:A:MET:HA	1:92:A:ALA:HB2	6	0.88
(1,132)	1:166:A:GLU:HG3	1:168:A:ALA:H	10	0.88
(2,5915)	1:130:A:PHE:HB2	1:131:A:PHE:H	3	0.87

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4767)	1:123:A:SER:HB3	1:122:A:CYS:H	8	0.87
(2,4764)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	10	0.87
(2,2957)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	2	0.87
(2,936)	1:175:A:ARG:HG2	1:175:A:ARG:HA	1	0.87
(2,81)	1:192:A:ARG:HA	1:137:A:VAL:HG12	9	0.87
(1,2968)	1:148:A:GLN:H	1:143:A:LEU:HD21	8	0.87
(1,2872)	1:131:A:PHE:HB2	1:136:A:ILE:HB	4	0.87
(1,2738)	1:143:A:LEU:HG	1:141:A:ILE:HG21	6	0.87
(1,2666)	1:115:A:LEU:HA	1:114:A:ARG:HG3	2	0.87
(1,2488)	1:137:A:VAL:HG23	1:140:A:GLY:H	2	0.87
(1,2488)	1:96:A:VAL:HG22	1:97:A:LEU:H	5	0.87
(1,2488)	1:137:A:VAL:HG23	1:140:A:GLY:H	9	0.87
(1,588)	1:164:A:ILE:HG13	1:165:A:ALA:H	1	0.87
(1,588)	1:164:A:ILE:HG13	1:165:A:ALA:H	10	0.87
(1,329)	1:166:A:GLU:HG3	1:168:A:ALA:H	4	0.87
(1,233)	1:116:A:ARG:HD3	1:116:A:ARG:HA	2	0.87
(1,233)	1:116:A:ARG:HD2	1:116:A:ARG:HA	8	0.87
(1,4)	1:136:A:ILE:HD13	1:164:A:ILE:HA	5	0.87
(1,4)	1:136:A:ILE:HD11	1:164:A:ILE:HA	8	0.87
(2,7788)	1:130:A:PHE:HB2	1:131:A:PHE:H	6	0.86
(2,6619)	1:176:A:ILE:HG21	1:175:A:ARG:HB3	8	0.86
(2,6313)	1:167:A:LYS:HG2	1:167:A:LYS:HE3	4	0.86
(2,1909)	1:142:A:THR:HG21	1:141:A:ILE:HG21	6	0.86
(2,1840)	1:191:A:VAL:HG11	1:186:A:SER:HA	6	0.86
(2,1840)	1:191:A:VAL:HG11	1:186:A:SER:HA	7	0.86
(2,1730)	1:192:A:ARG:HG2	1:192:A:ARG:H	1	0.86
(2,1647)	1:171:A:LYS:H	1:170:A:LYS:HB2	9	0.86
(2,1396)	1:112:A:PHE:H	1:111:A:GLY:H	7	0.86
(2,95)	1:159:A:PHE:HB2	1:135:A:GLU:H	7	0.86
(1,2666)	1:115:A:LEU:HA	1:114:A:ARG:HG3	5	0.86
(1,2488)	1:137:A:VAL:HG23	1:140:A:GLY:H	6	0.86
(1,2399)	1:189:A:ALA:H	1:186:A:SER:HA	8	0.86
(1,683)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	3	0.86
(1,683)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	9	0.86
(1,588)	1:164:A:ILE:HG13	1:165:A:ALA:H	7	0.86
(1,233)	1:116:A:ARG:HD2	1:116:A:ARG:HA	4	0.86
(1,227)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	5	0.86
(1,191)	1:98:A:LYS:HA	1:100:A:THR:HG22	3	0.86
(1,191)	1:93:A:MET:HA	1:92:A:ALA:HB2	10	0.86
(4,7)	1:116:A:ARG:H	1:182:A:GLU:O	5	0.85
(2,6313)	1:167:A:LYS:HG2	1:167:A:LYS:HE3	2	0.85
(2,5915)	1:130:A:PHE:HB2	1:131:A:PHE:H	6	0.85

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5448)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	1	0.85
(2,4007)	1:120:A:PHE:HB3	1:120:A:PHE:H	10	0.85
(2,1730)	1:192:A:ARG:HG2	1:192:A:ARG:H	7	0.85
(2,431)	1:126:A:GLU:HG3	1:127:A:ILE:H	7	0.85
(2,104)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	2	0.85
(2,81)	1:192:A:ARG:HA	1:137:A:VAL:HG11	8	0.85
(1,2968)	1:148:A:GLN:H	1:143:A:LEU:HD21	9	0.85
(1,2873)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	5	0.85
(1,2060)	1:115:A:LEU:HA	1:114:A:ARG:HG3	8	0.85
(1,683)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	6	0.85
(1,367)	1:110:A:ASP:HB2	1:107:A:THR:HG22	7	0.85
(1,329)	1:166:A:GLU:HG3	1:168:A:ALA:H	6	0.85
(1,221)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	6	0.85
(1,132)	1:166:A:GLU:HG3	1:168:A:ALA:H	3	0.85
(1,4)	1:136:A:ILE:HD13	1:164:A:ILE:HA	3	0.85
(2,8934)	1:162:A:GLN:HB2	1:163:A:GLU:H	6	0.84
(2,8175)	1:166:A:GLU:HG2	1:166:A:GLU:H	6	0.84
(2,7788)	1:130:A:PHE:HB2	1:131:A:PHE:H	7	0.84
(2,7409)	1:181:A:ILE:HG12	1:174:A:GLU:HB2	7	0.84
(2,7353)	1:192:A:ARG:HA	1:137:A:VAL:HG11	6	0.84
(2,7353)	1:192:A:ARG:HA	1:137:A:VAL:HG12	10	0.84
(2,7316)	1:191:A:VAL:HG11	1:186:A:SER:HA	4	0.84
(2,6313)	1:167:A:LYS:HG2	1:167:A:LYS:HE3	10	0.84
(2,5483)	1:192:A:ARG:HA	1:137:A:VAL:HG12	9	0.84
(2,5219)	1:162:A:GLN:HB2	1:163:A:GLU:H	6	0.84
(2,2019)	1:100:A:THR:HA	1:99:A:HIS:HB2	9	0.84
(2,1840)	1:191:A:VAL:HG11	1:186:A:SER:HA	10	0.84
(2,1200)	1:187:A:SER:H	1:184:A:PHE:HB2	3	0.84
(1,1696)	1:175:A:ARG:HB3	1:176:A:ILE:HD12	2	0.84
(1,1288)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	2	0.84
(1,757)	1:179:A:ARG:HB3	1:119:A:PRO:HD2	8	0.84
(1,588)	1:164:A:ILE:HG13	1:165:A:ALA:H	3	0.84
(1,588)	1:164:A:ILE:HG13	1:165:A:ALA:H	4	0.84
(1,295)	1:164:A:ILE:HD12	1:166:A:GLU:HB2	6	0.84
(1,221)	1:116:A:ARG:HD2	1:181:A:ILE:HD12	9	0.84
(2,9020)	1:185:A:LYS:H	1:185:A:LYS:HB2	10	0.83
(2,8032)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	9	0.83
(2,7340)	1:169:A:LEU:HB2	1:166:A:GLU:HA	2	0.83
(2,7320)	1:191:A:VAL:HG13	1:137:A:VAL:HG11	9	0.83
(2,7269)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	4	0.83
(2,6704)	1:139:A:ASN:H	1:141:A:ILE:HG22	6	0.83
(2,5915)	1:130:A:PHE:HB2	1:131:A:PHE:H	7	0.83

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5483)	1:192:A:ARG:HA	1:137:A:VAL:HG11	8	0.83
(2,5471)	1:169:A:LEU:HB2	1:166:A:GLU:HA	3	0.83
(2,5451)	1:191:A:VAL:HG13	1:137:A:VAL:HG11	9	0.83
(2,4764)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	6	0.83
(2,4764)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	8	0.83
(2,4007)	1:120:A:PHE:HB3	1:120:A:PHE:H	2	0.83
(2,3717)	1:142:A:THR:HG21	1:141:A:ILE:HG21	6	0.83
(2,2198)	1:120:A:PHE:HB3	1:120:A:PHE:H	10	0.83
(2,1909)	1:142:A:THR:HG21	1:141:A:ILE:HG21	8	0.83
(2,1730)	1:192:A:ARG:HG2	1:192:A:ARG:H	10	0.83
(2,54)	1:191:A:VAL:HG13	1:137:A:VAL:HG11	9	0.83
(1,2921)	1:176:A:ILE:HG23	1:175:A:ARG:HB2	1	0.83
(1,2488)	1:137:A:VAL:HG23	1:140:A:GLY:H	4	0.83
(1,718)	1:118:A:LEU:HG	1:154:A:GLU:H	7	0.83
(1,45)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	3	0.83
(1,45)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	9	0.83
(1,4)	1:136:A:ILE:HD11	1:164:A:ILE:HA	10	0.83
(2,9020)	1:185:A:LYS:H	1:185:A:LYS:HB2	1	0.82
(2,9020)	1:185:A:LYS:H	1:185:A:LYS:HB2	4	0.82
(2,7788)	1:130:A:PHE:HB2	1:131:A:PHE:H	8	0.82
(2,7788)	1:130:A:PHE:HB2	1:131:A:PHE:H	10	0.82
(2,7318)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	5	0.82
(2,7230)	1:150:A:ARG:HG2	1:151:A:SER:H	9	0.82
(2,6704)	1:139:A:ASN:H	1:141:A:ILE:HG22	8	0.82
(2,6619)	1:176:A:ILE:HG21	1:175:A:ARG:HB3	2	0.82
(2,6619)	1:176:A:ILE:HG21	1:175:A:ARG:HB3	6	0.82
(2,3649)	1:191:A:VAL:HG11	1:186:A:SER:HA	4	0.82
(2,3060)	1:139:A:ASN:H	1:141:A:ILE:HG22	6	0.82
(2,2957)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	3	0.82
(2,2957)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	5	0.82
(2,1840)	1:191:A:VAL:HG11	1:186:A:SER:HA	5	0.82
(2,1840)	1:191:A:VAL:HG11	1:186:A:SER:HA	9	0.82
(2,81)	1:192:A:ARG:HA	1:137:A:VAL:HG11	5	0.82
(2,53)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	3	0.82
(1,2735)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	10	0.82
(1,2488)	1:96:A:VAL:HG22	1:97:A:LEU:H	7	0.82
(1,2130)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	10	0.82
(1,1696)	1:175:A:ARG:HB3	1:176:A:ILE:HD12	3	0.82
(1,1516)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	10	0.82
(1,906)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	10	0.82
(1,757)	1:179:A:ARG:HB3	1:119:A:PRO:HD2	3	0.82
(1,541)	1:159:A:PHE:HA	1:135:A:GLU:H	2	0.82

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,541)	1:181:A:ILE:H	1:172:A:HIS:HA	8	0.82
(1,473)	1:157:A:VAL:HG23	1:114:A:ARG:HB3	6	0.82
(1,367)	1:110:A:ASP:HB2	1:107:A:THR:HG22	2	0.82
(1,233)	1:116:A:ARG:HD2	1:116:A:ARG:HA	5	0.82
(1,227)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	4	0.82
(1,191)	1:93:A:MET:HA	1:92:A:ALA:HB2	9	0.82
(1,45)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	6	0.82
(1,13)	1:181:A:ILE:HG12	1:175:A:ARG:HA	7	0.82
(1,4)	1:136:A:ILE:HD13	1:164:A:ILE:HA	9	0.82
(4,50)	1:183:A:ILE:H	1:181:A:ILE:O	6	0.81
(2,9020)	1:185:A:LYS:H	1:185:A:LYS:HB2	3	0.81
(2,8568)	1:139:A:ASN:H	1:158:A:GLN:HB2	5	0.81
(2,8017)	1:148:A:GLN:HB2	1:149:A:GLY:H	9	0.81
(2,7788)	1:130:A:PHE:HB2	1:131:A:PHE:H	5	0.81
(2,5915)	1:130:A:PHE:HB2	1:131:A:PHE:H	8	0.81
(2,5915)	1:130:A:PHE:HB2	1:131:A:PHE:H	10	0.81
(2,5400)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	3	0.81
(2,3060)	1:139:A:ASN:H	1:141:A:ILE:HG22	8	0.81
(2,2970)	1:111:A:GLY:HA3	1:109:A:ASN:H	7	0.81
(2,2198)	1:120:A:PHE:HB3	1:120:A:PHE:H	2	0.81
(2,2186)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	2	0.81
(2,1840)	1:191:A:VAL:HG11	1:186:A:SER:HA	3	0.81
(2,944)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	1	0.81
(2,837)	1:163:A:GLU:HG3	1:163:A:GLU:H	10	0.81
(2,110)	1:166:A:GLU:HB2	1:167:A:LYS:H	1	0.81
(2,42)	1:191:A:VAL:HG22	1:186:A:SER:HB2	1	0.81
(2,15)	1:189:A:ALA:HB2	1:186:A:SER:HA	9	0.81
(2,2)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	3	0.81
(1,2488)	1:137:A:VAL:HG23	1:140:A:GLY:H	3	0.81
(1,2415)	1:165:A:ALA:H	1:110:A:ASP:HB3	3	0.81
(1,2058)	1:115:A:LEU:HA	1:114:A:ARG:HG3	8	0.81
(1,1788)	1:132:A:SER:H	1:136:A:ILE:HB	8	0.81
(1,1429)	1:93:A:MET:HA	1:92:A:ALA:HB2	6	0.81
(1,683)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	8	0.81
(1,456)	1:165:A:ALA:HA	1:113:A:VAL:HG23	10	0.81
(1,329)	1:166:A:GLU:HG3	1:168:A:ALA:H	9	0.81
(1,221)	1:116:A:ARG:HD2	1:181:A:ILE:HD12	5	0.81
(2,7353)	1:192:A:ARG:HA	1:137:A:VAL:HG11	3	0.8
(2,6704)	1:139:A:ASN:H	1:141:A:ILE:HG22	4	0.8
(2,3717)	1:142:A:THR:HG21	1:141:A:ILE:HG21	8	0.8
(2,2957)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	10	0.8
(2,2186)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	3	0.8

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,15)	1:189:A:ALA:HB2	1:186:A:SER:HA	1	0.8
(1,3013)	1:189:A:ALA:H	1:186:A:SER:HA	9	0.8
(1,2921)	1:176:A:ILE:HG23	1:175:A:ARG:HB3	4	0.8
(1,2415)	1:165:A:ALA:H	1:110:A:ASP:HB3	6	0.8
(1,2296)	1:165:A:ALA:HA	1:113:A:VAL:HG21	8	0.8
(1,2222)	1:113:A:VAL:HG12	1:109:A:ASN:HA	9	0.8
(1,1429)	1:98:A:LYS:HA	1:100:A:THR:HG22	3	0.8
(1,1069)	1:168:A:ALA:HB1	1:167:A:LYS:H	3	0.8
(1,588)	1:165:A:ALA:H	1:134:A:LEU:HG	2	0.8
(1,329)	1:166:A:GLU:HG3	1:168:A:ALA:H	8	0.8
(1,4)	1:136:A:ILE:HD11	1:164:A:ILE:HA	1	0.8
(2,7316)	1:191:A:VAL:HG11	1:186:A:SER:HA	1	0.79
(2,7316)	1:191:A:VAL:HG11	1:186:A:SER:HA	2	0.79
(2,6704)	1:139:A:ASN:H	1:141:A:ILE:HG22	2	0.79
(2,6596)	1:123:A:SER:HB3	1:126:A:GLU:HB2	7	0.79
(2,5915)	1:130:A:PHE:HB2	1:131:A:PHE:H	5	0.79
(2,5483)	1:192:A:ARG:HA	1:137:A:VAL:HG11	5	0.79
(2,3060)	1:139:A:ASN:H	1:141:A:ILE:HG22	4	0.79
(2,2186)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	1	0.79
(2,2186)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	6	0.79
(2,1392)	1:110:A:ASP:HB3	1:111:A:GLY:H	9	0.79
(2,1236)	1:130:A:PHE:H	1:136:A:ILE:HG22	9	0.79
(2,232)	1:100:A:THR:HA	1:99:A:HIS:HB2	6	0.79
(2,232)	1:100:A:THR:HA	1:99:A:HIS:HB2	10	0.79
(2,104)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	5	0.79
(1,2666)	1:115:A:LEU:HA	1:114:A:ARG:HG3	3	0.79
(1,2352)	1:148:A:GLN:H	1:143:A:LEU:HD21	10	0.79
(1,1795)	1:122:A:CYS:H	1:127:A:ILE:HD13	9	0.79
(1,1788)	1:132:A:SER:H	1:136:A:ILE:HB	2	0.79
(1,1708)	1:136:A:ILE:HA	1:159:A:PHE:HB2	2	0.79
(1,1429)	1:93:A:MET:HA	1:92:A:ALA:HB2	10	0.79
(1,1093)	1:136:A:ILE:HA	1:159:A:PHE:HB2	2	0.79
(1,1069)	1:168:A:ALA:HB3	1:167:A:LYS:H	10	0.79
(1,473)	1:157:A:VAL:HG23	1:114:A:ARG:HB3	8	0.79
(1,13)	1:181:A:ILE:HG12	1:175:A:ARG:HA	8	0.79
(1,4)	1:136:A:ILE:HD11	1:164:A:ILE:HA	4	0.79
(2,9020)	1:185:A:LYS:H	1:185:A:LYS:HB2	9	0.78
(2,7353)	1:192:A:ARG:HA	1:137:A:VAL:HG13	1	0.78
(2,7314)	1:191:A:VAL:HG13	1:193:A:THR:H	7	0.78
(2,6706)	1:139:A:ASN:H	1:158:A:GLN:HB2	5	0.78
(2,6704)	1:139:A:ASN:H	1:141:A:ILE:HG22	7	0.78
(2,3420)	1:162:A:GLN:HB2	1:163:A:GLU:H	6	0.78

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3105)	1:181:A:ILE:HG22	1:122:A:CYS:H	10	0.78
(2,3060)	1:139:A:ASN:H	1:141:A:ILE:HG22	2	0.78
(2,2186)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	8	0.78
(2,738)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	9	0.78
(2,232)	1:100:A:THR:HA	1:99:A:HIS:HB2	2	0.78
(2,120)	1:142:A:THR:HG21	1:141:A:ILE:HG21	6	0.78
(2,15)	1:189:A:ALA:HB2	1:186:A:SER:HA	5	0.78
(1,2735)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	6	0.78
(1,2263)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	5	0.78
(1,2130)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	6	0.78
(1,1516)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	6	0.78
(1,1288)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	3	0.78
(1,935)	1:112:A:PHE:HB3	1:188:A:ARG:HG2	10	0.78
(1,906)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	6	0.78
(1,846)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	2	0.78
(1,841)	1:111:A:GLY:HA3	1:188:A:ARG:HG3	7	0.78
(1,588)	1:164:A:ILE:HG13	1:165:A:ALA:H	5	0.78
(1,588)	1:164:A:ILE:HG13	1:165:A:ALA:H	6	0.78
(1,484)	1:141:A:ILE:HA	1:156:A:PHE:HB3	4	0.78
(1,45)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	8	0.78
(2,7318)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	1	0.77
(2,7316)	1:191:A:VAL:HG11	1:186:A:SER:HA	6	0.77
(2,7316)	1:191:A:VAL:HG11	1:186:A:SER:HA	7	0.77
(2,7314)	1:191:A:VAL:HG12	1:193:A:THR:H	3	0.77
(2,7166)	1:185:A:LYS:H	1:185:A:LYS:HB2	10	0.77
(2,6704)	1:139:A:ASN:H	1:141:A:ILE:HG22	10	0.77
(2,4863)	1:139:A:ASN:H	1:141:A:ILE:HG22	6	0.77
(2,4863)	1:139:A:ASN:H	1:141:A:ILE:HG22	8	0.77
(2,4764)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	7	0.77
(2,3649)	1:191:A:VAL:HG11	1:186:A:SER:HA	1	0.77
(2,3649)	1:191:A:VAL:HG11	1:186:A:SER:HA	2	0.77
(2,3060)	1:139:A:ASN:H	1:141:A:ILE:HG22	7	0.77
(2,2961)	1:126:A:GLU:HB2	1:123:A:SER:HB3	7	0.77
(2,2950)	1:162:A:GLN:HG2	1:165:A:ALA:H	1	0.77
(2,2186)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	9	0.77
(2,837)	1:163:A:GLU:HG3	1:163:A:GLU:H	6	0.77
(2,53)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	4	0.77
(2,15)	1:189:A:ALA:HB2	1:186:A:SER:HA	8	0.77
(1,1708)	1:136:A:ILE:HA	1:159:A:PHE:HB2	7	0.77
(1,1696)	1:175:A:ARG:HB3	1:176:A:ILE:HD11	9	0.77
(1,1288)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	6	0.77
(1,1288)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	9	0.77

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1093)	1:136:A:ILE:HA	1:159:A:PHE:HB2	7	0.77
(1,614)	1:108:A:ALA:H	1:106:A:ASP:HB3	9	0.77
(1,588)	1:164:A:ILE:HG13	1:165:A:ALA:H	9	0.77
(1,397)	1:135:A:GLU:HA	1:136:A:ILE:HB	7	0.77
(2,7314)	1:191:A:VAL:HG13	1:193:A:THR:H	6	0.76
(2,7314)	1:191:A:VAL:HG13	1:193:A:THR:H	10	0.76
(2,7172)	1:187:A:SER:H	1:186:A:SER:HB2	1	0.76
(2,7166)	1:185:A:LYS:H	1:185:A:LYS:HB2	1	0.76
(2,7166)	1:185:A:LYS:H	1:185:A:LYS:HB2	4	0.76
(2,6704)	1:139:A:ASN:H	1:141:A:ILE:HG22	3	0.76
(2,3060)	1:139:A:ASN:H	1:141:A:ILE:HG22	10	0.76
(2,2962)	1:123:A:SER:HB3	1:143:A:LEU:HD23	8	0.76
(2,2957)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	6	0.76
(2,2950)	1:162:A:GLN:HG2	1:165:A:ALA:H	10	0.76
(2,1909)	1:142:A:THR:HG23	1:141:A:ILE:HG21	1	0.76
(2,1909)	1:142:A:THR:HG21	1:141:A:ILE:HG21	3	0.76
(2,1909)	1:142:A:THR:HG22	1:141:A:ILE:HG21	9	0.76
(2,1840)	1:191:A:VAL:HG11	1:186:A:SER:HA	8	0.76
(2,1560)	1:150:A:ARG:HG3	1:150:A:ARG:H	4	0.76
(2,1283)	1:105:A:PRO:HB3	1:106:A:ASP:H	2	0.76
(2,1283)	1:105:A:PRO:HB3	1:106:A:ASP:H	4	0.76
(2,95)	1:159:A:PHE:HB2	1:135:A:GLU:H	3	0.76
(1,2674)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	2	0.76
(1,2352)	1:148:A:GLN:H	1:143:A:LEU:HD21	2	0.76
(1,2222)	1:113:A:VAL:HG13	1:109:A:ASN:HA	6	0.76
(1,1795)	1:122:A:CYS:H	1:127:A:ILE:HD13	6	0.76
(1,1452)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	2	0.76
(1,854)	1:179:A:ARG:HD2	1:179:A:ARG:HA	6	0.76
(1,140)	1:163:A:GLU:HG3	1:163:A:GLU:HA	4	0.76
(2,7316)	1:191:A:VAL:HG11	1:186:A:SER:HA	10	0.75
(2,7166)	1:185:A:LYS:H	1:185:A:LYS:HB2	3	0.75
(2,7080)	1:162:A:GLN:HB2	1:163:A:GLU:H	6	0.75
(2,6704)	1:139:A:ASN:H	1:141:A:ILE:HG22	5	0.75
(2,4863)	1:139:A:ASN:H	1:141:A:ILE:HG22	4	0.75
(2,3649)	1:191:A:VAL:HG11	1:186:A:SER:HA	6	0.75
(2,3649)	1:191:A:VAL:HG11	1:186:A:SER:HA	7	0.75
(2,3060)	1:139:A:ASN:H	1:141:A:ILE:HG22	3	0.75
(2,2957)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	8	0.75
(2,120)	1:142:A:THR:HG21	1:141:A:ILE:HG21	8	0.75
(2,55)	1:191:A:VAL:HG13	1:190:A:GLU:H	4	0.75
(1,2488)	1:96:A:VAL:HG22	1:97:A:LEU:H	1	0.75
(1,2488)	1:137:A:VAL:HG23	1:140:A:GLY:H	8	0.75

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2399)	1:189:A:ALA:H	1:186:A:SER:HA	1	0.75
(1,1681)	1:168:A:ALA:HB1	1:167:A:LYS:H	3	0.75
(1,1681)	1:168:A:ALA:HB3	1:167:A:LYS:H	10	0.75
(1,1670)	1:133:A:GLY:HA3	1:134:A:LEU:HG	5	0.75
(1,1429)	1:93:A:MET:HA	1:92:A:ALA:HB2	9	0.75
(1,846)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	10	0.75
(1,683)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	1	0.75
(1,683)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	5	0.75
(1,413)	1:162:A:GLN:HG3	1:110:A:ASP:HA	1	0.75
(1,329)	1:166:A:GLU:HG3	1:168:A:ALA:H	10	0.75
(1,160)	1:102:A:PRO:HG2	1:101:A:GLY:HA3	10	0.75
(2,7353)	1:192:A:ARG:HA	1:137:A:VAL:HG12	2	0.74
(2,7353)	1:192:A:ARG:HA	1:137:A:VAL:HG13	7	0.74
(2,6704)	1:139:A:ASN:H	1:141:A:ILE:HG22	9	0.74
(2,3060)	1:139:A:ASN:H	1:141:A:ILE:HG22	5	0.74
(2,1909)	1:142:A:THR:HG21	1:141:A:ILE:HG21	4	0.74
(2,1638)	1:166:A:GLU:HB3	1:166:A:GLU:H	6	0.74
(2,1638)	1:166:A:GLU:HB3	1:166:A:GLU:H	9	0.74
(2,816)	1:161:A:SER:HB2	1:162:A:GLN:H	8	0.74
(2,431)	1:126:A:GLU:HG3	1:127:A:ILE:H	8	0.74
(2,104)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	7	0.74
(1,2528)	1:166:A:GLU:HB3	1:167:A:LYS:HA	3	0.74
(1,2528)	1:166:A:GLU:HB3	1:167:A:LYS:HA	10	0.74
(1,846)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	8	0.74
(1,683)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	7	0.74
(1,484)	1:141:A:ILE:HA	1:156:A:PHE:HB3	10	0.74
(1,459)	1:168:A:ALA:HB1	1:167:A:LYS:H	3	0.74
(1,456)	1:94:A:ASP:HA	1:164:A:ILE:HD13	8	0.74
(2,7316)	1:191:A:VAL:HG11	1:186:A:SER:HA	5	0.73
(2,7316)	1:191:A:VAL:HG11	1:186:A:SER:HA	9	0.73
(2,7314)	1:191:A:VAL:HG13	1:193:A:THR:H	8	0.73
(2,5818)	1:120:A:PHE:HB3	1:120:A:PHE:H	10	0.73
(2,4863)	1:139:A:ASN:H	1:141:A:ILE:HG22	2	0.73
(2,3717)	1:142:A:THR:HG23	1:141:A:ILE:HG21	1	0.73
(2,3717)	1:142:A:THR:HG21	1:141:A:ILE:HG21	3	0.73
(2,3717)	1:142:A:THR:HG22	1:141:A:ILE:HG21	9	0.73
(2,3060)	1:139:A:ASN:H	1:141:A:ILE:HG22	9	0.73
(2,2186)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	5	0.73
(2,2186)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	7	0.73
(2,1638)	1:166:A:GLU:HB3	1:166:A:GLU:H	4	0.73
(2,1283)	1:105:A:PRO:HB3	1:106:A:ASP:H	1	0.73
(2,418)	1:124:A:LYS:HA	1:124:A:LYS:HB2	5	0.73

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,418)	1:124:A:LYS:HA	1:124:A:LYS:HB2	8	0.73
(2,53)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	10	0.73
(1,2674)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	10	0.73
(1,2528)	1:166:A:GLU:HB3	1:167:A:LYS:HA	6	0.73
(1,2068)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	2	0.73
(1,1520)	1:141:A:ILE:HG21	1:143:A:LEU:HG	6	0.73
(1,1452)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	10	0.73
(1,1069)	1:168:A:ALA:HB3	1:167:A:LYS:H	8	0.73
(1,541)	1:181:A:ILE:H	1:172:A:HIS:HA	1	0.73
(1,484)	1:141:A:ILE:HA	1:156:A:PHE:HB3	5	0.73
(1,459)	1:168:A:ALA:HB3	1:167:A:LYS:H	10	0.73
(2,8567)	1:139:A:ASN:H	1:141:A:ILE:HG22	6	0.72
(2,7316)	1:191:A:VAL:HG11	1:186:A:SER:HA	3	0.72
(2,7314)	1:191:A:VAL:HG13	1:193:A:THR:H	9	0.72
(2,7166)	1:185:A:LYS:H	1:185:A:LYS:HB2	9	0.72
(2,6704)	1:139:A:ASN:H	1:141:A:ILE:HG22	1	0.72
(2,6604)	1:111:A:GLY:HA3	1:109:A:ASN:H	3	0.72
(2,5305)	1:185:A:LYS:H	1:185:A:LYS:HB2	10	0.72
(2,4863)	1:139:A:ASN:H	1:141:A:ILE:HG22	7	0.72
(2,3649)	1:191:A:VAL:HG11	1:186:A:SER:HA	10	0.72
(2,2981)	1:158:A:GLN:HG3	1:112:A:PHE:HA	1	0.72
(2,1862)	1:169:A:LEU:HB2	1:166:A:GLU:HA	2	0.72
(2,1283)	1:105:A:PRO:HB3	1:106:A:ASP:H	7	0.72
(2,1096)	1:190:A:GLU:HG2	1:190:A:GLU:H	4	0.72
(2,500)	1:130:A:PHE:HB2	1:131:A:PHE:H	2	0.72
(2,418)	1:124:A:LYS:HA	1:124:A:LYS:HB2	6	0.72
(2,232)	1:100:A:THR:HA	1:99:A:HIS:HB2	7	0.72
(2,232)	1:100:A:THR:HA	1:99:A:HIS:HB2	8	0.72
(1,2968)	1:148:A:GLN:H	1:143:A:LEU:HD21	10	0.72
(1,2674)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	8	0.72
(1,2352)	1:148:A:GLN:H	1:143:A:LEU:HD21	1	0.72
(1,1452)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	8	0.72
(1,1288)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	8	0.72
(1,1083)	1:175:A:ARG:HB3	1:176:A:ILE:HD12	6	0.72
(1,846)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	4	0.72
(1,846)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	7	0.72
(1,820)	1:93:A:MET:HA	1:92:A:ALA:HB2	6	0.72
(1,397)	1:135:A:GLU:HA	1:136:A:ILE:HB	2	0.72
(1,367)	1:110:A:ASP:HB2	1:107:A:THR:HG22	1	0.72
(1,329)	1:166:A:GLU:HG3	1:168:A:ALA:H	3	0.72
(1,295)	1:164:A:ILE:HD12	1:166:A:GLU:HB2	9	0.72
(1,160)	1:102:A:PRO:HG2	1:101:A:GLY:HA3	7	0.72

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	1	0.72
(1,45)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	5	0.72
(1,4)	1:136:A:ILE:HD11	1:164:A:ILE:HA	2	0.72
(2,8567)	1:139:A:ASN:H	1:141:A:ILE:HG22	8	0.71
(2,6604)	1:111:A:GLY:HA3	1:109:A:ASN:H	10	0.71
(2,6374)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	1	0.71
(2,5818)	1:120:A:PHE:HB3	1:120:A:PHE:H	2	0.71
(2,5499)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	6	0.71
(2,4863)	1:139:A:ASN:H	1:141:A:ILE:HG22	10	0.71
(2,3717)	1:142:A:THR:HG21	1:141:A:ILE:HG21	4	0.71
(2,3649)	1:191:A:VAL:HG11	1:186:A:SER:HA	5	0.71
(2,3060)	1:139:A:ASN:H	1:141:A:ILE:HG22	1	0.71
(2,2950)	1:162:A:GLN:HG2	1:165:A:ALA:H	3	0.71
(2,1909)	1:142:A:THR:HG22	1:141:A:ILE:HG21	5	0.71
(2,396)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	2	0.71
(2,232)	1:100:A:THR:HA	1:99:A:HIS:HB2	5	0.71
(2,226)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	5	0.71
(2,15)	1:189:A:ALA:HB2	1:186:A:SER:HA	2	0.71
(1,3066)	1:108:A:ALA:H	1:106:A:ASP:HB3	8	0.71
(1,2528)	1:162:A:GLN:HB2	1:163:A:GLU:HA	1	0.71
(1,2352)	1:148:A:GLN:H	1:143:A:LEU:HD21	4	0.71
(1,1795)	1:122:A:CYS:H	1:127:A:ILE:HD13	2	0.71
(1,1452)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	4	0.71
(1,820)	1:98:A:LYS:HA	1:100:A:THR:HG22	3	0.71
(1,423)	1:139:A:ASN:HB2	1:137:A:VAL:HG22	10	0.71
(1,377)	1:123:A:SER:HB3	1:181:A:ILE:HD11	8	0.71
(1,45)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	7	0.71
(2,9082)	1:150:A:ARG:HG2	1:151:A:SER:H	9	0.7
(2,8017)	1:148:A:GLN:HB2	1:149:A:GLY:H	5	0.7
(2,7353)	1:192:A:ARG:HA	1:137:A:VAL:HG12	9	0.7
(2,5305)	1:185:A:LYS:H	1:185:A:LYS:HB2	1	0.7
(2,5305)	1:185:A:LYS:H	1:185:A:LYS:HB2	4	0.7
(2,4863)	1:139:A:ASN:H	1:141:A:ILE:HG22	3	0.7
(2,4321)	1:148:A:GLN:HB2	1:149:A:GLY:H	9	0.7
(2,3649)	1:191:A:VAL:HG11	1:186:A:SER:HA	3	0.7
(2,3649)	1:191:A:VAL:HG11	1:186:A:SER:HA	9	0.7
(2,2186)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	10	0.7
(2,2019)	1:100:A:THR:HA	1:99:A:HIS:HB2	2	0.7
(2,2019)	1:100:A:THR:HA	1:99:A:HIS:HB2	6	0.7
(2,2019)	1:100:A:THR:HA	1:99:A:HIS:HB2	10	0.7
(2,1830)	1:191:A:VAL:HG22	1:186:A:SER:HB2	1	0.7
(2,396)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	1	0.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,396)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	3	0.7
(2,104)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	4	0.7
(2,85)	1:187:A:SER:HB3	1:189:A:ALA:H	5	0.7
(2,51)	1:191:A:VAL:HG11	1:186:A:SER:HA	4	0.7
(2,15)	1:189:A:ALA:HB2	1:186:A:SER:HA	7	0.7
(1,2674)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	4	0.7
(1,2674)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	7	0.7
(1,2399)	1:189:A:ALA:H	1:186:A:SER:HA	2	0.7
(1,2399)	1:189:A:ALA:H	1:186:A:SER:HA	5	0.7
(1,2324)	1:188:A:ARG:HA	1:186:A:SER:HA	3	0.7
(1,2298)	1:168:A:ALA:HB1	1:167:A:LYS:H	3	0.7
(1,2298)	1:168:A:ALA:HB3	1:167:A:LYS:H	10	0.7
(1,2068)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	10	0.7
(1,2060)	1:115:A:LEU:HA	1:114:A:ARG:HG3	2	0.7
(1,1795)	1:122:A:CYS:H	1:127:A:ILE:HD13	4	0.7
(1,1708)	1:136:A:ILE:HA	1:159:A:PHE:HB2	9	0.7
(1,1452)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	7	0.7
(1,1093)	1:136:A:ILE:HA	1:159:A:PHE:HB2	9	0.7
(1,1083)	1:175:A:ARG:HB3	1:176:A:ILE:HD11	8	0.7
(1,820)	1:93:A:MET:HA	1:92:A:ALA:HB2	10	0.7
(1,541)	1:181:A:ILE:H	1:172:A:HIS:HA	5	0.7
(1,367)	1:110:A:ASP:HB2	1:107:A:THR:HG22	4	0.7
(1,227)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	1	0.7
(1,160)	1:102:A:PRO:HG2	1:101:A:GLY:HA3	1	0.7
(2,8567)	1:139:A:ASN:H	1:141:A:ILE:HG22	4	0.69
(2,6619)	1:176:A:ILE:HG23	1:175:A:ARG:HB3	4	0.69
(2,5305)	1:185:A:LYS:H	1:185:A:LYS:HB2	3	0.69
(2,4863)	1:139:A:ASN:H	1:141:A:ILE:HG22	5	0.69
(2,4863)	1:139:A:ASN:H	1:141:A:ILE:HG22	9	0.69
(2,4537)	1:175:A:ARG:HG2	1:175:A:ARG:HA	1	0.69
(2,3508)	1:185:A:LYS:H	1:185:A:LYS:HB2	10	0.69
(2,3105)	1:181:A:ILE:HG22	1:122:A:CYS:H	8	0.69
(2,2957)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	7	0.69
(2,431)	1:126:A:GLU:HG3	1:127:A:ILE:H	1	0.69
(2,396)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	6	0.69
(2,15)	1:189:A:ALA:HB2	1:186:A:SER:HA	6	0.69
(1,2994)	1:150:A:ARG:H	1:143:A:LEU:HD21	7	0.69
(1,2921)	1:176:A:ILE:HG21	1:175:A:ARG:HB3	7	0.69
(1,2873)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	6	0.69
(1,2528)	1:166:A:GLU:HB3	1:167:A:LYS:HA	9	0.69
(1,2263)	1:139:A:ASN:HB2	1:137:A:VAL:HG22	10	0.69
(1,2068)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	8	0.69

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2060)	1:115:A:LEU:HA	1:114:A:ARG:HG3	5	0.69
(1,1795)	1:122:A:CYS:H	1:127:A:ILE:HD13	10	0.69
(1,1681)	1:168:A:ALA:HB3	1:167:A:LYS:H	8	0.69
(1,1364)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	10	0.69
(1,570)	1:150:A:ARG:HB3	1:151:A:SER:H	6	0.69
(1,541)	1:159:A:PHE:HA	1:135:A:GLU:H	3	0.69
(1,413)	1:162:A:GLN:HG3	1:110:A:ASP:HA	5	0.69
(1,397)	1:135:A:GLU:HA	1:136:A:ILE:HB	5	0.69
(1,365)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	10	0.69
(1,160)	1:102:A:PRO:HG2	1:101:A:GLY:HA3	5	0.69
(2,8567)	1:139:A:ASN:H	1:141:A:ILE:HG22	2	0.68
(2,8017)	1:148:A:GLN:HB2	1:149:A:GLY:H	2	0.68
(2,7353)	1:192:A:ARG:HA	1:137:A:VAL:HG11	8	0.68
(2,5243)	1:166:A:GLU:HB3	1:166:A:GLU:H	6	0.68
(2,5243)	1:166:A:GLU:HB3	1:166:A:GLU:H	9	0.68
(2,4777)	1:111:A:GLY:HA3	1:109:A:ASN:H	7	0.68
(2,3717)	1:142:A:THR:HG22	1:141:A:ILE:HG21	5	0.68
(2,3669)	1:169:A:LEU:HB2	1:166:A:GLU:HA	1	0.68
(2,3508)	1:185:A:LYS:H	1:185:A:LYS:HB2	4	0.68
(2,2950)	1:162:A:GLN:HG2	1:165:A:ALA:H	4	0.68
(2,2527)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	9	0.68
(2,2013)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	5	0.68
(2,1173)	1:111:A:GLY:HA3	1:109:A:ASN:H	3	0.68
(2,816)	1:161:A:SER:HB2	1:162:A:GLN:H	6	0.68
(2,396)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	8	0.68
(2,120)	1:142:A:THR:HG23	1:141:A:ILE:HG21	1	0.68
(2,120)	1:142:A:THR:HG21	1:141:A:ILE:HG21	3	0.68
(2,120)	1:142:A:THR:HG22	1:141:A:ILE:HG21	9	0.68
(2,55)	1:191:A:VAL:HG12	1:190:A:GLU:H	6	0.68
(1,3013)	1:189:A:ALA:H	1:186:A:SER:HA	8	0.68
(1,2968)	1:148:A:GLN:H	1:143:A:LEU:HD21	2	0.68
(1,2873)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	9	0.68
(1,2068)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	4	0.68
(1,2068)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	7	0.68
(1,1798)	1:165:A:ALA:H	1:110:A:ASP:HB3	3	0.68
(1,1708)	1:136:A:ILE:HA	1:159:A:PHE:HB2	8	0.68
(1,1364)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	4	0.68
(1,1364)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	5	0.68
(1,1364)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	7	0.68
(1,1093)	1:136:A:ILE:HA	1:159:A:PHE:HB2	8	0.68
(1,422)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	8	0.68
(1,397)	1:135:A:GLU:HA	1:136:A:ILE:HB	9	0.68

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:110:A:ASP:HB2	1:107:A:THR:HG22	5	0.68
(1,365)	1:143:A:LEU:HG	1:143:A:LEU:HD23	6	0.68
(1,227)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	2	0.68
(1,191)	1:98:A:LYS:HA	1:100:A:THR:HG23	8	0.68
(2,8567)	1:139:A:ASN:H	1:141:A:ILE:HG22	7	0.67
(2,7316)	1:191:A:VAL:HG11	1:186:A:SER:HA	8	0.67
(2,5931)	1:134:A:LEU:HG	1:134:A:LEU:HB2	1	0.67
(2,5931)	1:134:A:LEU:HG	1:134:A:LEU:HB2	2	0.67
(2,5931)	1:134:A:LEU:HG	1:134:A:LEU:HB2	3	0.67
(2,5931)	1:134:A:LEU:HG	1:134:A:LEU:HB2	4	0.67
(2,5931)	1:134:A:LEU:HG	1:134:A:LEU:HB2	7	0.67
(2,5471)	1:169:A:LEU:HB2	1:166:A:GLU:HA	2	0.67
(2,5305)	1:185:A:LYS:H	1:185:A:LYS:HB2	9	0.67
(2,5243)	1:166:A:GLU:HB3	1:166:A:GLU:H	4	0.67
(2,4997)	1:110:A:ASP:HB3	1:110:A:ASP:H	10	0.67
(2,4516)	1:171:A:LYS:HB3	1:171:A:LYS:H	3	0.67
(2,4516)	1:171:A:LYS:HB3	1:171:A:LYS:H	5	0.67
(2,4516)	1:171:A:LYS:HB3	1:171:A:LYS:H	8	0.67
(2,3508)	1:185:A:LYS:H	1:185:A:LYS:HB2	1	0.67
(2,3508)	1:185:A:LYS:H	1:185:A:LYS:HB2	3	0.67
(2,2705)	1:171:A:LYS:HB3	1:171:A:LYS:H	3	0.67
(2,2705)	1:171:A:LYS:HB3	1:171:A:LYS:H	8	0.67
(2,2511)	1:148:A:GLN:HB2	1:149:A:GLY:H	9	0.67
(2,2186)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	4	0.67
(2,1883)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	6	0.67
(2,1638)	1:166:A:GLU:HB3	1:166:A:GLU:H	2	0.67
(2,1638)	1:166:A:GLU:HB3	1:166:A:GLU:H	5	0.67
(2,1560)	1:150:A:ARG:HG3	1:150:A:ARG:H	8	0.67
(2,1236)	1:130:A:PHE:H	1:136:A:ILE:HG22	8	0.67
(2,1173)	1:111:A:GLY:HA3	1:109:A:ASN:H	10	0.67
(2,816)	1:161:A:SER:HB2	1:162:A:GLN:H	10	0.67
(2,396)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	9	0.67
(2,4)	1:164:A:ILE:HD11	1:161:A:SER:HB3	6	0.67
(1,2921)	1:176:A:ILE:HG21	1:175:A:ARG:HB3	9	0.67
(1,2528)	1:166:A:GLU:HB3	1:167:A:LYS:HA	8	0.67
(1,2352)	1:148:A:GLN:H	1:143:A:LEU:HD21	6	0.67
(1,1364)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	1	0.67
(1,1288)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	1	0.67
(1,1288)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	5	0.67
(1,1173)	1:189:A:ALA:H	1:186:A:SER:HA	9	0.67
(1,983)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	10	0.67
(1,484)	1:141:A:ILE:HA	1:156:A:PHE:HB3	1	0.67

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:157:A:VAL:HG23	1:114:A:ARG:HB3	2	0.67
(1,473)	1:175:A:ARG:HB3	1:176:A:ILE:HD11	10	0.67
(1,459)	1:168:A:ALA:HB3	1:167:A:LYS:H	8	0.67
(3,102)	1:158:A:GLN:HG3	1:112:A:PHE:HA	1	0.66
(2,8567)	1:139:A:ASN:H	1:141:A:ILE:HG22	10	0.66
(2,8464)	1:123:A:SER:HB3	1:126:A:GLU:HB2	8	0.66
(2,8246)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	1	0.66
(2,7410)	1:98:A:LYS:HB3	1:100:A:THR:HG23	9	0.66
(2,6942)	1:132:A:SER:HB2	1:133:A:GLY:H	2	0.66
(2,6509)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	4	0.66
(2,6509)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	10	0.66
(2,5931)	1:134:A:LEU:HG	1:134:A:LEU:HB2	5	0.66
(2,5931)	1:134:A:LEU:HG	1:134:A:LEU:HB2	8	0.66
(2,5931)	1:134:A:LEU:HG	1:134:A:LEU:HB2	9	0.66
(2,5931)	1:134:A:LEU:HG	1:134:A:LEU:HB2	10	0.66
(2,5446)	1:191:A:VAL:HG11	1:186:A:SER:HA	4	0.66
(2,5407)	1:181:A:ILE:HG12	1:175:A:ARG:HD2	3	0.66
(2,5252)	1:171:A:LYS:H	1:170:A:LYS:HB2	6	0.66
(2,4863)	1:139:A:ASN:H	1:141:A:ILE:HG22	1	0.66
(2,3822)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	5	0.66
(2,3605)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	7	0.66
(2,2705)	1:171:A:LYS:HB3	1:171:A:LYS:H	5	0.66
(2,1909)	1:142:A:THR:HG22	1:141:A:ILE:HG21	10	0.66
(2,1807)	1:113:A:VAL:HG12	1:113:A:VAL:HB	1	0.66
(2,1795)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	7	0.66
(2,1560)	1:150:A:ARG:HG3	1:150:A:ARG:H	7	0.66
(2,1236)	1:130:A:PHE:H	1:136:A:ILE:HG22	7	0.66
(2,120)	1:142:A:THR:HG21	1:141:A:ILE:HG21	4	0.66
(2,51)	1:191:A:VAL:HG11	1:186:A:SER:HA	1	0.66
(2,51)	1:191:A:VAL:HG11	1:186:A:SER:HA	2	0.66
(1,2320)	1:136:A:ILE:HA	1:159:A:PHE:HB2	2	0.66
(1,2058)	1:115:A:LEU:HA	1:114:A:ARG:HG3	2	0.66
(1,1798)	1:165:A:ALA:H	1:110:A:ASP:HB3	6	0.66
(1,1795)	1:122:A:CYS:H	1:127:A:ILE:HD13	3	0.66
(1,1788)	1:132:A:SER:H	1:136:A:ILE:HB	4	0.66
(1,1288)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	7	0.66
(1,1188)	1:165:A:ALA:H	1:110:A:ASP:HB3	8	0.66
(1,983)	1:143:A:LEU:HG	1:143:A:LEU:HD23	6	0.66
(1,820)	1:93:A:MET:HA	1:92:A:ALA:HB2	9	0.66
(1,570)	1:150:A:ARG:HB3	1:151:A:SER:H	2	0.66
(1,522)	1:169:A:LEU:H	1:169:A:LEU:HG	5	0.66
(1,522)	1:169:A:LEU:H	1:169:A:LEU:HG	7	0.66

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,522)	1:169:A:LEU:H	1:169:A:LEU:HG	8	0.66
(1,484)	1:141:A:ILE:HA	1:156:A:PHE:HB3	3	0.66
(1,456)	1:165:A:ALA:HA	1:113:A:VAL:HG23	7	0.66
(1,160)	1:102:A:PRO:HG2	1:101:A:GLY:HA3	4	0.66
(2,8567)	1:139:A:ASN:H	1:141:A:ILE:HG22	3	0.65
(2,7788)	1:130:A:PHE:HB2	1:131:A:PHE:H	1	0.65
(2,7353)	1:192:A:ARG:HA	1:137:A:VAL:HG11	5	0.65
(2,6509)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	2	0.65
(2,6509)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	3	0.65
(2,6509)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	7	0.65
(2,6165)	1:150:A:ARG:HG3	1:150:A:ARG:HD3	6	0.65
(2,5931)	1:134:A:LEU:HG	1:134:A:LEU:HB2	6	0.65
(2,3649)	1:191:A:VAL:HG11	1:186:A:SER:HA	8	0.65
(2,3605)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	8	0.65
(2,2933)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	2	0.65
(2,2933)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	3	0.65
(2,2933)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	5	0.65
(2,2933)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	6	0.65
(2,2933)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	7	0.65
(2,2933)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	9	0.65
(2,2498)	1:147:A:PHE:HB3	1:147:A:PHE:HA	7	0.65
(2,1795)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	8	0.65
(2,1638)	1:166:A:GLU:HB3	1:166:A:GLU:H	7	0.65
(2,1289)	1:114:A:ARG:H	1:186:A:SER:HB3	1	0.65
(2,431)	1:126:A:GLU:HG3	1:127:A:ILE:H	9	0.65
(2,226)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	1	0.65
(2,55)	1:191:A:VAL:HG11	1:190:A:GLU:H	5	0.65
(2,4)	1:164:A:ILE:HD11	1:161:A:SER:HB3	8	0.65
(1,2968)	1:148:A:GLN:H	1:143:A:LEU:HD21	1	0.65
(1,2921)	1:176:A:ILE:HG22	1:175:A:ARG:HB3	5	0.65
(1,2739)	1:143:A:LEU:HG	1:141:A:ILE:HG21	6	0.65
(1,2499)	1:181:A:ILE:HG21	1:181:A:ILE:H	6	0.65
(1,2058)	1:115:A:LEU:HA	1:114:A:ARG:HG3	5	0.65
(1,1795)	1:122:A:CYS:H	1:127:A:ILE:HD13	5	0.65
(1,1596)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	10	0.65
(1,1462)	1:175:A:ARG:HD2	1:178:A:HIS:HA	9	0.65
(1,1364)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	8	0.65
(1,1067)	1:165:A:ALA:HA	1:113:A:VAL:HG23	9	0.65
(1,541)	1:181:A:ILE:H	1:172:A:HIS:HA	4	0.65
(1,522)	1:169:A:LEU:H	1:169:A:LEU:HG	4	0.65
(1,397)	1:135:A:GLU:HA	1:136:A:ILE:HB	1	0.65
(1,288)	1:141:A:ILE:HG21	1:143:A:LEU:HG	6	0.65

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,221)	1:116:A:ARG:HD2	1:181:A:ILE:HD12	7	0.65
(1,160)	1:102:A:PRO:HG2	1:101:A:GLY:HA3	8	0.65
(1,160)	1:102:A:PRO:HG2	1:101:A:GLY:HA3	9	0.65
(1,3)	1:127:A:ILE:HD11	1:126:A:GLU:HB2	5	0.65
(2,8599)	1:114:A:ARG:H	1:186:A:SER:HB3	1	0.64
(2,8567)	1:139:A:ASN:H	1:141:A:ILE:HG22	5	0.64
(2,8282)	1:179:A:ARG:HG3	1:179:A:ARG:HB3	3	0.64
(2,6604)	1:111:A:GLY:HA3	1:109:A:ASN:H	6	0.64
(2,6509)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	1	0.64
(2,6509)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	6	0.64
(2,5915)	1:130:A:PHE:HB2	1:131:A:PHE:H	1	0.64
(2,5252)	1:171:A:LYS:H	1:170:A:LYS:HB2	3	0.64
(2,5252)	1:171:A:LYS:H	1:170:A:LYS:HB2	8	0.64
(2,4732)	1:192:A:ARG:HD3	1:192:A:ARG:HB2	6	0.64
(2,3508)	1:185:A:LYS:H	1:185:A:LYS:HB2	9	0.64
(2,2933)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	1	0.64
(2,2933)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	4	0.64
(2,2933)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	8	0.64
(2,2933)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	10	0.64
(2,2924)	1:192:A:ARG:HD3	1:192:A:ARG:HB2	6	0.64
(2,2498)	1:147:A:PHE:HB3	1:147:A:PHE:HA	9	0.64
(2,2019)	1:100:A:THR:HA	1:99:A:HIS:HB2	7	0.64
(2,2019)	1:100:A:THR:HA	1:99:A:HIS:HB2	8	0.64
(2,1909)	1:142:A:THR:HG22	1:141:A:ILE:HG21	7	0.64
(2,1560)	1:150:A:ARG:HG3	1:150:A:ARG:H	6	0.64
(2,396)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	7	0.64
(2,85)	1:187:A:SER:HB3	1:189:A:ALA:H	1	0.64
(2,85)	1:187:A:SER:HB3	1:189:A:ALA:H	2	0.64
(2,51)	1:191:A:VAL:HG11	1:186:A:SER:HA	6	0.64
(2,51)	1:191:A:VAL:HG11	1:186:A:SER:HA	7	0.64
(2,4)	1:164:A:ILE:HD11	1:161:A:SER:HB3	9	0.64
(1,3066)	1:108:A:ALA:H	1:106:A:ASP:HB3	4	0.64
(1,3066)	1:108:A:ALA:H	1:106:A:ASP:HB3	6	0.64
(1,2994)	1:150:A:ARG:H	1:143:A:LEU:HD21	8	0.64
(1,2873)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	3	0.64
(1,2379)	1:150:A:ARG:H	1:143:A:LEU:HD21	7	0.64
(1,2320)	1:136:A:ILE:HA	1:159:A:PHE:HB2	7	0.64
(1,2298)	1:168:A:ALA:HB3	1:167:A:LYS:H	8	0.64
(1,1596)	1:143:A:LEU:HG	1:143:A:LEU:HD23	6	0.64
(1,1364)	1:141:A:ILE:HG13	1:140:A:GLY:HA2	9	0.64
(1,910)	1:97:A:LEU:HD12	1:163:A:GLU:HB3	6	0.64
(1,473)	1:157:A:VAL:HG23	1:114:A:ARG:HB3	3	0.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,365)	1:143:A:LEU:HG	1:143:A:LEU:HD23	8	0.64
(1,365)	1:143:A:LEU:HG	1:143:A:LEU:HD23	9	0.64
(1,46)	1:167:A:LYS:HG2	1:134:A:LEU:HD11	9	0.64
(1,4)	1:136:A:ILE:HD11	1:164:A:ILE:HA	7	0.64
(2,8567)	1:139:A:ASN:H	1:141:A:ILE:HG22	9	0.63
(2,8017)	1:148:A:GLN:HB2	1:149:A:GLY:H	1	0.63
(2,7269)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	3	0.63
(2,6942)	1:132:A:SER:HB2	1:133:A:GLY:H	5	0.63
(2,6509)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	5	0.63
(2,6165)	1:150:A:ARG:HG3	1:150:A:ARG:HD3	2	0.63
(2,6165)	1:150:A:ARG:HG3	1:150:A:ARG:HD3	4	0.63
(2,6165)	1:150:A:ARG:HG3	1:150:A:ARG:HD3	8	0.63
(2,6165)	1:150:A:ARG:HG3	1:150:A:ARG:HD3	10	0.63
(2,5829)	1:124:A:LYS:HA	1:124:A:LYS:HB2	5	0.63
(2,5829)	1:124:A:LYS:HA	1:124:A:LYS:HB2	6	0.63
(2,5829)	1:124:A:LYS:HA	1:124:A:LYS:HB2	8	0.63
(2,4337)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	9	0.63
(2,4308)	1:147:A:PHE:HB3	1:147:A:PHE:HA	7	0.63
(2,4308)	1:147:A:PHE:HB3	1:147:A:PHE:HA	9	0.63
(2,3717)	1:142:A:THR:HG22	1:141:A:ILE:HG21	10	0.63
(2,3605)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	9	0.63
(2,2663)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	2	0.63
(2,2663)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	7	0.63
(2,2530)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	6	0.63
(2,2019)	1:100:A:THR:HA	1:99:A:HIS:HB2	5	0.63
(2,1795)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	9	0.63
(2,1699)	1:185:A:LYS:H	1:185:A:LYS:HB2	10	0.63
(2,1560)	1:150:A:ARG:HG3	1:150:A:ARG:H	2	0.63
(2,1283)	1:105:A:PRO:HB3	1:106:A:ASP:H	3	0.63
(2,396)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	5	0.63
(2,120)	1:142:A:THR:HG22	1:141:A:ILE:HG21	5	0.63
(2,55)	1:191:A:VAL:HG11	1:190:A:GLU:H	1	0.63
(2,55)	1:191:A:VAL:HG12	1:190:A:GLU:H	7	0.63
(2,4)	1:164:A:ILE:HD11	1:161:A:SER:HB3	1	0.63
(2,4)	1:164:A:ILE:HD11	1:161:A:SER:HB3	2	0.63
(2,4)	1:164:A:ILE:HD11	1:161:A:SER:HB3	5	0.63
(1,3030)	1:165:A:ALA:H	1:110:A:ASP:HB3	3	0.63
(1,3003)	1:108:A:ALA:H	1:109:A:ASN:HA	3	0.63
(1,2968)	1:148:A:GLN:H	1:143:A:LEU:HD21	4	0.63
(1,2921)	1:176:A:ILE:HG21	1:175:A:ARG:HB3	10	0.63
(1,2671)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	6	0.63
(1,2528)	1:166:A:GLU:HB3	1:167:A:LYS:HA	4	0.63

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2352)	1:148:A:GLN:H	1:143:A:LEU:HD22	3	0.63
(1,2324)	1:188:A:ARG:HA	1:186:A:SER:HA	10	0.63
(1,2263)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	6	0.63
(1,2060)	1:115:A:LEU:HA	1:114:A:ARG:HG3	3	0.63
(1,1708)	1:136:A:ILE:HA	1:159:A:PHE:HB2	6	0.63
(1,1093)	1:136:A:ILE:HA	1:159:A:PHE:HB2	6	0.63
(1,983)	1:143:A:LEU:HG	1:143:A:LEU:HD23	9	0.63
(1,683)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	10	0.63
(1,570)	1:150:A:ARG:HB3	1:151:A:SER:H	7	0.63
(1,397)	1:135:A:GLU:HA	1:136:A:ILE:HB	3	0.63
(1,365)	1:143:A:LEU:HG	1:143:A:LEU:HD23	3	0.63
(2,9034)	1:187:A:SER:HB3	1:188:A:ARG:H	5	0.62
(2,9034)	1:187:A:SER:HB3	1:188:A:ARG:H	7	0.62
(2,9034)	1:187:A:SER:HB3	1:188:A:ARG:H	9	0.62
(2,8282)	1:179:A:ARG:HG3	1:179:A:ARG:HB3	1	0.62
(2,8282)	1:179:A:ARG:HG3	1:179:A:ARG:HB3	4	0.62
(2,8282)	1:179:A:ARG:HG3	1:179:A:ARG:HB3	8	0.62
(2,6942)	1:132:A:SER:HB2	1:133:A:GLY:H	4	0.62
(2,6509)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	9	0.62
(2,6165)	1:150:A:ARG:HG3	1:150:A:ARG:HD3	7	0.62
(2,6159)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	9	0.62
(2,4741)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	3	0.62
(2,4741)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	6	0.62
(2,4516)	1:171:A:LYS:HB3	1:171:A:LYS:H	9	0.62
(2,3679)	1:187:A:SER:HB3	1:189:A:ALA:H	9	0.62
(2,3443)	1:166:A:GLU:HB3	1:166:A:GLU:H	9	0.62
(2,2705)	1:171:A:LYS:HB3	1:171:A:LYS:H	9	0.62
(2,2013)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	1	0.62
(2,1699)	1:185:A:LYS:H	1:185:A:LYS:HB2	1	0.62
(2,1699)	1:185:A:LYS:H	1:185:A:LYS:HB2	4	0.62
(2,95)	1:159:A:PHE:HB2	1:135:A:GLU:H	2	0.62
(1,3030)	1:165:A:ALA:H	1:110:A:ASP:HB3	6	0.62
(1,3003)	1:108:A:ALA:H	1:109:A:ASN:HA	10	0.62
(1,2994)	1:150:A:ARG:H	1:143:A:LEU:HD21	5	0.62
(1,2994)	1:150:A:ARG:H	1:143:A:LEU:HD21	9	0.62
(1,2432)	1:145:A:VAL:HA	1:151:A:SER:H	4	0.62
(1,1429)	1:98:A:LYS:HA	1:100:A:THR:HG23	8	0.62
(1,1364)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	2	0.62
(1,1364)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	3	0.62
(1,1364)	1:141:A:ILE:HG13	1:140:A:GLY:HA2	6	0.62
(1,983)	1:143:A:LEU:HG	1:143:A:LEU:HD23	8	0.62
(1,691)	1:166:A:GLU:HB3	1:168:A:ALA:H	4	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,570)	1:150:A:ARG:HB3	1:151:A:SER:H	8	0.62
(1,522)	1:100:A:THR:HG23	1:98:A:LYS:H	9	0.62
(1,423)	1:139:A:ASN:HB2	1:137:A:VAL:HG22	3	0.62
(2,8959)	1:166:A:GLU:HB3	1:166:A:GLU:H	9	0.61
(2,8567)	1:139:A:ASN:H	1:141:A:ILE:HG22	1	0.61
(2,7113)	1:171:A:LYS:H	1:170:A:LYS:HB2	6	0.61
(2,6509)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	8	0.61
(2,5499)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	7	0.61
(2,5499)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	9	0.61
(2,5446)	1:191:A:VAL:HG11	1:186:A:SER:HA	1	0.61
(2,5446)	1:191:A:VAL:HG11	1:186:A:SER:HA	2	0.61
(2,5243)	1:166:A:GLU:HB3	1:166:A:GLU:H	5	0.61
(2,4741)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	1	0.61
(2,4741)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	2	0.61
(2,4741)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	5	0.61
(2,4741)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	7	0.61
(2,4741)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	8	0.61
(2,4741)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	9	0.61
(2,4741)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	10	0.61
(2,4301)	1:145:A:VAL:HB	1:145:A:VAL:HG13	2	0.61
(2,3717)	1:142:A:THR:HG22	1:141:A:ILE:HG21	7	0.61
(2,3443)	1:166:A:GLU:HB3	1:166:A:GLU:H	6	0.61
(2,1867)	1:161:A:SER:HA	1:106:A:ASP:HB3	9	0.61
(2,1699)	1:185:A:LYS:H	1:185:A:LYS:HB2	3	0.61
(2,1560)	1:150:A:ARG:HG3	1:150:A:ARG:H	10	0.61
(2,1130)	1:192:A:ARG:HD3	1:192:A:ARG:HB2	6	0.61
(2,874)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	2	0.61
(2,874)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	7	0.61
(2,500)	1:130:A:PHE:HB2	1:131:A:PHE:H	4	0.61
(2,396)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	10	0.61
(2,51)	1:191:A:VAL:HG11	1:186:A:SER:HA	10	0.61
(1,2994)	1:150:A:ARG:H	1:143:A:LEU:HD21	3	0.61
(1,2263)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	9	0.61
(1,2222)	1:113:A:VAL:HG13	1:109:A:ASN:HA	8	0.61
(1,2065)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	6	0.61
(1,995)	1:123:A:SER:HB3	1:181:A:ILE:HD11	8	0.61
(1,983)	1:143:A:LEU:HG	1:143:A:LEU:HD23	3	0.61
(1,570)	1:150:A:ARG:HB3	1:151:A:SER:H	10	0.61
(1,522)	1:169:A:LEU:H	1:169:A:LEU:HG	1	0.61
(1,473)	1:175:A:ARG:HB3	1:176:A:ILE:HD11	7	0.61
(1,423)	1:139:A:ASN:HB2	1:137:A:VAL:HG22	8	0.61
(1,397)	1:135:A:GLU:HA	1:136:A:ILE:HB	4	0.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:135:A:GLU:HA	1:136:A:ILE:HB	10	0.61
(2,9034)	1:187:A:SER:HB3	1:188:A:ARG:H	1	0.6
(2,8959)	1:166:A:GLU:HB3	1:166:A:GLU:H	6	0.6
(2,6845)	1:110:A:ASP:HB3	1:110:A:ASP:H	10	0.6
(2,5499)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	2	0.6
(2,5243)	1:166:A:GLU:HB3	1:166:A:GLU:H	2	0.6
(2,4741)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	4	0.6
(2,4516)	1:171:A:LYS:HB3	1:171:A:LYS:H	1	0.6
(2,4516)	1:171:A:LYS:HB3	1:171:A:LYS:H	2	0.6
(2,3822)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	1	0.6
(2,3443)	1:166:A:GLU:HB3	1:166:A:GLU:H	4	0.6
(2,3056)	1:168:A:ALA:H	1:169:A:LEU:HB2	3	0.6
(2,2705)	1:171:A:LYS:HB3	1:171:A:LYS:H	1	0.6
(2,2530)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	4	0.6
(2,2530)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	8	0.6
(2,2530)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	10	0.6
(2,1173)	1:111:A:GLY:HA3	1:109:A:ASN:H	6	0.6
(2,816)	1:161:A:SER:HB2	1:162:A:GLN:H	9	0.6
(2,51)	1:191:A:VAL:HG11	1:186:A:SER:HA	5	0.6
(1,2968)	1:148:A:GLN:H	1:143:A:LEU:HD21	6	0.6
(1,2933)	1:136:A:ILE:HA	1:159:A:PHE:HB2	2	0.6
(1,2405)	1:132:A:SER:H	1:136:A:ILE:HB	9	0.6
(1,2379)	1:150:A:ARG:H	1:143:A:LEU:HD21	8	0.6
(1,1596)	1:143:A:LEU:HG	1:143:A:LEU:HD23	8	0.6
(1,1596)	1:143:A:LEU:HG	1:143:A:LEU:HD23	9	0.6
(1,1178)	1:132:A:SER:H	1:136:A:ILE:HB	9	0.6
(1,1034)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	1	0.6
(1,691)	1:166:A:GLU:HB2	1:168:A:ALA:H	6	0.6
(1,657)	1:96:A:VAL:HG21	1:96:A:VAL:HB	1	0.6
(1,473)	1:175:A:ARG:HB3	1:176:A:ILE:HD12	4	0.6
(1,365)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	4	0.6
(1,365)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	7	0.6
(1,295)	1:164:A:ILE:HD12	1:166:A:GLU:HB2	7	0.6
(1,45)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	10	0.6
(1,19)	1:96:A:VAL:HG21	1:96:A:VAL:HB	1	0.6
(2,8959)	1:166:A:GLU:HB3	1:166:A:GLU:H	4	0.59
(2,8382)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	4	0.59
(2,8382)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	10	0.59
(2,8038)	1:150:A:ARG:HG3	1:150:A:ARG:HD3	6	0.59
(2,7320)	1:191:A:VAL:HG13	1:137:A:VAL:HG11	4	0.59
(2,7113)	1:171:A:LYS:H	1:170:A:LYS:HB2	3	0.59
(2,7113)	1:171:A:LYS:H	1:170:A:LYS:HB2	8	0.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5807)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	2	0.59
(2,5451)	1:191:A:VAL:HG13	1:137:A:VAL:HG11	4	0.59
(2,5446)	1:191:A:VAL:HG11	1:186:A:SER:HA	6	0.59
(2,5446)	1:191:A:VAL:HG11	1:186:A:SER:HA	7	0.59
(2,5252)	1:171:A:LYS:H	1:170:A:LYS:HB2	4	0.59
(2,4321)	1:148:A:GLN:HB2	1:149:A:GLY:H	5	0.59
(2,3687)	1:116:A:ARG:HD2	1:183:A:ILE:HG23	6	0.59
(2,3616)	1:113:A:VAL:HG12	1:113:A:VAL:HB	1	0.59
(2,3605)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	2	0.59
(2,2726)	1:175:A:ARG:HG2	1:175:A:ARG:HA	1	0.59
(2,2705)	1:171:A:LYS:HB3	1:171:A:LYS:H	2	0.59
(2,2530)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	2	0.59
(2,2530)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	7	0.59
(2,1795)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	2	0.59
(2,976)	1:179:A:ARG:HD2	1:179:A:ARG:HB3	3	0.59
(2,54)	1:191:A:VAL:HG13	1:137:A:VAL:HG11	4	0.59
(2,51)	1:191:A:VAL:HG11	1:186:A:SER:HA	9	0.59
(2,15)	1:189:A:ALA:HB2	1:186:A:SER:HA	3	0.59
(1,3066)	1:108:A:ALA:H	1:106:A:ASP:HB3	2	0.59
(1,3066)	1:108:A:ALA:H	1:106:A:ASP:HB3	3	0.59
(1,3066)	1:108:A:ALA:H	1:106:A:ASP:HB3	7	0.59
(1,3003)	1:108:A:ALA:H	1:109:A:ASN:HA	6	0.59
(1,2910)	1:168:A:ALA:HB1	1:167:A:LYS:H	3	0.59
(1,2910)	1:168:A:ALA:HB3	1:167:A:LYS:H	10	0.59
(1,2399)	1:189:A:ALA:H	1:186:A:SER:HA	3	0.59
(1,2263)	1:139:A:ASN:HB2	1:137:A:VAL:HG22	8	0.59
(1,2058)	1:115:A:LEU:HA	1:114:A:ARG:HG3	3	0.59
(1,1696)	1:175:A:ARG:HB3	1:176:A:ILE:HD12	6	0.59
(1,1596)	1:143:A:LEU:HG	1:143:A:LEU:HD23	3	0.59
(1,1418)	1:169:A:LEU:HA	1:169:A:LEU:HD11	3	0.59
(1,1262)	1:96:A:VAL:HG21	1:96:A:VAL:HB	1	0.59
(1,1069)	1:168:A:ALA:HB1	1:167:A:LYS:H	6	0.59
(1,1067)	1:94:A:ASP:HA	1:164:A:ILE:HD13	6	0.59
(1,691)	1:166:A:GLU:HB2	1:168:A:ALA:H	9	0.59
(1,657)	1:96:A:VAL:HG21	1:96:A:VAL:HB	5	0.59
(1,456)	1:165:A:ALA:HA	1:113:A:VAL:HG23	3	0.59
(1,368)	1:169:A:LEU:HD21	1:167:A:LYS:H	9	0.59
(1,365)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	2	0.59
(1,54)	1:166:A:GLU:HB3	1:168:A:ALA:H	4	0.59
(1,19)	1:96:A:VAL:HG21	1:96:A:VAL:HB	5	0.59
(2,8382)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	2	0.58
(2,8382)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	3	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,8382)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	7	0.58
(2,8131)	1:163:A:GLU:HG3	1:163:A:GLU:H	7	0.58
(2,6619)	1:176:A:ILE:HG21	1:175:A:ARG:HB3	7	0.58
(2,6559)	1:192:A:ARG:HD3	1:192:A:ARG:HB2	6	0.58
(2,5840)	1:126:A:GLU:HG3	1:127:A:ILE:H	4	0.58
(2,5807)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	1	0.58
(2,5807)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	3	0.58
(2,5243)	1:166:A:GLU:HB3	1:166:A:GLU:H	7	0.58
(2,4474)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	2	0.58
(2,4474)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	7	0.58
(2,3728)	1:123:A:SER:HB3	1:181:A:ILE:HD11	8	0.58
(2,3691)	1:156:A:PHE:HB2	1:191:A:VAL:H	1	0.58
(2,3679)	1:187:A:SER:HB3	1:189:A:ALA:H	8	0.58
(2,2663)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	5	0.58
(2,2287)	1:130:A:PHE:HB2	1:131:A:PHE:H	2	0.58
(2,1699)	1:185:A:LYS:H	1:185:A:LYS:HB2	9	0.58
(2,396)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	4	0.58
(2,120)	1:142:A:THR:HG22	1:141:A:ILE:HG21	10	0.58
(2,51)	1:191:A:VAL:HG11	1:186:A:SER:HA	3	0.58
(1,2933)	1:136:A:ILE:HA	1:159:A:PHE:HB2	7	0.58
(1,2926)	1:179:A:ARG:HD2	1:179:A:ARG:HA	6	0.58
(1,2379)	1:150:A:ARG:H	1:143:A:LEU:HD21	5	0.58
(1,2379)	1:150:A:ARG:H	1:143:A:LEU:HD21	9	0.58
(1,1784)	1:189:A:ALA:H	1:186:A:SER:HA	9	0.58
(1,1034)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	4	0.58
(1,983)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	4	0.58
(1,983)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	7	0.58
(1,541)	1:181:A:ILE:H	1:172:A:HIS:HA	9	0.58
(1,447)	1:154:A:GLU:HG2	1:118:A:LEU:HD23	6	0.58
(1,397)	1:135:A:GLU:HA	1:136:A:ILE:HB	8	0.58
(1,133)	1:166:A:GLU:HG3	1:169:A:LEU:HD13	1	0.58
(1,33)	1:137:A:VAL:HG22	1:139:A:ASN:H	4	0.58
(1,33)	1:137:A:VAL:HG22	1:139:A:ASN:H	7	0.58
(2,9034)	1:187:A:SER:HB3	1:188:A:ARG:H	2	0.57
(2,9034)	1:187:A:SER:HB3	1:188:A:ARG:H	8	0.57
(2,8382)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	1	0.57
(2,8382)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	6	0.57
(2,8131)	1:163:A:GLU:HG3	1:163:A:GLU:H	4	0.57
(2,6701)	1:168:A:ALA:H	1:169:A:LEU:HB2	3	0.57
(2,5807)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	6	0.57
(2,5525)	1:142:A:THR:HG21	1:141:A:ILE:HG21	6	0.57
(2,4788)	1:158:A:GLN:HG3	1:112:A:PHE:HA	1	0.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4341)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	6	0.57
(2,4321)	1:148:A:GLN:HB2	1:149:A:GLY:H	2	0.57
(2,3286)	1:132:A:SER:HB2	1:133:A:GLY:H	2	0.57
(2,2984)	1:188:A:ARG:HD2	1:108:A:ALA:H	1	0.57
(2,874)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	5	0.57
(2,106)	1:93:A:MET:HB2	1:93:A:MET:HG2	4	0.57
(2,55)	1:191:A:VAL:HG11	1:190:A:GLU:H	8	0.57
(2,15)	1:189:A:ALA:HB2	1:186:A:SER:HA	10	0.57
(1,3050)	1:145:A:VAL:HA	1:151:A:SER:H	4	0.57
(1,3013)	1:189:A:ALA:H	1:186:A:SER:HA	1	0.57
(1,2994)	1:150:A:ARG:H	1:143:A:LEU:HD21	10	0.57
(1,2379)	1:150:A:ARG:H	1:143:A:LEU:HD21	3	0.57
(1,2320)	1:136:A:ILE:HA	1:159:A:PHE:HB2	9	0.57
(1,2263)	1:134:A:LEU:HD13	1:131:A:PHE:HB2	3	0.57
(1,1992)	1:158:A:GLN:HG3	1:161:A:SER:H	7	0.57
(1,1696)	1:175:A:ARG:HB3	1:176:A:ILE:HD11	8	0.57
(1,1262)	1:96:A:VAL:HG21	1:96:A:VAL:HB	5	0.57
(1,1083)	1:175:A:ARG:HB3	1:176:A:ILE:HD11	5	0.57
(1,983)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	2	0.57
(1,935)	1:110:A:ASP:HB3	1:188:A:ARG:HG2	3	0.57
(1,570)	1:150:A:ARG:HG2	1:151:A:SER:H	1	0.57
(1,368)	1:169:A:LEU:HD21	1:167:A:LYS:H	4	0.57
(1,297)	1:164:A:ILE:HD13	1:93:A:MET:HG3	3	0.57
(1,295)	1:164:A:ILE:HD12	1:166:A:GLU:HB2	2	0.57
(1,224)	1:116:A:ARG:HD2	1:116:A:ARG:HA	1	0.57
(1,160)	1:102:A:PRO:HG2	1:101:A:GLY:HA3	6	0.57
(1,54)	1:166:A:GLU:HB2	1:168:A:ALA:H	6	0.57
(1,54)	1:166:A:GLU:HB2	1:168:A:ALA:H	9	0.57
(2,8382)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	5	0.56
(2,8038)	1:150:A:ARG:HG3	1:150:A:ARG:HD3	2	0.56
(2,8038)	1:150:A:ARG:HG3	1:150:A:ARG:HD3	4	0.56
(2,8038)	1:150:A:ARG:HG3	1:150:A:ARG:HD3	7	0.56
(2,8038)	1:150:A:ARG:HG3	1:150:A:ARG:HD3	8	0.56
(2,8038)	1:150:A:ARG:HG3	1:150:A:ARG:HD3	10	0.56
(2,7131)	1:175:A:ARG:HG2	1:176:A:ILE:H	1	0.56
(2,6619)	1:176:A:ILE:HG21	1:175:A:ARG:HB3	9	0.56
(2,6569)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	2	0.56
(2,6569)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	3	0.56
(2,6569)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	5	0.56
(2,6569)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	6	0.56
(2,6409)	1:179:A:ARG:HG3	1:179:A:ARG:HB3	3	0.56
(2,5807)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	8	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5446)	1:191:A:VAL:HG11	1:186:A:SER:HA	10	0.56
(2,4789)	1:190:A:GLU:HG3	1:186:A:SER:HA	4	0.56
(2,3607)	1:164:A:ILE:HD13	1:91:A:ASN:HA	8	0.56
(2,3452)	1:171:A:LYS:H	1:170:A:LYS:HB2	6	0.56
(2,2970)	1:111:A:GLY:HA3	1:109:A:ASN:H	8	0.56
(2,2511)	1:148:A:GLN:HB2	1:149:A:GLY:H	5	0.56
(2,2471)	1:144:A:PRO:HD3	1:144:A:PRO:HA	9	0.56
(2,1873)	1:187:A:SER:HB3	1:189:A:ALA:H	9	0.56
(2,1243)	1:127:A:ILE:H	1:115:A:LEU:HD22	5	0.56
(2,426)	1:126:A:GLU:HG3	1:126:A:GLU:HB2	2	0.56
(2,129)	1:155:A:ALA:HB2	1:154:A:GLU:H	6	0.56
(2,120)	1:142:A:THR:HG22	1:141:A:ILE:HG21	7	0.56
(2,15)	1:189:A:ALA:HB2	1:186:A:SER:HA	4	0.56
(1,2994)	1:150:A:ARG:H	1:143:A:LEU:HD21	6	0.56
(1,2968)	1:148:A:GLN:H	1:143:A:LEU:HD22	3	0.56
(1,1596)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	4	0.56
(1,1596)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	7	0.56
(1,1188)	1:165:A:ALA:H	1:110:A:ASP:HB3	4	0.56
(1,1173)	1:189:A:ALA:H	1:186:A:SER:HA	8	0.56
(1,570)	1:150:A:ARG:HG2	1:151:A:SER:H	3	0.56
(1,522)	1:169:A:LEU:H	1:169:A:LEU:HG	2	0.56
(1,365)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	1	0.56
(2,8382)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	9	0.55
(2,7690)	1:120:A:PHE:HB3	1:120:A:PHE:H	10	0.55
(2,7320)	1:191:A:VAL:HG13	1:137:A:VAL:HG11	10	0.55
(2,6609)	1:95:A:TRP:HA	1:164:A:ILE:HG13	5	0.55
(2,6569)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	1	0.55
(2,6569)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	4	0.55
(2,6569)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	7	0.55
(2,6569)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	8	0.55
(2,6569)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	9	0.55
(2,6569)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	10	0.55
(2,5807)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	9	0.55
(2,5525)	1:142:A:THR:HG21	1:141:A:ILE:HG21	8	0.55
(2,5451)	1:191:A:VAL:HG13	1:137:A:VAL:HG11	10	0.55
(2,5446)	1:191:A:VAL:HG11	1:186:A:SER:HA	5	0.55
(2,4670)	1:187:A:SER:HB3	1:188:A:ARG:H	5	0.55
(2,4670)	1:187:A:SER:HB3	1:188:A:ARG:H	7	0.55
(2,3452)	1:171:A:LYS:H	1:170:A:LYS:HB2	3	0.55
(2,3452)	1:171:A:LYS:H	1:170:A:LYS:HB2	8	0.55
(2,3286)	1:132:A:SER:HB2	1:133:A:GLY:H	5	0.55
(2,2491)	1:145:A:VAL:HB	1:145:A:VAL:HG13	2	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1807)	1:113:A:VAL:HG11	1:113:A:VAL:HB	6	0.55
(2,426)	1:126:A:GLU:HG3	1:126:A:GLU:HB2	5	0.55
(2,55)	1:191:A:VAL:HG11	1:190:A:GLU:H	2	0.55
(2,54)	1:191:A:VAL:HG13	1:137:A:VAL:HG11	10	0.55
(1,2320)	1:136:A:ILE:HA	1:159:A:PHE:HB2	8	0.55
(1,1872)	1:113:A:VAL:HG11	1:186:A:SER:HB3	1	0.55
(1,1681)	1:168:A:ALA:HB1	1:167:A:LYS:H	6	0.55
(1,1596)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	2	0.55
(1,1563)	1:166:A:GLU:HG3	1:168:A:ALA:H	5	0.55
(1,1288)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	10	0.55
(1,983)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	1	0.55
(1,764)	1:166:A:GLU:HG3	1:168:A:ALA:H	5	0.55
(1,614)	1:108:A:ALA:H	1:106:A:ASP:HB3	8	0.55
(1,570)	1:150:A:ARG:HG2	1:151:A:SER:H	5	0.55
(1,570)	1:150:A:ARG:HB3	1:151:A:SER:H	9	0.55
(1,522)	1:100:A:THR:HG23	1:98:A:LYS:H	10	0.55
(1,295)	1:164:A:ILE:HD12	1:166:A:GLU:HB2	8	0.55
(1,295)	1:164:A:ILE:HD12	1:166:A:GLU:HB2	10	0.55
(1,191)	1:98:A:LYS:HA	1:100:A:THR:HG23	1	0.55
(1,191)	1:98:A:LYS:HA	1:100:A:THR:HG22	4	0.55
(1,46)	1:167:A:LYS:HG2	1:134:A:LEU:HD11	7	0.55
(2,9034)	1:187:A:SER:HB3	1:188:A:ARG:H	6	0.54
(2,8562)	1:168:A:ALA:H	1:169:A:LEU:HB2	3	0.54
(2,8382)	1:188:A:ARG:HD2	1:188:A:ARG:HG3	8	0.54
(2,7690)	1:120:A:PHE:HB3	1:120:A:PHE:H	2	0.54
(2,7230)	1:150:A:ARG:HG2	1:151:A:SER:H	2	0.54
(2,7113)	1:171:A:LYS:H	1:170:A:LYS:HB2	4	0.54
(2,6619)	1:176:A:ILE:HG22	1:175:A:ARG:HB3	5	0.54
(2,6616)	1:158:A:GLN:HG3	1:112:A:PHE:HA	1	0.54
(2,6409)	1:179:A:ARG:HG3	1:179:A:ARG:HB3	4	0.54
(2,6409)	1:179:A:ARG:HG3	1:179:A:ARG:HB3	8	0.54
(2,5446)	1:191:A:VAL:HG11	1:186:A:SER:HA	3	0.54
(2,5446)	1:191:A:VAL:HG11	1:186:A:SER:HA	9	0.54
(2,4670)	1:187:A:SER:HB3	1:188:A:ARG:H	9	0.54
(2,4341)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	2	0.54
(2,4341)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	4	0.54
(2,4341)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	7	0.54
(2,4341)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	8	0.54
(2,4341)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	10	0.54
(2,4098)	1:130:A:PHE:HB2	1:131:A:PHE:H	2	0.54
(2,3443)	1:166:A:GLU:HB3	1:166:A:GLU:H	2	0.54
(2,3443)	1:166:A:GLU:HB3	1:166:A:GLU:H	5	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2984)	1:188:A:ARG:HD2	1:108:A:ALA:H	5	0.54
(2,2970)	1:111:A:GLY:HA3	1:109:A:ASN:H	9	0.54
(2,2511)	1:148:A:GLN:HB2	1:149:A:GLY:H	2	0.54
(2,1560)	1:150:A:ARG:HG3	1:150:A:ARG:H	9	0.54
(2,1398)	1:112:A:PHE:H	1:112:A:PHE:HB3	7	0.54
(2,1283)	1:105:A:PRO:HB3	1:106:A:ASP:H	8	0.54
(2,1243)	1:127:A:ILE:H	1:115:A:LEU:HD22	9	0.54
(2,976)	1:179:A:ARG:HD2	1:179:A:ARG:HB3	1	0.54
(2,816)	1:161:A:SER:HB2	1:162:A:GLN:H	4	0.54
(2,100)	1:181:A:ILE:HG21	1:174:A:GLU:HA	7	0.54
(2,55)	1:191:A:VAL:HG13	1:190:A:GLU:H	3	0.54
(1,3066)	1:108:A:ALA:H	1:106:A:ASP:HB3	10	0.54
(1,2415)	1:165:A:ALA:H	1:110:A:ASP:HB3	8	0.54
(1,2352)	1:148:A:GLN:H	1:143:A:LEU:HD22	7	0.54
(1,2314)	1:179:A:ARG:HD2	1:179:A:ARG:HA	6	0.54
(1,2133)	1:97:A:LEU:HD12	1:163:A:GLU:HB3	6	0.54
(1,1961)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	10	0.54
(1,1548)	1:112:A:PHE:HB3	1:188:A:ARG:HG2	10	0.54
(1,1524)	1:93:A:MET:HB2	1:135:A:GLU:HB3	7	0.54
(1,1266)	1:127:A:ILE:HG21	1:127:A:ILE:HB	1	0.54
(1,1083)	1:175:A:ARG:HB3	1:176:A:ILE:HD11	10	0.54
(1,1069)	1:168:A:ALA:HB2	1:167:A:LYS:H	9	0.54
(1,927)	1:164:A:ILE:HA	1:91:A:ASN:HB3	1	0.54
(1,662)	1:127:A:ILE:HG21	1:127:A:ILE:HB	1	0.54
(1,369)	1:175:A:ARG:HB3	1:176:A:ILE:H	1	0.54
(1,46)	1:167:A:LYS:HG2	1:134:A:LEU:HD12	10	0.54
(2,8959)	1:166:A:GLU:HB3	1:166:A:GLU:H	2	0.53
(2,8959)	1:166:A:GLU:HB3	1:166:A:GLU:H	5	0.53
(2,7320)	1:191:A:VAL:HG13	1:137:A:VAL:HG12	2	0.53
(2,6409)	1:179:A:ARG:HG3	1:179:A:ARG:HB3	1	0.53
(2,6131)	1:147:A:PHE:HB3	1:147:A:PHE:HA	7	0.53
(2,5451)	1:191:A:VAL:HG13	1:137:A:VAL:HG12	2	0.53
(2,5252)	1:171:A:LYS:H	1:170:A:LYS:HB2	9	0.53
(2,4859)	1:168:A:ALA:H	1:169:A:LEU:HB2	3	0.53
(2,4670)	1:187:A:SER:HB3	1:188:A:ARG:H	1	0.53
(2,4474)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	5	0.53
(2,3986)	1:119:A:PRO:HB2	1:119:A:PRO:HA	4	0.53
(2,3691)	1:156:A:PHE:HB2	1:191:A:VAL:H	4	0.53
(2,3605)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	6	0.53
(2,3286)	1:132:A:SER:HB2	1:133:A:GLY:H	4	0.53
(2,3054)	1:167:A:LYS:HB3	1:168:A:ALA:H	7	0.53
(2,2492)	1:145:A:VAL:HB	1:145:A:VAL:HG21	2	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1795)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	6	0.53
(2,748)	1:151:A:SER:HB3	1:152:A:THR:H	4	0.53
(2,415)	1:123:A:SER:HB2	1:123:A:SER:HA	8	0.53
(2,106)	1:93:A:MET:HB2	1:93:A:MET:HG2	7	0.53
(2,104)	1:188:A:ARG:HG2	1:111:A:GLY:HA3	1	0.53
(2,55)	1:191:A:VAL:HG13	1:190:A:GLU:H	10	0.53
(2,54)	1:191:A:VAL:HG13	1:137:A:VAL:HG12	2	0.53
(2,51)	1:191:A:VAL:HG11	1:186:A:SER:HA	8	0.53
(2,4)	1:164:A:ILE:HD11	1:161:A:SER:HB3	10	0.53
(1,2528)	1:166:A:GLU:HB3	1:167:A:LYS:HA	2	0.53
(1,2515)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	2	0.53
(1,2405)	1:132:A:SER:H	1:136:A:ILE:HB	8	0.53
(1,2379)	1:150:A:ARG:H	1:143:A:LEU:HD21	10	0.53
(1,2210)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	10	0.53
(1,1961)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	4	0.53
(1,1961)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	5	0.53
(1,1961)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	7	0.53
(1,1266)	1:127:A:ILE:HG21	1:127:A:ILE:HB	5	0.53
(1,1178)	1:132:A:SER:H	1:136:A:ILE:HB	8	0.53
(1,820)	1:98:A:LYS:HA	1:100:A:THR:HG23	8	0.53
(1,662)	1:127:A:ILE:HG21	1:127:A:ILE:HB	5	0.53
(1,459)	1:168:A:ALA:HB1	1:167:A:LYS:H	6	0.53
(1,397)	1:135:A:GLU:HA	1:136:A:ILE:HB	6	0.53
(1,251)	1:112:A:PHE:HB2	1:191:A:VAL:HG22	8	0.53
(1,46)	1:167:A:LYS:HG2	1:134:A:LEU:HD12	6	0.53
(1,33)	1:137:A:VAL:HG22	1:139:A:ASN:H	5	0.53
(2,9026)	1:187:A:SER:H	1:186:A:SER:HB2	1	0.52
(2,8131)	1:163:A:GLU:HG3	1:163:A:GLU:H	9	0.52
(2,7104)	1:166:A:GLU:HB3	1:166:A:GLU:H	6	0.52
(2,7104)	1:166:A:GLU:HB3	1:166:A:GLU:H	9	0.52
(2,6619)	1:176:A:ILE:HG21	1:175:A:ARG:HB3	10	0.52
(2,6609)	1:95:A:TRP:HA	1:164:A:ILE:HG13	1	0.52
(2,6131)	1:147:A:PHE:HB3	1:147:A:PHE:HA	9	0.52
(2,5807)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	7	0.52
(2,5684)	1:105:A:PRO:HD3	1:104:A:SER:HB3	5	0.52
(2,4769)	1:123:A:SER:HB3	1:143:A:LEU:HD23	8	0.52
(2,4321)	1:148:A:GLN:HB2	1:149:A:GLY:H	1	0.52
(2,4281)	1:144:A:PRO:HD3	1:144:A:PRO:HA	9	0.52
(2,3640)	1:191:A:VAL:HG22	1:186:A:SER:HB2	1	0.52
(2,3443)	1:166:A:GLU:HB3	1:166:A:GLU:H	7	0.52
(2,1887)	1:156:A:PHE:HB2	1:191:A:VAL:H	1	0.52
(2,1873)	1:187:A:SER:HB3	1:189:A:ALA:H	8	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,915)	1:171:A:LYS:HB3	1:171:A:LYS:H	8	0.52
(2,47)	1:191:A:VAL:HG13	1:192:A:ARG:HA	1	0.52
(1,3013)	1:189:A:ALA:H	1:186:A:SER:HA	2	0.52
(1,3013)	1:189:A:ALA:H	1:186:A:SER:HA	5	0.52
(1,2994)	1:150:A:ARG:H	1:143:A:LEU:HD21	2	0.52
(1,2933)	1:136:A:ILE:HA	1:159:A:PHE:HB2	9	0.52
(1,2910)	1:168:A:ALA:HB3	1:167:A:LYS:H	8	0.52
(1,2820)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	10	0.52
(1,2379)	1:150:A:ARG:H	1:143:A:LEU:HD21	6	0.52
(1,2211)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	10	0.52
(1,2210)	1:143:A:LEU:HG	1:143:A:LEU:HD23	6	0.52
(1,1795)	1:122:A:CYS:H	1:127:A:ILE:HD13	1	0.52
(1,1706)	1:141:A:ILE:HA	1:140:A:GLY:H	8	0.52
(1,1645)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	1	0.52
(1,1601)	1:175:A:ARG:HB3	1:176:A:ILE:H	1	0.52
(1,1596)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	1	0.52
(1,1462)	1:175:A:ARG:HD2	1:178:A:HIS:HA	5	0.52
(1,1297)	1:166:A:GLU:HB3	1:168:A:ALA:H	4	0.52
(1,1188)	1:165:A:ALA:H	1:110:A:ASP:HB3	2	0.52
(1,783)	1:130:A:PHE:HB3	1:132:A:SER:H	9	0.52
(1,683)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	4	0.52
(1,541)	1:181:A:ILE:H	1:172:A:HIS:HA	7	0.52
(1,473)	1:157:A:VAL:HG23	1:114:A:ARG:HB3	1	0.52
(1,365)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	5	0.52
(1,46)	1:167:A:LYS:HG2	1:134:A:LEU:HD11	1	0.52
(2,8959)	1:166:A:GLU:HB3	1:166:A:GLU:H	7	0.51
(2,8131)	1:163:A:GLU:HG3	1:163:A:GLU:H	3	0.51
(2,7410)	1:98:A:LYS:HB3	1:100:A:THR:HG23	10	0.51
(2,7320)	1:191:A:VAL:HG13	1:137:A:VAL:HG11	8	0.51
(2,7104)	1:166:A:GLU:HB3	1:166:A:GLU:H	4	0.51
(2,5807)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	5	0.51
(2,5451)	1:191:A:VAL:HG13	1:137:A:VAL:HG11	8	0.51
(2,3691)	1:156:A:PHE:HB2	1:191:A:VAL:H	10	0.51
(2,3647)	1:191:A:VAL:HG13	1:193:A:THR:H	5	0.51
(2,3383)	1:154:A:GLU:HB3	1:154:A:GLU:H	2	0.51
(2,3383)	1:154:A:GLU:HB3	1:154:A:GLU:H	10	0.51
(2,915)	1:171:A:LYS:HB3	1:171:A:LYS:H	3	0.51
(2,915)	1:171:A:LYS:HB3	1:171:A:LYS:H	5	0.51
(2,129)	1:155:A:ALA:HB2	1:154:A:GLU:H	3	0.51
(2,54)	1:191:A:VAL:HG13	1:137:A:VAL:HG11	8	0.51
(1,2821)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	10	0.51
(1,2820)	1:143:A:LEU:HG	1:143:A:LEU:HD23	6	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2772)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	5	0.51
(1,2528)	1:166:A:GLU:HB3	1:167:A:LYS:HA	5	0.51
(1,2399)	1:189:A:ALA:H	1:186:A:SER:HA	4	0.51
(1,2213)	1:175:A:ARG:HB3	1:176:A:ILE:H	1	0.51
(1,2211)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	6	0.51
(1,2211)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	8	0.51
(1,1706)	1:174:A:GLU:HA	1:181:A:ILE:H	9	0.51
(1,1645)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	4	0.51
(1,1608)	1:174:A:GLU:HB2	1:181:A:ILE:HD13	7	0.51
(1,1188)	1:165:A:ALA:H	1:110:A:ASP:HB3	1	0.51
(1,988)	1:190:A:GLU:HG3	1:186:A:SER:HA	1	0.51
(1,988)	1:190:A:GLU:HG3	1:186:A:SER:HA	5	0.51
(1,983)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	5	0.51
(1,625)	1:97:A:LEU:H	1:99:A:HIS:HA	1	0.51
(1,368)	1:169:A:LEU:HD21	1:167:A:LYS:H	5	0.51
(1,368)	1:169:A:LEU:HD21	1:167:A:LYS:H	6	0.51
(1,251)	1:112:A:PHE:HB2	1:191:A:VAL:HG22	10	0.51
(1,224)	1:116:A:ARG:HD2	1:116:A:ARG:HA	3	0.51
(2,8439)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	2	0.5
(2,8439)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	3	0.5
(2,8439)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	6	0.5
(2,8004)	1:147:A:PHE:HB3	1:147:A:PHE:HA	7	0.5
(2,8004)	1:147:A:PHE:HB3	1:147:A:PHE:HA	9	0.5
(2,7273)	1:164:A:ILE:HD13	1:135:A:GLU:H	3	0.5
(2,6852)	1:112:A:PHE:H	1:112:A:PHE:HB3	7	0.5
(2,6345)	1:171:A:LYS:HB3	1:171:A:LYS:H	8	0.5
(2,5637)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	5	0.5
(2,3383)	1:154:A:GLU:HB3	1:154:A:GLU:H	5	0.5
(2,3095)	1:159:A:PHE:H	1:110:A:ASP:HA	7	0.5
(2,2950)	1:162:A:GLN:HG2	1:165:A:ALA:H	9	0.5
(2,2710)	1:173:A:LYS:HG2	1:173:A:LYS:HA	6	0.5
(2,2051)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	2	0.5
(2,1757)	1:173:A:LYS:HB2	1:172:A:HIS:H	10	0.5
(2,932)	1:174:A:GLU:HG3	1:175:A:ARG:H	6	0.5
(2,129)	1:155:A:ALA:HB2	1:154:A:GLU:H	10	0.5
(2,85)	1:187:A:SER:HB3	1:189:A:ALA:H	6	0.5
(2,85)	1:187:A:SER:HB3	1:189:A:ALA:H	7	0.5
(2,47)	1:191:A:VAL:HG12	1:192:A:ARG:HA	4	0.5
(1,3066)	1:108:A:ALA:H	1:106:A:ASP:HB3	1	0.5
(1,3066)	1:108:A:ALA:H	1:106:A:ASP:HB3	5	0.5
(1,2994)	1:150:A:ARG:H	1:143:A:LEU:HD21	1	0.5
(1,2933)	1:136:A:ILE:HA	1:159:A:PHE:HB2	8	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2821)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	6	0.5
(1,2821)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	8	0.5
(1,2405)	1:132:A:SER:H	1:136:A:ILE:HB	2	0.5
(1,2399)	1:189:A:ALA:H	1:186:A:SER:HA	10	0.5
(1,2320)	1:136:A:ILE:HA	1:159:A:PHE:HB2	6	0.5
(1,2298)	1:168:A:ALA:HB1	1:167:A:LYS:H	6	0.5
(1,2211)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	5	0.5
(1,1297)	1:166:A:GLU:HB2	1:168:A:ALA:H	6	0.5
(1,1297)	1:166:A:GLU:HB2	1:168:A:ALA:H	9	0.5
(1,1178)	1:132:A:SER:H	1:136:A:ILE:HB	2	0.5
(1,987)	1:175:A:ARG:HB3	1:176:A:ILE:H	1	0.5
(1,845)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	4	0.5
(1,837)	1:108:A:ALA:HA	1:109:A:ASN:H	10	0.5
(1,473)	1:157:A:VAL:HG23	1:114:A:ARG:HB3	5	0.5
(1,447)	1:154:A:GLU:HG2	1:118:A:LEU:HD23	3	0.5
(1,377)	1:123:A:SER:HB3	1:181:A:ILE:HD11	3	0.5
(1,227)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	3	0.5
(1,227)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	6	0.5
(1,13)	1:181:A:ILE:HG12	1:175:A:ARG:HA	2	0.5
(2,8439)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	1	0.49
(2,8439)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	5	0.49
(2,8439)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	7	0.49
(2,8439)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	8	0.49
(2,8439)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	9	0.49
(2,8439)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	10	0.49
(2,8131)	1:163:A:GLU:HG3	1:163:A:GLU:H	5	0.49
(2,7508)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	5	0.49
(2,6345)	1:171:A:LYS:HB3	1:171:A:LYS:H	3	0.49
(2,6345)	1:171:A:LYS:HB3	1:171:A:LYS:H	5	0.49
(2,5807)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	10	0.49
(2,5684)	1:105:A:PRO:HD3	1:104:A:SER:HB3	4	0.49
(2,5446)	1:191:A:VAL:HG11	1:186:A:SER:HA	8	0.49
(2,5400)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	7	0.49
(2,5086)	1:132:A:SER:HB2	1:133:A:GLY:H	2	0.49
(2,5003)	1:112:A:PHE:H	1:112:A:PHE:HB3	7	0.49
(2,4670)	1:187:A:SER:HB3	1:188:A:ARG:H	2	0.49
(2,4670)	1:187:A:SER:HB3	1:188:A:ARG:H	8	0.49
(2,3616)	1:113:A:VAL:HG11	1:113:A:VAL:HB	6	0.49
(2,3452)	1:171:A:LYS:H	1:170:A:LYS:HB2	4	0.49
(2,3383)	1:154:A:GLU:HB3	1:154:A:GLU:H	3	0.49
(2,3383)	1:154:A:GLU:HB3	1:154:A:GLU:H	4	0.49
(2,3383)	1:154:A:GLU:HB3	1:154:A:GLU:H	9	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3196)	1:110:A:ASP:HB3	1:110:A:ASP:H	10	0.49
(2,3095)	1:159:A:PHE:H	1:110:A:ASP:HA	3	0.49
(2,2984)	1:188:A:ARG:HD2	1:108:A:ALA:H	4	0.49
(2,2981)	1:158:A:GLN:HG3	1:112:A:PHE:HA	3	0.49
(2,2511)	1:148:A:GLN:HB2	1:149:A:GLY:H	1	0.49
(2,2466)	1:144:A:PRO:HB2	1:144:A:PRO:HA	9	0.49
(2,2177)	1:119:A:PRO:HB2	1:119:A:PRO:HA	4	0.49
(2,1797)	1:164:A:ILE:HD13	1:91:A:ASN:HA	8	0.49
(2,1758)	1:149:A:GLY:HA3	1:151:A:SER:H	9	0.49
(2,721)	1:148:A:GLN:HB2	1:149:A:GLY:H	9	0.49
(2,264)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	2	0.49
(2,47)	1:191:A:VAL:HG13	1:192:A:ARG:HA	2	0.49
(2,47)	1:191:A:VAL:HG13	1:192:A:ARG:HA	5	0.49
(2,2)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	7	0.49
(1,2821)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	5	0.49
(1,2528)	1:166:A:GLU:HB3	1:167:A:LYS:HA	7	0.49
(1,2399)	1:189:A:ALA:H	1:186:A:SER:HA	7	0.49
(1,1961)	1:141:A:ILE:HG13	1:140:A:GLY:HA2	9	0.49
(1,1788)	1:132:A:SER:H	1:136:A:ILE:HB	1	0.49
(1,1706)	1:141:A:ILE:HA	1:140:A:GLY:H	2	0.49
(1,1681)	1:168:A:ALA:HB2	1:167:A:LYS:H	9	0.49
(1,1462)	1:175:A:ARG:HD2	1:178:A:HIS:HA	10	0.49
(1,1083)	1:175:A:ARG:HB2	1:176:A:ILE:HD12	1	0.49
(1,1069)	1:168:A:ALA:HB3	1:167:A:LYS:H	1	0.49
(1,914)	1:93:A:MET:HB2	1:135:A:GLU:HB3	7	0.49
(1,845)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	2	0.49
(1,837)	1:92:A:ALA:HA	1:93:A:MET:H	4	0.49
(1,614)	1:108:A:ALA:H	1:106:A:ASP:HB3	6	0.49
(1,364)	1:96:A:VAL:HG12	1:93:A:MET:HG2	4	0.49
(1,251)	1:112:A:PHE:HB2	1:191:A:VAL:HG22	3	0.49
(1,224)	1:116:A:ARG:HD2	1:116:A:ARG:HA	9	0.49
(1,224)	1:116:A:ARG:HD2	1:116:A:ARG:HA	10	0.49
(1,45)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	4	0.49
(1,33)	1:137:A:VAL:HG22	1:139:A:ASN:H	3	0.49
(2,8724)	1:114:A:ARG:HG3	1:115:A:LEU:H	4	0.48
(2,8472)	1:111:A:GLY:HA3	1:109:A:ASN:H	3	0.48
(2,8439)	1:192:A:ARG:HG2	1:192:A:ARG:HD2	4	0.48
(2,7410)	1:98:A:LYS:HB3	1:100:A:THR:HG23	6	0.48
(2,7377)	1:181:A:ILE:HG21	1:174:A:GLU:HA	7	0.48
(2,7230)	1:150:A:ARG:HG2	1:151:A:SER:H	10	0.48
(2,7113)	1:171:A:LYS:H	1:170:A:LYS:HB2	9	0.48
(2,7042)	1:154:A:GLU:H	1:154:A:GLU:HB3	10	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6942)	1:132:A:SER:HB2	1:133:A:GLY:H	10	0.48
(2,5525)	1:142:A:THR:HG23	1:141:A:ILE:HG21	1	0.48
(2,5404)	1:164:A:ILE:HD13	1:135:A:GLU:H	3	0.48
(2,5400)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	8	0.48
(2,3647)	1:191:A:VAL:HG13	1:193:A:THR:H	4	0.48
(2,3514)	1:187:A:SER:H	1:186:A:SER:HB2	1	0.48
(2,3383)	1:154:A:GLU:HB3	1:154:A:GLU:H	8	0.48
(2,1887)	1:156:A:PHE:HB2	1:191:A:VAL:H	4	0.48
(2,1807)	1:113:A:VAL:HG13	1:113:A:VAL:HB	8	0.48
(2,1283)	1:105:A:PRO:HB3	1:106:A:ASP:H	9	0.48
(2,1243)	1:127:A:ILE:H	1:115:A:LEU:HD22	1	0.48
(2,1243)	1:127:A:ILE:H	1:115:A:LEU:HD22	3	0.48
(2,129)	1:155:A:ALA:HB2	1:154:A:GLU:H	2	0.48
(2,129)	1:155:A:ALA:HB2	1:154:A:GLU:H	7	0.48
(2,55)	1:191:A:VAL:HG11	1:190:A:GLU:H	9	0.48
(2,2)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	8	0.48
(1,2821)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	9	0.48
(1,2772)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	4	0.48
(1,2596)	1:163:A:GLU:HG3	1:163:A:GLU:HA	6	0.48
(1,2379)	1:150:A:ARG:H	1:143:A:LEU:HD21	2	0.48
(1,2211)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	3	0.48
(1,2211)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	9	0.48
(1,2210)	1:143:A:LEU:HG	1:143:A:LEU:HD23	8	0.48
(1,2210)	1:143:A:LEU:HG	1:143:A:LEU:HD23	9	0.48
(1,1596)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	5	0.48
(1,1429)	1:98:A:LYS:HA	1:100:A:THR:HG23	1	0.48
(1,1429)	1:98:A:LYS:HA	1:100:A:THR:HG22	4	0.48
(1,1083)	1:175:A:ARG:HB3	1:176:A:ILE:HD11	7	0.48
(1,837)	1:92:A:ALA:HA	1:93:A:MET:H	1	0.48
(1,837)	1:92:A:ALA:HA	1:93:A:MET:H	2	0.48
(1,837)	1:92:A:ALA:HA	1:93:A:MET:H	3	0.48
(1,837)	1:108:A:ALA:HA	1:109:A:ASN:H	6	0.48
(1,837)	1:92:A:ALA:HA	1:93:A:MET:H	8	0.48
(1,725)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	4	0.48
(1,691)	1:166:A:GLU:HB3	1:168:A:ALA:H	1	0.48
(1,614)	1:108:A:ALA:H	1:106:A:ASP:HB3	4	0.48
(1,459)	1:168:A:ALA:HB2	1:167:A:LYS:H	9	0.48
(1,224)	1:116:A:ARG:HD2	1:116:A:ARG:HA	7	0.48
(1,97)	1:119:A:PRO:HB2	1:119:A:PRO:HA	3	0.48
(1,97)	1:119:A:PRO:HB2	1:119:A:PRO:HA	10	0.48
(1,46)	1:167:A:LYS:HG2	1:134:A:LEU:HD11	2	0.48
(1,46)	1:167:A:LYS:HG2	1:134:A:LEU:HD12	8	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,7)	1:116:A:ARG:H	1:182:A:GLU:O	8	0.47
(2,8724)	1:114:A:ARG:HG3	1:115:A:LEU:H	6	0.47
(2,8472)	1:111:A:GLY:HA3	1:109:A:ASN:H	10	0.47
(2,8131)	1:163:A:GLU:HG3	1:163:A:GLU:H	1	0.47
(2,7997)	1:145:A:VAL:HB	1:145:A:VAL:HG13	2	0.47
(2,7042)	1:154:A:GLU:H	1:154:A:GLU:HB3	2	0.47
(2,7042)	1:154:A:GLU:H	1:154:A:GLU:HB3	5	0.47
(2,6609)	1:95:A:TRP:HA	1:164:A:ILE:HG13	4	0.47
(2,6587)	1:93:A:MET:HB2	1:164:A:ILE:HG12	4	0.47
(2,6124)	1:145:A:VAL:HB	1:145:A:VAL:HG13	2	0.47
(2,5539)	1:98:A:LYS:HB3	1:100:A:THR:HG23	9	0.47
(2,5525)	1:142:A:THR:HG21	1:141:A:ILE:HG21	3	0.47
(2,5525)	1:142:A:THR:HG22	1:141:A:ILE:HG21	9	0.47
(2,5086)	1:132:A:SER:HB2	1:133:A:GLY:H	5	0.47
(2,4516)	1:171:A:LYS:HB3	1:171:A:LYS:H	6	0.47
(2,4302)	1:145:A:VAL:HB	1:145:A:VAL:HG21	2	0.47
(2,4030)	1:126:A:GLU:HG3	1:127:A:ILE:H	4	0.47
(2,3986)	1:119:A:PRO:HB2	1:119:A:PRO:HA	3	0.47
(2,3095)	1:159:A:PHE:H	1:110:A:ASP:HA	2	0.47
(2,3042)	1:130:A:PHE:H	1:136:A:ILE:HG22	9	0.47
(2,2950)	1:162:A:GLN:HG2	1:165:A:ALA:H	8	0.47
(2,2705)	1:171:A:LYS:HB3	1:171:A:LYS:H	6	0.47
(2,2287)	1:130:A:PHE:HB2	1:131:A:PHE:H	4	0.47
(2,1781)	1:164:A:ILE:HG13	1:167:A:LYS:H	5	0.47
(2,1574)	1:155:A:ALA:H	1:154:A:GLU:HB2	2	0.47
(2,920)	1:173:A:LYS:HG2	1:173:A:LYS:HA	6	0.47
(2,915)	1:171:A:LYS:HB3	1:171:A:LYS:H	9	0.47
(2,129)	1:155:A:ALA:HB2	1:154:A:GLU:H	8	0.47
(2,63)	1:95:A:TRP:HB2	1:96:A:VAL:HG21	5	0.47
(2,4)	1:164:A:ILE:HD11	1:161:A:SER:HB3	4	0.47
(1,3081)	1:118:A:LEU:H	1:118:A:LEU:HD12	10	0.47
(1,2994)	1:150:A:ARG:H	1:143:A:LEU:HD22	4	0.47
(1,2968)	1:148:A:GLN:H	1:143:A:LEU:HD22	7	0.47
(1,2932)	1:141:A:ILE:HA	1:140:A:GLY:H	8	0.47
(1,2908)	1:165:A:ALA:HA	1:113:A:VAL:HG23	9	0.47
(1,2821)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	3	0.47
(1,2820)	1:143:A:LEU:HG	1:143:A:LEU:HD23	8	0.47
(1,2820)	1:143:A:LEU:HG	1:143:A:LEU:HD23	9	0.47
(1,2515)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	3	0.47
(1,2210)	1:143:A:LEU:HG	1:143:A:LEU:HD23	3	0.47
(1,1961)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	2	0.47
(1,1961)	1:141:A:ILE:HG13	1:140:A:GLY:HA2	6	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1868)	1:113:A:VAL:HG12	1:113:A:VAL:HB	1	0.47
(1,1784)	1:189:A:ALA:H	1:186:A:SER:HA	8	0.47
(1,1658)	1:143:A:LEU:HD23	1:123:A:SER:HA	8	0.47
(1,1563)	1:166:A:GLU:HG3	1:168:A:ALA:H	7	0.47
(1,1462)	1:175:A:ARG:HD2	1:178:A:HIS:HA	7	0.47
(1,1451)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	4	0.47
(1,1446)	1:108:A:ALA:HA	1:109:A:ASN:H	10	0.47
(1,1338)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	2	0.47
(1,1338)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	4	0.47
(1,1338)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.47
(1,1188)	1:165:A:ALA:H	1:110:A:ASP:HB3	5	0.47
(1,1083)	1:175:A:ARG:HB3	1:176:A:ILE:HD12	4	0.47
(1,988)	1:190:A:GLU:HG2	1:186:A:SER:HA	4	0.47
(1,845)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	8	0.47
(1,809)	1:169:A:LEU:HB2	1:169:A:LEU:HA	8	0.47
(1,809)	1:154:A:GLU:HG2	1:154:A:GLU:HA	9	0.47
(1,764)	1:166:A:GLU:HG3	1:168:A:ALA:H	7	0.47
(1,643)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	5	0.47
(1,368)	1:169:A:LEU:HD21	1:167:A:LYS:H	7	0.47
(1,224)	1:116:A:ARG:HD3	1:116:A:ARG:HA	2	0.47
(1,224)	1:116:A:ARG:HD2	1:116:A:ARG:HA	8	0.47
(1,33)	1:137:A:VAL:HG22	1:139:A:ASN:H	8	0.47
(1,12)	1:164:A:ILE:HD11	1:164:A:ILE:HB	9	0.47
(3,101)	1:126:A:GLU:HB2	1:123:A:SER:HB3	8	0.46
(2,8131)	1:163:A:GLU:HG3	1:163:A:GLU:H	2	0.46
(2,7360)	1:187:A:SER:HB3	1:189:A:ALA:H	9	0.46
(2,7340)	1:169:A:LEU:HB2	1:166:A:GLU:HA	1	0.46
(2,7105)	1:166:A:GLU:HB3	1:167:A:LYS:H	6	0.46
(2,7105)	1:166:A:GLU:HB3	1:167:A:LYS:H	9	0.46
(2,7042)	1:154:A:GLU:H	1:154:A:GLU:HB3	3	0.46
(2,7042)	1:154:A:GLU:H	1:154:A:GLU:HB3	4	0.46
(2,7042)	1:154:A:GLU:H	1:154:A:GLU:HB3	9	0.46
(2,6587)	1:93:A:MET:HB2	1:164:A:ILE:HG12	10	0.46
(2,6144)	1:148:A:GLN:HB2	1:149:A:GLY:H	9	0.46
(2,5807)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	4	0.46
(2,5400)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	9	0.46
(2,4670)	1:187:A:SER:HB3	1:188:A:ARG:H	6	0.46
(2,3986)	1:119:A:PRO:HB2	1:119:A:PRO:HA	7	0.46
(2,3986)	1:119:A:PRO:HB2	1:119:A:PRO:HA	10	0.46
(2,3691)	1:156:A:PHE:HB2	1:191:A:VAL:H	3	0.46
(2,3647)	1:191:A:VAL:HG13	1:193:A:THR:H	1	0.46
(2,3383)	1:154:A:GLU:HB3	1:154:A:GLU:H	1	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3383)	1:154:A:GLU:HB3	1:154:A:GLU:H	7	0.46
(2,3054)	1:167:A:LYS:HB3	1:168:A:ALA:H	2	0.46
(2,2982)	1:190:A:GLU:HG3	1:186:A:SER:HA	4	0.46
(2,2981)	1:158:A:GLN:HG3	1:112:A:PHE:HA	2	0.46
(2,2219)	1:126:A:GLU:HG3	1:127:A:ILE:H	4	0.46
(2,1887)	1:156:A:PHE:HB2	1:191:A:VAL:H	10	0.46
(2,1404)	1:114:A:ARG:H	1:113:A:VAL:HG13	9	0.46
(2,816)	1:161:A:SER:HB2	1:162:A:GLN:H	2	0.46
(2,95)	1:159:A:PHE:HB2	1:135:A:GLU:H	8	0.46
(2,63)	1:95:A:TRP:HB2	1:96:A:VAL:HG21	3	0.46
(2,2)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	9	0.46
(1,3081)	1:118:A:LEU:H	1:118:A:LEU:HD12	3	0.46
(1,3006)	1:117:A:GLY:H	1:118:A:LEU:HD12	6	0.46
(1,2846)	1:173:A:LYS:HA	1:172:A:HIS:H	4	0.46
(1,2846)	1:173:A:LYS:HA	1:172:A:HIS:H	6	0.46
(1,2846)	1:173:A:LYS:HA	1:172:A:HIS:H	10	0.46
(1,2820)	1:143:A:LEU:HG	1:143:A:LEU:HD23	3	0.46
(1,2706)	1:166:A:GLU:HA	1:159:A:PHE:HB2	7	0.46
(1,2515)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	6	0.46
(1,2515)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	9	0.46
(1,2493)	1:96:A:VAL:HG23	1:96:A:VAL:HB	4	0.46
(1,2493)	1:96:A:VAL:HG21	1:96:A:VAL:HB	7	0.46
(1,2379)	1:150:A:ARG:H	1:143:A:LEU:HD21	1	0.46
(1,2238)	1:173:A:LYS:HA	1:172:A:HIS:H	4	0.46
(1,2238)	1:173:A:LYS:HA	1:172:A:HIS:H	6	0.46
(1,2238)	1:173:A:LYS:HA	1:172:A:HIS:H	10	0.46
(1,1992)	1:158:A:GLN:HG2	1:161:A:SER:H	1	0.46
(1,1770)	1:108:A:ALA:H	1:109:A:ASN:HA	3	0.46
(1,1451)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	2	0.46
(1,1446)	1:92:A:ALA:HA	1:93:A:MET:H	4	0.46
(1,1338)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.46
(1,1338)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.46
(1,1338)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	5	0.46
(1,1338)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.46
(1,1338)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	8	0.46
(1,1338)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	9	0.46
(1,1338)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.46
(1,1069)	1:168:A:ALA:HB2	1:167:A:LYS:H	4	0.46
(1,1069)	1:168:A:ALA:HB1	1:167:A:LYS:H	7	0.46
(1,988)	1:190:A:GLU:HG3	1:186:A:SER:HA	7	0.46
(1,988)	1:190:A:GLU:HG3	1:186:A:SER:HA	10	0.46
(1,927)	1:164:A:ILE:HA	1:91:A:ASN:HB3	4	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,845)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	10	0.46
(1,837)	1:92:A:ALA:HA	1:93:A:MET:H	7	0.46
(1,837)	1:108:A:ALA:HA	1:109:A:ASN:H	9	0.46
(1,783)	1:130:A:PHE:HB3	1:132:A:SER:H	5	0.46
(1,732)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.46
(1,732)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	2	0.46
(1,732)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.46
(1,732)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	4	0.46
(1,732)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	5	0.46
(1,732)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.46
(1,732)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	8	0.46
(1,732)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	9	0.46
(1,732)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.46
(1,681)	1:134:A:LEU:HD13	1:133:A:GLY:H	3	0.46
(1,395)	1:135:A:GLU:HB3	1:135:A:GLU:HA	6	0.46
(1,368)	1:169:A:LEU:HD21	1:167:A:LYS:H	10	0.46
(1,224)	1:116:A:ARG:HD2	1:116:A:ARG:HA	4	0.46
(1,97)	1:105:A:PRO:HB2	1:105:A:PRO:HA	4	0.46
(1,97)	1:119:A:PRO:HB2	1:119:A:PRO:HA	5	0.46
(1,95)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	2	0.46
(1,95)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	4	0.46
(1,95)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.46
(1,54)	1:166:A:GLU:HB3	1:168:A:ALA:H	1	0.46
(1,33)	1:137:A:VAL:HG22	1:139:A:ASN:H	6	0.46
(1,33)	1:137:A:VAL:HG22	1:139:A:ASN:H	10	0.46
(1,12)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	2	0.46
(1,12)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	3	0.46
(1,12)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	7	0.46
(4,7)	1:116:A:ARG:H	1:182:A:GLU:O	4	0.45
(4,7)	1:116:A:ARG:H	1:182:A:GLU:O	7	0.45
(4,7)	1:116:A:ARG:H	1:182:A:GLU:O	10	0.45
(2,8701)	1:110:A:ASP:HB3	1:110:A:ASP:H	10	0.45
(2,8568)	1:139:A:ASN:H	1:158:A:GLN:HB2	7	0.45
(2,7280)	1:160:A:ALA:HB3	1:159:A:PHE:HB2	5	0.45
(2,7104)	1:166:A:GLU:HB3	1:166:A:GLU:H	5	0.45
(2,7042)	1:154:A:GLU:H	1:154:A:GLU:HB3	8	0.45
(2,6609)	1:95:A:TRP:HA	1:164:A:ILE:HG13	3	0.45
(2,6609)	1:95:A:TRP:HA	1:164:A:ILE:HG13	7	0.45
(2,6609)	1:95:A:TRP:HA	1:164:A:ILE:HG13	8	0.45
(2,6587)	1:93:A:MET:HB2	1:164:A:ILE:HG12	2	0.45
(2,6558)	1:192:A:ARG:HD2	1:192:A:ARG:HB2	3	0.45
(2,6345)	1:171:A:LYS:HB3	1:171:A:LYS:H	9	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5798)	1:119:A:PRO:HB2	1:119:A:PRO:HA	4	0.45
(2,5525)	1:142:A:THR:HG21	1:141:A:ILE:HG21	4	0.45
(2,5499)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	8	0.45
(2,5086)	1:132:A:SER:HB2	1:133:A:GLY:H	4	0.45
(2,4732)	1:192:A:ARG:HD3	1:192:A:ARG:HB2	3	0.45
(2,4276)	1:144:A:PRO:HB2	1:144:A:PRO:HA	9	0.45
(2,3986)	1:119:A:PRO:HB2	1:119:A:PRO:HA	2	0.45
(2,3986)	1:119:A:PRO:HB2	1:119:A:PRO:HA	5	0.45
(2,3986)	1:119:A:PRO:HB2	1:119:A:PRO:HA	8	0.45
(2,3054)	1:167:A:LYS:HB3	1:168:A:ALA:H	4	0.45
(2,2984)	1:188:A:ARG:HD2	1:108:A:ALA:H	2	0.45
(2,2924)	1:192:A:ARG:HD3	1:192:A:ARG:HB2	3	0.45
(2,2090)	1:110:A:ASP:HB2	1:110:A:ASP:HA	9	0.45
(2,2051)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	6	0.45
(2,1292)	1:111:A:GLY:HA3	1:159:A:PHE:H	6	0.45
(2,915)	1:171:A:LYS:HB3	1:171:A:LYS:H	1	0.45
(2,272)	1:105:A:PRO:HD3	1:104:A:SER:HB3	3	0.45
(2,129)	1:155:A:ALA:HB2	1:154:A:GLU:H	4	0.45
(2,9)	1:181:A:ILE:HG12	1:175:A:ARG:HD2	8	0.45
(1,3081)	1:118:A:LEU:H	1:118:A:LEU:HD12	2	0.45
(1,3081)	1:118:A:LEU:H	1:118:A:LEU:HD12	5	0.45
(1,2932)	1:174:A:GLU:HA	1:181:A:ILE:H	9	0.45
(1,2738)	1:143:A:LEU:HG	1:141:A:ILE:HG21	10	0.45
(1,2493)	1:96:A:VAL:HG21	1:96:A:VAL:HB	1	0.45
(1,2478)	1:181:A:ILE:HG12	1:175:A:ARG:HD2	3	0.45
(1,2415)	1:165:A:ALA:H	1:110:A:ASP:HB3	4	0.45
(1,2399)	1:189:A:ALA:H	1:186:A:SER:HA	6	0.45
(1,2298)	1:168:A:ALA:HB2	1:167:A:LYS:H	9	0.45
(1,1919)	1:166:A:GLU:HB3	1:167:A:LYS:HA	3	0.45
(1,1919)	1:166:A:GLU:HB3	1:167:A:LYS:HA	10	0.45
(1,1881)	1:127:A:ILE:HG21	1:127:A:ILE:HB	1	0.45
(1,1877)	1:96:A:VAL:HG21	1:96:A:VAL:HB	1	0.45
(1,1770)	1:108:A:ALA:H	1:109:A:ASN:HA	10	0.45
(1,1524)	1:93:A:MET:HB2	1:93:A:MET:HG2	8	0.45
(1,1446)	1:92:A:ALA:HA	1:93:A:MET:H	1	0.45
(1,1446)	1:92:A:ALA:HA	1:93:A:MET:H	3	0.45
(1,1446)	1:108:A:ALA:HA	1:109:A:ASN:H	6	0.45
(1,1418)	1:169:A:LEU:HA	1:169:A:LEU:HD11	1	0.45
(1,1175)	1:106:A:ASP:H	1:105:A:PRO:HD3	4	0.45
(1,1173)	1:189:A:ALA:H	1:186:A:SER:HA	1	0.45
(1,1067)	1:165:A:ALA:HA	1:113:A:VAL:HG23	10	0.45
(1,837)	1:92:A:ALA:HA	1:93:A:MET:H	5	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,809)	1:169:A:LEU:HB2	1:169:A:LEU:HA	7	0.45
(1,783)	1:130:A:PHE:HB3	1:132:A:SER:H	7	0.45
(1,764)	1:166:A:GLU:HG3	1:168:A:ALA:H	2	0.45
(1,732)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.45
(1,648)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	2	0.45
(1,648)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	3	0.45
(1,648)	1:164:A:ILE:HD11	1:164:A:ILE:HB	9	0.45
(1,522)	1:100:A:THR:HG22	1:98:A:LYS:H	3	0.45
(1,395)	1:135:A:GLU:HB3	1:135:A:GLU:HA	4	0.45
(1,395)	1:135:A:GLU:HB3	1:135:A:GLU:HA	7	0.45
(1,97)	1:105:A:PRO:HB2	1:105:A:PRO:HA	8	0.45
(1,97)	1:119:A:PRO:HB2	1:119:A:PRO:HA	9	0.45
(1,95)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.45
(1,95)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.45
(1,95)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	5	0.45
(1,95)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.45
(1,95)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	8	0.45
(1,95)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	9	0.45
(1,95)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.45
(1,19)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	3	0.45
(1,12)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	1	0.45
(1,12)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	6	0.45
(1,12)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	8	0.45
(4,7)	1:116:A:ARG:H	1:182:A:GLU:O	9	0.44
(2,9034)	1:187:A:SER:HB3	1:188:A:ARG:H	3	0.44
(2,8217)	1:171:A:LYS:HB3	1:171:A:LYS:H	3	0.44
(2,8217)	1:171:A:LYS:HB3	1:171:A:LYS:H	5	0.44
(2,8217)	1:171:A:LYS:HB3	1:171:A:LYS:H	8	0.44
(2,7105)	1:166:A:GLU:HB3	1:167:A:LYS:H	4	0.44
(2,7104)	1:166:A:GLU:HB3	1:166:A:GLU:H	2	0.44
(2,6609)	1:95:A:TRP:HA	1:164:A:ILE:HG13	9	0.44
(2,5637)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	1	0.44
(2,4777)	1:111:A:GLY:HA3	1:109:A:ASN:H	8	0.44
(2,4521)	1:173:A:LYS:HG2	1:173:A:LYS:HA	6	0.44
(2,3986)	1:119:A:PRO:HB2	1:119:A:PRO:HA	1	0.44
(2,3906)	1:111:A:GLY:HA3	1:112:A:PHE:H	10	0.44
(2,3218)	1:114:A:ARG:HG3	1:115:A:LEU:H	4	0.44
(2,3056)	1:168:A:ALA:H	1:169:A:LEU:HB2	1	0.44
(2,3050)	1:159:A:PHE:HA	1:135:A:GLU:H	6	0.44
(2,2950)	1:162:A:GLN:HG2	1:165:A:ALA:H	6	0.44
(2,2657)	1:166:A:GLU:HB2	1:166:A:GLU:HA	4	0.44
(2,2657)	1:166:A:GLU:HB2	1:166:A:GLU:HA	6	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2657)	1:166:A:GLU:HB2	1:166:A:GLU:HA	9	0.44
(2,2051)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	8	0.44
(2,1807)	1:113:A:VAL:HG13	1:113:A:VAL:HB	3	0.44
(2,1807)	1:113:A:VAL:HG13	1:113:A:VAL:HB	4	0.44
(2,1807)	1:113:A:VAL:HG13	1:113:A:VAL:HB	5	0.44
(2,1639)	1:166:A:GLU:HB3	1:167:A:LYS:H	6	0.44
(2,1639)	1:166:A:GLU:HB3	1:167:A:LYS:H	9	0.44
(2,1575)	1:154:A:GLU:HB3	1:154:A:GLU:H	10	0.44
(2,1574)	1:155:A:ALA:H	1:154:A:GLU:HB2	1	0.44
(2,915)	1:171:A:LYS:HB3	1:171:A:LYS:H	2	0.44
(2,264)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	6	0.44
(2,63)	1:95:A:TRP:HB2	1:96:A:VAL:HG21	7	0.44
(2,22)	1:113:A:VAL:HG12	1:112:A:PHE:H	7	0.44
(1,2933)	1:136:A:ILE:HA	1:159:A:PHE:HB2	6	0.44
(1,2932)	1:141:A:ILE:HA	1:140:A:GLY:H	2	0.44
(1,2846)	1:173:A:LYS:HA	1:172:A:HIS:H	8	0.44
(1,2585)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	9	0.44
(1,2510)	1:134:A:LEU:HD13	1:136:A:ILE:HB	7	0.44
(1,2493)	1:96:A:VAL:HG21	1:96:A:VAL:HB	2	0.44
(1,2493)	1:96:A:VAL:HG21	1:96:A:VAL:HB	3	0.44
(1,2493)	1:96:A:VAL:HG21	1:96:A:VAL:HB	5	0.44
(1,2493)	1:96:A:VAL:HG21	1:96:A:VAL:HB	6	0.44
(1,2493)	1:96:A:VAL:HG21	1:96:A:VAL:HB	8	0.44
(1,2493)	1:96:A:VAL:HG21	1:96:A:VAL:HB	10	0.44
(1,2238)	1:173:A:LYS:HA	1:172:A:HIS:H	8	0.44
(1,2211)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	1	0.44
(1,2211)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	4	0.44
(1,2210)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	4	0.44
(1,2210)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	7	0.44
(1,2031)	1:169:A:LEU:HA	1:169:A:LEU:HD11	3	0.44
(1,1961)	1:179:A:ARG:HB3	1:119:A:PRO:HD2	1	0.44
(1,1919)	1:166:A:GLU:HB3	1:167:A:LYS:HA	6	0.44
(1,1903)	1:134:A:LEU:HD13	1:136:A:ILE:HB	7	0.44
(1,1881)	1:127:A:ILE:HG21	1:127:A:ILE:HB	5	0.44
(1,1877)	1:96:A:VAL:HG21	1:96:A:VAL:HB	5	0.44
(1,1696)	1:175:A:ARG:HB3	1:176:A:ILE:HD11	5	0.44
(1,1681)	1:168:A:ALA:HB3	1:167:A:LYS:H	1	0.44
(1,1563)	1:166:A:GLU:HG3	1:168:A:ALA:H	2	0.44
(1,1524)	1:93:A:MET:HB2	1:135:A:GLU:HB3	4	0.44
(1,1451)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	8	0.44
(1,1446)	1:92:A:ALA:HA	1:93:A:MET:H	2	0.44
(1,1446)	1:92:A:ALA:HA	1:93:A:MET:H	8	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1288)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	4	0.44
(1,1284)	1:134:A:LEU:HD13	1:136:A:ILE:HB	7	0.44
(1,935)	1:110:A:ASP:HB3	1:188:A:ARG:HG2	6	0.44
(1,783)	1:130:A:PHE:HB3	1:132:A:SER:H	10	0.44
(1,678)	1:134:A:LEU:HD13	1:136:A:ILE:HB	7	0.44
(1,657)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	3	0.44
(1,648)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	7	0.44
(1,648)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	8	0.44
(1,643)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	7	0.44
(1,395)	1:135:A:GLU:HB3	1:135:A:GLU:HA	10	0.44
(1,364)	1:96:A:VAL:HG12	1:93:A:MET:HG2	7	0.44
(1,316)	1:98:A:LYS:HB3	1:100:A:THR:HG23	9	0.44
(1,295)	1:164:A:ILE:HD12	1:166:A:GLU:HB2	3	0.44
(1,97)	1:105:A:PRO:HB2	1:105:A:PRO:HA	2	0.44
(1,97)	1:119:A:PRO:HB2	1:119:A:PRO:HA	6	0.44
(1,40)	1:134:A:LEU:HD13	1:136:A:ILE:HB	7	0.44
(1,33)	1:137:A:VAL:HG22	1:139:A:ASN:H	1	0.44
(1,12)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	10	0.44
(4,11)	1:118:A:LEU:H	1:152:A:THR:O	6	0.43
(3,102)	1:158:A:GLN:HG3	1:112:A:PHE:HA	3	0.43
(2,8796)	1:132:A:SER:HB2	1:133:A:GLY:H	2	0.43
(2,8172)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	7	0.43
(2,7998)	1:145:A:VAL:HB	1:145:A:VAL:HG21	2	0.43
(2,7678)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	2	0.43
(2,7508)	1:98:A:LYS:HG2	1:98:A:LYS:HE3	1	0.43
(2,7042)	1:154:A:GLU:H	1:154:A:GLU:HB3	1	0.43
(2,7042)	1:154:A:GLU:H	1:154:A:GLU:HB3	7	0.43
(2,6609)	1:95:A:TRP:HA	1:164:A:ILE:HG13	10	0.43
(2,6587)	1:93:A:MET:HB2	1:164:A:ILE:HG12	1	0.43
(2,6345)	1:171:A:LYS:HB3	1:171:A:LYS:H	1	0.43
(2,5400)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	2	0.43
(2,4470)	1:166:A:GLU:HG2	1:166:A:GLU:HA	2	0.43
(2,4295)	1:144:A:PRO:HD2	1:143:A:LEU:HG	9	0.43
(2,4098)	1:130:A:PHE:HB2	1:131:A:PHE:H	4	0.43
(2,3986)	1:119:A:PRO:HB2	1:119:A:PRO:HA	6	0.43
(2,3986)	1:119:A:PRO:HB2	1:119:A:PRO:HA	9	0.43
(2,3906)	1:111:A:GLY:HA3	1:112:A:PHE:H	6	0.43
(2,3647)	1:191:A:VAL:HG13	1:193:A:THR:H	2	0.43
(2,3452)	1:171:A:LYS:H	1:170:A:LYS:HB2	9	0.43
(2,3383)	1:154:A:GLU:HB3	1:154:A:GLU:H	6	0.43
(2,3096)	1:111:A:GLY:HA3	1:159:A:PHE:H	6	0.43
(2,3095)	1:159:A:PHE:H	1:110:A:ASP:HA	4	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3095)	1:159:A:PHE:H	1:110:A:ASP:HA	9	0.43
(2,3054)	1:167:A:LYS:HB3	1:168:A:ALA:H	1	0.43
(2,2969)	1:116:A:ARG:HG2	1:154:A:GLU:HG2	6	0.43
(2,2659)	1:166:A:GLU:HG2	1:166:A:GLU:HA	2	0.43
(2,2051)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	9	0.43
(2,1807)	1:113:A:VAL:HG13	1:113:A:VAL:HB	9	0.43
(2,1575)	1:154:A:GLU:HB3	1:154:A:GLU:H	2	0.43
(2,1575)	1:154:A:GLU:HB3	1:154:A:GLU:H	5	0.43
(2,1256)	1:139:A:ASN:H	1:141:A:ILE:HG22	6	0.43
(2,932)	1:174:A:GLU:HG3	1:175:A:ARG:H	5	0.43
(2,932)	1:174:A:GLU:HG3	1:175:A:ARG:H	9	0.43
(2,307)	1:111:A:GLY:HA3	1:112:A:PHE:H	10	0.43
(2,129)	1:155:A:ALA:HB2	1:154:A:GLU:H	5	0.43
(2,129)	1:155:A:ALA:HB2	1:154:A:GLU:H	9	0.43
(2,5)	1:164:A:ILE:HD13	1:91:A:ASN:HA	8	0.43
(2,2)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	2	0.43
(1,2846)	1:173:A:LYS:HA	1:172:A:HIS:H	3	0.43
(1,2846)	1:173:A:LYS:HA	1:172:A:HIS:H	5	0.43
(1,2823)	1:175:A:ARG:HB3	1:176:A:ILE:H	1	0.43
(1,2821)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	1	0.43
(1,2821)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	2	0.43
(1,2821)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	4	0.43
(1,2820)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	4	0.43
(1,2820)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	7	0.43
(1,2706)	1:143:A:LEU:HA	1:122:A:CYS:HB2	6	0.43
(1,2596)	1:163:A:GLU:HG3	1:163:A:GLU:HA	1	0.43
(1,2585)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	10	0.43
(1,2510)	1:134:A:LEU:HD13	1:136:A:ILE:HB	2	0.43
(1,2510)	1:134:A:LEU:HD13	1:136:A:ILE:HB	4	0.43
(1,2493)	1:96:A:VAL:HG21	1:96:A:VAL:HB	9	0.43
(1,2483)	1:113:A:VAL:HG12	1:113:A:VAL:HB	1	0.43
(1,2432)	1:145:A:VAL:HA	1:151:A:SER:H	5	0.43
(1,2403)	1:96:A:VAL:HB	1:97:A:LEU:H	2	0.43
(1,2296)	1:165:A:ALA:HA	1:113:A:VAL:HG23	9	0.43
(1,2238)	1:173:A:LYS:HA	1:172:A:HIS:H	3	0.43
(1,2238)	1:173:A:LYS:HA	1:172:A:HIS:H	5	0.43
(1,2211)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	2	0.43
(1,2211)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	7	0.43
(1,2210)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	2	0.43
(1,1992)	1:158:A:GLN:HG2	1:161:A:SER:H	3	0.43
(1,1903)	1:134:A:LEU:HD13	1:136:A:ILE:HB	2	0.43
(1,1903)	1:134:A:LEU:HD13	1:136:A:ILE:HB	4	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1788)	1:132:A:SER:H	1:136:A:ILE:HB	10	0.43
(1,1597)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	10	0.43
(1,1451)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	10	0.43
(1,1446)	1:92:A:ALA:HA	1:93:A:MET:H	7	0.43
(1,1446)	1:108:A:ALA:HA	1:109:A:ASN:H	9	0.43
(1,1417)	1:169:A:LEU:HB2	1:169:A:LEU:HA	8	0.43
(1,1417)	1:154:A:GLU:HG2	1:154:A:GLU:HA	9	0.43
(1,1284)	1:134:A:LEU:HD13	1:136:A:ILE:HB	2	0.43
(1,1284)	1:134:A:LEU:HD13	1:136:A:ILE:HB	4	0.43
(1,1262)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	3	0.43
(1,984)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	10	0.43
(1,937)	1:98:A:LYS:HB3	1:100:A:THR:HG23	9	0.43
(1,809)	1:154:A:GLU:HG2	1:154:A:GLU:HA	10	0.43
(1,783)	1:130:A:PHE:HB3	1:132:A:SER:H	6	0.43
(1,783)	1:130:A:PHE:HB3	1:132:A:SER:H	8	0.43
(1,678)	1:134:A:LEU:HD13	1:136:A:ILE:HB	2	0.43
(1,678)	1:134:A:LEU:HD13	1:136:A:ILE:HB	4	0.43
(1,648)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	1	0.43
(1,648)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	6	0.43
(1,614)	1:108:A:ALA:H	1:106:A:ASP:HB3	2	0.43
(1,614)	1:108:A:ALA:H	1:106:A:ASP:HB3	3	0.43
(1,614)	1:108:A:ALA:H	1:106:A:ASP:HB3	7	0.43
(1,459)	1:168:A:ALA:HB3	1:167:A:LYS:H	1	0.43
(1,447)	1:154:A:GLU:HG2	1:118:A:LEU:HD23	2	0.43
(1,395)	1:135:A:GLU:HB3	1:135:A:GLU:HA	1	0.43
(1,395)	1:135:A:GLU:HB3	1:135:A:GLU:HA	2	0.43
(1,395)	1:135:A:GLU:HB3	1:135:A:GLU:HA	8	0.43
(1,395)	1:135:A:GLU:HB3	1:135:A:GLU:HA	9	0.43
(1,368)	1:169:A:LEU:HD21	1:167:A:LYS:H	8	0.43
(1,366)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	10	0.43
(1,251)	1:188:A:ARG:HD3	1:191:A:VAL:HG22	6	0.43
(1,153)	1:130:A:PHE:HB3	1:132:A:SER:H	9	0.43
(1,102)	1:181:A:ILE:HB	1:181:A:ILE:HA	8	0.43
(1,97)	1:105:A:PRO:HB2	1:105:A:PRO:HA	7	0.43
(1,40)	1:134:A:LEU:HD13	1:136:A:ILE:HB	2	0.43
(1,40)	1:134:A:LEU:HD13	1:136:A:ILE:HB	4	0.43
(1,33)	1:137:A:VAL:HG22	1:139:A:ASN:H	2	0.43
(1,12)	1:164:A:ILE:HD11	1:164:A:ILE:HB	4	0.43
(4,7)	1:116:A:ARG:H	1:182:A:GLU:O	2	0.42
(2,9082)	1:150:A:ARG:HG2	1:151:A:SER:H	2	0.42
(2,8172)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	2	0.42
(2,8035)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	6	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7678)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	1	0.42
(2,7678)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	3	0.42
(2,7669)	1:119:A:PRO:HB2	1:119:A:PRO:HA	4	0.42
(2,7514)	1:100:A:THR:HA	1:99:A:HIS:HB2	9	0.42
(2,7408)	1:155:A:ALA:HB2	1:154:A:GLU:H	6	0.42
(2,7360)	1:187:A:SER:HB3	1:189:A:ALA:H	8	0.42
(2,7320)	1:191:A:VAL:HG13	1:137:A:VAL:HG13	5	0.42
(2,7104)	1:166:A:GLU:HB3	1:166:A:GLU:H	7	0.42
(2,6706)	1:139:A:ASN:H	1:158:A:GLN:HB2	7	0.42
(2,6699)	1:168:A:ALA:H	1:167:A:LYS:HB3	7	0.42
(2,6609)	1:95:A:TRP:HA	1:164:A:ILE:HG13	6	0.42
(2,6592)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	1	0.42
(2,6558)	1:192:A:ARG:HD2	1:192:A:ARG:HB2	6	0.42
(2,6345)	1:171:A:LYS:HB3	1:171:A:LYS:H	2	0.42
(2,5525)	1:142:A:THR:HG22	1:141:A:ILE:HG21	5	0.42
(2,5451)	1:191:A:VAL:HG13	1:137:A:VAL:HG13	5	0.42
(2,5438)	1:191:A:VAL:HG22	1:186:A:SER:HB2	1	0.42
(2,4997)	1:110:A:ASP:HB3	1:110:A:ASP:H	2	0.42
(2,4899)	1:111:A:GLY:HA3	1:159:A:PHE:H	6	0.42
(2,4470)	1:166:A:GLU:HG2	1:166:A:GLU:HA	7	0.42
(2,3726)	1:155:A:ALA:HB2	1:154:A:GLU:H	6	0.42
(2,3616)	1:113:A:VAL:HG13	1:113:A:VAL:HB	8	0.42
(2,3605)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	10	0.42
(2,3218)	1:114:A:ARG:HG3	1:115:A:LEU:H	6	0.42
(2,3202)	1:112:A:PHE:H	1:112:A:PHE:HB3	7	0.42
(2,3095)	1:159:A:PHE:H	1:110:A:ASP:HA	1	0.42
(2,3095)	1:159:A:PHE:H	1:110:A:ASP:HA	8	0.42
(2,2992)	1:161:A:SER:H	1:159:A:PHE:HB2	5	0.42
(2,2950)	1:162:A:GLN:HG2	1:165:A:ALA:H	7	0.42
(2,2710)	1:173:A:LYS:HG2	1:173:A:LYS:HA	10	0.42
(2,2659)	1:166:A:GLU:HG2	1:166:A:GLU:HA	7	0.42
(2,2177)	1:119:A:PRO:HB2	1:119:A:PRO:HA	3	0.42
(2,2177)	1:119:A:PRO:HB2	1:119:A:PRO:HA	7	0.42
(2,2177)	1:119:A:PRO:HB2	1:119:A:PRO:HA	10	0.42
(2,2051)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	3	0.42
(2,1909)	1:142:A:THR:HG21	1:141:A:ILE:HG21	2	0.42
(2,1807)	1:113:A:VAL:HG13	1:113:A:VAL:HB	2	0.42
(2,1807)	1:113:A:VAL:HG13	1:113:A:VAL:HB	7	0.42
(2,1807)	1:113:A:VAL:HG13	1:113:A:VAL:HB	10	0.42
(2,1795)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	10	0.42
(2,1781)	1:164:A:ILE:HG13	1:167:A:LYS:H	10	0.42
(2,1639)	1:166:A:GLU:HB3	1:167:A:LYS:H	4	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1575)	1:154:A:GLU:HB3	1:154:A:GLU:H	3	0.42
(2,1575)	1:154:A:GLU:HB3	1:154:A:GLU:H	4	0.42
(2,1575)	1:154:A:GLU:HB3	1:154:A:GLU:H	9	0.42
(2,1404)	1:114:A:ARG:H	1:113:A:VAL:HG12	6	0.42
(2,1256)	1:139:A:ASN:H	1:141:A:ILE:HG22	8	0.42
(2,1130)	1:192:A:ARG:HD3	1:192:A:ARG:HB2	3	0.42
(2,868)	1:166:A:GLU:HB2	1:166:A:GLU:HA	6	0.42
(2,816)	1:161:A:SER:HB2	1:162:A:GLN:H	1	0.42
(2,307)	1:111:A:GLY:HA3	1:112:A:PHE:H	6	0.42
(2,264)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	8	0.42
(2,54)	1:191:A:VAL:HG13	1:137:A:VAL:HG13	5	0.42
(2,47)	1:191:A:VAL:HG13	1:192:A:ARG:HA	9	0.42
(1,3081)	1:118:A:LEU:H	1:118:A:LEU:HD12	9	0.42
(1,2846)	1:173:A:LYS:HA	1:172:A:HIS:H	2	0.42
(1,2821)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	7	0.42
(1,2820)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	2	0.42
(1,2738)	1:143:A:LEU:HG	1:141:A:ILE:HG21	4	0.42
(1,2738)	1:143:A:LEU:HG	1:141:A:ILE:HG21	7	0.42
(1,2596)	1:163:A:GLU:HG3	1:163:A:GLU:HA	10	0.42
(1,2585)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	4	0.42
(1,2585)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	5	0.42
(1,2585)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	7	0.42
(1,2515)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	8	0.42
(1,2510)	1:134:A:LEU:HD13	1:136:A:ILE:HB	6	0.42
(1,2432)	1:145:A:VAL:HA	1:151:A:SER:H	7	0.42
(1,2403)	1:96:A:VAL:HB	1:97:A:LEU:H	9	0.42
(1,2403)	1:97:A:LEU:H	1:163:A:GLU:HB2	10	0.42
(1,2379)	1:150:A:ARG:H	1:143:A:LEU:HD22	4	0.42
(1,2319)	1:141:A:ILE:HA	1:140:A:GLY:H	8	0.42
(1,2238)	1:173:A:LYS:HA	1:172:A:HIS:H	2	0.42
(1,2134)	1:97:A:LEU:HD12	1:163:A:GLU:HB3	6	0.42
(1,1976)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	9	0.42
(1,1976)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	10	0.42
(1,1919)	1:162:A:GLN:HB2	1:163:A:GLU:HA	1	0.42
(1,1903)	1:134:A:LEU:HD13	1:136:A:ILE:HB	6	0.42
(1,1788)	1:132:A:SER:H	1:136:A:ILE:HB	5	0.42
(1,1788)	1:132:A:SER:H	1:136:A:ILE:HB	6	0.42
(1,1597)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	6	0.42
(1,1597)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	8	0.42
(1,1524)	1:93:A:MET:HB2	1:93:A:MET:HG2	2	0.42
(1,1446)	1:92:A:ALA:HA	1:93:A:MET:H	5	0.42
(1,1284)	1:134:A:LEU:HD13	1:136:A:ILE:HB	6	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1069)	1:168:A:ALA:HB2	1:167:A:LYS:H	2	0.42
(1,984)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	8	0.42
(1,848)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	4	0.42
(1,809)	1:154:A:GLU:HG2	1:154:A:GLU:HA	4	0.42
(1,783)	1:130:A:PHE:HB3	1:132:A:SER:H	2	0.42
(1,678)	1:134:A:LEU:HD13	1:136:A:ILE:HB	6	0.42
(1,657)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	4	0.42
(1,657)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	8	0.42
(1,648)	1:164:A:ILE:HD11	1:164:A:ILE:HB	4	0.42
(1,648)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	10	0.42
(1,447)	1:154:A:GLU:HG2	1:118:A:LEU:HD23	10	0.42
(1,417)	1:107:A:THR:HB	1:110:A:ASP:HB3	1	0.42
(1,395)	1:135:A:GLU:HB3	1:135:A:GLU:HA	3	0.42
(1,395)	1:135:A:GLU:HB3	1:135:A:GLU:HA	5	0.42
(1,366)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	6	0.42
(1,366)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	8	0.42
(1,224)	1:116:A:ARG:HD2	1:116:A:ARG:HA	5	0.42
(1,102)	1:96:A:VAL:HB	1:96:A:VAL:HA	1	0.42
(1,102)	1:181:A:ILE:HB	1:181:A:ILE:HA	3	0.42
(1,97)	1:105:A:PRO:HB2	1:105:A:PRO:HA	1	0.42
(1,40)	1:134:A:LEU:HD13	1:136:A:ILE:HB	6	0.42
(1,25)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	3	0.42
(1,19)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	4	0.42
(1,19)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	8	0.42
(3,537)	1:118:A:LEU:HA	1:183:A:ILE:HG12	9	0.41
(2,8796)	1:132:A:SER:HB2	1:133:A:GLY:H	5	0.41
(2,8484)	1:190:A:GLU:HG3	1:186:A:SER:HA	4	0.41
(2,7678)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	6	0.41
(2,7280)	1:160:A:ALA:HB3	1:159:A:PHE:HB2	4	0.41
(2,7273)	1:164:A:ILE:HD13	1:135:A:GLU:H	9	0.41
(2,6701)	1:168:A:ALA:H	1:169:A:LEU:HB2	1	0.41
(2,6609)	1:95:A:TRP:HA	1:164:A:ILE:HG13	2	0.41
(2,6592)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	9	0.41
(2,5499)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	10	0.41
(2,4997)	1:110:A:ASP:HB3	1:110:A:ASP:H	1	0.41
(2,4997)	1:110:A:ASP:HB3	1:110:A:ASP:H	5	0.41
(2,4797)	1:161:A:SER:H	1:159:A:PHE:HB2	5	0.41
(2,4777)	1:111:A:GLY:HA3	1:109:A:ASN:H	9	0.41
(2,3906)	1:111:A:GLY:HA3	1:112:A:PHE:H	8	0.41
(2,3824)	1:98:A:LYS:HG3	1:98:A:LYS:HE3	2	0.41
(2,3691)	1:156:A:PHE:HB2	1:191:A:VAL:H	5	0.41
(2,3607)	1:164:A:ILE:HD13	1:91:A:ASN:HA	5	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3056)	1:168:A:ALA:H	1:169:A:LEU:HB2	2	0.41
(2,3054)	1:167:A:LYS:HB3	1:168:A:ALA:H	9	0.41
(2,3050)	1:159:A:PHE:HA	1:135:A:GLU:H	10	0.41
(2,2466)	1:144:A:PRO:HB2	1:144:A:PRO:HA	4	0.41
(2,2177)	1:119:A:PRO:HB2	1:119:A:PRO:HA	2	0.41
(2,1781)	1:164:A:ILE:HG13	1:167:A:LYS:H	3	0.41
(2,1575)	1:154:A:GLU:HB3	1:154:A:GLU:H	8	0.41
(2,1256)	1:139:A:ASN:H	1:141:A:ILE:HG22	4	0.41
(2,868)	1:166:A:GLU:HB2	1:166:A:GLU:HA	4	0.41
(2,868)	1:166:A:GLU:HB2	1:166:A:GLU:HA	9	0.41
(2,264)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	9	0.41
(2,47)	1:191:A:VAL:HG13	1:192:A:ARG:HA	7	0.41
(1,3081)	1:118:A:LEU:H	1:118:A:LEU:HD12	4	0.41
(1,3020)	1:132:A:SER:H	1:136:A:ILE:HB	9	0.41
(1,3013)	1:189:A:ALA:H	1:186:A:SER:HA	3	0.41
(1,2510)	1:134:A:LEU:HD13	1:136:A:ILE:HB	1	0.41
(1,2510)	1:134:A:LEU:HD13	1:136:A:ILE:HB	8	0.41
(1,2495)	1:127:A:ILE:HG21	1:127:A:ILE:HB	1	0.41
(1,2415)	1:165:A:ALA:H	1:110:A:ASP:HB3	2	0.41
(1,2403)	1:96:A:VAL:HB	1:97:A:LEU:H	6	0.41
(1,2101)	1:166:A:GLU:HA	1:159:A:PHE:HB2	7	0.41
(1,1992)	1:158:A:GLN:HG2	1:161:A:SER:H	9	0.41
(1,1976)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	4	0.41
(1,1976)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	5	0.41
(1,1976)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	7	0.41
(1,1903)	1:134:A:LEU:HD13	1:136:A:ILE:HB	1	0.41
(1,1903)	1:134:A:LEU:HD13	1:136:A:ILE:HB	8	0.41
(1,1788)	1:132:A:SER:H	1:136:A:ILE:HB	7	0.41
(1,1770)	1:108:A:ALA:H	1:109:A:ASN:HA	6	0.41
(1,1696)	1:175:A:ARG:HB3	1:176:A:ILE:HD11	10	0.41
(1,1681)	1:168:A:ALA:HB2	1:167:A:LYS:H	4	0.41
(1,1681)	1:168:A:ALA:HB1	1:167:A:LYS:H	7	0.41
(1,1597)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	5	0.41
(1,1524)	1:93:A:MET:HB2	1:135:A:GLU:HB3	9	0.41
(1,1417)	1:169:A:LEU:HB2	1:169:A:LEU:HA	7	0.41
(1,1370)	1:166:A:GLU:HG3	1:169:A:LEU:HD13	10	0.41
(1,1284)	1:134:A:LEU:HD13	1:136:A:ILE:HB	1	0.41
(1,1284)	1:134:A:LEU:HD13	1:136:A:ILE:HB	8	0.41
(1,1266)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	3	0.41
(1,1262)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	8	0.41
(1,1234)	1:97:A:LEU:H	1:99:A:HIS:HA	1	0.41
(1,1175)	1:106:A:ASP:H	1:105:A:PRO:HD3	3	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1091)	1:174:A:GLU:HA	1:181:A:ILE:H	9	0.41
(1,1057)	1:133:A:GLY:HA3	1:134:A:LEU:HG	6	0.41
(1,1057)	1:133:A:GLY:HA3	1:134:A:LEU:HG	10	0.41
(1,988)	1:190:A:GLU:HG3	1:186:A:SER:HA	8	0.41
(1,984)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	5	0.41
(1,984)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	6	0.41
(1,854)	1:156:A:PHE:HB3	1:142:A:THR:HB	8	0.41
(1,848)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	2	0.41
(1,845)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	7	0.41
(1,809)	1:154:A:GLU:HG2	1:154:A:GLU:HA	5	0.41
(1,783)	1:130:A:PHE:HB3	1:132:A:SER:H	4	0.41
(1,678)	1:134:A:LEU:HD13	1:136:A:ILE:HB	1	0.41
(1,678)	1:134:A:LEU:HD13	1:136:A:ILE:HB	8	0.41
(1,662)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	3	0.41
(1,657)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	2	0.41
(1,413)	1:162:A:GLN:HG3	1:110:A:ASP:HA	2	0.41
(1,366)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	5	0.41
(1,217)	1:115:A:LEU:HA	1:114:A:ARG:HG2	6	0.41
(1,205)	1:142:A:THR:HA	1:142:A:THR:HB	4	0.41
(1,205)	1:142:A:THR:HA	1:142:A:THR:HB	6	0.41
(1,205)	1:142:A:THR:HA	1:142:A:THR:HB	8	0.41
(1,46)	1:167:A:LYS:HG2	1:134:A:LEU:HD11	4	0.41
(1,40)	1:134:A:LEU:HD13	1:136:A:ILE:HB	1	0.41
(1,40)	1:134:A:LEU:HD13	1:136:A:ILE:HB	8	0.41
(1,33)	1:137:A:VAL:HG22	1:139:A:ASN:H	9	0.41
(1,19)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	2	0.41
(1,19)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	7	0.41
(1,19)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	9	0.41
(4,11)	1:118:A:LEU:H	1:152:A:THR:O	3	0.4
(3,537)	1:118:A:LEU:HA	1:183:A:ILE:HG12	10	0.4
(3,102)	1:158:A:GLN:HG3	1:112:A:PHE:HA	2	0.4
(2,8472)	1:111:A:GLY:HA3	1:109:A:ASN:H	6	0.4
(2,8217)	1:171:A:LYS:HB3	1:171:A:LYS:H	9	0.4
(2,7701)	1:124:A:LYS:HA	1:124:A:LYS:HB2	5	0.4
(2,7701)	1:124:A:LYS:HA	1:124:A:LYS:HB2	6	0.4
(2,7701)	1:124:A:LYS:HA	1:124:A:LYS:HB2	8	0.4
(2,7678)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	8	0.4
(2,7230)	1:150:A:ARG:HG2	1:151:A:SER:H	6	0.4
(2,6858)	1:114:A:ARG:H	1:113:A:VAL:HG13	9	0.4
(2,6587)	1:93:A:MET:HB2	1:164:A:ILE:HG12	3	0.4
(2,6587)	1:93:A:MET:HB2	1:164:A:ILE:HG12	6	0.4
(2,5183)	1:154:A:GLU:HB3	1:154:A:GLU:H	2	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5183)	1:154:A:GLU:HB3	1:154:A:GLU:H	10	0.4
(2,4997)	1:110:A:ASP:HB3	1:110:A:ASP:H	4	0.4
(2,3906)	1:111:A:GLY:HA3	1:112:A:PHE:H	9	0.4
(2,3607)	1:164:A:ILE:HD13	1:91:A:ASN:HA	2	0.4
(2,3607)	1:164:A:ILE:HD13	1:91:A:ASN:HA	10	0.4
(2,2177)	1:119:A:PRO:HB2	1:119:A:PRO:HA	5	0.4
(2,2177)	1:119:A:PRO:HB2	1:119:A:PRO:HA	8	0.4
(2,1887)	1:156:A:PHE:HB2	1:191:A:VAL:H	3	0.4
(2,1781)	1:164:A:ILE:HG13	1:167:A:LYS:H	8	0.4
(2,1757)	1:173:A:LYS:HB2	1:172:A:HIS:H	6	0.4
(2,1574)	1:155:A:ALA:H	1:154:A:GLU:HB2	3	0.4
(2,1404)	1:114:A:ARG:H	1:113:A:VAL:HG13	7	0.4
(2,1283)	1:105:A:PRO:HB3	1:106:A:ASP:H	5	0.4
(2,932)	1:174:A:GLU:HG3	1:175:A:ARG:H	4	0.4
(2,648)	1:144:A:PRO:HD2	1:143:A:LEU:HA	9	0.4
(2,307)	1:111:A:GLY:HA3	1:112:A:PHE:H	8	0.4
(2,264)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	3	0.4
(2,9)	1:181:A:ILE:HG12	1:175:A:ARG:HD2	10	0.4
(1,3081)	1:118:A:LEU:H	1:118:A:LEU:HD12	1	0.4
(1,3081)	1:118:A:LEU:H	1:118:A:LEU:HD12	6	0.4
(1,2974)	1:100:A:THR:HG23	1:98:A:LYS:H	2	0.4
(1,2908)	1:94:A:ASP:HA	1:164:A:ILE:HD13	6	0.4
(1,2738)	1:143:A:LEU:HG	1:141:A:ILE:HG21	2	0.4
(1,2596)	1:163:A:GLU:HG3	1:163:A:GLU:HA	2	0.4
(1,2585)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	6	0.4
(1,2510)	1:134:A:LEU:HD13	1:136:A:ILE:HB	9	0.4
(1,2510)	1:134:A:LEU:HD13	1:136:A:ILE:HB	10	0.4
(1,2495)	1:127:A:ILE:HG21	1:127:A:ILE:HB	5	0.4
(1,2403)	1:96:A:VAL:HB	1:97:A:LEU:H	3	0.4
(1,2319)	1:174:A:GLU:HA	1:181:A:ILE:H	9	0.4
(1,2298)	1:168:A:ALA:HB3	1:167:A:LYS:H	1	0.4
(1,2210)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	1	0.4
(1,2140)	1:93:A:MET:HB2	1:135:A:GLU:HB3	7	0.4
(1,2076)	1:159:A:PHE:HB2	1:166:A:GLU:H	1	0.4
(1,1992)	1:158:A:GLN:HG2	1:161:A:SER:H	6	0.4
(1,1919)	1:166:A:GLU:HB3	1:167:A:LYS:HA	9	0.4
(1,1903)	1:134:A:LEU:HD13	1:136:A:ILE:HB	9	0.4
(1,1903)	1:134:A:LEU:HD13	1:136:A:ILE:HB	10	0.4
(1,1798)	1:165:A:ALA:H	1:110:A:ASP:HB3	8	0.4
(1,1658)	1:143:A:LEU:HD23	1:123:A:SER:HA	7	0.4
(1,1524)	1:93:A:MET:HB2	1:93:A:MET:HG2	10	0.4
(1,1284)	1:134:A:LEU:HD13	1:136:A:ILE:HB	9	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1284)	1:134:A:LEU:HD13	1:136:A:ILE:HB	10	0.4
(1,1262)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	2	0.4
(1,1262)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	4	0.4
(1,1251)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	5	0.4
(1,1188)	1:165:A:ALA:H	1:110:A:ASP:HB3	10	0.4
(1,1173)	1:189:A:ALA:H	1:186:A:SER:HA	2	0.4
(1,1173)	1:189:A:ALA:H	1:186:A:SER:HA	5	0.4
(1,1091)	1:141:A:ILE:HA	1:140:A:GLY:H	2	0.4
(1,1088)	1:134:A:LEU:HD21	1:131:A:PHE:HB3	3	0.4
(1,988)	1:190:A:GLU:HG3	1:186:A:SER:HA	2	0.4
(1,914)	1:93:A:MET:HB2	1:93:A:MET:HG2	8	0.4
(1,848)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	8	0.4
(1,809)	1:154:A:GLU:HG2	1:154:A:GLU:HA	6	0.4
(1,783)	1:130:A:PHE:HB3	1:132:A:SER:H	1	0.4
(1,678)	1:134:A:LEU:HD13	1:136:A:ILE:HB	9	0.4
(1,678)	1:134:A:LEU:HD13	1:136:A:ILE:HB	10	0.4
(1,657)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	7	0.4
(1,657)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	9	0.4
(1,643)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	2	0.4
(1,504)	1:166:A:GLU:H	1:169:A:LEU:HD13	5	0.4
(1,459)	1:168:A:ALA:HB2	1:167:A:LYS:H	4	0.4
(1,459)	1:168:A:ALA:HB1	1:167:A:LYS:H	7	0.4
(1,377)	1:123:A:SER:HB3	1:181:A:ILE:HD11	1	0.4
(1,205)	1:142:A:THR:HA	1:142:A:THR:HB	5	0.4
(1,205)	1:142:A:THR:HA	1:142:A:THR:HB	7	0.4
(1,205)	1:142:A:THR:HA	1:142:A:THR:HB	9	0.4
(1,205)	1:142:A:THR:HA	1:142:A:THR:HB	10	0.4
(1,102)	1:181:A:ILE:HB	1:181:A:ILE:HA	5	0.4
(1,46)	1:167:A:LYS:HG2	1:134:A:LEU:HD11	3	0.4
(1,40)	1:134:A:LEU:HD13	1:136:A:ILE:HB	9	0.4
(1,40)	1:134:A:LEU:HD13	1:136:A:ILE:HB	10	0.4
(1,25)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	8	0.4
(2,8796)	1:132:A:SER:HB2	1:133:A:GLY:H	4	0.39
(2,8035)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	4	0.39
(2,8035)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	8	0.39
(2,7678)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	9	0.39
(2,7410)	1:98:A:LYS:HB3	1:100:A:THR:HG22	3	0.39
(2,7042)	1:154:A:GLU:H	1:154:A:GLU:HB3	6	0.39
(2,6629)	1:161:A:SER:H	1:159:A:PHE:HB2	5	0.39
(2,6592)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	2	0.39
(2,6587)	1:93:A:MET:HB2	1:164:A:ILE:HG12	9	0.39
(2,6559)	1:192:A:ARG:HD3	1:192:A:ARG:HB2	3	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5413)	1:160:A:ALA:HB3	1:159:A:PHE:HB2	5	0.39
(2,5404)	1:164:A:ILE:HD13	1:135:A:GLU:H	9	0.39
(2,5402)	1:164:A:ILE:HD13	1:91:A:ASN:HA	8	0.39
(2,5183)	1:154:A:GLU:HB3	1:154:A:GLU:H	5	0.39
(2,5009)	1:114:A:ARG:H	1:113:A:VAL:HG13	9	0.39
(2,4872)	1:157:A:VAL:HG21	1:158:A:GLN:H	7	0.39
(2,4872)	1:157:A:VAL:HG21	1:158:A:GLN:H	9	0.39
(2,3717)	1:142:A:THR:HG21	1:141:A:ILE:HG21	2	0.39
(2,3607)	1:164:A:ILE:HD13	1:91:A:ASN:HA	7	0.39
(2,3286)	1:132:A:SER:HB2	1:133:A:GLY:H	10	0.39
(2,3095)	1:159:A:PHE:H	1:110:A:ASP:HA	5	0.39
(2,2657)	1:166:A:GLU:HB2	1:166:A:GLU:HA	2	0.39
(2,2466)	1:144:A:PRO:HB2	1:144:A:PRO:HA	7	0.39
(2,2466)	1:144:A:PRO:HB2	1:144:A:PRO:HA	10	0.39
(2,2177)	1:119:A:PRO:HB2	1:119:A:PRO:HA	1	0.39
(2,2177)	1:119:A:PRO:HB2	1:119:A:PRO:HA	9	0.39
(2,2117)	1:115:A:LEU:HA	1:115:A:LEU:HB2	2	0.39
(2,2117)	1:115:A:LEU:HA	1:115:A:LEU:HB2	3	0.39
(2,2117)	1:115:A:LEU:HA	1:115:A:LEU:HB2	4	0.39
(2,2117)	1:115:A:LEU:HA	1:115:A:LEU:HB2	5	0.39
(2,2117)	1:115:A:LEU:HA	1:115:A:LEU:HB2	6	0.39
(2,2117)	1:115:A:LEU:HA	1:115:A:LEU:HB2	9	0.39
(2,1781)	1:164:A:ILE:HG13	1:167:A:LYS:H	6	0.39
(2,1638)	1:166:A:GLU:HB3	1:166:A:GLU:H	8	0.39
(2,1575)	1:154:A:GLU:HB3	1:154:A:GLU:H	1	0.39
(2,1575)	1:154:A:GLU:HB3	1:154:A:GLU:H	7	0.39
(2,1574)	1:155:A:ALA:H	1:154:A:GLU:HB2	9	0.39
(2,1256)	1:139:A:ASN:H	1:141:A:ILE:HG22	2	0.39
(2,1197)	1:145:A:VAL:H	1:143:A:LEU:HD11	4	0.39
(2,920)	1:173:A:LYS:HG2	1:173:A:LYS:HA	10	0.39
(2,424)	1:126:A:GLU:HG2	1:126:A:GLU:HB2	7	0.39
(2,307)	1:111:A:GLY:HA3	1:112:A:PHE:H	9	0.39
(2,272)	1:105:A:PRO:HD3	1:104:A:SER:HB3	6	0.39
(2,129)	1:155:A:ALA:HB2	1:154:A:GLU:H	1	0.39
(2,106)	1:93:A:MET:HB2	1:93:A:MET:HG2	1	0.39
(2,100)	1:181:A:ILE:HG21	1:174:A:GLU:HA	3	0.39
(2,47)	1:191:A:VAL:HG13	1:192:A:ARG:HA	6	0.39
(2,47)	1:191:A:VAL:HG13	1:192:A:ARG:HA	8	0.39
(2,47)	1:191:A:VAL:HG12	1:192:A:ARG:HA	10	0.39
(1,2820)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	1	0.39
(1,2773)	1:98:A:LYS:HB3	1:100:A:THR:HG23	9	0.39
(1,2596)	1:163:A:GLU:HG3	1:163:A:GLU:HA	5	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2596)	1:163:A:GLU:HG3	1:163:A:GLU:HA	9	0.39
(1,2510)	1:134:A:LEU:HD13	1:136:A:ILE:HB	3	0.39
(1,2415)	1:165:A:ALA:H	1:110:A:ASP:HB3	1	0.39
(1,2319)	1:141:A:ILE:HA	1:140:A:GLY:H	2	0.39
(1,1976)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	6	0.39
(1,1949)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.39
(1,1949)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	2	0.39
(1,1949)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	4	0.39
(1,1949)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	5	0.39
(1,1949)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.39
(1,1949)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	8	0.39
(1,1949)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	9	0.39
(1,1949)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.39
(1,1903)	1:134:A:LEU:HD13	1:136:A:ILE:HB	3	0.39
(1,1706)	1:174:A:GLU:HA	1:181:A:ILE:H	3	0.39
(1,1597)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	3	0.39
(1,1597)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	9	0.39
(1,1524)	1:93:A:MET:HB2	1:93:A:MET:HG2	6	0.39
(1,1455)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	4	0.39
(1,1284)	1:134:A:LEU:HD13	1:136:A:ILE:HB	3	0.39
(1,1266)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	8	0.39
(1,1262)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	7	0.39
(1,1262)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	9	0.39
(1,995)	1:123:A:SER:HB3	1:181:A:ILE:HD11	3	0.39
(1,984)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	3	0.39
(1,984)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	9	0.39
(1,914)	1:93:A:MET:HB2	1:135:A:GLU:HB3	4	0.39
(1,848)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	10	0.39
(1,820)	1:98:A:LYS:HA	1:100:A:THR:HG23	1	0.39
(1,820)	1:98:A:LYS:HA	1:100:A:THR:HG22	4	0.39
(1,691)	1:166:A:GLU:HB2	1:168:A:ALA:H	10	0.39
(1,681)	1:134:A:LEU:HD13	1:133:A:GLY:H	9	0.39
(1,678)	1:134:A:LEU:HD13	1:136:A:ILE:HB	3	0.39
(1,662)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	4	0.39
(1,662)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	8	0.39
(1,515)	1:112:A:PHE:H	1:169:A:LEU:HB2	3	0.39
(1,417)	1:107:A:THR:HB	1:110:A:ASP:HB3	4	0.39
(1,376)	1:174:A:GLU:HB2	1:181:A:ILE:HD13	8	0.39
(1,366)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	3	0.39
(1,366)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	9	0.39
(1,205)	1:142:A:THR:HA	1:142:A:THR:HB	1	0.39
(1,205)	1:142:A:THR:HA	1:142:A:THR:HB	2	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,178)	1:169:A:LEU:HB2	1:169:A:LEU:HA	8	0.39
(1,178)	1:154:A:GLU:HG2	1:154:A:GLU:HA	9	0.39
(1,102)	1:181:A:ILE:HB	1:181:A:ILE:HA	4	0.39
(1,40)	1:134:A:LEU:HD13	1:136:A:ILE:HB	3	0.39
(1,25)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	2	0.39
(1,25)	1:176:A:ILE:HG22	1:176:A:ILE:HG12	4	0.39
(1,25)	1:176:A:ILE:HG21	1:176:A:ILE:HG12	5	0.39
(1,12)	1:164:A:ILE:HD11	1:164:A:ILE:HB	5	0.39
(3,537)	1:118:A:LEU:HA	1:183:A:ILE:HG12	5	0.38
(3,537)	1:118:A:LEU:HA	1:183:A:ILE:HG12	6	0.38
(3,537)	1:118:A:LEU:HA	1:183:A:ILE:HG12	8	0.38
(2,8577)	1:157:A:VAL:HG21	1:158:A:GLN:H	7	0.38
(2,8577)	1:157:A:VAL:HG21	1:158:A:GLN:H	9	0.38
(2,8562)	1:168:A:ALA:H	1:169:A:LEU:HB2	1	0.38
(2,8217)	1:171:A:LYS:HB3	1:171:A:LYS:H	1	0.38
(2,8172)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	5	0.38
(2,8035)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	2	0.38
(2,8035)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	7	0.38
(2,8035)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	10	0.38
(2,8017)	1:148:A:GLN:HB2	1:149:A:GLY:H	3	0.38
(2,7992)	1:144:A:PRO:HD2	1:143:A:LEU:HG	9	0.38
(2,7408)	1:155:A:ALA:HB2	1:154:A:GLU:H	3	0.38
(2,6942)	1:132:A:SER:HB2	1:133:A:GLY:H	9	0.38
(2,6715)	1:157:A:VAL:HG21	1:158:A:GLN:H	7	0.38
(2,6715)	1:157:A:VAL:HG21	1:158:A:GLN:H	9	0.38
(2,6701)	1:168:A:ALA:H	1:169:A:LEU:HB2	2	0.38
(2,6587)	1:93:A:MET:HB2	1:164:A:ILE:HG12	7	0.38
(2,6587)	1:93:A:MET:HB2	1:164:A:ILE:HG12	8	0.38
(2,6162)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	6	0.38
(2,5808)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	9	0.38
(2,5798)	1:119:A:PRO:HB2	1:119:A:PRO:HA	3	0.38
(2,5798)	1:119:A:PRO:HB2	1:119:A:PRO:HA	7	0.38
(2,5798)	1:119:A:PRO:HB2	1:119:A:PRO:HA	10	0.38
(2,5498)	1:116:A:ARG:HD2	1:116:A:ARG:HA	1	0.38
(2,5183)	1:154:A:GLU:HB3	1:154:A:GLU:H	3	0.38
(2,5183)	1:154:A:GLU:HB3	1:154:A:GLU:H	4	0.38
(2,5183)	1:154:A:GLU:HB3	1:154:A:GLU:H	9	0.38
(2,4872)	1:157:A:VAL:HG21	1:158:A:GLN:H	1	0.38
(2,4872)	1:157:A:VAL:HG21	1:158:A:GLN:H	2	0.38
(2,4872)	1:157:A:VAL:HG21	1:158:A:GLN:H	3	0.38
(2,4872)	1:157:A:VAL:HG21	1:158:A:GLN:H	8	0.38
(2,4872)	1:157:A:VAL:HG21	1:158:A:GLN:H	10	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4470)	1:166:A:GLU:HG2	1:166:A:GLU:HA	5	0.38
(2,3726)	1:155:A:ALA:HB2	1:154:A:GLU:H	3	0.38
(2,3679)	1:187:A:SER:HB3	1:189:A:ALA:H	5	0.38
(2,3616)	1:113:A:VAL:HG13	1:113:A:VAL:HB	3	0.38
(2,3616)	1:113:A:VAL:HG13	1:113:A:VAL:HB	4	0.38
(2,3616)	1:113:A:VAL:HG13	1:113:A:VAL:HB	5	0.38
(2,3444)	1:166:A:GLU:HB3	1:167:A:LYS:H	6	0.38
(2,3444)	1:166:A:GLU:HB3	1:167:A:LYS:H	9	0.38
(2,3054)	1:167:A:LYS:HB3	1:168:A:ALA:H	3	0.38
(2,2981)	1:158:A:GLN:HG3	1:112:A:PHE:HA	9	0.38
(2,2659)	1:166:A:GLU:HG2	1:166:A:GLU:HA	5	0.38
(2,2466)	1:144:A:PRO:HB2	1:144:A:PRO:HA	1	0.38
(2,2466)	1:144:A:PRO:HB2	1:144:A:PRO:HA	2	0.38
(2,2466)	1:144:A:PRO:HB2	1:144:A:PRO:HA	8	0.38
(2,2177)	1:119:A:PRO:HB2	1:119:A:PRO:HA	6	0.38
(2,2117)	1:115:A:LEU:HA	1:115:A:LEU:HB2	1	0.38
(2,2117)	1:115:A:LEU:HA	1:115:A:LEU:HB2	7	0.38
(2,2117)	1:115:A:LEU:HA	1:115:A:LEU:HB2	8	0.38
(2,2117)	1:115:A:LEU:HA	1:115:A:LEU:HB2	10	0.38
(2,1781)	1:164:A:ILE:HG13	1:167:A:LYS:H	2	0.38
(2,1781)	1:164:A:ILE:HG13	1:167:A:LYS:H	9	0.38
(2,1749)	1:175:A:ARG:H	1:178:A:HIS:HA	3	0.38
(2,1667)	1:176:A:ILE:H	1:176:A:ILE:HD12	2	0.38
(2,1638)	1:166:A:GLU:HB3	1:166:A:GLU:H	3	0.38
(2,1574)	1:155:A:ALA:H	1:154:A:GLU:HB2	4	0.38
(2,1256)	1:139:A:ASN:H	1:141:A:ILE:HG22	7	0.38
(2,903)	1:169:A:LEU:HB2	1:169:A:LEU:HD13	2	0.38
(2,721)	1:148:A:GLN:HB2	1:149:A:GLY:H	5	0.38
(2,521)	1:134:A:LEU:HD11	1:134:A:LEU:HA	3	0.38
(2,106)	1:93:A:MET:HB2	1:93:A:MET:HG2	8	0.38
(2,63)	1:95:A:TRP:HB2	1:96:A:VAL:HG21	4	0.38
(2,53)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	5	0.38
(2,22)	1:113:A:VAL:HG12	1:112:A:PHE:H	2	0.38
(2,16)	1:113:A:VAL:HG12	1:113:A:VAL:HB	1	0.38
(2,9)	1:181:A:ILE:HG12	1:175:A:ARG:HD2	2	0.38
(1,3050)	1:145:A:VAL:HA	1:151:A:SER:H	5	0.38
(1,3025)	1:122:A:CYS:H	1:118:A:LEU:HD22	2	0.38
(1,2910)	1:168:A:ALA:HB1	1:167:A:LYS:H	6	0.38
(1,2738)	1:143:A:LEU:HG	1:141:A:ILE:HG21	3	0.38
(1,2675)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	4	0.38
(1,2636)	1:169:A:LEU:HA	1:169:A:LEU:HD11	3	0.38
(1,2510)	1:134:A:LEU:HD13	1:136:A:ILE:HB	5	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2101)	1:143:A:LEU:HA	1:122:A:CYS:HB2	6	0.38
(1,1992)	1:158:A:GLN:HG2	1:161:A:SER:H	2	0.38
(1,1949)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.38
(1,1949)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.38
(1,1919)	1:166:A:GLU:HB3	1:167:A:LYS:HA	8	0.38
(1,1918)	1:163:A:GLU:HB2	1:164:A:ILE:HG12	5	0.38
(1,1903)	1:134:A:LEU:HD13	1:136:A:ILE:HB	5	0.38
(1,1455)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	2	0.38
(1,1451)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	7	0.38
(1,1417)	1:154:A:GLU:HG2	1:154:A:GLU:HA	4	0.38
(1,1417)	1:154:A:GLU:HG2	1:154:A:GLU:HA	10	0.38
(1,1370)	1:166:A:GLU:HG3	1:169:A:LEU:HD13	1	0.38
(1,1297)	1:166:A:GLU:HB3	1:168:A:ALA:H	1	0.38
(1,1284)	1:134:A:LEU:HD13	1:136:A:ILE:HB	5	0.38
(1,1266)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	2	0.38
(1,1251)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	7	0.38
(1,1067)	1:94:A:ASP:HA	1:164:A:ILE:HD13	8	0.38
(1,927)	1:164:A:ILE:HA	1:91:A:ASN:HB2	5	0.38
(1,914)	1:93:A:MET:HB2	1:93:A:MET:HG2	2	0.38
(1,722)	1:148:A:GLN:HB3	1:147:A:PHE:H	7	0.38
(1,691)	1:166:A:GLU:HB2	1:168:A:ALA:H	8	0.38
(1,678)	1:134:A:LEU:HD13	1:136:A:ILE:HB	5	0.38
(1,662)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	2	0.38
(1,657)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	6	0.38
(1,648)	1:164:A:ILE:HD11	1:164:A:ILE:HB	5	0.38
(1,643)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	10	0.38
(1,614)	1:108:A:ALA:H	1:106:A:ASP:HB3	10	0.38
(1,522)	1:100:A:THR:HG23	1:98:A:LYS:H	6	0.38
(1,417)	1:107:A:THR:HB	1:110:A:ASP:HB3	7	0.38
(1,320)	1:97:A:LEU:HG	1:97:A:LEU:HD13	1	0.38
(1,320)	1:97:A:LEU:HG	1:97:A:LEU:HD13	3	0.38
(1,205)	1:142:A:THR:HA	1:142:A:THR:HB	3	0.38
(1,44)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	5	0.38
(1,40)	1:134:A:LEU:HD13	1:136:A:ILE:HB	5	0.38
(1,25)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	7	0.38
(1,25)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	9	0.38
(1,19)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	6	0.38
(4,11)	1:118:A:LEU:H	1:152:A:THR:O	5	0.37
(2,8577)	1:157:A:VAL:HG21	1:158:A:GLN:H	1	0.37
(2,8577)	1:157:A:VAL:HG21	1:158:A:GLN:H	2	0.37
(2,8577)	1:157:A:VAL:HG21	1:158:A:GLN:H	3	0.37
(2,8577)	1:157:A:VAL:HG21	1:158:A:GLN:H	8	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,8577)	1:157:A:VAL:HG21	1:158:A:GLN:H	10	0.37
(2,8431)	1:192:A:ARG:HD3	1:192:A:ARG:HB2	6	0.37
(2,8238)	1:175:A:ARG:HG2	1:175:A:ARG:HA	1	0.37
(2,8217)	1:171:A:LYS:HB3	1:171:A:LYS:H	2	0.37
(2,7973)	1:144:A:PRO:HB2	1:144:A:PRO:HA	9	0.37
(2,7408)	1:155:A:ALA:HB2	1:154:A:GLU:H	10	0.37
(2,7322)	1:191:A:VAL:HG13	1:190:A:GLU:H	4	0.37
(2,7280)	1:160:A:ALA:HB3	1:159:A:PHE:HB2	1	0.37
(2,7273)	1:164:A:ILE:HD13	1:135:A:GLU:H	2	0.37
(2,6858)	1:114:A:ARG:H	1:113:A:VAL:HG12	6	0.37
(2,6715)	1:157:A:VAL:HG21	1:158:A:GLN:H	1	0.37
(2,6715)	1:157:A:VAL:HG21	1:158:A:GLN:H	2	0.37
(2,6715)	1:157:A:VAL:HG21	1:158:A:GLN:H	3	0.37
(2,6715)	1:157:A:VAL:HG21	1:158:A:GLN:H	8	0.37
(2,6715)	1:157:A:VAL:HG21	1:158:A:GLN:H	10	0.37
(2,6300)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	2	0.37
(2,6300)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	7	0.37
(2,6125)	1:145:A:VAL:HB	1:145:A:VAL:HG21	2	0.37
(2,6105)	1:144:A:PRO:HD3	1:144:A:PRO:HA	9	0.37
(2,6100)	1:144:A:PRO:HB2	1:144:A:PRO:HA	9	0.37
(2,5808)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	5	0.37
(2,5808)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	6	0.37
(2,5808)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	7	0.37
(2,5808)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	8	0.37
(2,5808)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	10	0.37
(2,5525)	1:142:A:THR:HG22	1:141:A:ILE:HG21	10	0.37
(2,5498)	1:116:A:ARG:HD2	1:116:A:ARG:HA	2	0.37
(2,5244)	1:166:A:GLU:HB3	1:167:A:LYS:H	9	0.37
(2,5183)	1:154:A:GLU:HB3	1:154:A:GLU:H	8	0.37
(2,4859)	1:168:A:ALA:H	1:169:A:LEU:HB2	1	0.37
(2,4670)	1:187:A:SER:HB3	1:188:A:ARG:H	3	0.37
(2,4276)	1:144:A:PRO:HB2	1:144:A:PRO:HA	4	0.37
(2,3728)	1:123:A:SER:HB3	1:181:A:ILE:HD11	3	0.37
(2,3726)	1:155:A:ALA:HB2	1:154:A:GLU:H	10	0.37
(2,3707)	1:188:A:ARG:HB2	1:187:A:SER:H	5	0.37
(2,3068)	1:157:A:VAL:HG21	1:158:A:GLN:H	9	0.37
(2,2950)	1:162:A:GLN:HG2	1:165:A:ALA:H	2	0.37
(2,2657)	1:166:A:GLU:HB2	1:166:A:GLU:HA	5	0.37
(2,2657)	1:166:A:GLU:HB2	1:166:A:GLU:HA	7	0.37
(2,2466)	1:144:A:PRO:HB2	1:144:A:PRO:HA	3	0.37
(2,2466)	1:144:A:PRO:HB2	1:144:A:PRO:HA	5	0.37
(2,2466)	1:144:A:PRO:HB2	1:144:A:PRO:HA	6	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1918)	1:155:A:ALA:HB2	1:154:A:GLU:H	6	0.37
(2,1815)	1:176:A:ILE:HG22	1:120:A:PHE:H	3	0.37
(2,1815)	1:176:A:ILE:HG23	1:120:A:PHE:H	5	0.37
(2,1781)	1:164:A:ILE:HG13	1:167:A:LYS:H	4	0.37
(2,1667)	1:176:A:ILE:H	1:176:A:ILE:HD12	3	0.37
(2,1638)	1:166:A:GLU:HB3	1:166:A:GLU:H	10	0.37
(2,1256)	1:139:A:ASN:H	1:141:A:ILE:HG22	10	0.37
(2,1236)	1:130:A:PHE:H	1:136:A:ILE:HG22	10	0.37
(2,932)	1:174:A:GLU:HG3	1:175:A:ARG:H	10	0.37
(2,106)	1:93:A:MET:HB2	1:93:A:MET:HG2	5	0.37
(2,99)	1:188:A:ARG:HD3	1:191:A:VAL:HG22	10	0.37
(1,3050)	1:145:A:VAL:HA	1:151:A:SER:H	7	0.37
(1,2596)	1:163:A:GLU:HG3	1:163:A:GLU:HA	3	0.37
(1,2554)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	2	0.37
(1,2554)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	4	0.37
(1,2554)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	5	0.37
(1,2554)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.37
(1,2554)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	8	0.37
(1,2554)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	9	0.37
(1,2554)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.37
(1,2432)	1:145:A:VAL:HA	1:151:A:SER:H	8	0.37
(1,2405)	1:132:A:SER:H	1:136:A:ILE:HB	4	0.37
(1,2298)	1:168:A:ALA:HB2	1:167:A:LYS:H	4	0.37
(1,1950)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.37
(1,1950)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	2	0.37
(1,1950)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	4	0.37
(1,1950)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	5	0.37
(1,1950)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.37
(1,1950)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	8	0.37
(1,1950)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	9	0.37
(1,1950)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.37
(1,1868)	1:113:A:VAL:HG11	1:113:A:VAL:HB	6	0.37
(1,1681)	1:168:A:ALA:HB2	1:167:A:LYS:H	2	0.37
(1,1455)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	8	0.37
(1,1418)	1:169:A:LEU:HA	1:169:A:LEU:HD11	2	0.37
(1,1417)	1:154:A:GLU:HG2	1:154:A:GLU:HA	5	0.37
(1,1266)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	7	0.37
(1,1266)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	9	0.37
(1,1262)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	6	0.37
(1,1178)	1:132:A:SER:H	1:136:A:ILE:HB	4	0.37
(1,914)	1:93:A:MET:HB2	1:135:A:GLU:HB3	9	0.37
(1,845)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,662)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	7	0.37
(1,662)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	9	0.37
(1,643)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	3	0.37
(1,411)	1:164:A:ILE:HD13	1:135:A:GLU:HA	1	0.37
(1,377)	1:123:A:SER:HB3	1:181:A:ILE:HD11	6	0.37
(1,178)	1:169:A:LEU:HB2	1:169:A:LEU:HA	7	0.37
(1,159)	1:95:A:TRP:HA	1:96:A:VAL:H	5	0.37
(1,153)	1:130:A:PHE:HB3	1:132:A:SER:H	5	0.37
(4,11)	1:118:A:LEU:H	1:152:A:THR:O	7	0.36
(4,11)	1:118:A:LEU:H	1:152:A:THR:O	10	0.36
(2,9082)	1:150:A:ARG:HG2	1:151:A:SER:H	10	0.36
(2,7678)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	7	0.36
(2,7290)	1:96:A:VAL:HG22	1:97:A:LEU:H	6	0.36
(2,6587)	1:93:A:MET:HB2	1:164:A:ILE:HG12	5	0.36
(2,5808)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	1	0.36
(2,5808)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	2	0.36
(2,5808)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	4	0.36
(2,5798)	1:119:A:PRO:HB2	1:119:A:PRO:HA	2	0.36
(2,5798)	1:119:A:PRO:HB2	1:119:A:PRO:HA	5	0.36
(2,5798)	1:119:A:PRO:HB2	1:119:A:PRO:HA	8	0.36
(2,5413)	1:160:A:ALA:HB3	1:159:A:PHE:HB2	4	0.36
(2,5400)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	6	0.36
(2,5244)	1:166:A:GLU:HB3	1:167:A:LYS:H	6	0.36
(2,5009)	1:114:A:ARG:H	1:113:A:VAL:HG12	6	0.36
(2,4521)	1:173:A:LYS:HG2	1:173:A:LYS:HA	10	0.36
(2,3707)	1:188:A:ARG:HB2	1:187:A:SER:H	2	0.36
(2,3707)	1:188:A:ARG:HB2	1:187:A:SER:H	4	0.36
(2,3616)	1:113:A:VAL:HG13	1:113:A:VAL:HB	2	0.36
(2,3616)	1:113:A:VAL:HG13	1:113:A:VAL:HB	7	0.36
(2,3616)	1:113:A:VAL:HG13	1:113:A:VAL:HB	9	0.36
(2,3444)	1:166:A:GLU:HB3	1:167:A:LYS:H	4	0.36
(2,3068)	1:157:A:VAL:HG21	1:158:A:GLN:H	1	0.36
(2,3068)	1:157:A:VAL:HG21	1:158:A:GLN:H	2	0.36
(2,3068)	1:157:A:VAL:HG21	1:158:A:GLN:H	7	0.36
(2,3042)	1:130:A:PHE:H	1:136:A:ILE:HG22	8	0.36
(2,1862)	1:169:A:LEU:HB2	1:166:A:GLU:HA	1	0.36
(2,1806)	1:160:A:ALA:HB2	1:162:A:GLN:H	1	0.36
(2,1404)	1:114:A:ARG:H	1:113:A:VAL:HG12	8	0.36
(2,1256)	1:139:A:ASN:H	1:141:A:ILE:HG22	3	0.36
(2,1069)	1:187:A:SER:HB3	1:188:A:ARG:H	5	0.36
(2,1069)	1:187:A:SER:HB3	1:188:A:ARG:H	7	0.36
(2,1069)	1:187:A:SER:HB3	1:188:A:ARG:H	9	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,932)	1:174:A:GLU:HG3	1:175:A:ARG:H	1	0.36
(2,868)	1:166:A:GLU:HB2	1:166:A:GLU:HA	2	0.36
(2,721)	1:148:A:GLN:HB2	1:149:A:GLY:H	2	0.36
(2,106)	1:93:A:MET:HB2	1:93:A:MET:HG2	2	0.36
(2,100)	1:181:A:ILE:HG21	1:174:A:GLU:HA	1	0.36
(2,100)	1:181:A:ILE:HG21	1:174:A:GLU:HA	8	0.36
(2,2)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	6	0.36
(1,3030)	1:165:A:ALA:H	1:110:A:ASP:HB3	8	0.36
(1,2846)	1:173:A:LYS:HA	1:172:A:HIS:H	7	0.36
(1,2772)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	1	0.36
(1,2675)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	2	0.36
(1,2585)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	2	0.36
(1,2554)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.36
(1,2554)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.36
(1,2554)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.36
(1,2515)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	1	0.36
(1,2515)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	5	0.36
(1,2477)	1:164:A:ILE:HD11	1:164:A:ILE:HB	9	0.36
(1,2415)	1:165:A:ALA:H	1:110:A:ASP:HB3	5	0.36
(1,2298)	1:168:A:ALA:HB1	1:167:A:LYS:H	7	0.36
(1,2238)	1:173:A:LYS:HA	1:172:A:HIS:H	7	0.36
(1,2210)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	5	0.36
(1,1950)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.36
(1,1950)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.36
(1,1784)	1:189:A:ALA:H	1:186:A:SER:HA	1	0.36
(1,1550)	1:98:A:LYS:HB3	1:100:A:THR:HG23	9	0.36
(1,1455)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	10	0.36
(1,1447)	1:115:A:LEU:HA	1:114:A:ARG:HG3	10	0.36
(1,1417)	1:154:A:GLU:HG2	1:154:A:GLU:HA	6	0.36
(1,1410)	1:156:A:PHE:HA	1:141:A:ILE:HA	6	0.36
(1,1286)	1:134:A:LEU:HD13	1:133:A:GLY:H	3	0.36
(1,1159)	1:108:A:ALA:H	1:109:A:ASN:HA	3	0.36
(1,927)	1:164:A:ILE:HA	1:91:A:ASN:HB3	3	0.36
(1,927)	1:164:A:ILE:HA	1:91:A:ASN:HB3	9	0.36
(1,910)	1:141:A:ILE:HG21	1:143:A:LEU:HG	10	0.36
(1,838)	1:115:A:LEU:HA	1:114:A:ARG:HG3	1	0.36
(1,838)	1:115:A:LEU:HA	1:114:A:ARG:HG3	10	0.36
(1,810)	1:169:A:LEU:HA	1:169:A:LEU:HD11	3	0.36
(1,691)	1:166:A:GLU:HB2	1:168:A:ALA:H	3	0.36
(1,681)	1:134:A:LEU:HD13	1:133:A:GLY:H	8	0.36
(1,657)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.36
(1,643)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	4	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:168:A:ALA:HB2	1:167:A:LYS:H	2	0.36
(1,447)	1:154:A:GLU:HG2	1:118:A:LEU:HD23	1	0.36
(1,411)	1:164:A:ILE:HD13	1:93:A:MET:HA	9	0.36
(1,191)	1:98:A:LYS:HA	1:100:A:THR:HG23	5	0.36
(1,191)	1:98:A:LYS:HA	1:100:A:THR:HG23	7	0.36
(1,153)	1:130:A:PHE:HB3	1:132:A:SER:H	7	0.36
(1,54)	1:166:A:GLU:HB2	1:168:A:ALA:H	10	0.36
(1,25)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	6	0.36
(1,19)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.36
(4,7)	1:116:A:ARG:H	1:182:A:GLU:O	3	0.35
(2,8562)	1:168:A:ALA:H	1:169:A:LEU:HB2	2	0.35
(2,7678)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	5	0.35
(2,7669)	1:119:A:PRO:HB2	1:119:A:PRO:HA	3	0.35
(2,7669)	1:119:A:PRO:HB2	1:119:A:PRO:HA	7	0.35
(2,7669)	1:119:A:PRO:HB2	1:119:A:PRO:HA	10	0.35
(2,7608)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	2	0.35
(2,7408)	1:155:A:ALA:HB2	1:154:A:GLU:H	2	0.35
(2,7230)	1:150:A:ARG:HG2	1:151:A:SER:H	8	0.35
(2,6858)	1:114:A:ARG:H	1:113:A:VAL:HG13	7	0.35
(2,6845)	1:110:A:ASP:HB3	1:110:A:ASP:H	2	0.35
(2,6699)	1:168:A:ALA:H	1:167:A:LYS:HB3	2	0.35
(2,6527)	1:190:A:GLU:HG2	1:190:A:GLU:H	4	0.35
(2,6162)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	4	0.35
(2,6162)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	8	0.35
(2,6162)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	10	0.35
(2,6144)	1:148:A:GLN:HB2	1:149:A:GLY:H	5	0.35
(2,5866)	1:127:A:ILE:HG23	1:127:A:ILE:HG12	1	0.35
(2,5808)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	3	0.35
(2,5798)	1:119:A:PRO:HB2	1:119:A:PRO:HA	1	0.35
(2,5798)	1:119:A:PRO:HB2	1:119:A:PRO:HA	9	0.35
(2,5643)	1:100:A:THR:HA	1:99:A:HIS:HB2	9	0.35
(2,5525)	1:142:A:THR:HG22	1:141:A:ILE:HG21	7	0.35
(2,5487)	1:187:A:SER:HB3	1:189:A:ALA:H	9	0.35
(2,5444)	1:191:A:VAL:HG13	1:193:A:THR:H	5	0.35
(2,5404)	1:164:A:ILE:HD13	1:135:A:GLU:H	2	0.35
(2,5235)	1:164:A:ILE:H	1:164:A:ILE:HG21	5	0.35
(2,5183)	1:154:A:GLU:HB3	1:154:A:GLU:H	1	0.35
(2,5183)	1:154:A:GLU:HB3	1:154:A:GLU:H	7	0.35
(2,4872)	1:157:A:VAL:HG21	1:158:A:GLN:H	4	0.35
(2,4872)	1:157:A:VAL:HG21	1:158:A:GLN:H	5	0.35
(2,4733)	1:192:A:ARG:HB2	1:192:A:ARG:H	6	0.35
(2,4276)	1:144:A:PRO:HB2	1:144:A:PRO:HA	7	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4276)	1:144:A:PRO:HB2	1:144:A:PRO:HA	10	0.35
(2,3726)	1:155:A:ALA:HB2	1:154:A:GLU:H	2	0.35
(2,3707)	1:188:A:ARG:HB2	1:187:A:SER:H	3	0.35
(2,3616)	1:113:A:VAL:HG13	1:113:A:VAL:HB	10	0.35
(2,3435)	1:164:A:ILE:H	1:164:A:ILE:HG21	5	0.35
(2,3208)	1:114:A:ARG:H	1:113:A:VAL:HG13	9	0.35
(2,3068)	1:157:A:VAL:HG21	1:158:A:GLN:H	3	0.35
(2,3068)	1:157:A:VAL:HG21	1:158:A:GLN:H	8	0.35
(2,3068)	1:157:A:VAL:HG21	1:158:A:GLN:H	10	0.35
(2,2970)	1:111:A:GLY:HA3	1:109:A:ASN:H	2	0.35
(2,2970)	1:111:A:GLY:HA3	1:109:A:ASN:H	4	0.35
(2,2051)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	10	0.35
(2,1887)	1:156:A:PHE:HB2	1:191:A:VAL:H	5	0.35
(2,1838)	1:191:A:VAL:HG13	1:193:A:THR:H	5	0.35
(2,1781)	1:164:A:ILE:HG13	1:167:A:LYS:H	1	0.35
(2,1749)	1:175:A:ARG:H	1:178:A:HIS:HA	2	0.35
(2,1749)	1:175:A:ARG:H	1:178:A:HIS:HA	8	0.35
(2,1575)	1:154:A:GLU:HB3	1:154:A:GLU:H	6	0.35
(2,1292)	1:111:A:GLY:HA3	1:159:A:PHE:H	10	0.35
(2,1283)	1:105:A:PRO:HB3	1:106:A:ASP:H	6	0.35
(2,1256)	1:139:A:ASN:H	1:141:A:ILE:HG22	5	0.35
(2,868)	1:166:A:GLU:HB2	1:166:A:GLU:HA	7	0.35
(2,106)	1:93:A:MET:HB2	1:93:A:MET:HG2	9	0.35
(2,47)	1:191:A:VAL:HG12	1:192:A:ARG:HA	3	0.35
(2,22)	1:113:A:VAL:HG13	1:112:A:PHE:H	8	0.35
(1,2820)	1:134:A:LEU:HD21	1:134:A:LEU:HB2	5	0.35
(1,2738)	1:143:A:LEU:HG	1:141:A:ILE:HG21	5	0.35
(1,2675)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	8	0.35
(1,2555)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.35
(1,2555)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	2	0.35
(1,2555)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.35
(1,2555)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	4	0.35
(1,2555)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	5	0.35
(1,2555)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.35
(1,2555)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.35
(1,2555)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	8	0.35
(1,2555)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	9	0.35
(1,2555)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.35
(1,2515)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	7	0.35
(1,2477)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	2	0.35
(1,2477)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	3	0.35
(1,2477)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	7	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1976)	1:119:A:PRO:HB2	1:119:A:PRO:HD2	2	0.35
(1,1918)	1:163:A:GLU:HB2	1:96:A:VAL:HG13	3	0.35
(1,1864)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	2	0.35
(1,1864)	1:164:A:ILE:HD11	1:164:A:ILE:HB	9	0.35
(1,1696)	1:175:A:ARG:HB3	1:176:A:ILE:HD11	7	0.35
(1,1658)	1:143:A:LEU:HD23	1:123:A:SER:HA	5	0.35
(1,1597)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	1	0.35
(1,1597)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	4	0.35
(1,1524)	1:93:A:MET:HB2	1:135:A:GLU:HB3	1	0.35
(1,1524)	1:93:A:MET:HB2	1:135:A:GLU:HB3	5	0.35
(1,1462)	1:175:A:ARG:HD2	1:178:A:HIS:HA	4	0.35
(1,1447)	1:115:A:LEU:HA	1:114:A:ARG:HG3	1	0.35
(1,1447)	1:115:A:LEU:HA	1:114:A:ARG:HG3	7	0.35
(1,1345)	1:181:A:ILE:HB	1:181:A:ILE:HA	8	0.35
(1,1266)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	6	0.35
(1,1262)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.35
(1,1159)	1:108:A:ALA:H	1:109:A:ASN:HA	10	0.35
(1,1106)	1:161:A:SER:H	1:110:A:ASP:HB3	4	0.35
(1,994)	1:174:A:GLU:HB2	1:181:A:ILE:HD13	7	0.35
(1,984)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	1	0.35
(1,984)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	4	0.35
(1,914)	1:93:A:MET:HB2	1:93:A:MET:HG2	10	0.35
(1,845)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	1	0.35
(1,838)	1:115:A:LEU:HA	1:114:A:ARG:HG3	7	0.35
(1,803)	1:156:A:PHE:HA	1:141:A:ILE:HA	6	0.35
(1,783)	1:130:A:PHE:HB3	1:132:A:SER:H	3	0.35
(1,691)	1:166:A:GLU:HB2	1:168:A:ALA:H	7	0.35
(1,682)	1:134:A:LEU:HD13	1:134:A:LEU:HB3	5	0.35
(1,662)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	6	0.35
(1,643)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	1	0.35
(1,643)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	9	0.35
(1,614)	1:108:A:ALA:H	1:106:A:ASP:HB3	1	0.35
(1,541)	1:181:A:ILE:H	1:172:A:HIS:HA	10	0.35
(1,411)	1:164:A:ILE:HD13	1:93:A:MET:HA	3	0.35
(1,411)	1:164:A:ILE:HD13	1:135:A:GLU:HA	4	0.35
(1,377)	1:123:A:SER:HB3	1:181:A:ILE:HD11	10	0.35
(1,376)	1:174:A:GLU:HB2	1:181:A:ILE:HD13	6	0.35
(1,366)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	1	0.35
(1,366)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	4	0.35
(1,297)	1:164:A:ILE:HD13	1:93:A:MET:HG3	1	0.35
(1,227)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	10	0.35
(1,179)	1:169:A:LEU:HA	1:169:A:LEU:HD11	3	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,178)	1:154:A:GLU:HG2	1:154:A:GLU:HA	10	0.35
(1,153)	1:130:A:PHE:HB3	1:132:A:SER:H	10	0.35
(1,54)	1:166:A:GLU:HB2	1:168:A:ALA:H	8	0.35
(2,8577)	1:157:A:VAL:HG21	1:158:A:GLN:H	4	0.34
(2,7669)	1:119:A:PRO:HB2	1:119:A:PRO:HA	2	0.34
(2,7608)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	3	0.34
(2,7608)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	10	0.34
(2,7408)	1:155:A:ALA:HB2	1:154:A:GLU:H	7	0.34
(2,7408)	1:155:A:ALA:HB2	1:154:A:GLU:H	8	0.34
(2,7344)	1:109:A:ASN:HA	1:108:A:ALA:HB1	1	0.34
(2,7290)	1:96:A:VAL:HG22	1:97:A:LEU:H	8	0.34
(2,7273)	1:164:A:ILE:HD13	1:135:A:GLU:H	10	0.34
(2,7230)	1:150:A:ARG:HG2	1:151:A:SER:H	7	0.34
(2,6845)	1:110:A:ASP:HB3	1:110:A:ASP:H	1	0.34
(2,6845)	1:110:A:ASP:HB3	1:110:A:ASP:H	5	0.34
(2,6715)	1:157:A:VAL:HG21	1:158:A:GLN:H	4	0.34
(2,6699)	1:168:A:ALA:H	1:167:A:LYS:HB3	4	0.34
(2,6592)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	3	0.34
(2,6592)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	5	0.34
(2,6162)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	2	0.34
(2,6162)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	7	0.34
(2,5866)	1:127:A:ILE:HG23	1:127:A:ILE:HG12	5	0.34
(2,5798)	1:119:A:PRO:HB2	1:119:A:PRO:HA	6	0.34
(2,5473)	1:109:A:ASN:HA	1:108:A:ALA:HB1	1	0.34
(2,5244)	1:166:A:GLU:HB3	1:167:A:LYS:H	4	0.34
(2,5235)	1:164:A:ILE:H	1:164:A:ILE:HG21	10	0.34
(2,5009)	1:114:A:ARG:H	1:113:A:VAL:HG13	7	0.34
(2,4859)	1:168:A:ALA:H	1:169:A:LEU:HB2	2	0.34
(2,4788)	1:158:A:GLN:HG3	1:112:A:PHE:HA	3	0.34
(2,4276)	1:144:A:PRO:HB2	1:144:A:PRO:HA	1	0.34
(2,4276)	1:144:A:PRO:HB2	1:144:A:PRO:HA	2	0.34
(2,4276)	1:144:A:PRO:HB2	1:144:A:PRO:HA	8	0.34
(2,3926)	1:115:A:LEU:HA	1:115:A:LEU:HB2	2	0.34
(2,3926)	1:115:A:LEU:HA	1:115:A:LEU:HB2	3	0.34
(2,3926)	1:115:A:LEU:HA	1:115:A:LEU:HB2	4	0.34
(2,3926)	1:115:A:LEU:HA	1:115:A:LEU:HB2	5	0.34
(2,3926)	1:115:A:LEU:HA	1:115:A:LEU:HB2	6	0.34
(2,3926)	1:115:A:LEU:HA	1:115:A:LEU:HB2	8	0.34
(2,3926)	1:115:A:LEU:HA	1:115:A:LEU:HB2	9	0.34
(2,3926)	1:115:A:LEU:HA	1:115:A:LEU:HB2	10	0.34
(2,3906)	1:111:A:GLY:HA3	1:112:A:PHE:H	3	0.34
(2,3726)	1:155:A:ALA:HB2	1:154:A:GLU:H	7	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3726)	1:155:A:ALA:HB2	1:154:A:GLU:H	8	0.34
(2,3707)	1:188:A:ARG:HB2	1:187:A:SER:H	1	0.34
(2,3707)	1:188:A:ARG:HB2	1:187:A:SER:H	6	0.34
(2,3707)	1:188:A:ARG:HB2	1:187:A:SER:H	10	0.34
(2,3647)	1:191:A:VAL:HG13	1:193:A:THR:H	7	0.34
(2,3435)	1:164:A:ILE:H	1:164:A:ILE:HG21	10	0.34
(2,3042)	1:130:A:PHE:H	1:136:A:ILE:HG22	7	0.34
(2,1901)	1:188:A:ARG:HB2	1:187:A:SER:H	5	0.34
(2,1815)	1:176:A:ILE:HG22	1:120:A:PHE:H	10	0.34
(2,1806)	1:160:A:ALA:HB2	1:162:A:GLN:H	7	0.34
(2,1256)	1:139:A:ASN:H	1:141:A:ILE:HG22	9	0.34
(2,1106)	1:191:A:VAL:HG11	1:191:A:VAL:HA	4	0.34
(2,1106)	1:191:A:VAL:HG11	1:191:A:VAL:HA	10	0.34
(2,1069)	1:187:A:SER:HB3	1:188:A:ARG:H	1	0.34
(2,932)	1:174:A:GLU:HG3	1:175:A:ARG:H	8	0.34
(2,925)	1:173:A:LYS:HG2	1:174:A:GLU:H	4	0.34
(2,868)	1:166:A:GLU:HB2	1:166:A:GLU:HA	5	0.34
(2,307)	1:111:A:GLY:HA3	1:112:A:PHE:H	3	0.34
(2,300)	1:110:A:ASP:HB2	1:110:A:ASP:HA	9	0.34
(2,264)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	10	0.34
(2,120)	1:142:A:THR:HG21	1:141:A:ILE:HG21	2	0.34
(2,95)	1:159:A:PHE:HB2	1:135:A:GLU:H	9	0.34
(2,22)	1:113:A:VAL:HG12	1:112:A:PHE:H	4	0.34
(1,3020)	1:132:A:SER:H	1:136:A:ILE:HB	8	0.34
(1,3003)	1:108:A:ALA:H	1:109:A:ASN:HA	8	0.34
(1,2974)	1:100:A:THR:HG23	1:98:A:LYS:H	5	0.34
(1,2898)	1:144:A:PRO:HD2	1:118:A:LEU:HD22	7	0.34
(1,2675)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	10	0.34
(1,2585)	1:179:A:ARG:HB3	1:119:A:PRO:HD2	1	0.34
(1,2477)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	1	0.34
(1,2477)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	6	0.34
(1,2477)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	8	0.34
(1,2285)	1:144:A:PRO:HD2	1:118:A:LEU:HD22	7	0.34
(1,1919)	1:166:A:GLU:HB3	1:167:A:LYS:HA	4	0.34
(1,1864)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	3	0.34
(1,1864)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	7	0.34
(1,1864)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	8	0.34
(1,1696)	1:175:A:ARG:HB3	1:176:A:ILE:HD12	4	0.34
(1,1668)	1:144:A:PRO:HD2	1:118:A:LEU:HD22	7	0.34
(1,1597)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	2	0.34
(1,1597)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	7	0.34
(1,1462)	1:116:A:ARG:HD2	1:116:A:ARG:HA	6	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1451)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.34
(1,1410)	1:156:A:PHE:HA	1:141:A:ILE:HA	2	0.34
(1,1410)	1:156:A:PHE:HA	1:141:A:ILE:HA	7	0.34
(1,1410)	1:156:A:PHE:HA	1:141:A:ILE:HA	8	0.34
(1,1348)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	2	0.34
(1,1348)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	4	0.34
(1,1348)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.34
(1,1348)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	8	0.34
(1,1348)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.34
(1,1345)	1:96:A:VAL:HB	1:96:A:VAL:HA	1	0.34
(1,1345)	1:181:A:ILE:HB	1:181:A:ILE:HA	3	0.34
(1,1259)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	6	0.34
(1,1251)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	2	0.34
(1,1057)	1:133:A:GLY:HA3	1:134:A:LEU:HG	8	0.34
(1,984)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	2	0.34
(1,982)	1:96:A:VAL:HG12	1:93:A:MET:HG2	4	0.34
(1,914)	1:93:A:MET:HB2	1:93:A:MET:HG2	6	0.34
(1,869)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	9	0.34
(1,845)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	5	0.34
(1,803)	1:156:A:PHE:HA	1:141:A:ILE:HA	7	0.34
(1,614)	1:108:A:ALA:H	1:106:A:ASP:HB3	5	0.34
(1,447)	1:154:A:GLU:HG2	1:118:A:LEU:HD23	9	0.34
(1,444)	1:144:A:PRO:HD2	1:118:A:LEU:HD22	7	0.34
(1,366)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	2	0.34
(1,178)	1:154:A:GLU:HG2	1:154:A:GLU:HA	4	0.34
(1,159)	1:95:A:TRP:HA	1:96:A:VAL:H	4	0.34
(1,153)	1:130:A:PHE:HB3	1:132:A:SER:H	6	0.34
(1,105)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.34
(1,105)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	2	0.34
(1,105)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	4	0.34
(1,105)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	5	0.34
(1,105)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.34
(1,105)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	8	0.34
(1,105)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	9	0.34
(1,105)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.34
(1,25)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.34
(1,8)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	5	0.34
(4,40)	1:168:A:ALA:H	1:164:A:ILE:O	7	0.33
(4,30)	1:157:A:VAL:H	1:113:A:VAL:O	4	0.33
(4,11)	1:118:A:LEU:H	1:152:A:THR:O	8	0.33
(2,8724)	1:114:A:ARG:HG3	1:115:A:LEU:H	8	0.33
(2,8577)	1:157:A:VAL:HG21	1:158:A:GLN:H	5	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7678)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	10	0.33
(2,7669)	1:119:A:PRO:HB2	1:119:A:PRO:HA	5	0.33
(2,7669)	1:119:A:PRO:HB2	1:119:A:PRO:HA	8	0.33
(2,7377)	1:181:A:ILE:HG21	1:174:A:GLU:HA	3	0.33
(2,7290)	1:96:A:VAL:HG22	1:97:A:LEU:H	9	0.33
(2,7044)	1:154:A:GLU:HG2	1:154:A:GLU:H	6	0.33
(2,6845)	1:110:A:ASP:HB3	1:110:A:ASP:H	4	0.33
(2,6740)	1:97:A:LEU:H	1:92:A:ALA:H	5	0.33
(2,6715)	1:157:A:VAL:HG21	1:158:A:GLN:H	5	0.33
(2,6604)	1:111:A:GLY:HA3	1:109:A:ASN:H	7	0.33
(2,6350)	1:173:A:LYS:HG2	1:173:A:LYS:HA	6	0.33
(2,6144)	1:148:A:GLN:HB2	1:149:A:GLY:H	2	0.33
(2,5404)	1:164:A:ILE:HD13	1:135:A:GLU:H	10	0.33
(2,4872)	1:157:A:VAL:HG21	1:158:A:GLN:H	6	0.33
(2,4792)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	4	0.33
(2,4792)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	10	0.33
(2,4768)	1:126:A:GLU:HB2	1:123:A:SER:HB3	8	0.33
(2,4733)	1:192:A:ARG:HB2	1:192:A:ARG:H	5	0.33
(2,4477)	1:166:A:GLU:HG2	1:166:A:GLU:H	1	0.33
(2,4470)	1:166:A:GLU:HG2	1:166:A:GLU:HA	1	0.33
(2,4276)	1:144:A:PRO:HB2	1:144:A:PRO:HA	3	0.33
(2,4276)	1:144:A:PRO:HB2	1:144:A:PRO:HA	5	0.33
(2,4276)	1:144:A:PRO:HB2	1:144:A:PRO:HA	6	0.33
(2,3926)	1:115:A:LEU:HA	1:115:A:LEU:HB2	1	0.33
(2,3926)	1:115:A:LEU:HA	1:115:A:LEU:HB2	7	0.33
(2,3914)	1:113:A:VAL:HG13	1:113:A:VAL:HB	1	0.33
(2,3647)	1:191:A:VAL:HG12	1:193:A:THR:H	3	0.33
(2,3096)	1:111:A:GLY:HA3	1:159:A:PHE:H	10	0.33
(2,3095)	1:159:A:PHE:H	1:110:A:ASP:HA	6	0.33
(2,3054)	1:167:A:LYS:HB3	1:168:A:ALA:H	6	0.33
(2,3050)	1:159:A:PHE:HA	1:135:A:GLU:H	8	0.33
(2,2666)	1:166:A:GLU:HG2	1:166:A:GLU:H	1	0.33
(2,2659)	1:166:A:GLU:HG2	1:166:A:GLU:HA	1	0.33
(2,2657)	1:166:A:GLU:HB2	1:166:A:GLU:HA	3	0.33
(2,2657)	1:166:A:GLU:HB2	1:166:A:GLU:HA	10	0.33
(2,1918)	1:155:A:ALA:HB2	1:154:A:GLU:H	3	0.33
(2,1901)	1:188:A:ARG:HB2	1:187:A:SER:H	4	0.33
(2,1861)	1:154:A:GLU:HG2	1:118:A:LEU:H	4	0.33
(2,1844)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	8	0.33
(2,1815)	1:176:A:ILE:HG21	1:120:A:PHE:H	4	0.33
(2,1797)	1:164:A:ILE:HD13	1:91:A:ASN:HA	2	0.33
(2,1797)	1:164:A:ILE:HD13	1:91:A:ASN:HA	5	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1797)	1:164:A:ILE:HD13	1:91:A:ASN:HA	10	0.33
(2,1781)	1:164:A:ILE:HG13	1:167:A:LYS:H	7	0.33
(2,1560)	1:150:A:ARG:HG3	1:150:A:ARG:H	5	0.33
(2,1396)	1:112:A:PHE:H	1:111:A:GLY:H	4	0.33
(2,1106)	1:191:A:VAL:HG11	1:191:A:VAL:HA	3	0.33
(2,903)	1:169:A:LEU:HB2	1:169:A:LEU:HD13	1	0.33
(2,521)	1:134:A:LEU:HD11	1:134:A:LEU:HA	9	0.33
(2,424)	1:126:A:GLU:HG2	1:126:A:GLU:HB2	3	0.33
(2,106)	1:93:A:MET:HB2	1:93:A:MET:HG2	6	0.33
(2,106)	1:93:A:MET:HB2	1:93:A:MET:HG2	10	0.33
(2,53)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	1	0.33
(1,3050)	1:145:A:VAL:HA	1:151:A:SER:H	8	0.33
(1,3013)	1:189:A:ALA:H	1:186:A:SER:HA	4	0.33
(1,2932)	1:174:A:GLU:HA	1:181:A:ILE:H	3	0.33
(1,2916)	1:134:A:LEU:HD12	1:167:A:LYS:HB2	5	0.33
(1,2910)	1:168:A:ALA:HB2	1:167:A:LYS:H	9	0.33
(1,2772)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	2	0.33
(1,2738)	1:143:A:LEU:HG	1:141:A:ILE:HG21	8	0.33
(1,2588)	1:166:A:GLU:HG3	1:168:A:ALA:H	5	0.33
(1,2527)	1:163:A:GLU:HB2	1:164:A:ILE:HG12	5	0.33
(1,2483)	1:113:A:VAL:HG11	1:113:A:VAL:HB	6	0.33
(1,2298)	1:168:A:ALA:HB2	1:167:A:LYS:H	2	0.33
(1,2072)	1:175:A:ARG:HD2	1:178:A:HIS:HA	9	0.33
(1,1992)	1:158:A:GLN:HG2	1:161:A:SER:H	10	0.33
(1,1976)	1:179:A:ARG:HB3	1:119:A:PRO:HD2	1	0.33
(1,1864)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	1	0.33
(1,1864)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	6	0.33
(1,1548)	1:110:A:ASP:HB3	1:188:A:ARG:HG2	3	0.33
(1,1348)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.33
(1,1348)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.33
(1,1348)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	5	0.33
(1,1348)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.33
(1,1348)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	9	0.33
(1,1266)	1:96:A:VAL:HG23	1:93:A:MET:HG3	4	0.33
(1,1266)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.33
(1,1106)	1:161:A:SER:H	1:110:A:ASP:HB3	5	0.33
(1,1057)	1:133:A:GLY:HA3	1:134:A:LEU:HG	9	0.33
(1,984)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	7	0.33
(1,910)	1:141:A:ILE:HG21	1:143:A:LEU:HG	4	0.33
(1,868)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	9	0.33
(1,848)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	7	0.33
(1,809)	1:169:A:LEU:HB2	1:169:A:LEU:HA	3	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,803)	1:156:A:PHE:HA	1:141:A:ILE:HA	2	0.33
(1,803)	1:156:A:PHE:HA	1:141:A:ILE:HA	8	0.33
(1,742)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.33
(1,742)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	2	0.33
(1,742)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.33
(1,742)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	4	0.33
(1,742)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	5	0.33
(1,742)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.33
(1,742)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.33
(1,742)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	8	0.33
(1,742)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	9	0.33
(1,742)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.33
(1,681)	1:134:A:LEU:HD13	1:133:A:GLY:H	10	0.33
(1,662)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.33
(1,653)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	6	0.33
(1,504)	1:166:A:GLU:H	1:169:A:LEU:HD13	7	0.33
(1,456)	1:165:A:ALA:HA	1:113:A:VAL:HG23	2	0.33
(1,447)	1:154:A:GLU:HG2	1:118:A:LEU:HD23	4	0.33
(1,376)	1:174:A:GLU:HB2	1:181:A:ILE:HD13	1	0.33
(1,376)	1:174:A:GLU:HB2	1:181:A:ILE:HD13	2	0.33
(1,366)	1:134:A:LEU:HD22	1:134:A:LEU:HD12	7	0.33
(1,320)	1:169:A:LEU:HB2	1:169:A:LEU:HD11	2	0.33
(1,178)	1:154:A:GLU:HG2	1:154:A:GLU:HA	5	0.33
(1,159)	1:95:A:TRP:HA	1:96:A:VAL:H	1	0.33
(1,159)	1:95:A:TRP:HA	1:96:A:VAL:H	2	0.33
(1,153)	1:130:A:PHE:HB3	1:132:A:SER:H	8	0.33
(1,105)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.33
(1,105)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.33
(1,99)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	2	0.33
(1,99)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	3	0.33
(1,54)	1:166:A:GLU:HB2	1:168:A:ALA:H	3	0.33
(1,54)	1:166:A:GLU:HB2	1:168:A:ALA:H	7	0.33
(1,39)	1:134:A:LEU:HD11	1:134:A:LEU:HG	5	0.33
(4,40)	1:168:A:ALA:H	1:164:A:ILE:O	2	0.32
(4,40)	1:168:A:ALA:H	1:164:A:ILE:O	9	0.32
(4,11)	1:118:A:LEU:H	1:152:A:THR:O	2	0.32
(4,11)	1:118:A:LEU:H	1:152:A:THR:O	4	0.32
(3,102)	1:158:A:GLN:HG3	1:112:A:PHE:HA	9	0.32
(2,9010)	1:183:A:ILE:H	1:183:A:ILE:HG12	6	0.32
(2,8985)	1:175:A:ARG:HG2	1:176:A:ILE:H	1	0.32
(2,8577)	1:157:A:VAL:HG21	1:158:A:GLN:H	6	0.32
(2,8131)	1:163:A:GLU:HG3	1:163:A:GLU:H	10	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7669)	1:119:A:PRO:HB2	1:119:A:PRO:HA	1	0.32
(2,7669)	1:119:A:PRO:HB2	1:119:A:PRO:HA	9	0.32
(2,7608)	1:114:A:ARG:HD3	1:114:A:ARG:HG2	9	0.32
(2,7379)	1:126:A:GLU:HA	1:136:A:ILE:HB	7	0.32
(2,7290)	1:96:A:VAL:HG22	1:97:A:LEU:H	2	0.32
(2,7273)	1:164:A:ILE:HD13	1:135:A:GLU:H	5	0.32
(2,7269)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	7	0.32
(2,6751)	1:151:A:SER:H	1:151:A:SER:HB2	7	0.32
(2,6699)	1:168:A:ALA:H	1:167:A:LYS:HB3	1	0.32
(2,6592)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	10	0.32
(2,6300)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	5	0.32
(2,5539)	1:98:A:LYS:HB3	1:100:A:THR:HG23	10	0.32
(2,5498)	1:116:A:ARG:HD2	1:116:A:ARG:HA	3	0.32
(2,5444)	1:191:A:VAL:HG13	1:193:A:THR:H	4	0.32
(2,5243)	1:166:A:GLU:HB3	1:166:A:GLU:H	3	0.32
(2,5243)	1:166:A:GLU:HB3	1:166:A:GLU:H	8	0.32
(2,5235)	1:164:A:ILE:H	1:164:A:ILE:HG21	7	0.32
(2,5183)	1:154:A:GLU:HB3	1:154:A:GLU:H	6	0.32
(2,4899)	1:111:A:GLY:HA3	1:159:A:PHE:H	10	0.32
(2,4792)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	5	0.32
(2,4496)	1:169:A:LEU:HD22	1:169:A:LEU:HA	2	0.32
(2,3679)	1:187:A:SER:HB3	1:189:A:ALA:H	1	0.32
(2,3679)	1:187:A:SER:HB3	1:189:A:ALA:H	2	0.32
(2,3647)	1:191:A:VAL:HG13	1:193:A:THR:H	10	0.32
(2,3622)	1:113:A:VAL:HG12	1:112:A:PHE:H	7	0.32
(2,3435)	1:164:A:ILE:H	1:164:A:ILE:HG21	4	0.32
(2,3435)	1:164:A:ILE:H	1:164:A:ILE:HG21	7	0.32
(2,3208)	1:114:A:ARG:H	1:113:A:VAL:HG12	6	0.32
(2,3068)	1:157:A:VAL:HG21	1:158:A:GLN:H	4	0.32
(2,3068)	1:157:A:VAL:HG21	1:158:A:GLN:H	5	0.32
(2,2925)	1:192:A:ARG:HB2	1:192:A:ARG:H	6	0.32
(2,2657)	1:166:A:GLU:HB2	1:166:A:GLU:HA	8	0.32
(2,2205)	1:123:A:SER:HB2	1:123:A:SER:HA	8	0.32
(2,1918)	1:155:A:ALA:HB2	1:154:A:GLU:H	10	0.32
(2,1901)	1:188:A:ARG:HB2	1:187:A:SER:H	2	0.32
(2,1901)	1:188:A:ARG:HB2	1:187:A:SER:H	3	0.32
(2,1873)	1:187:A:SER:HB3	1:189:A:ALA:H	5	0.32
(2,1838)	1:191:A:VAL:HG13	1:193:A:THR:H	4	0.32
(2,1806)	1:160:A:ALA:HB2	1:162:A:GLN:H	9	0.32
(2,1797)	1:164:A:ILE:HD13	1:91:A:ASN:HA	7	0.32
(2,1600)	1:159:A:PHE:H	1:158:A:GLN:HG3	2	0.32
(2,1574)	1:155:A:ALA:H	1:154:A:GLU:HB2	10	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1560)	1:150:A:ARG:HG3	1:150:A:ARG:H	1	0.32
(2,1396)	1:112:A:PHE:H	1:111:A:GLY:H	2	0.32
(2,1256)	1:139:A:ASN:H	1:141:A:ILE:HG22	1	0.32
(2,418)	1:124:A:LYS:HA	1:124:A:LYS:HB2	2	0.32
(2,418)	1:124:A:LYS:HA	1:124:A:LYS:HB2	4	0.32
(2,99)	1:188:A:ARG:HD3	1:191:A:VAL:HG22	3	0.32
(2,25)	1:96:A:VAL:HG22	1:161:A:SER:H	8	0.32
(1,3013)	1:189:A:ALA:H	1:186:A:SER:HA	10	0.32
(1,2974)	1:100:A:THR:HG23	1:98:A:LYS:H	1	0.32
(1,2477)	1:164:A:ILE:HD11	1:164:A:ILE:HB	4	0.32
(1,2477)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	10	0.32
(1,2432)	1:145:A:VAL:HA	1:151:A:SER:H	3	0.32
(1,2403)	1:96:A:VAL:HB	1:97:A:LEU:H	4	0.32
(1,2324)	1:188:A:ARG:HA	1:186:A:SER:HA	4	0.32
(1,2324)	1:188:A:ARG:HA	1:186:A:SER:HA	7	0.32
(1,2069)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	4	0.32
(1,1881)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	3	0.32
(1,1864)	1:164:A:ILE:HD11	1:164:A:ILE:HB	4	0.32
(1,1864)	1:164:A:ILE:HD12	1:164:A:ILE:HG13	10	0.32
(1,1704)	1:166:A:GLU:HB2	1:166:A:GLU:HA	2	0.32
(1,1702)	1:134:A:LEU:HD21	1:131:A:PHE:HB3	3	0.32
(1,1410)	1:156:A:PHE:HA	1:141:A:ILE:HA	9	0.32
(1,1345)	1:181:A:ILE:HB	1:181:A:ILE:HA	5	0.32
(1,1175)	1:106:A:ASP:H	1:105:A:PRO:HD3	10	0.32
(1,1159)	1:108:A:ALA:H	1:109:A:ASN:HA	6	0.32
(1,1091)	1:137:A:VAL:HA	1:140:A:GLY:H	8	0.32
(1,927)	1:164:A:ILE:HA	1:91:A:ASN:HB3	10	0.32
(1,869)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	10	0.32
(1,868)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	8	0.32
(1,854)	1:179:A:ARG:HD2	1:179:A:ARG:HA	5	0.32
(1,845)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	3	0.32
(1,681)	1:134:A:LEU:HD13	1:133:A:GLY:H	1	0.32
(1,681)	1:134:A:LEU:HD13	1:133:A:GLY:H	6	0.32
(1,545)	1:168:A:ALA:H	1:169:A:LEU:HB2	3	0.32
(1,411)	1:164:A:ILE:HD13	1:93:A:MET:HA	10	0.32
(1,320)	1:169:A:LEU:HB2	1:169:A:LEU:HD11	5	0.32
(1,320)	1:169:A:LEU:HB2	1:169:A:LEU:HD11	6	0.32
(1,178)	1:154:A:GLU:HG2	1:154:A:GLU:HA	6	0.32
(1,159)	1:95:A:TRP:HA	1:96:A:VAL:H	9	0.32
(1,153)	1:130:A:PHE:HB3	1:132:A:SER:H	2	0.32
(1,153)	1:130:A:PHE:HB3	1:132:A:SER:H	4	0.32
(1,140)	1:190:A:GLU:HG2	1:190:A:GLU:HA	10	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,133)	1:166:A:GLU:HG3	1:169:A:LEU:HD13	5	0.32
(1,8)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	7	0.32
(4,30)	1:157:A:VAL:H	1:113:A:VAL:O	10	0.31
(3,537)	1:118:A:LEU:HA	1:183:A:ILE:HG12	4	0.31
(2,8430)	1:192:A:ARG:HD2	1:192:A:ARG:HB2	3	0.31
(2,7825)	1:135:A:GLU:HA	1:135:A:GLU:HG2	4	0.31
(2,7825)	1:135:A:GLU:HA	1:135:A:GLU:HG2	8	0.31
(2,7669)	1:119:A:PRO:HB2	1:119:A:PRO:HA	6	0.31
(2,7408)	1:155:A:ALA:HB2	1:154:A:GLU:H	4	0.31
(2,7379)	1:126:A:GLU:HA	1:136:A:ILE:HB	10	0.31
(2,7372)	1:156:A:PHE:HB2	1:191:A:VAL:H	1	0.31
(2,7290)	1:96:A:VAL:HG22	1:97:A:LEU:H	3	0.31
(2,7271)	1:164:A:ILE:HD13	1:91:A:ASN:HA	8	0.31
(2,7269)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	8	0.31
(2,6858)	1:114:A:ARG:H	1:113:A:VAL:HG12	8	0.31
(2,6751)	1:151:A:SER:H	1:151:A:SER:HB2	4	0.31
(2,6715)	1:157:A:VAL:HG21	1:158:A:GLN:H	6	0.31
(2,6616)	1:158:A:GLN:HG3	1:112:A:PHE:HA	3	0.31
(2,5952)	1:135:A:GLU:HA	1:135:A:GLU:HG2	8	0.31
(2,5487)	1:187:A:SER:HB3	1:189:A:ALA:H	8	0.31
(2,5473)	1:109:A:ASN:HA	1:108:A:ALA:HB1	4	0.31
(2,5471)	1:169:A:LEU:HB2	1:166:A:GLU:HA	1	0.31
(2,5413)	1:160:A:ALA:HB3	1:159:A:PHE:HB2	1	0.31
(2,5243)	1:166:A:GLU:HB3	1:166:A:GLU:H	10	0.31
(2,5235)	1:164:A:ILE:H	1:164:A:ILE:HG21	2	0.31
(2,5235)	1:164:A:ILE:H	1:164:A:ILE:HG21	4	0.31
(2,5235)	1:164:A:ILE:H	1:164:A:ILE:HG21	6	0.31
(2,5086)	1:132:A:SER:HB2	1:133:A:GLY:H	10	0.31
(2,4792)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	7	0.31
(2,4792)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	8	0.31
(2,4788)	1:158:A:GLN:HG3	1:112:A:PHE:HA	2	0.31
(2,4496)	1:169:A:LEU:HD22	1:169:A:LEU:HA	1	0.31
(2,3906)	1:111:A:GLY:HA3	1:112:A:PHE:H	1	0.31
(2,3906)	1:111:A:GLY:HA3	1:112:A:PHE:H	5	0.31
(2,3726)	1:155:A:ALA:HB2	1:154:A:GLU:H	4	0.31
(2,3707)	1:188:A:ARG:HB2	1:187:A:SER:H	8	0.31
(2,3707)	1:188:A:ARG:HB2	1:187:A:SER:H	9	0.31
(2,3647)	1:191:A:VAL:HG13	1:193:A:THR:H	6	0.31
(2,3607)	1:164:A:ILE:HD13	1:91:A:ASN:HA	6	0.31
(2,3435)	1:164:A:ILE:H	1:164:A:ILE:HG21	2	0.31
(2,3435)	1:164:A:ILE:H	1:164:A:ILE:HG21	6	0.31
(2,3179)	1:106:A:ASP:H	1:105:A:PRO:HD2	3	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2984)	1:188:A:ARG:HD2	1:108:A:ALA:H	10	0.31
(2,2202)	1:122:A:CYS:HA	1:122:A:CYS:HB2	4	0.31
(2,2202)	1:122:A:CYS:HA	1:122:A:CYS:HB2	5	0.31
(2,2202)	1:122:A:CYS:HA	1:122:A:CYS:HB2	6	0.31
(2,2202)	1:122:A:CYS:HA	1:122:A:CYS:HB2	7	0.31
(2,2202)	1:122:A:CYS:HA	1:122:A:CYS:HB2	9	0.31
(2,2202)	1:122:A:CYS:HA	1:122:A:CYS:HB2	10	0.31
(2,1901)	1:188:A:ARG:HB2	1:187:A:SER:H	1	0.31
(2,1901)	1:188:A:ARG:HB2	1:187:A:SER:H	6	0.31
(2,1861)	1:154:A:GLU:HG2	1:118:A:LEU:H	5	0.31
(2,1861)	1:154:A:GLU:HG2	1:118:A:LEU:H	6	0.31
(2,1664)	1:175:A:ARG:HG2	1:176:A:ILE:H	2	0.31
(2,1069)	1:187:A:SER:HB3	1:188:A:ARG:H	2	0.31
(2,915)	1:171:A:LYS:HB3	1:171:A:LYS:H	6	0.31
(2,748)	1:151:A:SER:HB3	1:152:A:THR:H	5	0.31
(2,748)	1:151:A:SER:HB3	1:152:A:THR:H	7	0.31
(2,387)	1:119:A:PRO:HB2	1:119:A:PRO:HA	4	0.31
(2,307)	1:111:A:GLY:HA3	1:112:A:PHE:H	1	0.31
(2,307)	1:111:A:GLY:HA3	1:112:A:PHE:H	5	0.31
(2,63)	1:95:A:TRP:HB2	1:96:A:VAL:HG21	9	0.31
(2,63)	1:95:A:TRP:HB2	1:96:A:VAL:HG21	10	0.31
(2,22)	1:113:A:VAL:HG12	1:112:A:PHE:H	5	0.31
(1,3020)	1:132:A:SER:H	1:136:A:ILE:HB	2	0.31
(1,3013)	1:189:A:ALA:H	1:186:A:SER:HA	7	0.31
(1,3003)	1:108:A:ALA:H	1:109:A:ASN:HA	9	0.31
(1,2738)	1:143:A:LEU:HG	1:141:A:ILE:HG21	9	0.31
(1,2403)	1:97:A:LEU:H	1:163:A:GLU:HB2	8	0.31
(1,2377)	1:146:A:ASP:H	1:143:A:LEU:HD21	5	0.31
(1,2140)	1:93:A:MET:HB2	1:93:A:MET:HG2	8	0.31
(1,2069)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	2	0.31
(1,1981)	1:166:A:GLU:HG3	1:168:A:ALA:H	5	0.31
(1,1798)	1:165:A:ALA:H	1:110:A:ASP:HB3	4	0.31
(1,1784)	1:189:A:ALA:H	1:186:A:SER:HA	2	0.31
(1,1784)	1:189:A:ALA:H	1:186:A:SER:HA	5	0.31
(1,1623)	1:119:A:PRO:HB3	1:119:A:PRO:HA	5	0.31
(1,1623)	1:119:A:PRO:HB3	1:119:A:PRO:HA	7	0.31
(1,1623)	1:119:A:PRO:HB3	1:119:A:PRO:HA	8	0.31
(1,1520)	1:141:A:ILE:HG21	1:143:A:LEU:HG	10	0.31
(1,1486)	1:143:A:LEU:HA	1:143:A:LEU:HB2	2	0.31
(1,1451)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	1	0.31
(1,1451)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	5	0.31
(1,1410)	1:156:A:PHE:HA	1:141:A:ILE:HA	5	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:181:A:ILE:HB	1:181:A:ILE:HA	4	0.31
(1,1251)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	10	0.31
(1,1175)	1:106:A:ASP:H	1:105:A:PRO:HD3	6	0.31
(1,1106)	1:161:A:SER:H	1:110:A:ASP:HB3	10	0.31
(1,869)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	3	0.31
(1,868)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	10	0.31
(1,809)	1:169:A:LEU:HB2	1:169:A:LEU:HA	1	0.31
(1,803)	1:156:A:PHE:HA	1:141:A:ILE:HA	5	0.31
(1,803)	1:156:A:PHE:HA	1:141:A:ILE:HA	9	0.31
(1,681)	1:134:A:LEU:HD13	1:133:A:GLY:H	7	0.31
(1,458)	1:136:A:ILE:HG13	1:159:A:PHE:HA	6	0.31
(1,411)	1:164:A:ILE:HD13	1:135:A:GLU:HA	5	0.31
(1,320)	1:169:A:LEU:HB2	1:169:A:LEU:HD11	9	0.31
(1,295)	1:164:A:ILE:HD12	1:166:A:GLU:HB2	5	0.31
(1,247)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	9	0.31
(1,160)	1:102:A:PRO:HG2	1:101:A:GLY:HA3	3	0.31
(1,159)	1:159:A:PHE:HA	1:137:A:VAL:H	7	0.31
(1,153)	1:130:A:PHE:HB3	1:132:A:SER:H	1	0.31
(4,40)	1:168:A:ALA:H	1:164:A:ILE:O	8	0.3
(4,23)	1:144:A:PRO:O	1:152:A:THR:OG1	1	0.3
(4,7)	1:116:A:ARG:H	1:182:A:GLU:O	1	0.3
(2,8714)	1:114:A:ARG:H	1:113:A:VAL:HG13	9	0.3
(2,8608)	1:151:A:SER:H	1:151:A:SER:HB2	7	0.3
(2,8461)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	1	0.3
(2,7978)	1:144:A:PRO:HD3	1:144:A:PRO:HA	9	0.3
(2,7825)	1:135:A:GLU:HA	1:135:A:GLU:HG2	1	0.3
(2,7825)	1:135:A:GLU:HA	1:135:A:GLU:HG2	5	0.3
(2,7825)	1:135:A:GLU:HA	1:135:A:GLU:HG2	9	0.3
(2,7825)	1:135:A:GLU:HA	1:135:A:GLU:HG2	10	0.3
(2,7678)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	4	0.3
(2,7408)	1:155:A:ALA:HB2	1:154:A:GLU:H	5	0.3
(2,7408)	1:155:A:ALA:HB2	1:154:A:GLU:H	9	0.3
(2,7377)	1:181:A:ILE:HG21	1:174:A:GLU:HA	1	0.3
(2,7377)	1:181:A:ILE:HG21	1:174:A:GLU:HA	8	0.3
(2,7344)	1:109:A:ASN:HA	1:108:A:ALA:HB1	4	0.3
(2,7322)	1:191:A:VAL:HG12	1:190:A:GLU:H	6	0.3
(2,6751)	1:151:A:SER:H	1:151:A:SER:HB2	10	0.3
(2,6699)	1:168:A:ALA:H	1:167:A:LYS:HB3	9	0.3
(2,6627)	1:111:A:GLY:H	1:188:A:ARG:HG2	8	0.3
(2,5952)	1:135:A:GLU:HA	1:135:A:GLU:HG2	4	0.3
(2,5498)	1:116:A:ARG:HD2	1:116:A:ARG:HA	9	0.3
(2,5498)	1:116:A:ARG:HD2	1:116:A:ARG:HA	10	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5444)	1:191:A:VAL:HG13	1:193:A:THR:H	1	0.3
(2,5404)	1:164:A:ILE:HD13	1:135:A:GLU:H	5	0.3
(2,5361)	1:149:A:GLY:HA3	1:151:A:SER:H	9	0.3
(2,5235)	1:164:A:ILE:H	1:164:A:ILE:HG21	1	0.3
(2,5235)	1:164:A:ILE:H	1:164:A:ILE:HG21	3	0.3
(2,5009)	1:114:A:ARG:H	1:113:A:VAL:HG12	8	0.3
(2,4776)	1:116:A:ARG:HG2	1:154:A:GLU:HG2	6	0.3
(2,4772)	1:155:A:ALA:HA	1:155:A:ALA:HB3	5	0.3
(2,4733)	1:192:A:ARG:HB2	1:192:A:ARG:H	3	0.3
(2,4247)	1:144:A:PRO:HD2	1:143:A:LEU:HA	9	0.3
(2,3906)	1:111:A:GLY:HA3	1:112:A:PHE:H	2	0.3
(2,3726)	1:155:A:ALA:HB2	1:154:A:GLU:H	5	0.3
(2,3726)	1:155:A:ALA:HB2	1:154:A:GLU:H	9	0.3
(2,3695)	1:181:A:ILE:HG21	1:174:A:GLU:HA	7	0.3
(2,3435)	1:164:A:ILE:H	1:164:A:ILE:HG21	1	0.3
(2,3435)	1:164:A:ILE:H	1:164:A:ILE:HG21	3	0.3
(2,3286)	1:132:A:SER:HB2	1:133:A:GLY:H	9	0.3
(2,3208)	1:114:A:ARG:H	1:113:A:VAL:HG13	7	0.3
(2,3068)	1:157:A:VAL:HG21	1:158:A:GLN:H	6	0.3
(2,2925)	1:192:A:ARG:HB2	1:192:A:ARG:H	5	0.3
(2,2202)	1:122:A:CYS:HA	1:122:A:CYS:HB2	2	0.3
(2,2202)	1:122:A:CYS:HA	1:122:A:CYS:HB2	3	0.3
(2,2097)	1:111:A:GLY:HA3	1:112:A:PHE:H	10	0.3
(2,1918)	1:155:A:ALA:HB2	1:154:A:GLU:H	2	0.3
(2,1901)	1:188:A:ARG:HB2	1:187:A:SER:H	10	0.3
(2,1838)	1:191:A:VAL:HG13	1:193:A:THR:H	1	0.3
(2,1806)	1:160:A:ALA:HB2	1:162:A:GLN:H	5	0.3
(2,1664)	1:175:A:ARG:HG2	1:176:A:ILE:H	8	0.3
(2,1574)	1:155:A:ALA:H	1:154:A:GLU:HB2	6	0.3
(2,1562)	1:150:A:ARG:H	1:151:A:SER:H	9	0.3
(2,1560)	1:150:A:ARG:HG3	1:150:A:ARG:H	3	0.3
(2,1327)	1:96:A:VAL:HG13	1:97:A:LEU:H	9	0.3
(2,1069)	1:187:A:SER:HB3	1:188:A:ARG:H	8	0.3
(2,871)	1:166:A:GLU:HG3	1:166:A:GLU:HA	3	0.3
(2,868)	1:166:A:GLU:HB2	1:166:A:GLU:HA	3	0.3
(2,868)	1:166:A:GLU:HB2	1:166:A:GLU:HA	10	0.3
(2,721)	1:148:A:GLN:HB2	1:149:A:GLY:H	1	0.3
(2,595)	1:139:A:ASN:HA	1:140:A:GLY:HA3	3	0.3
(2,521)	1:134:A:LEU:HD11	1:134:A:LEU:HA	6	0.3
(2,521)	1:134:A:LEU:HD11	1:134:A:LEU:HA	8	0.3
(2,307)	1:111:A:GLY:HA3	1:112:A:PHE:H	2	0.3
(2,100)	1:181:A:ILE:HG21	1:174:A:GLU:HA	2	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:107:A:THR:HB	1:110:A:ASP:HA	8	0.3
(1,2451)	1:108:A:ALA:H	1:106:A:ASP:HB3	9	0.3
(1,2377)	1:146:A:ASP:H	1:143:A:LEU:HD21	7	0.3
(1,2207)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	1	0.3
(1,2140)	1:93:A:MET:HB2	1:135:A:GLU:HB3	4	0.3
(1,2069)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	8	0.3
(1,1881)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	8	0.3
(1,1868)	1:113:A:VAL:HG13	1:113:A:VAL:HB	8	0.3
(1,1850)	1:118:A:LEU:H	1:118:A:LEU:HD12	10	0.3
(1,1706)	1:174:A:GLU:HA	1:181:A:ILE:H	1	0.3
(1,1623)	1:119:A:PRO:HB3	1:119:A:PRO:HA	1	0.3
(1,1623)	1:119:A:PRO:HB3	1:119:A:PRO:HA	9	0.3
(1,1623)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.3
(1,1530)	1:165:A:ALA:HB3	1:113:A:VAL:HG23	9	0.3
(1,1486)	1:143:A:LEU:HA	1:143:A:LEU:HB2	1	0.3
(1,1455)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	7	0.3
(1,1410)	1:156:A:PHE:HA	1:141:A:ILE:HA	4	0.3
(1,1251)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	3	0.3
(1,1067)	1:165:A:ALA:HA	1:113:A:VAL:HG23	7	0.3
(1,1012)	1:119:A:PRO:HB3	1:119:A:PRO:HA	5	0.3
(1,1012)	1:119:A:PRO:HB3	1:119:A:PRO:HA	7	0.3
(1,1012)	1:119:A:PRO:HB3	1:119:A:PRO:HA	8	0.3
(1,935)	1:112:A:PHE:HB3	1:188:A:ARG:HG2	8	0.3
(1,935)	1:112:A:PHE:HB3	1:188:A:ARG:HG2	9	0.3
(1,927)	1:164:A:ILE:HA	1:91:A:ASN:HB3	6	0.3
(1,914)	1:93:A:MET:HB2	1:135:A:GLU:HB3	1	0.3
(1,914)	1:93:A:MET:HB2	1:135:A:GLU:HB3	5	0.3
(1,848)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.3
(1,803)	1:156:A:PHE:HA	1:141:A:ILE:HA	4	0.3
(1,739)	1:181:A:ILE:HB	1:181:A:ILE:HA	4	0.3
(1,739)	1:181:A:ILE:HB	1:181:A:ILE:HA	5	0.3
(1,625)	1:97:A:LEU:H	1:99:A:HIS:HA	2	0.3
(1,598)	1:116:A:ARG:H	1:181:A:ILE:HD12	1	0.3
(1,411)	1:164:A:ILE:HD13	1:93:A:MET:HA	7	0.3
(1,377)	1:123:A:SER:HB3	1:181:A:ILE:HD11	2	0.3
(1,376)	1:174:A:GLU:HB2	1:181:A:ILE:HD13	4	0.3
(1,320)	1:169:A:LEU:HB2	1:169:A:LEU:HD11	4	0.3
(1,320)	1:97:A:LEU:HG	1:97:A:LEU:HD13	8	0.3
(1,320)	1:169:A:LEU:HB2	1:169:A:LEU:HD11	10	0.3
(1,316)	1:98:A:LYS:HB3	1:100:A:THR:HG23	10	0.3
(1,248)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	9	0.3
(1,247)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	8	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,99)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	1	0.3
(1,39)	1:134:A:LEU:HD11	1:134:A:LEU:HG	6	0.3
(1,39)	1:134:A:LEU:HD11	1:134:A:LEU:HG	8	0.3
(1,39)	1:134:A:LEU:HD11	1:134:A:LEU:HG	10	0.3
(1,25)	1:176:A:ILE:HG22	1:176:A:ILE:HG12	1	0.3
(2,8697)	1:110:A:ASP:HA	1:110:A:ASP:H	7	0.29
(2,8608)	1:151:A:SER:H	1:151:A:SER:HB2	4	0.29
(2,8560)	1:168:A:ALA:H	1:167:A:LYS:HB3	7	0.29
(2,8503)	1:187:A:SER:H	1:184:A:PHE:HB2	5	0.29
(2,8461)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	9	0.29
(2,7973)	1:144:A:PRO:HB2	1:144:A:PRO:HA	4	0.29
(2,7825)	1:135:A:GLU:HA	1:135:A:GLU:HG2	2	0.29
(2,7825)	1:135:A:GLU:HA	1:135:A:GLU:HG2	3	0.29
(2,7825)	1:135:A:GLU:HA	1:135:A:GLU:HG2	6	0.29
(2,7825)	1:135:A:GLU:HA	1:135:A:GLU:HG2	7	0.29
(2,7356)	1:175:A:ARG:HA	1:179:A:ARG:H	4	0.29
(2,7344)	1:109:A:ASN:HA	1:108:A:ALA:HB1	7	0.29
(2,7290)	1:96:A:VAL:HG22	1:97:A:LEU:H	10	0.29
(2,7273)	1:164:A:ILE:HD13	1:135:A:GLU:H	6	0.29
(2,7273)	1:164:A:ILE:HD13	1:135:A:GLU:H	7	0.29
(2,6751)	1:151:A:SER:H	1:151:A:SER:HB2	5	0.29
(2,6345)	1:171:A:LYS:HB3	1:171:A:LYS:H	6	0.29
(2,6100)	1:144:A:PRO:HB2	1:144:A:PRO:HA	4	0.29
(2,5952)	1:135:A:GLU:HA	1:135:A:GLU:HG2	1	0.29
(2,5952)	1:135:A:GLU:HA	1:135:A:GLU:HG2	5	0.29
(2,5952)	1:135:A:GLU:HA	1:135:A:GLU:HG2	9	0.29
(2,5952)	1:135:A:GLU:HA	1:135:A:GLU:HG2	10	0.29
(2,5821)	1:122:A:CYS:HA	1:121:A:GLY:H	6	0.29
(2,5539)	1:98:A:LYS:HB3	1:100:A:THR:HG23	6	0.29
(2,5499)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	3	0.29
(2,5499)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	4	0.29
(2,5498)	1:116:A:ARG:HD2	1:116:A:ARG:HA	7	0.29
(2,5498)	1:116:A:ARG:HD2	1:116:A:ARG:HA	8	0.29
(2,5473)	1:109:A:ASN:HA	1:108:A:ALA:HB1	7	0.29
(2,5327)	1:190:A:GLU:HB3	1:190:A:GLU:H	4	0.29
(2,4898)	1:159:A:PHE:H	1:110:A:ASP:HA	7	0.29
(2,4792)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	6	0.29
(2,4733)	1:192:A:ARG:HB2	1:192:A:ARG:H	10	0.29
(2,4468)	1:166:A:GLU:HB2	1:166:A:GLU:HA	6	0.29
(2,4468)	1:166:A:GLU:HB2	1:166:A:GLU:HA	9	0.29
(2,4436)	1:163:A:GLU:HG3	1:163:A:GLU:H	4	0.29
(2,4436)	1:163:A:GLU:HG3	1:163:A:GLU:H	7	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3647)	1:191:A:VAL:HG13	1:193:A:THR:H	8	0.29
(2,3635)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	8	0.29
(2,3218)	1:114:A:ARG:HG3	1:115:A:LEU:H	8	0.29
(2,2965)	1:155:A:ALA:HA	1:155:A:ALA:HB3	5	0.29
(2,2202)	1:122:A:CYS:HA	1:122:A:CYS:HB2	1	0.29
(2,2097)	1:111:A:GLY:HA3	1:112:A:PHE:H	6	0.29
(2,1918)	1:155:A:ALA:HB2	1:154:A:GLU:H	7	0.29
(2,1918)	1:155:A:ALA:HB2	1:154:A:GLU:H	8	0.29
(2,1396)	1:112:A:PHE:H	1:111:A:GLY:H	5	0.29
(2,1327)	1:96:A:VAL:HG13	1:97:A:LEU:H	8	0.29
(2,1283)	1:105:A:PRO:HB3	1:106:A:ASP:H	10	0.29
(2,1173)	1:111:A:GLY:HA3	1:109:A:ASN:H	7	0.29
(2,868)	1:166:A:GLU:HB2	1:166:A:GLU:HA	8	0.29
(2,748)	1:151:A:SER:HB3	1:152:A:THR:H	8	0.29
(2,677)	1:144:A:PRO:HB2	1:144:A:PRO:HA	9	0.29
(2,424)	1:126:A:GLU:HG2	1:126:A:GLU:HB2	6	0.29
(2,100)	1:181:A:ILE:HG21	1:174:A:GLU:HA	10	0.29
(2,95)	1:159:A:PHE:HB2	1:135:A:GLU:H	6	0.29
(2,63)	1:95:A:TRP:HB2	1:96:A:VAL:HG21	1	0.29
(1,2974)	1:100:A:THR:HG23	1:98:A:LYS:H	7	0.29
(1,2898)	1:144:A:PRO:HD2	1:118:A:LEU:HD22	8	0.29
(1,2675)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	7	0.29
(1,2527)	1:163:A:GLU:HB2	1:96:A:VAL:HG13	3	0.29
(1,2495)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	3	0.29
(1,2415)	1:165:A:ALA:H	1:110:A:ASP:HB3	10	0.29
(1,2377)	1:146:A:ASP:H	1:143:A:LEU:HD21	8	0.29
(1,2377)	1:146:A:ASP:H	1:143:A:LEU:HD21	10	0.29
(1,2285)	1:144:A:PRO:HD2	1:118:A:LEU:HD22	8	0.29
(1,2207)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	2	0.29
(1,2207)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	4	0.29
(1,2207)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	7	0.29
(1,2207)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	9	0.29
(1,2140)	1:93:A:MET:HB2	1:93:A:MET:HG2	2	0.29
(1,2069)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	10	0.29
(1,2031)	1:169:A:LEU:HA	1:169:A:LEU:HD11	1	0.29
(1,1881)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	2	0.29
(1,1877)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	3	0.29
(1,1850)	1:118:A:LEU:H	1:118:A:LEU:HD12	3	0.29
(1,1841)	1:134:A:LEU:HD12	1:167:A:LYS:H	5	0.29
(1,1668)	1:144:A:PRO:HD2	1:118:A:LEU:HD22	8	0.29
(1,1623)	1:119:A:PRO:HB3	1:119:A:PRO:HA	2	0.29
(1,1623)	1:119:A:PRO:HB3	1:119:A:PRO:HA	3	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1623)	1:119:A:PRO:HB3	1:119:A:PRO:HA	6	0.29
(1,1451)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	3	0.29
(1,1429)	1:98:A:LYS:HA	1:100:A:THR:HG23	5	0.29
(1,1429)	1:98:A:LYS:HA	1:100:A:THR:HG23	7	0.29
(1,1410)	1:156:A:PHE:HA	1:141:A:ILE:HA	10	0.29
(1,1297)	1:166:A:GLU:HB2	1:168:A:ALA:H	10	0.29
(1,1286)	1:134:A:LEU:HD13	1:133:A:GLY:H	9	0.29
(1,1251)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	4	0.29
(1,1251)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	9	0.29
(1,1173)	1:189:A:ALA:H	1:186:A:SER:HA	3	0.29
(1,1106)	1:161:A:SER:H	1:110:A:ASP:HB3	2	0.29
(1,1091)	1:174:A:GLU:HA	1:181:A:ILE:H	3	0.29
(1,1012)	1:119:A:PRO:HB3	1:119:A:PRO:HA	9	0.29
(1,1012)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.29
(1,995)	1:123:A:SER:HB3	1:181:A:ILE:HD11	1	0.29
(1,988)	1:190:A:GLU:HG3	1:186:A:SER:HA	9	0.29
(1,982)	1:96:A:VAL:HG12	1:93:A:MET:HG2	7	0.29
(1,939)	1:97:A:LEU:HG	1:97:A:LEU:HD13	1	0.29
(1,939)	1:97:A:LEU:HG	1:97:A:LEU:HD13	3	0.29
(1,927)	1:164:A:ILE:HA	1:91:A:ASN:HB3	7	0.29
(1,868)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	3	0.29
(1,444)	1:144:A:PRO:HD2	1:118:A:LEU:HD22	8	0.29
(1,417)	1:107:A:THR:HB	1:110:A:ASP:HB3	2	0.29
(1,377)	1:123:A:SER:HB3	1:181:A:ILE:HD11	5	0.29
(1,377)	1:123:A:SER:HB3	1:181:A:ILE:HD11	9	0.29
(1,248)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	8	0.29
(1,222)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	2	0.29
(1,159)	1:95:A:TRP:HA	1:96:A:VAL:H	3	0.29
(1,99)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	6	0.29
(1,99)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	8	0.29
(1,39)	1:134:A:LEU:HD11	1:134:A:LEU:HG	3	0.29
(4,48)	1:183:A:ILE:H	1:171:A:LYS:O	6	0.28
(4,40)	1:168:A:ALA:H	1:164:A:ILE:O	3	0.28
(4,30)	1:157:A:VAL:H	1:113:A:VAL:O	3	0.28
(4,25)	1:148:A:GLN:N	1:146:A:ASP:OD2	2	0.28
(4,25)	1:148:A:GLN:N	1:146:A:ASP:OD2	3	0.28
(4,25)	1:148:A:GLN:N	1:146:A:ASP:OD2	6	0.28
(4,25)	1:148:A:GLN:N	1:146:A:ASP:OD2	7	0.28
(4,25)	1:148:A:GLN:N	1:146:A:ASP:OD2	8	0.28
(4,25)	1:148:A:GLN:N	1:146:A:ASP:OD2	9	0.28
(4,24)	1:146:A:ASP:OD2	1:148:A:GLN:N	2	0.28
(4,24)	1:146:A:ASP:OD2	1:148:A:GLN:N	3	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,24)	1:146:A:ASP:OD2	1:148:A:GLN:N	6	0.28
(4,24)	1:146:A:ASP:OD2	1:148:A:GLN:N	7	0.28
(4,24)	1:146:A:ASP:OD2	1:148:A:GLN:N	8	0.28
(4,24)	1:146:A:ASP:OD2	1:148:A:GLN:N	9	0.28
(3,537)	1:118:A:LEU:HA	1:183:A:ILE:HG12	3	0.28
(2,9104)	1:122:A:CYS:H	1:151:A:SER:HB2	4	0.28
(2,9082)	1:150:A:ARG:HG2	1:151:A:SER:H	6	0.28
(2,8781)	1:127:A:ILE:H	1:127:A:ILE:HG13	4	0.28
(2,8608)	1:151:A:SER:H	1:151:A:SER:HB2	10	0.28
(2,8464)	1:123:A:SER:HB3	1:126:A:GLU:HB2	2	0.28
(2,8430)	1:192:A:ARG:HD2	1:192:A:ARG:HB2	6	0.28
(2,8222)	1:173:A:LYS:HG2	1:173:A:LYS:HA	6	0.28
(2,8131)	1:163:A:GLU:HG3	1:163:A:GLU:H	6	0.28
(2,7514)	1:100:A:THR:HA	1:99:A:HIS:HB2	2	0.28
(2,7514)	1:100:A:THR:HA	1:99:A:HIS:HB2	6	0.28
(2,7514)	1:100:A:THR:HA	1:99:A:HIS:HB2	10	0.28
(2,7269)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	9	0.28
(2,6751)	1:151:A:SER:H	1:151:A:SER:HB2	3	0.28
(2,6751)	1:151:A:SER:H	1:151:A:SER:HB2	9	0.28
(2,6714)	1:108:A:ALA:H	1:189:A:ALA:H	8	0.28
(2,6616)	1:158:A:GLN:HG3	1:112:A:PHE:HA	2	0.28
(2,6592)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	6	0.28
(2,6461)	1:182:A:GLU:HB2	1:182:A:GLU:HG3	1	0.28
(2,6461)	1:182:A:GLU:HB2	1:182:A:GLU:HG3	2	0.28
(2,6461)	1:182:A:GLU:HB2	1:182:A:GLU:HG3	5	0.28
(2,5952)	1:135:A:GLU:HA	1:135:A:GLU:HG2	2	0.28
(2,5952)	1:135:A:GLU:HA	1:135:A:GLU:HG2	3	0.28
(2,5952)	1:135:A:GLU:HA	1:135:A:GLU:HG2	6	0.28
(2,5952)	1:135:A:GLU:HA	1:135:A:GLU:HG2	7	0.28
(2,5537)	1:155:A:ALA:HB2	1:154:A:GLU:H	6	0.28
(2,5473)	1:109:A:ASN:HA	1:108:A:ALA:HB1	2	0.28
(2,5473)	1:109:A:ASN:HA	1:108:A:ALA:HB1	5	0.28
(2,5404)	1:164:A:ILE:HD13	1:135:A:GLU:H	7	0.28
(2,5327)	1:190:A:GLU:HB3	1:190:A:GLU:H	3	0.28
(2,5327)	1:190:A:GLU:HB3	1:190:A:GLU:H	10	0.28
(2,4898)	1:159:A:PHE:H	1:110:A:ASP:HA	3	0.28
(2,4772)	1:155:A:ALA:HA	1:155:A:ALA:HB3	3	0.28
(2,4772)	1:155:A:ALA:HA	1:155:A:ALA:HB3	4	0.28
(2,4733)	1:192:A:ARG:HB2	1:192:A:ARG:H	2	0.28
(2,4468)	1:166:A:GLU:HB2	1:166:A:GLU:HA	4	0.28
(2,4321)	1:148:A:GLN:HB2	1:149:A:GLY:H	3	0.28
(2,3707)	1:188:A:ARG:HB2	1:187:A:SER:H	7	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3682)	1:134:A:LEU:HA	1:136:A:ILE:H	3	0.28
(2,3676)	1:175:A:ARG:HA	1:179:A:ARG:H	4	0.28
(2,3647)	1:191:A:VAL:HG13	1:193:A:THR:H	9	0.28
(2,3054)	1:167:A:LYS:HB3	1:168:A:ALA:H	8	0.28
(2,2625)	1:163:A:GLU:HG3	1:163:A:GLU:H	4	0.28
(2,2625)	1:163:A:GLU:HG3	1:163:A:GLU:H	7	0.28
(2,2437)	1:144:A:PRO:HD2	1:143:A:LEU:HA	9	0.28
(2,2102)	1:113:A:VAL:HB	1:113:A:VAL:HG22	1	0.28
(2,1901)	1:188:A:ARG:HB2	1:187:A:SER:H	9	0.28
(2,1806)	1:160:A:ALA:HB2	1:162:A:GLN:H	8	0.28
(2,1106)	1:191:A:VAL:HG11	1:191:A:VAL:HA	1	0.28
(2,1069)	1:187:A:SER:HB3	1:188:A:ARG:H	6	0.28
(2,871)	1:166:A:GLU:HG3	1:166:A:GLU:HA	5	0.28
(2,595)	1:139:A:ASN:HA	1:140:A:GLY:HA3	10	0.28
(2,418)	1:124:A:LYS:HA	1:124:A:LYS:HB2	1	0.28
(2,27)	1:181:A:ILE:HG21	1:174:A:GLU:H	3	0.28
(2,16)	1:113:A:VAL:HG11	1:113:A:VAL:HB	6	0.28
(1,3050)	1:145:A:VAL:HA	1:151:A:SER:H	3	0.28
(1,2992)	1:146:A:ASP:H	1:143:A:LEU:HD21	5	0.28
(1,2974)	1:100:A:THR:HG23	1:98:A:LYS:H	8	0.28
(1,2910)	1:168:A:ALA:HB3	1:167:A:LYS:H	1	0.28
(1,2817)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	1	0.28
(1,2746)	1:93:A:MET:HB2	1:135:A:GLU:HB3	7	0.28
(1,2477)	1:164:A:ILE:HD11	1:164:A:ILE:HB	5	0.28
(1,2403)	1:96:A:VAL:HB	1:97:A:LEU:H	1	0.28
(1,2324)	1:188:A:ARG:HA	1:186:A:SER:HA	6	0.28
(1,2319)	1:174:A:GLU:HA	1:181:A:ILE:H	3	0.28
(1,2207)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	8	0.28
(1,2140)	1:93:A:MET:HB2	1:135:A:GLU:HB3	9	0.28
(1,1961)	1:179:A:ARG:HB3	1:119:A:PRO:HD2	8	0.28
(1,1917)	1:166:A:GLU:HB2	1:168:A:ALA:H	9	0.28
(1,1881)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	7	0.28
(1,1881)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	9	0.28
(1,1864)	1:164:A:ILE:HD11	1:164:A:ILE:HB	5	0.28
(1,1850)	1:118:A:LEU:H	1:118:A:LEU:HD12	2	0.28
(1,1850)	1:118:A:LEU:H	1:118:A:LEU:HD12	5	0.28
(1,1706)	1:174:A:GLU:HA	1:181:A:ILE:H	7	0.28
(1,1670)	1:133:A:GLY:HA3	1:134:A:LEU:HG	6	0.28
(1,1670)	1:133:A:GLY:HA3	1:134:A:LEU:HG	10	0.28
(1,1658)	1:143:A:LEU:HD23	1:123:A:SER:HA	4	0.28
(1,1530)	1:164:A:ILE:HD13	1:93:A:MET:HG3	10	0.28
(1,1520)	1:141:A:ILE:HG21	1:143:A:LEU:HG	4	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1520)	1:141:A:ILE:HG21	1:143:A:LEU:HG	7	0.28
(1,1417)	1:169:A:LEU:HB2	1:169:A:LEU:HA	3	0.28
(1,1410)	1:156:A:PHE:HA	1:141:A:ILE:HA	1	0.28
(1,1297)	1:166:A:GLU:HB2	1:168:A:ALA:H	8	0.28
(1,1251)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	1	0.28
(1,1057)	1:133:A:GLY:HA3	1:134:A:LEU:HG	3	0.28
(1,1027)	1:164:A:ILE:HD13	1:135:A:GLU:HA	1	0.28
(1,1012)	1:119:A:PRO:HB3	1:119:A:PRO:HA	1	0.28
(1,1012)	1:119:A:PRO:HB3	1:119:A:PRO:HA	2	0.28
(1,1012)	1:119:A:PRO:HB3	1:119:A:PRO:HA	6	0.28
(1,988)	1:190:A:GLU:HG3	1:186:A:SER:HA	3	0.28
(1,937)	1:98:A:LYS:HB3	1:100:A:THR:HG23	10	0.28
(1,910)	1:141:A:ILE:HG21	1:143:A:LEU:HG	3	0.28
(1,846)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.28
(1,803)	1:156:A:PHE:HA	1:141:A:ILE:HA	1	0.28
(1,803)	1:156:A:PHE:HA	1:141:A:ILE:HA	10	0.28
(1,731)	1:119:A:PRO:HB3	1:119:A:PRO:HA	8	0.28
(1,691)	1:166:A:GLU:HB2	1:168:A:ALA:H	2	0.28
(1,681)	1:134:A:LEU:HD13	1:133:A:GLY:H	4	0.28
(1,618)	1:166:A:GLU:H	1:169:A:LEU:HD13	5	0.28
(1,458)	1:136:A:ILE:HG13	1:159:A:PHE:HA	10	0.28
(1,376)	1:174:A:GLU:HB2	1:181:A:ILE:HD13	3	0.28
(1,251)	1:112:A:PHE:HB2	1:191:A:VAL:HG22	4	0.28
(1,247)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	10	0.28
(1,222)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	3	0.28
(1,222)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	7	0.28
(1,222)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	10	0.28
(1,99)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	4	0.28
(1,99)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	7	0.28
(1,99)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	9	0.28
(1,39)	1:134:A:LEU:HD11	1:134:A:LEU:HG	1	0.28
(1,39)	1:134:A:LEU:HD11	1:134:A:LEU:HG	2	0.28
(1,39)	1:134:A:LEU:HD11	1:134:A:LEU:HG	4	0.28
(1,39)	1:134:A:LEU:HD11	1:134:A:LEU:HG	9	0.28
(1,8)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	2	0.28
(4,40)	1:168:A:ALA:H	1:164:A:ILE:O	4	0.27
(4,25)	1:148:A:GLN:N	1:146:A:ASP:OD2	1	0.27
(4,25)	1:148:A:GLN:N	1:146:A:ASP:OD2	5	0.27
(4,25)	1:148:A:GLN:N	1:146:A:ASP:OD2	10	0.27
(4,24)	1:146:A:ASP:OD2	1:148:A:GLN:N	1	0.27
(4,24)	1:146:A:ASP:OD2	1:148:A:GLN:N	5	0.27
(4,24)	1:146:A:ASP:OD2	1:148:A:GLN:N	10	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,8708)	1:112:A:PHE:H	1:112:A:PHE:HB3	7	0.27
(2,8697)	1:110:A:ASP:HA	1:110:A:ASP:H	2	0.27
(2,8697)	1:110:A:ASP:HA	1:110:A:ASP:H	4	0.27
(2,8608)	1:151:A:SER:H	1:151:A:SER:HB2	5	0.27
(2,8461)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	2	0.27
(2,8182)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	10	0.27
(2,7973)	1:144:A:PRO:HB2	1:144:A:PRO:HA	7	0.27
(2,7973)	1:144:A:PRO:HB2	1:144:A:PRO:HA	10	0.27
(2,7788)	1:130:A:PHE:HB2	1:131:A:PHE:H	2	0.27
(2,7569)	1:107:A:THR:HA	1:107:A:THR:HG22	1	0.27
(2,7569)	1:107:A:THR:HA	1:107:A:THR:HG22	2	0.27
(2,7569)	1:107:A:THR:HA	1:107:A:THR:HG22	3	0.27
(2,7569)	1:107:A:THR:HA	1:107:A:THR:HG22	4	0.27
(2,7569)	1:107:A:THR:HA	1:107:A:THR:HG22	5	0.27
(2,7569)	1:107:A:THR:HA	1:107:A:THR:HG22	10	0.27
(2,7344)	1:109:A:ASN:HA	1:108:A:ALA:HB1	2	0.27
(2,7344)	1:109:A:ASN:HA	1:108:A:ALA:HB1	5	0.27
(2,7322)	1:191:A:VAL:HG11	1:190:A:GLU:H	5	0.27
(2,7273)	1:164:A:ILE:HD13	1:135:A:GLU:H	1	0.27
(2,7273)	1:164:A:ILE:HD13	1:135:A:GLU:H	4	0.27
(2,7105)	1:166:A:GLU:HB3	1:167:A:LYS:H	7	0.27
(2,6740)	1:97:A:LEU:H	1:92:A:ALA:H	7	0.27
(2,6699)	1:168:A:ALA:H	1:167:A:LYS:HB3	3	0.27
(2,6627)	1:111:A:GLY:H	1:188:A:ARG:HG2	9	0.27
(2,6592)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	8	0.27
(2,6144)	1:148:A:GLN:HB2	1:149:A:GLY:H	1	0.27
(2,6100)	1:144:A:PRO:HB2	1:144:A:PRO:HA	7	0.27
(2,6100)	1:144:A:PRO:HB2	1:144:A:PRO:HA	10	0.27
(2,5821)	1:122:A:CYS:HA	1:121:A:GLY:H	8	0.27
(2,5821)	1:122:A:CYS:HA	1:121:A:GLY:H	9	0.27
(2,5498)	1:116:A:ARG:HD2	1:116:A:ARG:HA	4	0.27
(2,5444)	1:191:A:VAL:HG13	1:193:A:THR:H	2	0.27
(2,5404)	1:164:A:ILE:HD13	1:135:A:GLU:H	6	0.27
(2,5328)	1:190:A:GLU:HB3	1:191:A:VAL:H	7	0.27
(2,4772)	1:155:A:ALA:HA	1:155:A:ALA:HB3	2	0.27
(2,4772)	1:155:A:ALA:HA	1:155:A:ALA:HB3	7	0.27
(2,4772)	1:155:A:ALA:HA	1:155:A:ALA:HB3	8	0.27
(2,4772)	1:155:A:ALA:HA	1:155:A:ALA:HB3	10	0.27
(2,4755)	1:164:A:ILE:HD11	1:161:A:SER:HB2	3	0.27
(2,4733)	1:192:A:ARG:HB2	1:192:A:ARG:H	1	0.27
(2,4733)	1:192:A:ARG:HB2	1:192:A:ARG:H	7	0.27
(2,4012)	1:122:A:CYS:HA	1:122:A:CYS:HB2	3	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4012)	1:122:A:CYS:HA	1:122:A:CYS:HB2	4	0.27
(2,4012)	1:122:A:CYS:HA	1:122:A:CYS:HB2	5	0.27
(2,4012)	1:122:A:CYS:HA	1:122:A:CYS:HB2	6	0.27
(2,4012)	1:122:A:CYS:HA	1:122:A:CYS:HB2	7	0.27
(2,4012)	1:122:A:CYS:HA	1:122:A:CYS:HB2	9	0.27
(2,4012)	1:122:A:CYS:HA	1:122:A:CYS:HB2	10	0.27
(2,3728)	1:123:A:SER:HB3	1:181:A:ILE:HD11	1	0.27
(2,3622)	1:113:A:VAL:HG12	1:112:A:PHE:H	2	0.27
(2,3607)	1:164:A:ILE:HD13	1:91:A:ASN:HA	9	0.27
(2,2992)	1:161:A:SER:H	1:159:A:PHE:HB2	1	0.27
(2,2970)	1:111:A:GLY:HA3	1:109:A:ASN:H	5	0.27
(2,2965)	1:155:A:ALA:HA	1:155:A:ALA:HB3	3	0.27
(2,2965)	1:155:A:ALA:HA	1:155:A:ALA:HB3	4	0.27
(2,2925)	1:192:A:ARG:HB2	1:192:A:ARG:H	3	0.27
(2,2097)	1:111:A:GLY:HA3	1:112:A:PHE:H	8	0.27
(2,1923)	1:135:A:GLU:HA	1:164:A:ILE:HA	8	0.27
(2,1901)	1:188:A:ARG:HB2	1:187:A:SER:H	8	0.27
(2,1861)	1:154:A:GLU:HG2	1:118:A:LEU:H	10	0.27
(2,1838)	1:191:A:VAL:HG13	1:193:A:THR:H	2	0.27
(2,1822)	1:181:A:ILE:HG23	1:183:A:ILE:H	6	0.27
(2,1815)	1:176:A:ILE:HG22	1:120:A:PHE:H	7	0.27
(2,1813)	1:113:A:VAL:HG12	1:112:A:PHE:H	7	0.27
(2,1806)	1:160:A:ALA:HB2	1:162:A:GLN:H	2	0.27
(2,1777)	1:166:A:GLU:H	1:169:A:LEU:HB2	5	0.27
(2,1327)	1:96:A:VAL:HG13	1:97:A:LEU:H	6	0.27
(2,1243)	1:127:A:ILE:H	1:115:A:LEU:HD22	4	0.27
(2,1243)	1:127:A:ILE:H	1:115:A:LEU:HD22	10	0.27
(2,1169)	1:115:A:LEU:HD23	1:114:A:ARG:HA	3	0.27
(2,1169)	1:115:A:LEU:HD23	1:114:A:ARG:HA	4	0.27
(2,932)	1:174:A:GLU:HG3	1:175:A:ARG:H	2	0.27
(2,871)	1:166:A:GLU:HG3	1:166:A:GLU:HA	8	0.27
(2,829)	1:163:A:GLU:HB2	1:163:A:GLU:HG2	10	0.27
(2,595)	1:139:A:ASN:HA	1:140:A:GLY:HA3	8	0.27
(2,521)	1:134:A:LEU:HD11	1:134:A:LEU:HA	10	0.27
(2,76)	1:107:A:THR:HB	1:110:A:ASP:HA	1	0.27
(2,5)	1:164:A:ILE:HD13	1:91:A:ASN:HA	2	0.27
(2,5)	1:164:A:ILE:HD13	1:91:A:ASN:HA	5	0.27
(2,5)	1:164:A:ILE:HD13	1:91:A:ASN:HA	10	0.27
(1,3030)	1:165:A:ALA:H	1:110:A:ASP:HB3	4	0.27
(1,3013)	1:189:A:ALA:H	1:186:A:SER:HA	6	0.27
(1,2992)	1:146:A:ASP:H	1:143:A:LEU:HD21	7	0.27
(1,2817)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	2	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2817)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	4	0.27
(1,2817)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	7	0.27
(1,2817)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	9	0.27
(1,2738)	1:143:A:LEU:HG	1:141:A:ILE:HG21	1	0.27
(1,2706)	1:174:A:GLU:HA	1:175:A:ARG:HD2	8	0.27
(1,2377)	1:146:A:ASP:H	1:143:A:LEU:HD21	2	0.27
(1,2207)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	5	0.27
(1,2207)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	6	0.27
(1,2207)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	10	0.27
(1,2076)	1:150:A:ARG:HD3	1:149:A:GLY:H	8	0.27
(1,1961)	1:179:A:ARG:HB3	1:119:A:PRO:HD2	3	0.27
(1,1918)	1:163:A:GLU:HB2	1:164:A:ILE:HG12	4	0.27
(1,1908)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	2	0.27
(1,1877)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	4	0.27
(1,1877)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	8	0.27
(1,1798)	1:165:A:ALA:H	1:110:A:ASP:HB3	2	0.27
(1,1623)	1:119:A:PRO:HB3	1:119:A:PRO:HA	4	0.27
(1,1486)	1:143:A:LEU:HA	1:143:A:LEU:HB2	3	0.27
(1,1486)	1:169:A:LEU:HB2	1:166:A:GLU:HA	10	0.27
(1,1478)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	8	0.27
(1,1477)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	8	0.27
(1,1455)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.27
(1,1410)	1:156:A:PHE:HA	1:141:A:ILE:HA	3	0.27
(1,1337)	1:119:A:PRO:HB3	1:119:A:PRO:HA	5	0.27
(1,1337)	1:119:A:PRO:HB3	1:119:A:PRO:HA	7	0.27
(1,1337)	1:119:A:PRO:HB3	1:119:A:PRO:HA	8	0.27
(1,1327)	1:148:A:GLN:HB3	1:147:A:PHE:H	7	0.27
(1,1259)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	7	0.27
(1,1175)	1:106:A:ASP:H	1:105:A:PRO:HD2	9	0.27
(1,1012)	1:119:A:PRO:HB3	1:119:A:PRO:HA	3	0.27
(1,995)	1:123:A:SER:HB3	1:181:A:ILE:HD11	6	0.27
(1,869)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	2	0.27
(1,848)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	1	0.27
(1,809)	1:154:A:GLU:HG2	1:154:A:GLU:HA	2	0.27
(1,731)	1:119:A:PRO:HB3	1:119:A:PRO:HA	5	0.27
(1,731)	1:119:A:PRO:HB3	1:119:A:PRO:HA	7	0.27
(1,684)	1:167:A:LYS:HG2	1:134:A:LEU:HD11	9	0.27
(1,681)	1:134:A:LEU:HD13	1:133:A:GLY:H	5	0.27
(1,653)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	7	0.27
(1,541)	1:181:A:ILE:H	1:172:A:HIS:HA	6	0.27
(1,447)	1:154:A:GLU:HG2	1:118:A:LEU:HD23	7	0.27
(1,413)	1:162:A:GLN:HG3	1:110:A:ASP:HA	4	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:164:A:ILE:HD13	1:135:A:GLU:HA	6	0.27
(1,320)	1:169:A:LEU:HB2	1:169:A:LEU:HD11	7	0.27
(1,251)	1:188:A:ARG:HD3	1:191:A:VAL:HG22	1	0.27
(1,248)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	10	0.27
(1,247)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	3	0.27
(1,222)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	4	0.27
(1,222)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	8	0.27
(1,222)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	9	0.27
(1,39)	1:134:A:LEU:HD11	1:134:A:LEU:HG	7	0.27
(4,50)	1:183:A:ILE:H	1:181:A:ILE:O	4	0.26
(4,30)	1:157:A:VAL:H	1:113:A:VAL:O	5	0.26
(3,618)	1:152:A:THR:HB	1:117:A:GLY:H	2	0.26
(2,8960)	1:166:A:GLU:HB3	1:167:A:LYS:H	6	0.26
(2,8960)	1:166:A:GLU:HB3	1:167:A:LYS:H	9	0.26
(2,8781)	1:127:A:ILE:H	1:127:A:ILE:HG13	9	0.26
(2,8714)	1:114:A:ARG:H	1:113:A:VAL:HG12	6	0.26
(2,8697)	1:110:A:ASP:HA	1:110:A:ASP:H	1	0.26
(2,8697)	1:110:A:ASP:HA	1:110:A:ASP:H	5	0.26
(2,8608)	1:151:A:SER:H	1:151:A:SER:HB2	3	0.26
(2,8608)	1:151:A:SER:H	1:151:A:SER:HB2	9	0.26
(2,8017)	1:148:A:GLN:HB2	1:149:A:GLY:H	4	0.26
(2,7973)	1:144:A:PRO:HB2	1:144:A:PRO:HA	1	0.26
(2,7973)	1:144:A:PRO:HB2	1:144:A:PRO:HA	2	0.26
(2,7973)	1:144:A:PRO:HB2	1:144:A:PRO:HA	8	0.26
(2,7713)	1:126:A:GLU:HG3	1:127:A:ILE:H	7	0.26
(2,7569)	1:107:A:THR:HA	1:107:A:THR:HG22	6	0.26
(2,7569)	1:107:A:THR:HA	1:107:A:THR:HG22	7	0.26
(2,7394)	1:142:A:THR:HG21	1:141:A:ILE:HG21	6	0.26
(2,7372)	1:156:A:PHE:HB2	1:191:A:VAL:H	4	0.26
(2,7322)	1:191:A:VAL:HG11	1:190:A:GLU:H	1	0.26
(2,7280)	1:160:A:ALA:HB3	1:159:A:PHE:HB2	7	0.26
(2,7105)	1:166:A:GLU:HB3	1:167:A:LYS:H	2	0.26
(2,7096)	1:164:A:ILE:H	1:164:A:ILE:HG21	5	0.26
(2,6714)	1:108:A:ALA:H	1:189:A:ALA:H	9	0.26
(2,6621)	1:166:A:GLU:HA	1:169:A:LEU:HD11	2	0.26
(2,6461)	1:182:A:GLU:HB2	1:182:A:GLU:HG3	7	0.26
(2,6461)	1:182:A:GLU:HB2	1:182:A:GLU:HG3	8	0.26
(2,6461)	1:182:A:GLU:HB2	1:182:A:GLU:HG3	9	0.26
(2,6185)	1:155:A:ALA:HA	1:155:A:ALA:HB1	2	0.26
(2,6185)	1:155:A:ALA:HA	1:155:A:ALA:HB1	4	0.26
(2,6185)	1:155:A:ALA:HA	1:155:A:ALA:HB1	5	0.26
(2,6185)	1:155:A:ALA:HA	1:155:A:ALA:HB1	7	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6100)	1:144:A:PRO:HB2	1:144:A:PRO:HA	1	0.26
(2,6100)	1:144:A:PRO:HB2	1:144:A:PRO:HA	2	0.26
(2,6100)	1:144:A:PRO:HB2	1:144:A:PRO:HA	8	0.26
(2,5915)	1:130:A:PHE:HB2	1:131:A:PHE:H	2	0.26
(2,5404)	1:164:A:ILE:HD13	1:135:A:GLU:H	1	0.26
(2,5400)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	10	0.26
(2,5235)	1:164:A:ILE:H	1:164:A:ILE:HG21	9	0.26
(2,4898)	1:159:A:PHE:H	1:110:A:ASP:HA	2	0.26
(2,4797)	1:161:A:SER:H	1:159:A:PHE:HB2	1	0.26
(2,4650)	1:183:A:ILE:HG21	1:184:A:PHE:HA	10	0.26
(2,4012)	1:122:A:CYS:HA	1:122:A:CYS:HB2	2	0.26
(2,3906)	1:111:A:GLY:HA3	1:112:A:PHE:H	4	0.26
(2,3716)	1:188:A:ARG:HG2	1:189:A:ALA:H	2	0.26
(2,3716)	1:188:A:ARG:HG2	1:189:A:ALA:H	6	0.26
(2,3716)	1:188:A:ARG:HG2	1:189:A:ALA:H	7	0.26
(2,3682)	1:134:A:LEU:HA	1:136:A:ILE:H	5	0.26
(2,3682)	1:134:A:LEU:HA	1:136:A:ILE:H	6	0.26
(2,3682)	1:134:A:LEU:HA	1:136:A:ILE:H	8	0.26
(2,3682)	1:134:A:LEU:HA	1:136:A:ILE:H	10	0.26
(2,3581)	1:108:A:ALA:H	1:188:A:ARG:HG3	8	0.26
(2,3443)	1:166:A:GLU:HB3	1:166:A:GLU:H	8	0.26
(2,3435)	1:164:A:ILE:H	1:164:A:ILE:HG21	9	0.26
(2,3054)	1:167:A:LYS:HB3	1:168:A:ALA:H	5	0.26
(2,2965)	1:155:A:ALA:HA	1:155:A:ALA:HB3	2	0.26
(2,2965)	1:155:A:ALA:HA	1:155:A:ALA:HB3	8	0.26
(2,2965)	1:155:A:ALA:HA	1:155:A:ALA:HB3	10	0.26
(2,2954)	1:110:A:ASP:HB2	1:107:A:THR:HB	7	0.26
(2,2925)	1:192:A:ARG:HB2	1:192:A:ARG:H	10	0.26
(2,2097)	1:111:A:GLY:HA3	1:112:A:PHE:H	9	0.26
(2,1923)	1:135:A:GLU:HA	1:164:A:ILE:HA	2	0.26
(2,1918)	1:155:A:ALA:HB2	1:154:A:GLU:H	4	0.26
(2,1873)	1:187:A:SER:HB3	1:189:A:ALA:H	1	0.26
(2,1873)	1:187:A:SER:HB3	1:189:A:ALA:H	2	0.26
(2,1861)	1:154:A:GLU:HG2	1:118:A:LEU:H	3	0.26
(2,1806)	1:160:A:ALA:HB2	1:162:A:GLN:H	4	0.26
(2,1616)	1:162:A:GLN:HG3	1:162:A:GLN:H	6	0.26
(2,1600)	1:159:A:PHE:H	1:158:A:GLN:HG3	9	0.26
(2,903)	1:169:A:LEU:HB2	1:169:A:LEU:HD13	3	0.26
(2,871)	1:166:A:GLU:HG3	1:166:A:GLU:HA	1	0.26
(2,595)	1:139:A:ASN:HA	1:140:A:GLY:HA3	4	0.26
(2,595)	1:139:A:ASN:HA	1:140:A:GLY:HA3	6	0.26
(2,307)	1:111:A:GLY:HA3	1:112:A:PHE:H	4	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:107:A:THR:HB	1:110:A:ASP:HA	6	0.26
(2,74)	1:169:A:LEU:HB2	1:166:A:GLU:HA	3	0.26
(2,18)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	6	0.26
(2,5)	1:164:A:ILE:HD13	1:91:A:ASN:HA	7	0.26
(2,2)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	10	0.26
(1,2992)	1:146:A:ASP:H	1:143:A:LEU:HD21	8	0.26
(1,2992)	1:146:A:ASP:H	1:143:A:LEU:HD21	10	0.26
(1,2974)	1:100:A:THR:HG22	1:98:A:LYS:H	4	0.26
(1,2958)	1:189:A:ALA:HB2	1:190:A:GLU:H	7	0.26
(1,2908)	1:165:A:ALA:HA	1:113:A:VAL:HG23	10	0.26
(1,2817)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	8	0.26
(1,2674)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.26
(1,2588)	1:166:A:GLU:HG3	1:168:A:ALA:H	7	0.26
(1,2526)	1:166:A:GLU:HB3	1:168:A:ALA:H	4	0.26
(1,2495)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	4	0.26
(1,2495)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	8	0.26
(1,2483)	1:113:A:VAL:HG13	1:113:A:VAL:HB	8	0.26
(1,2432)	1:145:A:VAL:HA	1:151:A:SER:H	2	0.26
(1,2432)	1:145:A:VAL:HA	1:151:A:SER:H	6	0.26
(1,2377)	1:146:A:ASP:H	1:143:A:LEU:HD21	6	0.26
(1,2140)	1:93:A:MET:HB2	1:93:A:MET:HG2	6	0.26
(1,2140)	1:93:A:MET:HB2	1:93:A:MET:HG2	10	0.26
(1,2133)	1:143:A:LEU:HG	1:141:A:ILE:HG21	10	0.26
(1,2076)	1:159:A:PHE:HB2	1:166:A:GLU:H	3	0.26
(1,1959)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	2	0.26
(1,1959)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	4	0.26
(1,1881)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	6	0.26
(1,1877)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	2	0.26
(1,1877)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	7	0.26
(1,1869)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	6	0.26
(1,1798)	1:165:A:ALA:H	1:110:A:ASP:HB3	1	0.26
(1,1704)	1:166:A:GLU:HB2	1:166:A:GLU:HA	3	0.26
(1,1478)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	7	0.26
(1,1452)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.26
(1,1417)	1:169:A:LEU:HB2	1:169:A:LEU:HA	1	0.26
(1,1337)	1:119:A:PRO:HB3	1:119:A:PRO:HA	9	0.26
(1,1337)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.26
(1,1297)	1:166:A:GLU:HB2	1:168:A:ALA:H	3	0.26
(1,1027)	1:164:A:ILE:HD13	1:93:A:MET:HA	3	0.26
(1,1027)	1:164:A:ILE:HD13	1:135:A:GLU:HA	4	0.26
(1,1027)	1:164:A:ILE:HD13	1:93:A:MET:HA	9	0.26
(1,1012)	1:119:A:PRO:HB3	1:119:A:PRO:HA	4	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,985)	1:169:A:LEU:HD21	1:167:A:LYS:H	9	0.26
(1,917)	1:166:A:GLU:HB2	1:167:A:LYS:H	1	0.26
(1,910)	1:141:A:ILE:HG21	1:143:A:LEU:HG	5	0.26
(1,848)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	5	0.26
(1,803)	1:156:A:PHE:HA	1:141:A:ILE:HA	3	0.26
(1,731)	1:119:A:PRO:HB3	1:119:A:PRO:HA	1	0.26
(1,731)	1:119:A:PRO:HB3	1:119:A:PRO:HA	6	0.26
(1,731)	1:119:A:PRO:HB3	1:119:A:PRO:HA	9	0.26
(1,731)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.26
(1,681)	1:134:A:LEU:HD13	1:133:A:GLY:H	2	0.26
(1,595)	1:145:A:VAL:HA	1:151:A:SER:H	4	0.26
(1,417)	1:107:A:THR:HB	1:110:A:ASP:HB3	5	0.26
(1,377)	1:123:A:SER:HB3	1:181:A:ILE:HD11	4	0.26
(1,316)	1:98:A:LYS:HB3	1:100:A:THR:HG23	6	0.26
(1,248)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	3	0.26
(1,222)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	1	0.26
(1,222)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	5	0.26
(1,153)	1:130:A:PHE:HB3	1:132:A:SER:H	3	0.26
(1,99)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	5	0.26
(1,99)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	10	0.26
(1,3)	1:127:A:ILE:HD11	1:126:A:GLU:HB2	7	0.26
(4,40)	1:168:A:ALA:H	1:164:A:ILE:O	6	0.25
(4,30)	1:157:A:VAL:H	1:113:A:VAL:O	1	0.25
(4,25)	1:148:A:GLN:N	1:146:A:ASP:OD2	4	0.25
(4,24)	1:146:A:ASP:OD2	1:148:A:GLN:N	4	0.25
(4,8)	1:116:A:ARG:N	1:182:A:GLU:O	5	0.25
(3,618)	1:152:A:THR:HB	1:117:A:GLY:H	8	0.25
(2,9104)	1:122:A:CYS:H	1:151:A:SER:HB2	5	0.25
(2,8959)	1:166:A:GLU:HB3	1:166:A:GLU:H	8	0.25
(2,8796)	1:132:A:SER:HB2	1:133:A:GLY:H	10	0.25
(2,8779)	1:127:A:ILE:H	1:127:A:ILE:HG12	7	0.25
(2,8503)	1:187:A:SER:H	1:184:A:PHE:HB2	9	0.25
(2,7973)	1:144:A:PRO:HB2	1:144:A:PRO:HA	3	0.25
(2,7973)	1:144:A:PRO:HB2	1:144:A:PRO:HA	5	0.25
(2,7973)	1:144:A:PRO:HB2	1:144:A:PRO:HA	6	0.25
(2,7408)	1:155:A:ALA:HB2	1:154:A:GLU:H	1	0.25
(2,7379)	1:126:A:GLU:HA	1:136:A:ILE:HB	4	0.25
(2,7372)	1:156:A:PHE:HB2	1:191:A:VAL:H	10	0.25
(2,7356)	1:175:A:ARG:HA	1:179:A:ARG:H	6	0.25
(2,7356)	1:175:A:ARG:HA	1:179:A:ARG:H	9	0.25
(2,7322)	1:191:A:VAL:HG12	1:190:A:GLU:H	7	0.25
(2,7269)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	2	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7193)	1:190:A:GLU:HB3	1:190:A:GLU:H	4	0.25
(2,7096)	1:164:A:ILE:H	1:164:A:ILE:HG21	10	0.25
(2,6751)	1:151:A:SER:H	1:151:A:SER:HB2	1	0.25
(2,6638)	1:187:A:SER:H	1:184:A:PHE:HB2	5	0.25
(2,6461)	1:182:A:GLU:HB2	1:182:A:GLU:HG3	6	0.25
(2,6350)	1:173:A:LYS:HG2	1:173:A:LYS:HA	10	0.25
(2,6185)	1:155:A:ALA:HA	1:155:A:ALA:HB1	1	0.25
(2,6185)	1:155:A:ALA:HA	1:155:A:ALA:HB1	3	0.25
(2,6185)	1:155:A:ALA:HA	1:155:A:ALA:HB1	6	0.25
(2,6185)	1:155:A:ALA:HA	1:155:A:ALA:HB1	8	0.25
(2,6185)	1:155:A:ALA:HA	1:155:A:ALA:HB1	9	0.25
(2,6185)	1:155:A:ALA:HA	1:155:A:ALA:HB1	10	0.25
(2,6100)	1:144:A:PRO:HB2	1:144:A:PRO:HA	3	0.25
(2,6100)	1:144:A:PRO:HB2	1:144:A:PRO:HA	5	0.25
(2,6100)	1:144:A:PRO:HB2	1:144:A:PRO:HA	6	0.25
(2,5821)	1:122:A:CYS:HA	1:121:A:GLY:H	1	0.25
(2,5721)	1:111:A:GLY:HA3	1:112:A:PHE:H	10	0.25
(2,5499)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	1	0.25
(2,5404)	1:164:A:ILE:HD13	1:135:A:GLU:H	4	0.25
(2,5328)	1:190:A:GLU:HB3	1:191:A:VAL:H	9	0.25
(2,4934)	1:96:A:VAL:HG13	1:97:A:LEU:H	9	0.25
(2,4792)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	2	0.25
(2,4792)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	9	0.25
(2,4772)	1:155:A:ALA:HA	1:155:A:ALA:HB3	1	0.25
(2,4772)	1:155:A:ALA:HA	1:155:A:ALA:HB3	9	0.25
(2,4733)	1:192:A:ARG:HB2	1:192:A:ARG:H	9	0.25
(2,4650)	1:183:A:ILE:HG21	1:184:A:PHE:HA	4	0.25
(2,4430)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	2	0.25
(2,4430)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	5	0.25
(2,4430)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	6	0.25
(2,4012)	1:122:A:CYS:HA	1:122:A:CYS:HB2	1	0.25
(2,3726)	1:155:A:ALA:HB2	1:154:A:GLU:H	1	0.25
(2,3716)	1:188:A:ARG:HG2	1:189:A:ALA:H	5	0.25
(2,3682)	1:134:A:LEU:HA	1:136:A:ILE:H	9	0.25
(2,3633)	1:181:A:ILE:HG23	1:183:A:ILE:H	6	0.25
(2,3608)	1:164:A:ILE:HD11	1:161:A:SER:H	5	0.25
(2,3607)	1:164:A:ILE:HD13	1:91:A:ASN:HA	3	0.25
(2,3443)	1:166:A:GLU:HB3	1:166:A:GLU:H	3	0.25
(2,3443)	1:166:A:GLU:HB3	1:166:A:GLU:H	10	0.25
(2,3435)	1:164:A:ILE:H	1:164:A:ILE:HG21	8	0.25
(2,3208)	1:114:A:ARG:H	1:113:A:VAL:HG12	8	0.25
(2,2992)	1:161:A:SER:H	1:159:A:PHE:HB2	4	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2965)	1:155:A:ALA:HA	1:155:A:ALA:HB3	7	0.25
(2,2925)	1:192:A:ARG:HB2	1:192:A:ARG:H	2	0.25
(2,2511)	1:148:A:GLN:HB2	1:149:A:GLY:H	3	0.25
(2,1923)	1:135:A:GLU:HA	1:164:A:ILE:HA	1	0.25
(2,1923)	1:135:A:GLU:HA	1:164:A:ILE:HA	5	0.25
(2,1923)	1:135:A:GLU:HA	1:164:A:ILE:HA	7	0.25
(2,1918)	1:155:A:ALA:HB2	1:154:A:GLU:H	9	0.25
(2,1901)	1:188:A:ARG:HB2	1:187:A:SER:H	7	0.25
(2,1868)	1:150:A:ARG:HA	1:151:A:SER:H	4	0.25
(2,1861)	1:154:A:GLU:HG2	1:118:A:LEU:H	2	0.25
(2,1861)	1:154:A:GLU:HG2	1:118:A:LEU:H	8	0.25
(2,1861)	1:154:A:GLU:HG2	1:118:A:LEU:H	9	0.25
(2,1664)	1:175:A:ARG:HG2	1:176:A:ILE:H	3	0.25
(2,1327)	1:96:A:VAL:HG13	1:97:A:LEU:H	2	0.25
(2,1327)	1:96:A:VAL:HG13	1:97:A:LEU:H	3	0.25
(2,1327)	1:96:A:VAL:HG13	1:97:A:LEU:H	10	0.25
(2,871)	1:166:A:GLU:HG3	1:166:A:GLU:HA	10	0.25
(2,700)	1:145:A:VAL:HB	1:146:A:ASP:H	4	0.25
(2,595)	1:139:A:ASN:HA	1:140:A:GLY:HA3	5	0.25
(2,418)	1:124:A:LYS:HA	1:124:A:LYS:HB2	9	0.25
(2,365)	1:116:A:ARG:HD2	1:116:A:ARG:HB3	6	0.25
(2,80)	1:156:A:PHE:HA	1:141:A:ILE:HA	6	0.25
(2,76)	1:107:A:THR:HB	1:110:A:ASP:HA	2	0.25
(2,76)	1:107:A:THR:HB	1:110:A:ASP:HA	5	0.25
(2,63)	1:95:A:TRP:HB2	1:96:A:VAL:HG21	2	0.25
(1,2992)	1:146:A:ASP:H	1:143:A:LEU:HD21	2	0.25
(1,2958)	1:189:A:ALA:HB2	1:190:A:GLU:H	3	0.25
(1,2958)	1:189:A:ALA:HB2	1:190:A:GLU:H	10	0.25
(1,2949)	1:145:A:VAL:H	1:143:A:LEU:HD21	4	0.25
(1,2910)	1:168:A:ALA:HB2	1:167:A:LYS:H	4	0.25
(1,2910)	1:168:A:ALA:HB1	1:167:A:LYS:H	7	0.25
(1,2846)	1:152:A:THR:HA	1:117:A:GLY:H	1	0.25
(1,2817)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	5	0.25
(1,2817)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	6	0.25
(1,2817)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	10	0.25
(1,2675)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.25
(1,2495)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	2	0.25
(1,2495)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	7	0.25
(1,2495)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	9	0.25
(1,2388)	1:108:A:ALA:H	1:109:A:ASN:HA	3	0.25
(1,2377)	1:146:A:ASP:H	1:143:A:LEU:HD21	1	0.25
(1,2337)	1:145:A:VAL:H	1:143:A:LEU:HD21	4	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2238)	1:152:A:THR:HA	1:117:A:GLY:H	1	0.25
(1,1959)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.25
(1,1959)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.25
(1,1959)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	5	0.25
(1,1959)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.25
(1,1959)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.25
(1,1959)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	8	0.25
(1,1959)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	9	0.25
(1,1959)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.25
(1,1877)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	9	0.25
(1,1868)	1:113:A:VAL:HG13	1:113:A:VAL:HB	4	0.25
(1,1859)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	5	0.25
(1,1850)	1:118:A:LEU:H	1:118:A:LEU:HD12	9	0.25
(1,1725)	1:145:A:VAL:H	1:143:A:LEU:HD21	4	0.25
(1,1563)	1:166:A:GLU:HG3	1:168:A:ALA:H	4	0.25
(1,1530)	1:164:A:ILE:HD13	1:93:A:MET:HG3	6	0.25
(1,1524)	1:93:A:MET:HB2	1:93:A:MET:HG2	3	0.25
(1,1520)	1:141:A:ILE:HG21	1:143:A:LEU:HG	2	0.25
(1,1477)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	7	0.25
(1,1337)	1:119:A:PRO:HB3	1:119:A:PRO:HA	1	0.25
(1,1337)	1:119:A:PRO:HB3	1:119:A:PRO:HA	2	0.25
(1,1337)	1:119:A:PRO:HB3	1:119:A:PRO:HA	6	0.25
(1,1297)	1:166:A:GLU:HB2	1:168:A:ALA:H	7	0.25
(1,1286)	1:134:A:LEU:HD13	1:133:A:GLY:H	8	0.25
(1,1112)	1:145:A:VAL:H	1:143:A:LEU:HD21	4	0.25
(1,1014)	1:135:A:GLU:HA	1:136:A:ILE:HB	7	0.25
(1,995)	1:123:A:SER:HB3	1:181:A:ILE:HD11	10	0.25
(1,988)	1:190:A:GLU:HG3	1:186:A:SER:HA	6	0.25
(1,958)	1:96:A:VAL:HG23	1:96:A:VAL:HB	4	0.25
(1,958)	1:96:A:VAL:HG21	1:96:A:VAL:HB	7	0.25
(1,937)	1:98:A:LYS:HB3	1:100:A:THR:HG23	6	0.25
(1,910)	1:97:A:LEU:HD12	1:163:A:GLU:HB3	2	0.25
(1,869)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	7	0.25
(1,868)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	2	0.25
(1,846)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	1	0.25
(1,764)	1:166:A:GLU:HG3	1:168:A:ALA:H	4	0.25
(1,731)	1:119:A:PRO:HB3	1:119:A:PRO:HA	2	0.25
(1,731)	1:119:A:PRO:HB3	1:119:A:PRO:HA	3	0.25
(1,641)	1:141:A:ILE:HD12	1:125:A:GLU:H	8	0.25
(1,606)	1:185:A:LYS:HB3	1:185:A:LYS:H	8	0.25
(1,482)	1:141:A:ILE:HA	1:140:A:GLY:H	8	0.25
(1,447)	1:154:A:GLU:HG2	1:118:A:LEU:HD23	8	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:164:A:ILE:HD13	1:93:A:MET:HA	2	0.25
(1,343)	1:120:A:PHE:HA	1:120:A:PHE:HB2	2	0.25
(1,343)	1:159:A:PHE:HB2	1:159:A:PHE:HA	10	0.25
(1,178)	1:169:A:LEU:HB2	1:169:A:LEU:HA	3	0.25
(1,54)	1:166:A:GLU:HB2	1:168:A:ALA:H	2	0.25
(1,32)	1:141:A:ILE:HG21	1:141:A:ILE:HB	2	0.25
(1,8)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	10	0.25
(4,44)	1:182:A:GLU:H	1:116:A:ARG:O	6	0.24
(4,40)	1:168:A:ALA:H	1:164:A:ILE:O	1	0.24
(4,40)	1:168:A:ALA:H	1:164:A:ILE:O	5	0.24
(4,40)	1:168:A:ALA:H	1:164:A:ILE:O	10	0.24
(3,618)	1:152:A:THR:HB	1:117:A:GLY:H	9	0.24
(3,537)	1:118:A:LEU:HA	1:183:A:ILE:HG12	1	0.24
(2,9054)	1:192:A:ARG:HG2	1:192:A:ARG:H	3	0.24
(2,8960)	1:166:A:GLU:HB3	1:167:A:LYS:H	4	0.24
(2,8959)	1:166:A:GLU:HB3	1:166:A:GLU:H	3	0.24
(2,8895)	1:154:A:GLU:H	1:154:A:GLU:HB3	2	0.24
(2,8895)	1:154:A:GLU:H	1:154:A:GLU:HB3	10	0.24
(2,8779)	1:127:A:ILE:H	1:127:A:ILE:HG12	8	0.24
(2,8714)	1:114:A:ARG:H	1:113:A:VAL:HG13	7	0.24
(2,8217)	1:171:A:LYS:HB3	1:171:A:LYS:H	6	0.24
(2,8182)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	2	0.24
(2,7569)	1:107:A:THR:HA	1:107:A:THR:HG22	8	0.24
(2,7413)	1:181:A:ILE:HD12	1:183:A:ILE:H	3	0.24
(2,7377)	1:181:A:ILE:HG21	1:174:A:GLU:HA	2	0.24
(2,7307)	1:191:A:VAL:HG22	1:186:A:SER:HB2	1	0.24
(2,7200)	1:192:A:ARG:HG2	1:192:A:ARG:H	3	0.24
(2,7193)	1:190:A:GLU:HB3	1:190:A:GLU:H	3	0.24
(2,7193)	1:190:A:GLU:HB3	1:190:A:GLU:H	10	0.24
(2,6751)	1:151:A:SER:H	1:151:A:SER:HB2	8	0.24
(2,6733)	1:150:A:ARG:HB2	1:147:A:PHE:H	1	0.24
(2,6629)	1:161:A:SER:H	1:159:A:PHE:HB2	1	0.24
(2,6461)	1:182:A:GLU:HB2	1:182:A:GLU:HG3	10	0.24
(2,6072)	1:144:A:PRO:HD2	1:143:A:LEU:HA	9	0.24
(2,5721)	1:111:A:GLY:HA3	1:112:A:PHE:H	6	0.24
(2,5537)	1:155:A:ALA:HB2	1:154:A:GLU:H	3	0.24
(2,5402)	1:164:A:ILE:HD13	1:91:A:ASN:HA	5	0.24
(2,5328)	1:190:A:GLU:HB3	1:191:A:VAL:H	6	0.24
(2,5235)	1:164:A:ILE:H	1:164:A:ILE:HG21	8	0.24
(2,4997)	1:110:A:ASP:HB3	1:110:A:ASP:H	8	0.24
(2,4934)	1:96:A:VAL:HG13	1:97:A:LEU:H	8	0.24
(2,4797)	1:161:A:SER:H	1:159:A:PHE:HB2	4	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4733)	1:192:A:ARG:HB2	1:192:A:ARG:H	8	0.24
(2,4650)	1:183:A:ILE:HG21	1:184:A:PHE:HA	5	0.24
(2,4468)	1:166:A:GLU:HB2	1:166:A:GLU:HA	2	0.24
(2,4430)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	1	0.24
(2,4430)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	4	0.24
(2,4430)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	7	0.24
(2,4430)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	9	0.24
(2,4430)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	10	0.24
(2,3868)	1:105:A:PRO:HD3	1:104:A:SER:HB3	5	0.24
(2,3728)	1:123:A:SER:HB3	1:181:A:ILE:HD11	6	0.24
(2,3716)	1:188:A:ARG:HG2	1:189:A:ALA:H	1	0.24
(2,3682)	1:134:A:LEU:HA	1:136:A:ILE:H	1	0.24
(2,3682)	1:134:A:LEU:HA	1:136:A:ILE:H	4	0.24
(2,3676)	1:175:A:ARG:HA	1:179:A:ARG:H	6	0.24
(2,3676)	1:175:A:ARG:HA	1:179:A:ARG:H	9	0.24
(2,3622)	1:113:A:VAL:HG13	1:112:A:PHE:H	8	0.24
(2,3470)	1:175:A:ARG:HB3	1:176:A:ILE:H	5	0.24
(2,3050)	1:159:A:PHE:HA	1:135:A:GLU:H	9	0.24
(2,2965)	1:155:A:ALA:HA	1:155:A:ALA:HB3	1	0.24
(2,2965)	1:155:A:ALA:HA	1:155:A:ALA:HB3	9	0.24
(2,2947)	1:164:A:ILE:HD11	1:161:A:SER:HB2	3	0.24
(2,2925)	1:192:A:ARG:HB2	1:192:A:ARG:H	1	0.24
(2,2925)	1:192:A:ARG:HB2	1:192:A:ARG:H	7	0.24
(2,2578)	1:157:A:VAL:HG21	1:157:A:VAL:HA	4	0.24
(2,2578)	1:157:A:VAL:HG21	1:157:A:VAL:HA	5	0.24
(2,1921)	1:143:A:LEU:HG	1:123:A:SER:HA	8	0.24
(2,1918)	1:155:A:ALA:HB2	1:154:A:GLU:H	5	0.24
(2,1815)	1:176:A:ILE:HG22	1:120:A:PHE:H	2	0.24
(2,1815)	1:176:A:ILE:HG22	1:120:A:PHE:H	9	0.24
(2,1806)	1:160:A:ALA:HB2	1:162:A:GLN:H	3	0.24
(2,1797)	1:164:A:ILE:HD13	1:91:A:ASN:HA	6	0.24
(2,1777)	1:166:A:GLU:H	1:169:A:LEU:HB2	7	0.24
(2,1729)	1:191:A:VAL:HG13	1:191:A:VAL:H	1	0.24
(2,1664)	1:175:A:ARG:HG2	1:176:A:ILE:H	6	0.24
(2,1639)	1:166:A:GLU:HB3	1:167:A:LYS:H	2	0.24
(2,1639)	1:166:A:GLU:HB3	1:167:A:LYS:H	7	0.24
(2,829)	1:163:A:GLU:HB2	1:163:A:GLU:HG2	8	0.24
(2,816)	1:161:A:SER:HB2	1:162:A:GLN:H	3	0.24
(2,387)	1:119:A:PRO:HB2	1:119:A:PRO:HA	3	0.24
(2,387)	1:119:A:PRO:HB2	1:119:A:PRO:HA	7	0.24
(2,387)	1:119:A:PRO:HB2	1:119:A:PRO:HA	10	0.24
(2,239)	1:100:A:THR:HG22	1:100:A:THR:HB	4	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,225)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	8	0.24
(2,101)	1:151:A:SER:HB2	1:151:A:SER:HA	2	0.24
(2,25)	1:96:A:VAL:HG22	1:161:A:SER:H	1	0.24
(1,2992)	1:146:A:ASP:H	1:143:A:LEU:HD21	6	0.24
(1,2958)	1:189:A:ALA:HB2	1:190:A:GLU:H	4	0.24
(1,2958)	1:189:A:ALA:HB2	1:190:A:GLU:H	6	0.24
(1,2932)	1:174:A:GLU:HA	1:181:A:ILE:H	1	0.24
(1,2926)	1:156:A:PHE:HB3	1:142:A:THR:HB	8	0.24
(1,2773)	1:98:A:LYS:HB3	1:100:A:THR:HG23	10	0.24
(1,2739)	1:143:A:LEU:HG	1:141:A:ILE:HG21	10	0.24
(1,2636)	1:169:A:LEU:HA	1:169:A:LEU:HD11	1	0.24
(1,2635)	1:169:A:LEU:HB2	1:169:A:LEU:HA	4	0.24
(1,2576)	1:141:A:ILE:HG12	1:158:A:GLN:H	4	0.24
(1,2526)	1:166:A:GLU:HB2	1:168:A:ALA:H	6	0.24
(1,2515)	1:114:A:ARG:HG3	1:115:A:LEU:HD23	10	0.24
(1,2388)	1:108:A:ALA:H	1:109:A:ASN:HA	10	0.24
(1,2207)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	3	0.24
(1,1919)	1:166:A:GLU:HB3	1:167:A:LYS:HA	2	0.24
(1,1881)	1:96:A:VAL:HG23	1:93:A:MET:HG3	4	0.24
(1,1881)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.24
(1,1868)	1:183:A:ILE:HG22	1:113:A:VAL:HB	5	0.24
(1,1868)	1:113:A:VAL:HG13	1:113:A:VAL:HB	9	0.24
(1,1676)	1:156:A:PHE:HB2	1:157:A:VAL:HG21	8	0.24
(1,1598)	1:169:A:LEU:HD21	1:167:A:LYS:H	9	0.24
(1,1520)	1:141:A:ILE:HG21	1:143:A:LEU:HG	3	0.24
(1,1478)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	6	0.24
(1,1477)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	6	0.24
(1,1455)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	1	0.24
(1,1342)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	6	0.24
(1,1342)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	7	0.24
(1,1337)	1:119:A:PRO:HB3	1:119:A:PRO:HA	3	0.24
(1,1315)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	2	0.24
(1,1270)	1:141:A:ILE:HG21	1:141:A:ILE:HB	2	0.24
(1,1270)	1:141:A:ILE:HG21	1:141:A:ILE:HB	7	0.24
(1,1183)	1:166:A:GLU:HB2	1:167:A:LYS:H	1	0.24
(1,1175)	1:106:A:ASP:H	1:105:A:PRO:HD2	1	0.24
(1,1106)	1:161:A:SER:H	1:110:A:ASP:HB3	1	0.24
(1,958)	1:96:A:VAL:HG21	1:96:A:VAL:HB	1	0.24
(1,939)	1:169:A:LEU:HB2	1:169:A:LEU:HD11	2	0.24
(1,939)	1:169:A:LEU:HB2	1:169:A:LEU:HD11	5	0.24
(1,939)	1:169:A:LEU:HB2	1:169:A:LEU:HD11	6	0.24
(1,848)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	3	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	5	0.24
(1,458)	1:136:A:ILE:HG13	1:159:A:PHE:HA	2	0.24
(1,376)	1:174:A:GLU:HB2	1:181:A:ILE:HD13	9	0.24
(1,223)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	2	0.24
(1,223)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	3	0.24
(1,43)	1:134:A:LEU:HD13	1:133:A:GLY:H	3	0.24
(1,32)	1:141:A:ILE:HG21	1:141:A:ILE:HB	7	0.24
(1,32)	1:141:A:ILE:HG21	1:141:A:ILE:HB	9	0.24
(1,8)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	3	0.24
(4,23)	1:144:A:PRO:O	1:152:A:THR:OG1	9	0.23
(4,1)	1:113:A:VAL:H	1:157:A:VAL:O	6	0.23
(3,618)	1:152:A:THR:HB	1:117:A:GLY:H	3	0.23
(2,9104)	1:122:A:CYS:H	1:151:A:SER:HB2	10	0.23
(2,8959)	1:166:A:GLU:HB3	1:166:A:GLU:H	10	0.23
(2,8895)	1:154:A:GLU:H	1:154:A:GLU:HB3	3	0.23
(2,8895)	1:154:A:GLU:H	1:154:A:GLU:HB3	4	0.23
(2,8895)	1:154:A:GLU:H	1:154:A:GLU:HB3	5	0.23
(2,8781)	1:127:A:ILE:H	1:127:A:ILE:HG13	3	0.23
(2,8781)	1:127:A:ILE:H	1:127:A:ILE:HG13	6	0.23
(2,8608)	1:151:A:SER:H	1:151:A:SER:HB2	1	0.23
(2,8578)	1:143:A:LEU:H	1:141:A:ILE:HB	10	0.23
(2,8495)	1:161:A:SER:H	1:159:A:PHE:HB2	5	0.23
(2,8461)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	3	0.23
(2,8461)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	5	0.23
(2,8405)	1:191:A:VAL:HG22	1:191:A:VAL:HB	3	0.23
(2,8182)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	4	0.23
(2,8182)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	6	0.23
(2,8182)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	8	0.23
(2,7394)	1:142:A:THR:HG21	1:141:A:ILE:HG21	8	0.23
(2,7377)	1:181:A:ILE:HG21	1:174:A:GLU:HA	10	0.23
(2,7360)	1:187:A:SER:HB3	1:189:A:ALA:H	5	0.23
(2,7273)	1:164:A:ILE:HD13	1:135:A:GLU:H	8	0.23
(2,7096)	1:164:A:ILE:H	1:164:A:ILE:HG21	7	0.23
(2,6740)	1:97:A:LEU:H	1:92:A:ALA:H	1	0.23
(2,6699)	1:168:A:ALA:H	1:167:A:LYS:HB3	6	0.23
(2,6461)	1:182:A:GLU:HB2	1:182:A:GLU:HG3	3	0.23
(2,6461)	1:182:A:GLU:HB2	1:182:A:GLU:HG3	4	0.23
(2,5537)	1:155:A:ALA:HB2	1:154:A:GLU:H	10	0.23
(2,5519)	1:150:A:ARG:HB2	1:150:A:ARG:HA	3	0.23
(2,5519)	1:150:A:ARG:HB2	1:150:A:ARG:HA	5	0.23
(2,5499)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	5	0.23
(2,5498)	1:116:A:ARG:HD2	1:116:A:ARG:HA	5	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5466)	1:166:A:GLU:HG2	1:166:A:GLU:H	1	0.23
(2,5402)	1:164:A:ILE:HD13	1:91:A:ASN:HA	2	0.23
(2,5402)	1:164:A:ILE:HD13	1:91:A:ASN:HA	10	0.23
(2,5328)	1:190:A:GLU:HB3	1:191:A:VAL:H	2	0.23
(2,5328)	1:190:A:GLU:HB3	1:191:A:VAL:H	5	0.23
(2,5327)	1:190:A:GLU:HB3	1:190:A:GLU:H	1	0.23
(2,5327)	1:190:A:GLU:HB3	1:190:A:GLU:H	7	0.23
(2,4788)	1:158:A:GLN:HG3	1:112:A:PHE:HA	9	0.23
(2,4777)	1:111:A:GLY:HA3	1:109:A:ASN:H	4	0.23
(2,4772)	1:155:A:ALA:HA	1:155:A:ALA:HB3	6	0.23
(2,4650)	1:183:A:ILE:HG21	1:184:A:PHE:HA	3	0.23
(2,4650)	1:183:A:ILE:HG21	1:184:A:PHE:HA	9	0.23
(2,4586)	1:179:A:ARG:HG3	1:179:A:ARG:HD2	5	0.23
(2,4436)	1:163:A:GLU:HG3	1:163:A:GLU:H	3	0.23
(2,4436)	1:163:A:GLU:HG3	1:163:A:GLU:H	9	0.23
(2,4433)	1:163:A:GLU:HB3	1:164:A:ILE:H	5	0.23
(2,4430)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	3	0.23
(2,3731)	1:135:A:GLU:HA	1:164:A:ILE:HA	8	0.23
(2,3716)	1:188:A:ARG:HG2	1:189:A:ALA:H	4	0.23
(2,3568)	1:188:A:ARG:HG2	1:188:A:ARG:H	9	0.23
(2,3532)	1:190:A:GLU:HB3	1:190:A:GLU:H	4	0.23
(2,3532)	1:190:A:GLU:HB3	1:190:A:GLU:H	10	0.23
(2,3196)	1:110:A:ASP:HB3	1:110:A:ASP:H	2	0.23
(2,3196)	1:110:A:ASP:HB3	1:110:A:ASP:H	5	0.23
(2,3095)	1:159:A:PHE:H	1:110:A:ASP:HA	10	0.23
(2,3050)	1:159:A:PHE:HA	1:135:A:GLU:H	2	0.23
(2,3050)	1:159:A:PHE:HA	1:135:A:GLU:H	7	0.23
(2,2997)	1:145:A:VAL:H	1:155:A:ALA:HA	4	0.23
(2,2984)	1:188:A:ARG:HD2	1:108:A:ALA:H	3	0.23
(2,2660)	1:166:A:GLU:HG3	1:166:A:GLU:HA	3	0.23
(2,1923)	1:135:A:GLU:HA	1:164:A:ILE:HA	4	0.23
(2,1923)	1:135:A:GLU:HA	1:164:A:ILE:HA	6	0.23
(2,1923)	1:135:A:GLU:HA	1:164:A:ILE:HA	9	0.23
(2,1923)	1:135:A:GLU:HA	1:164:A:ILE:HA	10	0.23
(2,1867)	1:161:A:SER:HA	1:106:A:ASP:HB3	3	0.23
(2,1867)	1:161:A:SER:HA	1:106:A:ASP:HB3	8	0.23
(2,1749)	1:175:A:ARG:H	1:178:A:HIS:HA	1	0.23
(2,1667)	1:176:A:ILE:H	1:176:A:ILE:HD11	9	0.23
(2,1379)	1:107:A:THR:HG21	1:107:A:THR:H	9	0.23
(2,1169)	1:115:A:LEU:HD23	1:114:A:ARG:HA	1	0.23
(2,881)	1:167:A:LYS:HA	1:167:A:LYS:HG2	5	0.23
(2,880)	1:167:A:LYS:HB2	1:167:A:LYS:HA	2	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,880)	1:167:A:LYS:HB2	1:167:A:LYS:HA	6	0.23
(2,880)	1:167:A:LYS:HB2	1:167:A:LYS:HA	8	0.23
(2,880)	1:167:A:LYS:HB2	1:167:A:LYS:HA	10	0.23
(2,871)	1:166:A:GLU:HG3	1:166:A:GLU:HA	6	0.23
(2,816)	1:161:A:SER:HB2	1:162:A:GLN:H	5	0.23
(2,387)	1:119:A:PRO:HB2	1:119:A:PRO:HA	2	0.23
(2,299)	1:108:A:ALA:HB3	1:108:A:ALA:H	7	0.23
(2,239)	1:100:A:THR:HG22	1:100:A:THR:HB	3	0.23
(2,225)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	1	0.23
(2,225)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	4	0.23
(2,225)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	5	0.23
(2,225)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	10	0.23
(2,139)	1:102:A:PRO:HA	1:103:A:ASN:H	2	0.23
(2,80)	1:156:A:PHE:HA	1:141:A:ILE:HA	2	0.23
(2,80)	1:156:A:PHE:HA	1:141:A:ILE:HA	7	0.23
(2,80)	1:156:A:PHE:HA	1:141:A:ILE:HA	8	0.23
(2,69)	1:166:A:GLU:HG2	1:166:A:GLU:H	1	0.23
(2,27)	1:181:A:ILE:HG21	1:174:A:GLU:H	4	0.23
(2,25)	1:96:A:VAL:HG22	1:161:A:SER:H	4	0.23
(2,18)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	1	0.23
(1,3030)	1:165:A:ALA:H	1:110:A:ASP:HB3	2	0.23
(1,2958)	1:189:A:ALA:HB2	1:190:A:GLU:H	2	0.23
(1,2958)	1:189:A:ALA:HB2	1:190:A:GLU:H	8	0.23
(1,2958)	1:189:A:ALA:HB2	1:190:A:GLU:H	9	0.23
(1,2932)	1:174:A:GLU:HA	1:181:A:ILE:H	7	0.23
(1,2847)	1:119:A:PRO:HB3	1:119:A:PRO:HA	5	0.23
(1,2847)	1:119:A:PRO:HB3	1:119:A:PRO:HA	7	0.23
(1,2847)	1:119:A:PRO:HB3	1:119:A:PRO:HA	8	0.23
(1,2706)	1:143:A:LEU:HA	1:122:A:CYS:HB2	4	0.23
(1,2674)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	1	0.23
(1,2666)	1:115:A:LEU:HA	1:114:A:ARG:HG3	10	0.23
(1,2588)	1:166:A:GLU:HG3	1:168:A:ALA:H	2	0.23
(1,2566)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.23
(1,2566)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	2	0.23
(1,2566)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.23
(1,2566)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	4	0.23
(1,2566)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	5	0.23
(1,2566)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.23
(1,2566)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.23
(1,2566)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	8	0.23
(1,2566)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	9	0.23
(1,2566)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2526)	1:166:A:GLU:HB2	1:168:A:ALA:H	9	0.23
(1,2432)	1:145:A:VAL:HA	1:151:A:SER:H	10	0.23
(1,2403)	1:96:A:VAL:HB	1:97:A:LEU:H	7	0.23
(1,2377)	1:146:A:ASP:H	1:143:A:LEU:HD21	9	0.23
(1,2296)	1:165:A:ALA:HA	1:113:A:VAL:HG23	10	0.23
(1,2219)	1:174:A:GLU:HB2	1:181:A:ILE:HD13	7	0.23
(1,2133)	1:143:A:LEU:HG	1:141:A:ILE:HG21	4	0.23
(1,2076)	1:150:A:ARG:HD3	1:149:A:GLY:H	2	0.23
(1,2076)	1:150:A:ARG:HD3	1:149:A:GLY:H	6	0.23
(1,2069)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	7	0.23
(1,2068)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.23
(1,2030)	1:169:A:LEU:HB2	1:169:A:LEU:HA	4	0.23
(1,1981)	1:166:A:GLU:HG3	1:168:A:ALA:H	7	0.23
(1,1918)	1:163:A:GLU:HB2	1:164:A:ILE:HG12	1	0.23
(1,1877)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	6	0.23
(1,1859)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	7	0.23
(1,1850)	1:118:A:LEU:H	1:118:A:LEU:HD12	1	0.23
(1,1850)	1:118:A:LEU:H	1:118:A:LEU:HD12	4	0.23
(1,1850)	1:118:A:LEU:H	1:118:A:LEU:HD12	6	0.23
(1,1571)	1:96:A:VAL:HG23	1:96:A:VAL:HB	4	0.23
(1,1563)	1:166:A:GLU:HG3	1:168:A:ALA:H	6	0.23
(1,1486)	1:169:A:LEU:HB2	1:166:A:GLU:HA	5	0.23
(1,1486)	1:169:A:LEU:HB2	1:166:A:GLU:HA	8	0.23
(1,1478)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	9	0.23
(1,1477)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	9	0.23
(1,1455)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	5	0.23
(1,1452)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	1	0.23
(1,1342)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	4	0.23
(1,1342)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	9	0.23
(1,1337)	1:119:A:PRO:HB3	1:119:A:PRO:HA	4	0.23
(1,1289)	1:167:A:LYS:HG2	1:134:A:LEU:HD11	9	0.23
(1,1270)	1:141:A:ILE:HG21	1:141:A:ILE:HB	9	0.23
(1,1269)	1:137:A:VAL:HG22	1:140:A:GLY:H	10	0.23
(1,1259)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	8	0.23
(1,1175)	1:106:A:ASP:H	1:105:A:PRO:HD2	7	0.23
(1,1148)	1:146:A:ASP:H	1:143:A:LEU:HD21	5	0.23
(1,985)	1:169:A:LEU:HD21	1:167:A:LYS:H	4	0.23
(1,958)	1:96:A:VAL:HG21	1:96:A:VAL:HB	2	0.23
(1,958)	1:96:A:VAL:HG21	1:96:A:VAL:HB	3	0.23
(1,958)	1:96:A:VAL:HG21	1:96:A:VAL:HB	5	0.23
(1,958)	1:96:A:VAL:HG21	1:96:A:VAL:HB	6	0.23
(1,958)	1:96:A:VAL:HG21	1:96:A:VAL:HB	8	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:96:A:VAL:HG21	1:96:A:VAL:HB	10	0.23
(1,939)	1:169:A:LEU:HB2	1:169:A:LEU:HD11	9	0.23
(1,927)	1:164:A:ILE:HA	1:91:A:ASN:HB3	2	0.23
(1,869)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	6	0.23
(1,868)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	7	0.23
(1,764)	1:166:A:GLU:HG3	1:168:A:ALA:H	6	0.23
(1,731)	1:119:A:PRO:HB3	1:119:A:PRO:HA	4	0.23
(1,722)	1:148:A:GLN:HB3	1:147:A:PHE:H	10	0.23
(1,668)	1:141:A:ILE:HG21	1:141:A:ILE:HB	2	0.23
(1,653)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	8	0.23
(1,376)	1:174:A:GLU:HB2	1:181:A:ILE:HD13	5	0.23
(1,304)	1:150:A:ARG:HB2	1:150:A:ARG:HA	3	0.23
(1,288)	1:141:A:ILE:HG21	1:143:A:LEU:HG	10	0.23
(1,247)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	2	0.23
(1,226)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	2	0.23
(1,226)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	3	0.23
(1,223)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	7	0.23
(1,223)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	10	0.23
(1,222)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	6	0.23
(1,178)	1:169:A:LEU:HB2	1:169:A:LEU:HA	1	0.23
(1,32)	1:181:A:ILE:HG21	1:181:A:ILE:HB	6	0.23
(1,8)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	1	0.23
(1,8)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	4	0.23
(1,8)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	9	0.23
(4,50)	1:183:A:ILE:H	1:181:A:ILE:O	7	0.22
(4,36)	1:160:A:ALA:H	1:135:A:GLU:O	6	0.22
(4,30)	1:157:A:VAL:H	1:113:A:VAL:O	8	0.22
(3,618)	1:152:A:THR:HB	1:117:A:GLY:H	4	0.22
(2,9104)	1:122:A:CYS:H	1:151:A:SER:HB2	9	0.22
(2,9082)	1:150:A:ARG:HG2	1:151:A:SER:H	7	0.22
(2,9082)	1:150:A:ARG:HG2	1:151:A:SER:H	8	0.22
(2,8895)	1:154:A:GLU:H	1:154:A:GLU:HB3	9	0.22
(2,8779)	1:127:A:ILE:H	1:127:A:ILE:HG12	2	0.22
(2,8779)	1:127:A:ILE:H	1:127:A:ILE:HG12	3	0.22
(2,8608)	1:151:A:SER:H	1:151:A:SER:HB2	8	0.22
(2,8578)	1:143:A:LEU:H	1:141:A:ILE:HB	5	0.22
(2,8560)	1:168:A:ALA:H	1:167:A:LYS:HB3	2	0.22
(2,8503)	1:187:A:SER:H	1:184:A:PHE:HB2	8	0.22
(2,8414)	1:191:A:VAL:HG13	1:192:A:ARG:HA	4	0.22
(2,8405)	1:191:A:VAL:HG22	1:191:A:VAL:HB	4	0.22
(2,7514)	1:100:A:THR:HA	1:99:A:HIS:HB2	7	0.22
(2,7514)	1:100:A:THR:HA	1:99:A:HIS:HB2	8	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7379)	1:126:A:GLU:HA	1:136:A:ILE:HB	2	0.22
(2,7356)	1:175:A:ARG:HA	1:179:A:ARG:H	5	0.22
(2,7356)	1:175:A:ARG:HA	1:179:A:ARG:H	7	0.22
(2,7280)	1:160:A:ALA:HB3	1:159:A:PHE:HB2	3	0.22
(2,7096)	1:164:A:ILE:H	1:164:A:ILE:HG21	2	0.22
(2,7096)	1:164:A:ILE:H	1:164:A:ILE:HG21	4	0.22
(2,7096)	1:164:A:ILE:H	1:164:A:ILE:HG21	6	0.22
(2,6733)	1:150:A:ARG:HB2	1:147:A:PHE:H	3	0.22
(2,6733)	1:150:A:ARG:HB2	1:147:A:PHE:H	9	0.22
(2,6629)	1:161:A:SER:H	1:159:A:PHE:HB2	4	0.22
(2,5829)	1:124:A:LYS:HA	1:124:A:LYS:HB2	2	0.22
(2,5829)	1:124:A:LYS:HA	1:124:A:LYS:HB2	4	0.22
(2,5821)	1:122:A:CYS:HA	1:121:A:GLY:H	3	0.22
(2,5821)	1:122:A:CYS:HA	1:121:A:GLY:H	7	0.22
(2,5721)	1:111:A:GLY:HA3	1:112:A:PHE:H	8	0.22
(2,5643)	1:100:A:THR:HA	1:99:A:HIS:HB2	6	0.22
(2,5519)	1:150:A:ARG:HB2	1:150:A:ARG:HA	7	0.22
(2,5502)	1:156:A:PHE:HB2	1:191:A:VAL:H	1	0.22
(2,5482)	1:150:A:ARG:HA	1:151:A:SER:H	4	0.22
(2,5402)	1:164:A:ILE:HD13	1:91:A:ASN:HA	7	0.22
(2,5327)	1:190:A:GLU:HB3	1:190:A:GLU:H	5	0.22
(2,5086)	1:132:A:SER:HB2	1:133:A:GLY:H	9	0.22
(2,4997)	1:110:A:ASP:HB3	1:110:A:ASP:H	6	0.22
(2,4997)	1:110:A:ASP:HB3	1:110:A:ASP:H	7	0.22
(2,4934)	1:96:A:VAL:HG13	1:97:A:LEU:H	6	0.22
(2,4898)	1:159:A:PHE:H	1:110:A:ASP:HA	4	0.22
(2,4898)	1:159:A:PHE:H	1:110:A:ASP:HA	9	0.22
(2,4869)	1:108:A:ALA:H	1:188:A:ARG:HG2	3	0.22
(2,4869)	1:108:A:ALA:H	1:188:A:ARG:HG2	10	0.22
(2,4777)	1:111:A:GLY:HA3	1:109:A:ASN:H	2	0.22
(2,4733)	1:192:A:ARG:HB2	1:192:A:ARG:H	4	0.22
(2,4496)	1:169:A:LEU:HD22	1:169:A:LEU:HA	3	0.22
(2,4468)	1:166:A:GLU:HB2	1:166:A:GLU:HA	5	0.22
(2,4468)	1:166:A:GLU:HB2	1:166:A:GLU:HA	7	0.22
(2,3728)	1:123:A:SER:HB3	1:181:A:ILE:HD11	10	0.22
(2,3716)	1:188:A:ARG:HG2	1:189:A:ALA:H	8	0.22
(2,3698)	1:151:A:SER:HB2	1:151:A:SER:HA	2	0.22
(2,3682)	1:134:A:LEU:HA	1:136:A:ILE:H	2	0.22
(2,3682)	1:134:A:LEU:HA	1:136:A:ILE:H	7	0.22
(2,3668)	1:154:A:GLU:HG2	1:118:A:LEU:H	4	0.22
(2,3622)	1:113:A:VAL:HG12	1:112:A:PHE:H	4	0.22
(2,3608)	1:164:A:ILE:HD11	1:161:A:SER:H	10	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3568)	1:188:A:ARG:HG2	1:188:A:ARG:H	8	0.22
(2,3564)	1:149:A:GLY:HA3	1:151:A:SER:H	9	0.22
(2,3532)	1:190:A:GLU:HB3	1:190:A:GLU:H	3	0.22
(2,3470)	1:175:A:ARG:HB3	1:176:A:ILE:H	4	0.22
(2,3470)	1:175:A:ARG:HB3	1:176:A:ILE:H	10	0.22
(2,3197)	1:110:A:ASP:HB3	1:111:A:GLY:H	9	0.22
(2,3196)	1:110:A:ASP:HB3	1:110:A:ASP:H	1	0.22
(2,3050)	1:159:A:PHE:HA	1:135:A:GLU:H	4	0.22
(2,2984)	1:188:A:ARG:HD2	1:108:A:ALA:H	6	0.22
(2,2965)	1:155:A:ALA:HA	1:155:A:ALA:HB3	6	0.22
(2,2925)	1:192:A:ARG:HB2	1:192:A:ARG:H	9	0.22
(2,2625)	1:163:A:GLU:HG3	1:163:A:GLU:H	3	0.22
(2,2625)	1:163:A:GLU:HG3	1:163:A:GLU:H	9	0.22
(2,1861)	1:154:A:GLU:HG2	1:118:A:LEU:H	1	0.22
(2,1777)	1:166:A:GLU:H	1:169:A:LEU:HB2	6	0.22
(2,1729)	1:191:A:VAL:HG12	1:191:A:VAL:H	5	0.22
(2,1374)	1:106:A:ASP:H	1:105:A:PRO:HD2	3	0.22
(2,1207)	1:172:A:HIS:H	1:171:A:LYS:H	1	0.22
(2,1207)	1:172:A:HIS:H	1:171:A:LYS:H	10	0.22
(2,1169)	1:115:A:LEU:HD23	1:114:A:ARG:HA	5	0.22
(2,1169)	1:115:A:LEU:HD23	1:114:A:ARG:HA	10	0.22
(2,880)	1:167:A:LYS:HB2	1:167:A:LYS:HA	3	0.22
(2,880)	1:167:A:LYS:HB2	1:167:A:LYS:HA	4	0.22
(2,748)	1:151:A:SER:HB3	1:152:A:THR:H	3	0.22
(2,595)	1:139:A:ASN:HA	1:140:A:GLY:HA3	7	0.22
(2,490)	1:129:A:GLN:HG3	1:129:A:GLN:HB2	9	0.22
(2,418)	1:124:A:LYS:HA	1:124:A:LYS:HB2	3	0.22
(2,387)	1:119:A:PRO:HB2	1:119:A:PRO:HA	5	0.22
(2,387)	1:119:A:PRO:HB2	1:119:A:PRO:HA	8	0.22
(2,126)	1:115:A:LEU:HA	1:115:A:LEU:HD21	5	0.22
(2,126)	1:115:A:LEU:HA	1:115:A:LEU:HD21	8	0.22
(2,93)	1:116:A:ARG:HD2	1:116:A:ARG:H	6	0.22
(2,85)	1:187:A:SER:HB3	1:189:A:ALA:H	3	0.22
(1,3050)	1:145:A:VAL:HA	1:151:A:SER:H	6	0.22
(1,2992)	1:146:A:ASP:H	1:143:A:LEU:HD21	1	0.22
(1,2847)	1:119:A:PRO:HB3	1:119:A:PRO:HA	9	0.22
(1,2846)	1:152:A:THR:HA	1:117:A:GLY:H	9	0.22
(1,2817)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	3	0.22
(1,2675)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	1	0.22
(1,2675)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	5	0.22
(1,2674)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	5	0.22
(1,2666)	1:115:A:LEU:HA	1:114:A:ARG:HG3	1	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2666)	1:115:A:LEU:HA	1:114:A:ARG:HG3	7	0.22
(1,2635)	1:169:A:LEU:HB2	1:169:A:LEU:HA	6	0.22
(1,2495)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	6	0.22
(1,2472)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	5	0.22
(1,2377)	1:146:A:ASP:H	1:143:A:LEU:HD21	4	0.22
(1,2239)	1:119:A:PRO:HB3	1:119:A:PRO:HA	8	0.22
(1,2238)	1:152:A:THR:HA	1:117:A:GLY:H	9	0.22
(1,2140)	1:93:A:MET:HB2	1:135:A:GLU:HB3	5	0.22
(1,2101)	1:174:A:GLU:HA	1:175:A:ARG:HD2	8	0.22
(1,2076)	1:159:A:PHE:HB2	1:166:A:GLU:H	5	0.22
(1,2031)	1:169:A:LEU:HA	1:169:A:LEU:HD11	2	0.22
(1,2003)	1:130:A:PHE:HB3	1:132:A:SER:H	9	0.22
(1,1919)	1:166:A:GLU:HB3	1:167:A:LYS:HA	5	0.22
(1,1918)	1:163:A:GLU:HB2	1:96:A:VAL:HG13	7	0.22
(1,1798)	1:165:A:ALA:H	1:110:A:ASP:HB3	5	0.22
(1,1670)	1:133:A:GLY:HA3	1:134:A:LEU:HG	8	0.22
(1,1598)	1:169:A:LEU:HD21	1:167:A:LYS:H	4	0.22
(1,1571)	1:96:A:VAL:HG21	1:96:A:VAL:HB	7	0.22
(1,1478)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	1	0.22
(1,1478)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	10	0.22
(1,1477)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	1	0.22
(1,1452)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	5	0.22
(1,1417)	1:154:A:GLU:HG2	1:154:A:GLU:HA	2	0.22
(1,1315)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	3	0.22
(1,1286)	1:134:A:LEU:HD13	1:133:A:GLY:H	6	0.22
(1,1286)	1:134:A:LEU:HD13	1:133:A:GLY:H	10	0.22
(1,1270)	1:181:A:ILE:HG21	1:181:A:ILE:HB	6	0.22
(1,1270)	1:141:A:ILE:HG21	1:141:A:ILE:HB	10	0.22
(1,1260)	1:183:A:ILE:HG21	1:184:A:PHE:HA	10	0.22
(1,1148)	1:146:A:ASP:H	1:143:A:LEU:HD21	7	0.22
(1,1067)	1:165:A:ALA:HA	1:113:A:VAL:HG23	3	0.22
(1,1027)	1:164:A:ILE:HD13	1:93:A:MET:HA	10	0.22
(1,958)	1:96:A:VAL:HG21	1:96:A:VAL:HB	9	0.22
(1,939)	1:169:A:LEU:HB2	1:169:A:LEU:HD11	4	0.22
(1,910)	1:141:A:ILE:HG21	1:143:A:LEU:HG	9	0.22
(1,868)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	6	0.22
(1,846)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	3	0.22
(1,810)	1:169:A:LEU:HA	1:169:A:LEU:HD11	1	0.22
(1,668)	1:141:A:ILE:HG21	1:141:A:ILE:HB	7	0.22
(1,668)	1:141:A:ILE:HG21	1:141:A:ILE:HB	9	0.22
(1,641)	1:141:A:ILE:HD12	1:125:A:GLU:H	9	0.22
(1,618)	1:166:A:GLU:H	1:169:A:LEU:HD13	7	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:185:A:LYS:HB3	1:185:A:LYS:H	6	0.22
(1,482)	1:141:A:ILE:HA	1:140:A:GLY:H	2	0.22
(1,458)	1:136:A:ILE:HG13	1:159:A:PHE:HA	7	0.22
(1,338)	1:96:A:VAL:HG21	1:96:A:VAL:HB	5	0.22
(1,304)	1:150:A:ARG:HB2	1:150:A:ARG:HA	5	0.22
(1,248)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	2	0.22
(1,226)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	7	0.22
(1,226)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	10	0.22
(1,223)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	4	0.22
(1,223)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	8	0.22
(1,223)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	9	0.22
(1,32)	1:141:A:ILE:HG21	1:141:A:ILE:HB	10	0.22
(4,50)	1:183:A:ILE:H	1:181:A:ILE:O	2	0.21
(4,34)	1:159:A:PHE:H	1:111:A:GLY:O	6	0.21
(3,618)	1:152:A:THR:HB	1:117:A:GLY:H	1	0.21
(3,537)	1:118:A:LEU:HA	1:183:A:ILE:HG12	2	0.21
(2,8968)	1:171:A:LYS:H	1:170:A:LYS:HB2	6	0.21
(2,8895)	1:154:A:GLU:H	1:154:A:GLU:HB3	8	0.21
(2,8781)	1:127:A:ILE:H	1:127:A:ILE:HG13	8	0.21
(2,8781)	1:127:A:ILE:H	1:127:A:ILE:HG13	10	0.21
(2,8724)	1:114:A:ARG:HG3	1:115:A:LEU:H	9	0.21
(2,8688)	1:107:A:THR:HB	1:107:A:THR:H	1	0.21
(2,8688)	1:107:A:THR:HB	1:107:A:THR:H	5	0.21
(2,8578)	1:143:A:LEU:H	1:141:A:ILE:HB	4	0.21
(2,8560)	1:168:A:ALA:H	1:167:A:LYS:HB3	4	0.21
(2,8405)	1:191:A:VAL:HG22	1:191:A:VAL:HB	10	0.21
(2,8222)	1:173:A:LYS:HG2	1:173:A:LYS:HA	10	0.21
(2,7721)	1:127:A:ILE:HD12	1:127:A:ILE:HB	1	0.21
(2,7721)	1:127:A:ILE:HD12	1:127:A:ILE:HB	5	0.21
(2,7679)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	9	0.21
(2,7514)	1:100:A:THR:HA	1:99:A:HIS:HB2	5	0.21
(2,7413)	1:181:A:ILE:HD12	1:183:A:ILE:H	8	0.21
(2,7379)	1:126:A:GLU:HA	1:136:A:ILE:HB	1	0.21
(2,7379)	1:126:A:GLU:HA	1:136:A:ILE:HB	5	0.21
(2,7379)	1:126:A:GLU:HA	1:136:A:ILE:HB	8	0.21
(2,7356)	1:175:A:ARG:HA	1:179:A:ARG:H	10	0.21
(2,7344)	1:109:A:ASN:HA	1:108:A:ALA:HB1	9	0.21
(2,7300)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	8	0.21
(2,7180)	1:187:A:SER:HB3	1:188:A:ARG:H	5	0.21
(2,7180)	1:187:A:SER:HB3	1:188:A:ARG:H	7	0.21
(2,7180)	1:187:A:SER:HB3	1:188:A:ARG:H	9	0.21
(2,7096)	1:164:A:ILE:H	1:164:A:ILE:HG21	1	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7096)	1:164:A:ILE:H	1:164:A:ILE:HG21	3	0.21
(2,6784)	1:97:A:LEU:HB2	1:98:A:LYS:H	2	0.21
(2,6638)	1:187:A:SER:H	1:184:A:PHE:HB2	9	0.21
(2,6592)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	7	0.21
(2,6533)	1:191:A:VAL:HG22	1:191:A:VAL:HB	3	0.21
(2,5721)	1:111:A:GLY:HA3	1:112:A:PHE:H	9	0.21
(2,5643)	1:100:A:THR:HA	1:99:A:HIS:HB2	2	0.21
(2,5643)	1:100:A:THR:HA	1:99:A:HIS:HB2	10	0.21
(2,5537)	1:155:A:ALA:HB2	1:154:A:GLU:H	2	0.21
(2,5519)	1:150:A:ARG:HB2	1:150:A:ARG:HA	1	0.21
(2,5519)	1:150:A:ARG:HB2	1:150:A:ARG:HA	4	0.21
(2,5519)	1:150:A:ARG:HB2	1:150:A:ARG:HA	6	0.21
(2,5473)	1:109:A:ASN:HA	1:108:A:ALA:HB1	3	0.21
(2,5473)	1:109:A:ASN:HA	1:108:A:ALA:HB1	9	0.21
(2,5404)	1:164:A:ILE:HD13	1:135:A:GLU:H	8	0.21
(2,5327)	1:190:A:GLU:HB3	1:190:A:GLU:H	6	0.21
(2,5327)	1:190:A:GLU:HB3	1:190:A:GLU:H	8	0.21
(2,5327)	1:190:A:GLU:HB3	1:190:A:GLU:H	9	0.21
(2,4997)	1:110:A:ASP:HB3	1:110:A:ASP:H	3	0.21
(2,4898)	1:159:A:PHE:H	1:110:A:ASP:HA	1	0.21
(2,4898)	1:159:A:PHE:H	1:110:A:ASP:HA	8	0.21
(2,4869)	1:108:A:ALA:H	1:188:A:ARG:HG2	6	0.21
(2,4792)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	3	0.21
(2,4650)	1:183:A:ILE:HG21	1:184:A:PHE:HA	8	0.21
(2,4586)	1:179:A:ARG:HG3	1:179:A:ARG:HD2	4	0.21
(2,4586)	1:179:A:ARG:HG3	1:179:A:ARG:HD2	8	0.21
(2,4579)	1:179:A:ARG:HG2	1:179:A:ARG:HB3	6	0.21
(2,4477)	1:166:A:GLU:HG2	1:166:A:GLU:H	3	0.21
(2,4433)	1:163:A:GLU:HB3	1:164:A:ILE:H	2	0.21
(2,4015)	1:123:A:SER:HB2	1:123:A:SER:HA	8	0.21
(2,3731)	1:135:A:GLU:HA	1:164:A:ILE:HA	1	0.21
(2,3731)	1:135:A:GLU:HA	1:164:A:ILE:HA	2	0.21
(2,3731)	1:135:A:GLU:HA	1:164:A:ILE:HA	5	0.21
(2,3731)	1:135:A:GLU:HA	1:164:A:ILE:HA	7	0.21
(2,3716)	1:188:A:ARG:HG2	1:189:A:ALA:H	10	0.21
(2,3676)	1:175:A:ARG:HA	1:179:A:ARG:H	5	0.21
(2,3676)	1:175:A:ARG:HA	1:179:A:ARG:H	7	0.21
(2,3652)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	8	0.21
(2,3607)	1:164:A:ILE:HD13	1:91:A:ASN:HA	4	0.21
(2,3196)	1:110:A:ASP:HB3	1:110:A:ASP:H	4	0.21
(2,3179)	1:106:A:ASP:H	1:105:A:PRO:HD2	4	0.21
(2,3054)	1:167:A:LYS:HB3	1:168:A:ALA:H	10	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2925)	1:192:A:ARG:HB2	1:192:A:ARG:H	8	0.21
(2,2776)	1:179:A:ARG:HG3	1:179:A:ARG:HD2	5	0.21
(2,2666)	1:166:A:GLU:HG2	1:166:A:GLU:H	3	0.21
(2,2578)	1:157:A:VAL:HG21	1:157:A:VAL:HA	1	0.21
(2,2578)	1:157:A:VAL:HG21	1:157:A:VAL:HA	3	0.21
(2,1853)	1:95:A:TRP:HB3	1:91:A:ASN:HB3	2	0.21
(2,1853)	1:95:A:TRP:HB3	1:91:A:ASN:HB3	8	0.21
(2,1852)	1:95:A:TRP:HB2	1:96:A:VAL:HG21	5	0.21
(2,1813)	1:113:A:VAL:HG12	1:112:A:PHE:H	2	0.21
(2,1396)	1:112:A:PHE:H	1:111:A:GLY:H	1	0.21
(2,1215)	1:110:A:ASP:H	1:188:A:ARG:HG2	9	0.21
(2,1207)	1:172:A:HIS:H	1:171:A:LYS:H	6	0.21
(2,1169)	1:115:A:LEU:HD23	1:114:A:ARG:HA	2	0.21
(2,1169)	1:115:A:LEU:HD23	1:114:A:ARG:HA	8	0.21
(2,1168)	1:155:A:ALA:HA	1:155:A:ALA:HB3	5	0.21
(2,880)	1:167:A:LYS:HB2	1:167:A:LYS:HA	9	0.21
(2,871)	1:166:A:GLU:HG3	1:166:A:GLU:HA	2	0.21
(2,871)	1:166:A:GLU:HG3	1:166:A:GLU:HA	9	0.21
(2,829)	1:163:A:GLU:HB2	1:163:A:GLU:HG2	1	0.21
(2,829)	1:163:A:GLU:HB2	1:163:A:GLU:HG2	3	0.21
(2,677)	1:144:A:PRO:HB2	1:144:A:PRO:HA	4	0.21
(2,521)	1:134:A:LEU:HD11	1:134:A:LEU:HA	5	0.21
(2,387)	1:119:A:PRO:HB2	1:119:A:PRO:HA	1	0.21
(2,387)	1:119:A:PRO:HB2	1:119:A:PRO:HA	9	0.21
(2,126)	1:115:A:LEU:HA	1:115:A:LEU:HD21	2	0.21
(2,126)	1:115:A:LEU:HA	1:115:A:LEU:HD21	4	0.21
(2,126)	1:115:A:LEU:HA	1:115:A:LEU:HD21	10	0.21
(2,111)	1:188:A:ARG:HB2	1:189:A:ALA:H	3	0.21
(2,100)	1:181:A:ILE:HG21	1:174:A:GLU:HA	4	0.21
(2,80)	1:156:A:PHE:HA	1:141:A:ILE:HA	9	0.21
(2,76)	1:107:A:THR:HB	1:110:A:ASP:HA	9	0.21
(2,76)	1:107:A:THR:HB	1:110:A:ASP:HA	10	0.21
(2,63)	1:95:A:TRP:HB2	1:96:A:VAL:HG21	8	0.21
(2,27)	1:181:A:ILE:HG21	1:174:A:GLU:H	7	0.21
(2,27)	1:181:A:ILE:HG21	1:174:A:GLU:H	8	0.21
(2,16)	1:113:A:VAL:HG13	1:113:A:VAL:HB	8	0.21
(1,3050)	1:145:A:VAL:HA	1:151:A:SER:H	2	0.21
(1,3030)	1:165:A:ALA:H	1:110:A:ASP:HB3	1	0.21
(1,2958)	1:189:A:ALA:HB2	1:190:A:GLU:H	1	0.21
(1,2958)	1:189:A:ALA:HB2	1:190:A:GLU:H	5	0.21
(1,2910)	1:168:A:ALA:HB2	1:167:A:LYS:H	2	0.21
(1,2847)	1:119:A:PRO:HB3	1:119:A:PRO:HA	1	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2847)	1:119:A:PRO:HB3	1:119:A:PRO:HA	2	0.21
(1,2847)	1:119:A:PRO:HB3	1:119:A:PRO:HA	6	0.21
(1,2847)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.21
(1,2773)	1:98:A:LYS:HB3	1:100:A:THR:HG23	6	0.21
(1,2739)	1:143:A:LEU:HG	1:141:A:ILE:HG21	4	0.21
(1,2739)	1:143:A:LEU:HG	1:141:A:ILE:HG21	7	0.21
(1,2680)	1:175:A:ARG:HD2	1:178:A:HIS:HA	9	0.21
(1,2527)	1:163:A:GLU:HB2	1:164:A:ILE:HG12	4	0.21
(1,2483)	1:113:A:VAL:HG13	1:113:A:VAL:HB	4	0.21
(1,2316)	1:156:A:PHE:HB2	1:141:A:ILE:HG23	10	0.21
(1,2239)	1:119:A:PRO:HB3	1:119:A:PRO:HA	5	0.21
(1,2239)	1:119:A:PRO:HB3	1:119:A:PRO:HA	7	0.21
(1,2140)	1:93:A:MET:HB2	1:135:A:GLU:HB3	1	0.21
(1,2111)	1:175:A:ARG:HD2	1:178:A:HIS:HA	9	0.21
(1,2030)	1:169:A:LEU:HB2	1:169:A:LEU:HA	6	0.21
(1,1981)	1:166:A:GLU:HG3	1:168:A:ALA:H	2	0.21
(1,1948)	1:119:A:PRO:HB3	1:119:A:PRO:HA	5	0.21
(1,1948)	1:119:A:PRO:HB3	1:119:A:PRO:HA	7	0.21
(1,1948)	1:119:A:PRO:HB3	1:119:A:PRO:HA	8	0.21
(1,1917)	1:163:A:GLU:HB2	1:96:A:VAL:H	4	0.21
(1,1908)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	3	0.21
(1,1877)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.21
(1,1826)	1:184:A:PHE:H	1:186:A:SER:HB3	8	0.21
(1,1759)	1:146:A:ASP:H	1:143:A:LEU:HD21	5	0.21
(1,1670)	1:133:A:GLY:HA3	1:134:A:LEU:HG	9	0.21
(1,1571)	1:96:A:VAL:HG21	1:96:A:VAL:HB	1	0.21
(1,1552)	1:97:A:LEU:HG	1:97:A:LEU:HD13	1	0.21
(1,1552)	1:97:A:LEU:HG	1:97:A:LEU:HD13	3	0.21
(1,1552)	1:97:A:LEU:HG	1:97:A:LEU:HD11	7	0.21
(1,1550)	1:98:A:LYS:HB3	1:100:A:THR:HG23	10	0.21
(1,1520)	1:141:A:ILE:HG21	1:143:A:LEU:HG	5	0.21
(1,1477)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	10	0.21
(1,1455)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	3	0.21
(1,1342)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	5	0.21
(1,1342)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	10	0.21
(1,1315)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	9	0.21
(1,1315)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	10	0.21
(1,1286)	1:134:A:LEU:HD13	1:133:A:GLY:H	1	0.21
(1,1270)	1:141:A:ILE:HG21	1:141:A:ILE:HB	3	0.21
(1,1270)	1:141:A:ILE:HG21	1:141:A:ILE:HB	4	0.21
(1,1269)	1:137:A:VAL:HG22	1:140:A:GLY:H	5	0.21
(1,1260)	1:183:A:ILE:HG21	1:184:A:PHE:HA	4	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1259)	1:113:A:VAL:HG11	1:168:A:ALA:HB2	4	0.21
(1,1178)	1:132:A:SER:H	1:136:A:ILE:HB	1	0.21
(1,1148)	1:146:A:ASP:H	1:143:A:LEU:HD21	8	0.21
(1,1148)	1:146:A:ASP:H	1:143:A:LEU:HD21	10	0.21
(1,1027)	1:164:A:ILE:HD13	1:135:A:GLU:HA	5	0.21
(1,939)	1:97:A:LEU:HG	1:97:A:LEU:HD13	8	0.21
(1,939)	1:169:A:LEU:HB2	1:169:A:LEU:HD11	10	0.21
(1,910)	1:97:A:LEU:HD11	1:163:A:GLU:HB3	7	0.21
(1,869)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	1	0.21
(1,841)	1:111:A:GLY:HA3	1:188:A:ARG:HG3	2	0.21
(1,820)	1:98:A:LYS:HA	1:100:A:THR:HG23	5	0.21
(1,820)	1:98:A:LYS:HA	1:100:A:THR:HG23	7	0.21
(1,668)	1:181:A:ILE:HG21	1:181:A:ILE:HB	6	0.21
(1,625)	1:97:A:LEU:H	1:99:A:HIS:HA	4	0.21
(1,304)	1:150:A:ARG:HB2	1:150:A:ARG:HA	1	0.21
(1,304)	1:150:A:ARG:HB2	1:150:A:ARG:HA	7	0.21
(1,247)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	7	0.21
(1,226)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	4	0.21
(1,226)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	8	0.21
(1,226)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	9	0.21
(1,223)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	1	0.21
(1,223)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	5	0.21
(1,179)	1:169:A:LEU:HA	1:169:A:LEU:HD11	1	0.21
(1,32)	1:141:A:ILE:HG21	1:141:A:ILE:HB	3	0.21
(1,32)	1:141:A:ILE:HG21	1:141:A:ILE:HB	4	0.21
(3,618)	1:152:A:THR:HB	1:117:A:GLY:H	5	0.2
(2,9104)	1:122:A:CYS:H	1:151:A:SER:HB2	7	0.2
(2,8781)	1:127:A:ILE:H	1:127:A:ILE:HG13	2	0.2
(2,8781)	1:127:A:ILE:H	1:127:A:ILE:HG13	5	0.2
(2,8714)	1:114:A:ARG:H	1:113:A:VAL:HG12	8	0.2
(2,8578)	1:143:A:LEU:H	1:141:A:ILE:HB	6	0.2
(2,8461)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	10	0.2
(2,7679)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	5	0.2
(2,7679)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	6	0.2
(2,7679)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	7	0.2
(2,7679)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	8	0.2
(2,7679)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	10	0.2
(2,7413)	1:181:A:ILE:HD12	1:183:A:ILE:H	7	0.2
(2,7399)	1:166:A:GLU:HG2	1:168:A:ALA:H	7	0.2
(2,7344)	1:109:A:ASN:HA	1:108:A:ALA:HB1	3	0.2
(2,7105)	1:166:A:GLU:HB3	1:167:A:LYS:H	5	0.2
(2,6784)	1:97:A:LEU:HB2	1:98:A:LYS:H	5	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6784)	1:97:A:LEU:HB2	1:98:A:LYS:H	6	0.2
(2,6740)	1:97:A:LEU:H	1:92:A:ALA:H	4	0.2
(2,6616)	1:158:A:GLN:HG3	1:112:A:PHE:HA	9	0.2
(2,6596)	1:123:A:SER:HB3	1:126:A:GLU:HB2	8	0.2
(2,6533)	1:191:A:VAL:HG22	1:191:A:VAL:HB	4	0.2
(2,5539)	1:98:A:LYS:HB3	1:100:A:THR:HG22	3	0.2
(2,5537)	1:155:A:ALA:HB2	1:154:A:GLU:H	7	0.2
(2,5537)	1:155:A:ALA:HB2	1:154:A:GLU:H	8	0.2
(2,5506)	1:181:A:ILE:HG21	1:174:A:GLU:HA	7	0.2
(2,5473)	1:109:A:ASN:HA	1:108:A:ALA:HB1	8	0.2
(2,5413)	1:160:A:ALA:HB3	1:159:A:PHE:HB2	7	0.2
(2,5328)	1:190:A:GLU:HB3	1:191:A:VAL:H	1	0.2
(2,5328)	1:190:A:GLU:HB3	1:191:A:VAL:H	8	0.2
(2,5327)	1:190:A:GLU:HB3	1:190:A:GLU:H	2	0.2
(2,4934)	1:96:A:VAL:HG13	1:97:A:LEU:H	2	0.2
(2,4934)	1:96:A:VAL:HG13	1:97:A:LEU:H	3	0.2
(2,4650)	1:183:A:ILE:HG21	1:184:A:PHE:HA	2	0.2
(2,4579)	1:179:A:ARG:HG2	1:179:A:ARG:HB3	2	0.2
(2,4579)	1:179:A:ARG:HG2	1:179:A:ARG:HB3	7	0.2
(2,4579)	1:179:A:ARG:HG2	1:179:A:ARG:HB3	9	0.2
(2,4579)	1:179:A:ARG:HG2	1:179:A:ARG:HB3	10	0.2
(2,4477)	1:166:A:GLU:HG2	1:166:A:GLU:H	2	0.2
(2,4477)	1:166:A:GLU:HG2	1:166:A:GLU:H	8	0.2
(2,4477)	1:166:A:GLU:HG2	1:166:A:GLU:H	10	0.2
(2,4436)	1:163:A:GLU:HG3	1:163:A:GLU:H	5	0.2
(2,3911)	1:113:A:VAL:HB	1:113:A:VAL:HG22	1	0.2
(2,3903)	1:110:A:ASP:HB3	1:110:A:ASP:HA	6	0.2
(2,3868)	1:105:A:PRO:HD3	1:104:A:SER:HB3	4	0.2
(2,3716)	1:188:A:ARG:HG2	1:189:A:ALA:H	3	0.2
(2,3716)	1:188:A:ARG:HG2	1:189:A:ALA:H	9	0.2
(2,3676)	1:175:A:ARG:HA	1:179:A:ARG:H	10	0.2
(2,3674)	1:150:A:ARG:HA	1:151:A:SER:H	4	0.2
(2,3668)	1:154:A:GLU:HG2	1:118:A:LEU:H	5	0.2
(2,3668)	1:154:A:GLU:HG2	1:118:A:LEU:H	6	0.2
(2,3622)	1:113:A:VAL:HG12	1:112:A:PHE:H	5	0.2
(2,3608)	1:164:A:ILE:HD11	1:161:A:SER:H	8	0.2
(2,3184)	1:107:A:THR:HG21	1:107:A:THR:H	9	0.2
(2,3182)	1:107:A:THR:HA	1:108:A:ALA:H	8	0.2
(2,3050)	1:159:A:PHE:HA	1:135:A:GLU:H	5	0.2
(2,2776)	1:179:A:ARG:HG3	1:179:A:ARG:HD2	4	0.2
(2,2660)	1:166:A:GLU:HG3	1:166:A:GLU:HA	5	0.2
(2,2097)	1:111:A:GLY:HA3	1:112:A:PHE:H	3	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1923)	1:135:A:GLU:HA	1:164:A:ILE:HA	3	0.2
(2,1918)	1:155:A:ALA:HB2	1:154:A:GLU:H	1	0.2
(2,1861)	1:154:A:GLU:HG2	1:118:A:LEU:H	7	0.2
(2,1853)	1:95:A:TRP:HB3	1:91:A:ASN:HB3	6	0.2
(2,1852)	1:95:A:TRP:HB2	1:96:A:VAL:HG21	3	0.2
(2,1806)	1:160:A:ALA:HB2	1:162:A:GLN:H	10	0.2
(2,1797)	1:164:A:ILE:HD13	1:91:A:ASN:HA	9	0.2
(2,1207)	1:172:A:HIS:H	1:171:A:LYS:H	4	0.2
(2,1207)	1:172:A:HIS:H	1:171:A:LYS:H	9	0.2
(2,1021)	1:181:A:ILE:HG12	1:181:A:ILE:HD13	4	0.2
(2,1021)	1:181:A:ILE:HG12	1:181:A:ILE:HD13	5	0.2
(2,1021)	1:181:A:ILE:HG12	1:181:A:ILE:HD13	6	0.2
(2,1021)	1:181:A:ILE:HG12	1:181:A:ILE:HD13	9	0.2
(2,1021)	1:181:A:ILE:HG12	1:181:A:ILE:HD13	10	0.2
(2,880)	1:167:A:LYS:HB2	1:167:A:LYS:HA	1	0.2
(2,880)	1:167:A:LYS:HB2	1:167:A:LYS:HA	7	0.2
(2,871)	1:166:A:GLU:HG3	1:166:A:GLU:HA	7	0.2
(2,829)	1:163:A:GLU:HB2	1:163:A:GLU:HG2	9	0.2
(2,418)	1:124:A:LYS:HA	1:124:A:LYS:HB2	10	0.2
(2,387)	1:119:A:PRO:HB2	1:119:A:PRO:HA	6	0.2
(2,225)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	9	0.2
(2,139)	1:102:A:PRO:HA	1:103:A:ASN:H	5	0.2
(2,126)	1:115:A:LEU:HA	1:115:A:LEU:HD21	1	0.2
(2,126)	1:115:A:LEU:HA	1:115:A:LEU:HD21	3	0.2
(2,126)	1:115:A:LEU:HA	1:115:A:LEU:HD21	7	0.2
(2,80)	1:156:A:PHE:HA	1:141:A:ILE:HA	5	0.2
(2,76)	1:107:A:THR:HB	1:110:A:ASP:HA	4	0.2
(2,18)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	7	0.2
(1,3006)	1:117:A:GLY:H	1:118:A:LEU:HD12	3	0.2
(1,2992)	1:146:A:ASP:H	1:143:A:LEU:HD21	4	0.2
(1,2992)	1:146:A:ASP:H	1:143:A:LEU:HD21	9	0.2
(1,2847)	1:119:A:PRO:HB3	1:119:A:PRO:HA	3	0.2
(1,2677)	1:156:A:PHE:HB3	1:141:A:ILE:HG23	8	0.2
(1,2675)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	3	0.2
(1,2674)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	3	0.2
(1,2635)	1:169:A:LEU:HB2	1:169:A:LEU:HA	9	0.2
(1,2495)	1:127:A:ILE:HG22	1:127:A:ILE:HG13	10	0.2
(1,2483)	1:183:A:ILE:HG22	1:113:A:VAL:HB	5	0.2
(1,2483)	1:113:A:VAL:HG13	1:113:A:VAL:HB	9	0.2
(1,2472)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	7	0.2
(1,2405)	1:132:A:SER:H	1:136:A:ILE:HB	1	0.2
(1,2388)	1:108:A:ALA:H	1:109:A:ASN:HA	6	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2377)	1:146:A:ASP:H	1:143:A:LEU:HD21	3	0.2
(1,2239)	1:119:A:PRO:HB3	1:119:A:PRO:HA	1	0.2
(1,2239)	1:119:A:PRO:HB3	1:119:A:PRO:HA	6	0.2
(1,2239)	1:119:A:PRO:HB3	1:119:A:PRO:HA	9	0.2
(1,2239)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.2
(1,2076)	1:159:A:PHE:HB2	1:166:A:GLU:H	4	0.2
(1,2072)	1:175:A:ARG:HD2	1:178:A:HIS:HA	5	0.2
(1,2069)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	9	0.2
(1,2068)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	1	0.2
(1,2068)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	5	0.2
(1,1956)	1:181:A:ILE:HB	1:181:A:ILE:HA	2	0.2
(1,1956)	1:181:A:ILE:HB	1:181:A:ILE:HA	8	0.2
(1,1948)	1:119:A:PRO:HB3	1:119:A:PRO:HA	1	0.2
(1,1948)	1:119:A:PRO:HB3	1:119:A:PRO:HA	9	0.2
(1,1948)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.2
(1,1919)	1:166:A:GLU:HB3	1:167:A:LYS:HA	7	0.2
(1,1908)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	6	0.2
(1,1908)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	9	0.2
(1,1805)	1:158:A:GLN:H	1:141:A:ILE:HG23	4	0.2
(1,1759)	1:146:A:ASP:H	1:143:A:LEU:HD21	7	0.2
(1,1700)	1:114:A:ARG:HG3	1:114:A:ARG:HD2	5	0.2
(1,1625)	1:135:A:GLU:HA	1:136:A:ILE:HB	7	0.2
(1,1571)	1:96:A:VAL:HG21	1:96:A:VAL:HB	2	0.2
(1,1571)	1:96:A:VAL:HG21	1:96:A:VAL:HB	3	0.2
(1,1571)	1:96:A:VAL:HG21	1:96:A:VAL:HB	5	0.2
(1,1571)	1:96:A:VAL:HG21	1:96:A:VAL:HB	6	0.2
(1,1571)	1:96:A:VAL:HG21	1:96:A:VAL:HB	8	0.2
(1,1571)	1:96:A:VAL:HG21	1:96:A:VAL:HB	10	0.2
(1,1552)	1:97:A:LEU:HG	1:97:A:LEU:HD11	4	0.2
(1,1552)	1:97:A:LEU:HG	1:97:A:LEU:HD13	6	0.2
(1,1548)	1:110:A:ASP:HB3	1:188:A:ARG:HG2	6	0.2
(1,1537)	1:150:A:ARG:HB2	1:150:A:ARG:HA	3	0.2
(1,1478)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	3	0.2
(1,1478)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	5	0.2
(1,1452)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	3	0.2
(1,1442)	1:144:A:PRO:HD2	1:118:A:LEU:HD11	2	0.2
(1,1442)	1:144:A:PRO:HD2	1:118:A:LEU:HD11	5	0.2
(1,1339)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	6	0.2
(1,1315)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	8	0.2
(1,1304)	1:166:A:GLU:HB2	1:169:A:LEU:HD13	5	0.2
(1,1286)	1:134:A:LEU:HD13	1:133:A:GLY:H	7	0.2
(1,1270)	1:141:A:ILE:HG21	1:141:A:ILE:HB	1	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1270)	1:141:A:ILE:HG21	1:141:A:ILE:HB	5	0.2
(1,1234)	1:97:A:LEU:H	1:99:A:HIS:HA	2	0.2
(1,1175)	1:106:A:ASP:H	1:105:A:PRO:HD2	8	0.2
(1,1173)	1:189:A:ALA:H	1:186:A:SER:HA	4	0.2
(1,1148)	1:146:A:ASP:H	1:143:A:LEU:HD21	2	0.2
(1,1091)	1:174:A:GLU:HA	1:181:A:ILE:H	1	0.2
(1,1027)	1:164:A:ILE:HD13	1:93:A:MET:HA	7	0.2
(1,1014)	1:135:A:GLU:HA	1:136:A:ILE:HB	2	0.2
(1,995)	1:123:A:SER:HB3	1:181:A:ILE:HD11	2	0.2
(1,919)	1:165:A:ALA:HB3	1:113:A:VAL:HG23	9	0.2
(1,914)	1:93:A:MET:HB2	1:93:A:MET:HG2	3	0.2
(1,868)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	1	0.2
(1,764)	1:166:A:GLU:HG3	1:168:A:ALA:H	9	0.2
(1,691)	1:166:A:GLU:HB2	1:168:A:ALA:H	5	0.2
(1,668)	1:141:A:ILE:HG21	1:141:A:ILE:HB	10	0.2
(1,653)	1:113:A:VAL:HG11	1:168:A:ALA:HB2	4	0.2
(1,606)	1:114:A:ARG:HG3	1:115:A:LEU:H	5	0.2
(1,380)	1:134:A:LEU:HG	1:167:A:LYS:H	5	0.2
(1,304)	1:150:A:ARG:HB2	1:150:A:ARG:HA	4	0.2
(1,304)	1:150:A:ARG:HB2	1:150:A:ARG:HA	6	0.2
(1,288)	1:141:A:ILE:HG21	1:143:A:LEU:HG	4	0.2
(1,288)	1:141:A:ILE:HG21	1:143:A:LEU:HG	7	0.2
(1,248)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	7	0.2
(1,226)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	1	0.2
(1,226)	1:116:A:ARG:HG2	1:116:A:ARG:HD3	5	0.2
(1,32)	1:141:A:ILE:HG21	1:141:A:ILE:HB	1	0.2
(1,32)	1:141:A:ILE:HG21	1:141:A:ILE:HB	5	0.2
(4,34)	1:159:A:PHE:H	1:111:A:GLY:O	10	0.19
(2,8968)	1:171:A:LYS:H	1:170:A:LYS:HB2	3	0.19
(2,8968)	1:171:A:LYS:H	1:170:A:LYS:HB2	8	0.19
(2,8951)	1:164:A:ILE:H	1:164:A:ILE:HG21	5	0.19
(2,8895)	1:154:A:GLU:H	1:154:A:GLU:HB3	1	0.19
(2,8895)	1:154:A:GLU:H	1:154:A:GLU:HB3	7	0.19
(2,8779)	1:127:A:ILE:H	1:127:A:ILE:HG12	6	0.19
(2,8779)	1:127:A:ILE:H	1:127:A:ILE:HG12	9	0.19
(2,8779)	1:127:A:ILE:H	1:127:A:ILE:HG12	10	0.19
(2,8701)	1:110:A:ASP:HB3	1:110:A:ASP:H	2	0.19
(2,8701)	1:110:A:ASP:HB3	1:110:A:ASP:H	5	0.19
(2,8688)	1:107:A:THR:HB	1:107:A:THR:H	8	0.19
(2,8578)	1:143:A:LEU:H	1:141:A:ILE:HB	1	0.19
(2,8578)	1:143:A:LEU:H	1:141:A:ILE:HB	3	0.19
(2,8560)	1:168:A:ALA:H	1:167:A:LYS:HB3	1	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,8464)	1:123:A:SER:HB3	1:126:A:GLU:HB2	10	0.19
(2,8405)	1:191:A:VAL:HG22	1:191:A:VAL:HB	5	0.19
(2,8175)	1:166:A:GLU:HG2	1:166:A:GLU:H	1	0.19
(2,7679)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	1	0.19
(2,7679)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	2	0.19
(2,7679)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	4	0.19
(2,7413)	1:181:A:ILE:HD12	1:183:A:ILE:H	1	0.19
(2,7413)	1:181:A:ILE:HD12	1:183:A:ILE:H	6	0.19
(2,7372)	1:156:A:PHE:HB2	1:191:A:VAL:H	3	0.19
(2,7344)	1:109:A:ASN:HA	1:108:A:ALA:HB1	8	0.19
(2,7322)	1:191:A:VAL:HG11	1:190:A:GLU:H	8	0.19
(2,7320)	1:191:A:VAL:HG13	1:137:A:VAL:HG12	7	0.19
(2,7269)	1:164:A:ILE:HD11	1:159:A:PHE:HB2	6	0.19
(2,7193)	1:190:A:GLU:HB3	1:190:A:GLU:H	1	0.19
(2,7193)	1:190:A:GLU:HB3	1:190:A:GLU:H	7	0.19
(2,7180)	1:187:A:SER:HB3	1:188:A:ARG:H	1	0.19
(2,6784)	1:97:A:LEU:HB2	1:98:A:LYS:H	1	0.19
(2,6784)	1:97:A:LEU:HB2	1:98:A:LYS:H	3	0.19
(2,6784)	1:97:A:LEU:HB2	1:98:A:LYS:H	4	0.19
(2,6784)	1:97:A:LEU:HB2	1:98:A:LYS:H	7	0.19
(2,6784)	1:97:A:LEU:HB2	1:98:A:LYS:H	8	0.19
(2,6784)	1:97:A:LEU:HB2	1:98:A:LYS:H	9	0.19
(2,6784)	1:97:A:LEU:HB2	1:98:A:LYS:H	10	0.19
(2,6533)	1:191:A:VAL:HG22	1:191:A:VAL:HB	10	0.19
(2,5866)	1:127:A:ILE:HG23	1:127:A:ILE:HG12	4	0.19
(2,5840)	1:126:A:GLU:HG3	1:127:A:ILE:H	10	0.19
(2,5676)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	2	0.19
(2,5519)	1:150:A:ARG:HB2	1:150:A:ARG:HA	8	0.19
(2,5519)	1:150:A:ARG:HB2	1:150:A:ARG:HA	10	0.19
(2,5496)	1:183:A:ILE:HG12	1:116:A:ARG:HD2	6	0.19
(2,5473)	1:109:A:ASN:HA	1:108:A:ALA:HB1	6	0.19
(2,5451)	1:191:A:VAL:HG13	1:137:A:VAL:HG12	7	0.19
(2,5355)	1:158:A:GLN:H	1:141:A:ILE:HB	8	0.19
(2,4934)	1:96:A:VAL:HG13	1:97:A:LEU:H	10	0.19
(2,4477)	1:166:A:GLU:HG2	1:166:A:GLU:H	7	0.19
(2,4433)	1:163:A:GLU:HB3	1:164:A:ILE:H	10	0.19
(2,4390)	1:157:A:VAL:HG21	1:157:A:VAL:HA	4	0.19
(2,4390)	1:157:A:VAL:HG21	1:157:A:VAL:HA	5	0.19
(2,3903)	1:110:A:ASP:HB3	1:110:A:ASP:HA	3	0.19
(2,3793)	1:97:A:LEU:HD12	1:97:A:LEU:H	8	0.19
(2,3731)	1:135:A:GLU:HA	1:164:A:ILE:HA	4	0.19
(2,3731)	1:135:A:GLU:HA	1:164:A:ILE:HA	6	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3731)	1:135:A:GLU:HA	1:164:A:ILE:HA	9	0.19
(2,3731)	1:135:A:GLU:HA	1:164:A:ILE:HA	10	0.19
(2,3608)	1:164:A:ILE:HD11	1:161:A:SER:H	2	0.19
(2,3608)	1:164:A:ILE:HD11	1:161:A:SER:H	9	0.19
(2,3606)	1:164:A:ILE:HD12	1:164:A:ILE:HA	5	0.19
(2,3470)	1:175:A:ARG:HB3	1:176:A:ILE:H	7	0.19
(2,3470)	1:175:A:ARG:HB3	1:176:A:ILE:H	9	0.19
(2,3444)	1:166:A:GLU:HB3	1:167:A:LYS:H	7	0.19
(2,3091)	1:181:A:ILE:H	1:116:A:ARG:H	4	0.19
(2,3066)	1:108:A:ALA:H	1:188:A:ARG:HG2	3	0.19
(2,3066)	1:108:A:ALA:H	1:188:A:ARG:HG2	10	0.19
(2,2961)	1:126:A:GLU:HB2	1:123:A:SER:HB3	8	0.19
(2,2925)	1:192:A:ARG:HB2	1:192:A:ARG:H	4	0.19
(2,2861)	1:187:A:SER:HB3	1:188:A:ARG:H	7	0.19
(2,2776)	1:179:A:ARG:HG3	1:179:A:ARG:HD2	8	0.19
(2,2666)	1:166:A:GLU:HG2	1:166:A:GLU:H	2	0.19
(2,2666)	1:166:A:GLU:HG2	1:166:A:GLU:H	7	0.19
(2,2666)	1:166:A:GLU:HG2	1:166:A:GLU:H	8	0.19
(2,2666)	1:166:A:GLU:HG2	1:166:A:GLU:H	10	0.19
(2,2663)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	4	0.19
(2,2663)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	6	0.19
(2,2663)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	9	0.19
(2,2660)	1:166:A:GLU:HG3	1:166:A:GLU:HA	1	0.19
(2,2660)	1:166:A:GLU:HG3	1:166:A:GLU:HA	8	0.19
(2,2625)	1:163:A:GLU:HG3	1:163:A:GLU:H	5	0.19
(2,2578)	1:157:A:VAL:HG21	1:157:A:VAL:HA	2	0.19
(2,2459)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	1	0.19
(2,2210)	1:126:A:GLU:HB2	1:126:A:GLU:HA	1	0.19
(2,2210)	1:126:A:GLU:HB2	1:126:A:GLU:HA	3	0.19
(2,2210)	1:126:A:GLU:HB2	1:126:A:GLU:HA	8	0.19
(2,2210)	1:126:A:GLU:HB2	1:126:A:GLU:HA	9	0.19
(2,2090)	1:110:A:ASP:HB2	1:110:A:ASP:HA	1	0.19
(2,2090)	1:110:A:ASP:HB2	1:110:A:ASP:HA	2	0.19
(2,2090)	1:110:A:ASP:HB2	1:110:A:ASP:HA	5	0.19
(2,2090)	1:110:A:ASP:HB2	1:110:A:ASP:HA	10	0.19
(2,1893)	1:151:A:SER:HB2	1:151:A:SER:HA	2	0.19
(2,1853)	1:95:A:TRP:HB3	1:91:A:ASN:HB3	10	0.19
(2,1844)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	9	0.19
(2,1647)	1:171:A:LYS:H	1:170:A:LYS:HB2	10	0.19
(2,1404)	1:114:A:ARG:H	1:113:A:VAL:HG13	10	0.19
(2,1215)	1:110:A:ASP:H	1:188:A:ARG:HG2	8	0.19
(2,1169)	1:115:A:LEU:HD23	1:114:A:ARG:HA	7	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1168)	1:155:A:ALA:HA	1:155:A:ALA:HB3	3	0.19
(2,1021)	1:181:A:ILE:HG12	1:181:A:ILE:HD13	1	0.19
(2,1021)	1:181:A:ILE:HG12	1:181:A:ILE:HD13	2	0.19
(2,1021)	1:181:A:ILE:HG12	1:181:A:ILE:HD13	3	0.19
(2,996)	1:181:A:ILE:HD12	1:181:A:ILE:HB	6	0.19
(2,871)	1:166:A:GLU:HG3	1:166:A:GLU:HA	4	0.19
(2,677)	1:144:A:PRO:HB2	1:144:A:PRO:HA	7	0.19
(2,677)	1:144:A:PRO:HB2	1:144:A:PRO:HA	10	0.19
(2,139)	1:102:A:PRO:HA	1:103:A:ASN:H	1	0.19
(2,139)	1:102:A:PRO:HA	1:103:A:ASN:H	3	0.19
(2,139)	1:102:A:PRO:HA	1:103:A:ASN:H	4	0.19
(2,80)	1:156:A:PHE:HA	1:141:A:ILE:HA	4	0.19
(2,59)	1:148:A:GLN:HB3	1:147:A:PHE:H	7	0.19
(2,54)	1:191:A:VAL:HG13	1:137:A:VAL:HG12	7	0.19
(2,27)	1:181:A:ILE:HG21	1:174:A:GLU:H	1	0.19
(2,27)	1:181:A:ILE:HG21	1:174:A:GLU:H	2	0.19
(2,18)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	2	0.19
(2,18)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	3	0.19
(1,2908)	1:94:A:ASP:HA	1:164:A:ILE:HD13	8	0.19
(1,2847)	1:119:A:PRO:HB3	1:119:A:PRO:HA	4	0.19
(1,2746)	1:93:A:MET:HB2	1:93:A:MET:HG2	8	0.19
(1,2635)	1:169:A:LEU:HB2	1:169:A:LEU:HA	5	0.19
(1,2553)	1:119:A:PRO:HB3	1:119:A:PRO:HA	5	0.19
(1,2553)	1:119:A:PRO:HB3	1:119:A:PRO:HA	7	0.19
(1,2553)	1:119:A:PRO:HB3	1:119:A:PRO:HA	8	0.19
(1,2319)	1:174:A:GLU:HA	1:181:A:ILE:H	1	0.19
(1,2314)	1:156:A:PHE:HB3	1:142:A:THR:HB	8	0.19
(1,2239)	1:119:A:PRO:HB3	1:119:A:PRO:HA	2	0.19
(1,2239)	1:119:A:PRO:HB3	1:119:A:PRO:HA	3	0.19
(1,2133)	1:143:A:LEU:HG	1:141:A:ILE:HG21	3	0.19
(1,2030)	1:169:A:LEU:HB2	1:169:A:LEU:HA	9	0.19
(1,1956)	1:96:A:VAL:HB	1:96:A:VAL:HA	1	0.19
(1,1956)	1:181:A:ILE:HB	1:181:A:ILE:HA	3	0.19
(1,1956)	1:96:A:VAL:HB	1:96:A:VAL:HA	7	0.19
(1,1948)	1:119:A:PRO:HB3	1:119:A:PRO:HA	2	0.19
(1,1948)	1:119:A:PRO:HB3	1:119:A:PRO:HA	3	0.19
(1,1948)	1:119:A:PRO:HB3	1:119:A:PRO:HA	6	0.19
(1,1869)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	7	0.19
(1,1859)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	2	0.19
(1,1826)	1:184:A:PHE:H	1:186:A:SER:HB3	10	0.19
(1,1784)	1:189:A:ALA:H	1:186:A:SER:HA	3	0.19
(1,1759)	1:146:A:ASP:H	1:143:A:LEU:HD21	8	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1759)	1:146:A:ASP:H	1:143:A:LEU:HD21	10	0.19
(1,1638)	1:164:A:ILE:HD13	1:135:A:GLU:HA	1	0.19
(1,1571)	1:96:A:VAL:HG21	1:96:A:VAL:HB	9	0.19
(1,1563)	1:166:A:GLU:HG3	1:168:A:ALA:H	9	0.19
(1,1552)	1:97:A:LEU:HG	1:97:A:LEU:HD11	10	0.19
(1,1537)	1:150:A:ARG:HB2	1:150:A:ARG:HA	5	0.19
(1,1537)	1:150:A:ARG:HB2	1:150:A:ARG:HA	7	0.19
(1,1478)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	2	0.19
(1,1477)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	3	0.19
(1,1477)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	5	0.19
(1,1339)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	9	0.19
(1,1270)	1:141:A:ILE:HG21	1:141:A:ILE:HB	8	0.19
(1,1260)	1:183:A:ILE:HG21	1:184:A:PHE:HA	3	0.19
(1,1260)	1:183:A:ILE:HG21	1:184:A:PHE:HA	5	0.19
(1,1260)	1:183:A:ILE:HG21	1:184:A:PHE:HA	9	0.19
(1,1173)	1:189:A:ALA:H	1:186:A:SER:HA	7	0.19
(1,1173)	1:189:A:ALA:H	1:186:A:SER:HA	10	0.19
(1,1148)	1:146:A:ASP:H	1:143:A:LEU:HD21	6	0.19
(1,1091)	1:174:A:GLU:HA	1:181:A:ILE:H	7	0.19
(1,1090)	1:166:A:GLU:HB2	1:166:A:GLU:HA	2	0.19
(1,1087)	1:114:A:ARG:HG3	1:114:A:ARG:HD2	5	0.19
(1,995)	1:123:A:SER:HB3	1:181:A:ILE:HD11	5	0.19
(1,869)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	5	0.19
(1,869)	1:114:A:ARG:HD3	1:114:A:ARG:HB3	8	0.19
(1,668)	1:141:A:ILE:HG21	1:141:A:ILE:HB	3	0.19
(1,668)	1:141:A:ILE:HG21	1:141:A:ILE:HB	4	0.19
(1,645)	1:164:A:ILE:HD13	1:91:A:ASN:HB3	6	0.19
(1,641)	1:141:A:ILE:HD13	1:125:A:GLU:H	2	0.19
(1,376)	1:174:A:GLU:HB2	1:181:A:ILE:HD13	10	0.19
(1,304)	1:150:A:ARG:HB2	1:150:A:ARG:HA	10	0.19
(1,247)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	6	0.19
(1,223)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	6	0.19
(1,207)	1:154:A:GLU:HB2	1:144:A:PRO:HD2	3	0.19
(1,178)	1:154:A:GLU:HG2	1:154:A:GLU:HA	2	0.19
(1,94)	1:119:A:PRO:HB3	1:119:A:PRO:HA	7	0.19
(1,94)	1:119:A:PRO:HB3	1:119:A:PRO:HA	8	0.19
(1,32)	1:141:A:ILE:HG21	1:141:A:ILE:HB	8	0.19
(4,41)	1:168:A:ALA:N	1:164:A:ILE:O	8	0.18
(4,10)	1:117:A:GLY:N	1:153:A:GLY:O	5	0.18
(4,10)	1:117:A:GLY:N	1:153:A:GLY:O	6	0.18
(4,10)	1:117:A:GLY:N	1:153:A:GLY:O	7	0.18
(4,4)	1:114:A:ARG:N	1:184:A:PHE:O	2	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,627)	1:108:A:ALA:H	1:189:A:ALA:H	8	0.18
(3,625)	1:139:A:ASN:H	1:128:A:VAL:HA	9	0.18
(3,618)	1:152:A:THR:HB	1:117:A:GLY:H	6	0.18
(3,618)	1:152:A:THR:HB	1:117:A:GLY:H	10	0.18
(3,499)	1:139:A:ASN:H	1:128:A:VAL:HA	9	0.18
(2,9104)	1:122:A:CYS:H	1:151:A:SER:HB2	2	0.18
(2,9104)	1:122:A:CYS:H	1:151:A:SER:HB2	3	0.18
(2,8951)	1:164:A:ILE:H	1:164:A:ILE:HG21	10	0.18
(2,8701)	1:110:A:ASP:HB3	1:110:A:ASP:H	1	0.18
(2,8688)	1:107:A:THR:HB	1:107:A:THR:H	7	0.18
(2,8566)	1:139:A:ASN:H	1:141:A:ILE:HD12	6	0.18
(2,8503)	1:187:A:SER:H	1:184:A:PHE:HB2	7	0.18
(2,8431)	1:192:A:ARG:HD3	1:192:A:ARG:HB2	3	0.18
(2,8405)	1:191:A:VAL:HG22	1:191:A:VAL:HB	1	0.18
(2,7693)	1:122:A:CYS:HA	1:121:A:GLY:H	6	0.18
(2,7679)	1:119:A:PRO:HB3	1:119:A:PRO:HG2	3	0.18
(2,7388)	1:150:A:ARG:HB2	1:150:A:ARG:HA	3	0.18
(2,7379)	1:126:A:GLU:HA	1:136:A:ILE:HB	3	0.18
(2,7344)	1:109:A:ASN:HA	1:108:A:ALA:HB1	6	0.18
(2,7322)	1:191:A:VAL:HG11	1:190:A:GLU:H	2	0.18
(2,7290)	1:96:A:VAL:HG22	1:97:A:LEU:H	5	0.18
(2,7193)	1:190:A:GLU:HB3	1:190:A:GLU:H	5	0.18
(2,6740)	1:97:A:LEU:H	1:92:A:ALA:H	3	0.18
(2,6733)	1:150:A:ARG:HB2	1:147:A:PHE:H	5	0.18
(2,6638)	1:187:A:SER:H	1:184:A:PHE:HB2	8	0.18
(2,6599)	1:155:A:ALA:HA	1:155:A:ALA:HB3	5	0.18
(2,6558)	1:192:A:ARG:HD2	1:192:A:ARG:HB2	4	0.18
(2,6533)	1:191:A:VAL:HG22	1:191:A:VAL:HB	5	0.18
(2,5829)	1:124:A:LYS:HA	1:124:A:LYS:HB2	1	0.18
(2,5519)	1:150:A:ARG:HB2	1:150:A:ARG:HA	2	0.18
(2,5519)	1:150:A:ARG:HB2	1:150:A:ARG:HA	9	0.18
(2,5444)	1:191:A:VAL:HG13	1:193:A:THR:H	7	0.18
(2,5432)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	8	0.18
(2,4907)	1:151:A:SER:H	1:151:A:SER:HB2	7	0.18
(2,4898)	1:159:A:PHE:H	1:110:A:ASP:HA	5	0.18
(2,4657)	1:183:A:ILE:HA	1:183:A:ILE:HD11	9	0.18
(2,4650)	1:183:A:ILE:HG21	1:184:A:PHE:HA	6	0.18
(2,4496)	1:169:A:LEU:HD22	1:169:A:LEU:HA	7	0.18
(2,4468)	1:166:A:GLU:HB2	1:166:A:GLU:HA	3	0.18
(2,4468)	1:166:A:GLU:HB2	1:166:A:GLU:HA	10	0.18
(2,4436)	1:163:A:GLU:HG3	1:163:A:GLU:H	1	0.18
(2,3903)	1:110:A:ASP:HB3	1:110:A:ASP:HA	7	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3679)	1:187:A:SER:HB3	1:189:A:ALA:H	6	0.18
(2,3679)	1:187:A:SER:HB3	1:189:A:ALA:H	7	0.18
(2,3606)	1:164:A:ILE:HD12	1:164:A:ILE:HA	10	0.18
(2,3532)	1:190:A:GLU:HB3	1:190:A:GLU:H	7	0.18
(2,3444)	1:166:A:GLU:HB3	1:167:A:LYS:H	2	0.18
(2,3104)	1:151:A:SER:H	1:151:A:SER:HB2	7	0.18
(2,3091)	1:181:A:ILE:H	1:116:A:ARG:H	10	0.18
(2,3050)	1:159:A:PHE:HA	1:135:A:GLU:H	1	0.18
(2,2969)	1:116:A:ARG:HG2	1:154:A:GLU:HG2	3	0.18
(2,2861)	1:187:A:SER:HB3	1:188:A:ARG:H	5	0.18
(2,2861)	1:187:A:SER:HB3	1:188:A:ARG:H	9	0.18
(2,2660)	1:166:A:GLU:HG3	1:166:A:GLU:HA	10	0.18
(2,2459)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	2	0.18
(2,2459)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	4	0.18
(2,2459)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	7	0.18
(2,2459)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	9	0.18
(2,2172)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	6	0.18
(2,2090)	1:110:A:ASP:HB2	1:110:A:ASP:HA	4	0.18
(2,2012)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	8	0.18
(2,1870)	1:175:A:ARG:HA	1:179:A:ARG:H	4	0.18
(2,1853)	1:95:A:TRP:HB3	1:91:A:ASN:HB3	9	0.18
(2,1852)	1:95:A:TRP:HB2	1:96:A:VAL:HG21	7	0.18
(2,1844)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	6	0.18
(2,1813)	1:113:A:VAL:HG13	1:112:A:PHE:H	8	0.18
(2,1797)	1:164:A:ILE:HD13	1:91:A:ASN:HA	3	0.18
(2,1639)	1:166:A:GLU:HB3	1:167:A:LYS:H	5	0.18
(2,1207)	1:172:A:HIS:H	1:171:A:LYS:H	2	0.18
(2,1207)	1:172:A:HIS:H	1:171:A:LYS:H	5	0.18
(2,1207)	1:172:A:HIS:H	1:171:A:LYS:H	8	0.18
(2,1168)	1:155:A:ALA:HA	1:155:A:ALA:HB3	2	0.18
(2,1168)	1:155:A:ALA:HA	1:155:A:ALA:HB3	4	0.18
(2,1168)	1:155:A:ALA:HA	1:155:A:ALA:HB3	10	0.18
(2,1106)	1:191:A:VAL:HG11	1:191:A:VAL:HA	5	0.18
(2,1069)	1:187:A:SER:HB3	1:188:A:ARG:H	3	0.18
(2,1067)	1:187:A:SER:HB2	1:187:A:SER:HA	2	0.18
(2,1067)	1:187:A:SER:HB2	1:187:A:SER:HA	6	0.18
(2,1021)	1:181:A:ILE:HG12	1:181:A:ILE:HD13	8	0.18
(2,829)	1:163:A:GLU:HB2	1:163:A:GLU:HG2	6	0.18
(2,720)	1:148:A:GLN:HB2	1:148:A:GLN:HG2	2	0.18
(2,720)	1:148:A:GLN:HB2	1:148:A:GLN:HG2	4	0.18
(2,720)	1:148:A:GLN:HB2	1:148:A:GLN:HG2	5	0.18
(2,720)	1:148:A:GLN:HB2	1:148:A:GLN:HG2	10	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,677)	1:144:A:PRO:HB2	1:144:A:PRO:HA	1	0.18
(2,677)	1:144:A:PRO:HB2	1:144:A:PRO:HA	2	0.18
(2,677)	1:144:A:PRO:HB2	1:144:A:PRO:HA	8	0.18
(2,595)	1:139:A:ASN:HA	1:140:A:GLY:HA3	1	0.18
(2,521)	1:134:A:LEU:HD11	1:134:A:LEU:HA	7	0.18
(2,418)	1:124:A:LYS:HA	1:124:A:LYS:HB2	7	0.18
(2,228)	1:98:A:LYS:HG3	1:98:A:LYS:HE3	2	0.18
(2,225)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	6	0.18
(2,111)	1:188:A:ARG:HB2	1:189:A:ALA:H	4	0.18
(2,111)	1:188:A:ARG:HB2	1:189:A:ALA:H	10	0.18
(2,106)	1:93:A:MET:HB2	1:93:A:MET:HG2	3	0.18
(2,100)	1:181:A:ILE:HG21	1:174:A:GLU:HA	9	0.18
(2,80)	1:156:A:PHE:HA	1:141:A:ILE:HA	1	0.18
(2,80)	1:156:A:PHE:HA	1:141:A:ILE:HA	10	0.18
(2,25)	1:96:A:VAL:HG22	1:161:A:SER:H	5	0.18
(2,22)	1:113:A:VAL:HG12	1:112:A:PHE:H	3	0.18
(2,22)	1:113:A:VAL:HG12	1:112:A:PHE:H	9	0.18
(2,18)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	4	0.18
(2,6)	1:164:A:ILE:HD11	1:161:A:SER:H	5	0.18
(2,5)	1:164:A:ILE:HD13	1:91:A:ASN:HA	6	0.18
(1,3050)	1:145:A:VAL:HA	1:151:A:SER:H	10	0.18
(1,3030)	1:165:A:ALA:H	1:110:A:ASP:HB3	5	0.18
(1,3020)	1:132:A:SER:H	1:136:A:ILE:HB	4	0.18
(1,2928)	1:156:A:PHE:HB2	1:141:A:ILE:HG23	10	0.18
(1,2746)	1:93:A:MET:HB2	1:135:A:GLU:HB3	4	0.18
(1,2739)	1:143:A:LEU:HG	1:141:A:ILE:HG21	2	0.18
(1,2635)	1:169:A:LEU:HB2	1:169:A:LEU:HA	8	0.18
(1,2585)	1:179:A:ARG:HB3	1:119:A:PRO:HD2	8	0.18
(1,2553)	1:119:A:PRO:HB3	1:119:A:PRO:HA	1	0.18
(1,2553)	1:119:A:PRO:HB3	1:119:A:PRO:HA	9	0.18
(1,2553)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.18
(1,2527)	1:163:A:GLU:HB2	1:164:A:ILE:HG12	1	0.18
(1,2319)	1:174:A:GLU:HA	1:181:A:ILE:H	7	0.18
(1,2239)	1:119:A:PRO:HB3	1:119:A:PRO:HA	4	0.18
(1,2181)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	7	0.18
(1,2101)	1:143:A:LEU:HA	1:122:A:CYS:HB2	4	0.18
(1,2097)	1:143:A:LEU:HA	1:143:A:LEU:HB2	2	0.18
(1,2068)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	3	0.18
(1,2030)	1:169:A:LEU:HB2	1:169:A:LEU:HA	5	0.18
(1,1956)	1:181:A:ILE:HB	1:181:A:ILE:HA	9	0.18
(1,1826)	1:184:A:PHE:H	1:186:A:SER:HB3	5	0.18
(1,1826)	1:184:A:PHE:H	1:186:A:SER:HB3	7	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1700)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	2	0.18
(1,1700)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	10	0.18
(1,1563)	1:166:A:GLU:HG3	1:168:A:ALA:H	8	0.18
(1,1552)	1:97:A:LEU:HG	1:97:A:LEU:HD13	5	0.18
(1,1550)	1:98:A:LYS:HB3	1:100:A:THR:HG23	6	0.18
(1,1537)	1:150:A:ARG:HB2	1:150:A:ARG:HA	1	0.18
(1,1520)	1:141:A:ILE:HG21	1:143:A:LEU:HG	8	0.18
(1,1478)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	4	0.18
(1,1477)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	2	0.18
(1,1442)	1:144:A:PRO:HD2	1:118:A:LEU:HD11	6	0.18
(1,1370)	1:166:A:GLU:HG3	1:169:A:LEU:HD13	8	0.18
(1,1363)	1:144:A:PRO:HB2	1:144:A:PRO:HB3	4	0.18
(1,1363)	1:144:A:PRO:HB2	1:144:A:PRO:HB3	10	0.18
(1,1315)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	1	0.18
(1,1315)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	4	0.18
(1,1315)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	7	0.18
(1,1297)	1:166:A:GLU:HB2	1:168:A:ALA:H	2	0.18
(1,1253)	1:164:A:ILE:HD13	1:91:A:ASN:HB3	6	0.18
(1,1175)	1:106:A:ASP:H	1:105:A:PRO:HD2	2	0.18
(1,1106)	1:161:A:SER:H	1:110:A:ASP:HB3	8	0.18
(1,1087)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	2	0.18
(1,1027)	1:164:A:ILE:HD13	1:135:A:GLU:HA	6	0.18
(1,1014)	1:135:A:GLU:HA	1:136:A:ILE:HB	5	0.18
(1,995)	1:123:A:SER:HB3	1:181:A:ILE:HD11	9	0.18
(1,985)	1:169:A:LEU:HD21	1:167:A:LYS:H	5	0.18
(1,985)	1:169:A:LEU:HD21	1:167:A:LYS:H	6	0.18
(1,939)	1:169:A:LEU:HB2	1:169:A:LEU:HD11	7	0.18
(1,919)	1:164:A:ILE:HD13	1:93:A:MET:HG3	10	0.18
(1,764)	1:166:A:GLU:HG3	1:168:A:ALA:H	8	0.18
(1,684)	1:167:A:LYS:HG2	1:134:A:LEU:HD11	7	0.18
(1,684)	1:167:A:LYS:HG2	1:134:A:LEU:HD12	10	0.18
(1,668)	1:141:A:ILE:HG21	1:141:A:ILE:HB	1	0.18
(1,668)	1:141:A:ILE:HG21	1:141:A:ILE:HB	5	0.18
(1,641)	1:141:A:ILE:HD12	1:125:A:GLU:H	6	0.18
(1,641)	1:141:A:ILE:HD12	1:125:A:GLU:H	10	0.18
(1,458)	1:136:A:ILE:HG13	1:159:A:PHE:HA	4	0.18
(1,316)	1:98:A:LYS:HB3	1:100:A:THR:HG22	3	0.18
(1,304)	1:150:A:ARG:HB2	1:150:A:ARG:HA	2	0.18
(1,304)	1:150:A:ARG:HB2	1:150:A:ARG:HA	8	0.18
(1,297)	1:164:A:ILE:HD13	1:93:A:MET:HG3	9	0.18
(1,248)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	6	0.18
(1,226)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	6	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,191)	1:98:A:LYS:HA	1:100:A:THR:HG23	2	0.18
(1,106)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	2	0.18
(1,106)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	4	0.18
(1,106)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.18
(1,94)	1:119:A:PRO:HB3	1:119:A:PRO:HA	5	0.18
(1,94)	1:119:A:PRO:HB3	1:119:A:PRO:HA	9	0.18
(1,84)	1:115:A:LEU:HG	1:115:A:LEU:HB2	8	0.18
(1,41)	1:134:A:LEU:HD11	1:134:A:LEU:HA	3	0.18
(1,10)	1:164:A:ILE:HD13	1:91:A:ASN:HB3	6	0.18
(1,3)	1:127:A:ILE:HD11	1:126:A:GLU:HB2	2	0.18
(4,48)	1:183:A:ILE:H	1:171:A:LYS:O	8	0.17
(4,30)	1:157:A:VAL:H	1:113:A:VAL:O	7	0.17
(4,10)	1:117:A:GLY:N	1:153:A:GLY:O	8	0.17
(4,1)	1:113:A:VAL:H	1:157:A:VAL:O	5	0.17
(4,1)	1:113:A:VAL:H	1:157:A:VAL:O	7	0.17
(3,625)	1:139:A:ASN:H	1:128:A:VAL:HA	5	0.17
(3,618)	1:152:A:THR:HB	1:117:A:GLY:H	7	0.17
(3,499)	1:139:A:ASN:H	1:128:A:VAL:HA	5	0.17
(2,8701)	1:110:A:ASP:HB3	1:110:A:ASP:H	4	0.17
(2,8578)	1:143:A:LEU:H	1:141:A:ILE:HB	8	0.17
(2,8576)	1:108:A:ALA:H	1:102:A:PRO:HG3	4	0.17
(2,8563)	1:168:A:ALA:H	1:95:A:TRP:HB2	9	0.17
(2,8560)	1:168:A:ALA:H	1:167:A:LYS:HB3	9	0.17
(2,8462)	1:119:A:PRO:HB2	1:120:A:PHE:H	1	0.17
(2,8405)	1:191:A:VAL:HG22	1:191:A:VAL:HB	8	0.17
(2,8352)	1:183:A:ILE:HG21	1:184:A:PHE:HA	10	0.17
(2,8120)	1:163:A:GLU:HB3	1:163:A:GLU:HA	3	0.17
(2,8032)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	3	0.17
(2,7788)	1:130:A:PHE:HB2	1:131:A:PHE:H	4	0.17
(2,7498)	1:96:A:VAL:HG22	1:97:A:LEU:H	6	0.17
(2,7413)	1:181:A:ILE:HD12	1:183:A:ILE:H	2	0.17
(2,7388)	1:150:A:ARG:HB2	1:150:A:ARG:HA	5	0.17
(2,7320)	1:191:A:VAL:HG13	1:137:A:VAL:HG13	1	0.17
(2,7230)	1:150:A:ARG:HG2	1:151:A:SER:H	1	0.17
(2,7193)	1:190:A:GLU:HB3	1:190:A:GLU:H	6	0.17
(2,7193)	1:190:A:GLU:HB3	1:190:A:GLU:H	8	0.17
(2,7193)	1:190:A:GLU:HB3	1:190:A:GLU:H	9	0.17
(2,7096)	1:164:A:ILE:H	1:164:A:ILE:HG21	9	0.17
(2,6845)	1:110:A:ASP:HB3	1:110:A:ASP:H	8	0.17
(2,6753)	1:164:A:ILE:H	1:91:A:ASN:HA	5	0.17
(2,6751)	1:151:A:SER:H	1:151:A:SER:HB2	6	0.17
(2,6714)	1:108:A:ALA:H	1:189:A:ALA:H	2	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6699)	1:168:A:ALA:H	1:167:A:LYS:HB3	8	0.17
(2,6599)	1:155:A:ALA:HA	1:155:A:ALA:HB3	3	0.17
(2,6593)	1:119:A:PRO:HB2	1:120:A:PHE:H	1	0.17
(2,6519)	1:189:A:ALA:HB1	1:190:A:GLU:H	7	0.17
(2,6366)	1:175:A:ARG:HG2	1:175:A:ARG:HA	1	0.17
(2,5866)	1:127:A:ILE:HG23	1:127:A:ILE:HG12	6	0.17
(2,5821)	1:122:A:CYS:HA	1:121:A:GLY:H	2	0.17
(2,5821)	1:122:A:CYS:HA	1:121:A:GLY:H	4	0.17
(2,5821)	1:122:A:CYS:HA	1:121:A:GLY:H	5	0.17
(2,5542)	1:181:A:ILE:HD12	1:183:A:ILE:H	3	0.17
(2,5537)	1:155:A:ALA:HB2	1:154:A:GLU:H	4	0.17
(2,5502)	1:156:A:PHE:HB2	1:191:A:VAL:H	4	0.17
(2,5451)	1:191:A:VAL:HG13	1:137:A:VAL:HG13	1	0.17
(2,5444)	1:191:A:VAL:HG12	1:193:A:THR:H	3	0.17
(2,5355)	1:158:A:GLN:H	1:141:A:ILE:HB	3	0.17
(2,5244)	1:166:A:GLU:HB3	1:167:A:LYS:H	7	0.17
(2,4847)	1:146:A:ASP:H	1:150:A:ARG:H	4	0.17
(2,4481)	1:167:A:LYS:HB2	1:167:A:LYS:HA	2	0.17
(2,4481)	1:167:A:LYS:HB2	1:167:A:LYS:HA	6	0.17
(2,4481)	1:167:A:LYS:HB2	1:167:A:LYS:HA	8	0.17
(2,4481)	1:167:A:LYS:HB2	1:167:A:LYS:HA	10	0.17
(2,4468)	1:166:A:GLU:HB2	1:166:A:GLU:HA	8	0.17
(2,4436)	1:163:A:GLU:HG3	1:163:A:GLU:H	2	0.17
(2,4433)	1:163:A:GLU:HB3	1:164:A:ILE:H	6	0.17
(2,3903)	1:110:A:ASP:HB3	1:110:A:ASP:HA	8	0.17
(2,3728)	1:123:A:SER:HB3	1:181:A:ILE:HD11	2	0.17
(2,3668)	1:154:A:GLU:HG2	1:118:A:LEU:H	10	0.17
(2,3608)	1:164:A:ILE:HD11	1:161:A:SER:H	3	0.17
(2,3608)	1:164:A:ILE:HD11	1:161:A:SER:H	4	0.17
(2,3606)	1:164:A:ILE:HD12	1:164:A:ILE:HA	1	0.17
(2,3606)	1:164:A:ILE:HD12	1:164:A:ILE:HA	3	0.17
(2,3606)	1:164:A:ILE:HD12	1:164:A:ILE:HA	4	0.17
(2,3532)	1:190:A:GLU:HB3	1:190:A:GLU:H	1	0.17
(2,3218)	1:114:A:ARG:HG3	1:115:A:LEU:H	9	0.17
(2,3091)	1:181:A:ILE:H	1:116:A:ARG:H	2	0.17
(2,3091)	1:181:A:ILE:H	1:116:A:ARG:H	6	0.17
(2,3091)	1:181:A:ILE:H	1:116:A:ARG:H	8	0.17
(2,3091)	1:181:A:ILE:H	1:116:A:ARG:H	9	0.17
(2,3066)	1:108:A:ALA:H	1:188:A:ARG:HG2	6	0.17
(2,2969)	1:116:A:ARG:HG2	1:154:A:GLU:HG2	7	0.17
(2,2969)	1:116:A:ARG:HG2	1:154:A:GLU:HG2	10	0.17
(2,2958)	1:119:A:PRO:HB2	1:120:A:PHE:H	1	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2841)	1:183:A:ILE:HG21	1:184:A:PHE:HA	10	0.17
(2,2625)	1:163:A:GLU:HG3	1:163:A:GLU:H	1	0.17
(2,2578)	1:157:A:VAL:HG21	1:157:A:VAL:HA	7	0.17
(2,2578)	1:157:A:VAL:HG21	1:157:A:VAL:HA	9	0.17
(2,2578)	1:157:A:VAL:HG21	1:157:A:VAL:HA	10	0.17
(2,2510)	1:148:A:GLN:HB2	1:148:A:GLN:HG2	4	0.17
(2,2459)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	8	0.17
(2,2210)	1:126:A:GLU:HB2	1:126:A:GLU:HA	6	0.17
(2,2172)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	2	0.17
(2,2172)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	4	0.17
(2,2172)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	5	0.17
(2,2097)	1:111:A:GLY:HA3	1:112:A:PHE:H	1	0.17
(2,2097)	1:111:A:GLY:HA3	1:112:A:PHE:H	5	0.17
(2,2012)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	1	0.17
(2,2012)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	4	0.17
(2,2012)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	5	0.17
(2,2012)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	10	0.17
(2,1867)	1:161:A:SER:HA	1:106:A:ASP:HB3	10	0.17
(2,1838)	1:191:A:VAL:HG12	1:193:A:THR:H	3	0.17
(2,1838)	1:191:A:VAL:HG13	1:193:A:THR:H	7	0.17
(2,1813)	1:113:A:VAL:HG12	1:112:A:PHE:H	4	0.17
(2,1796)	1:164:A:ILE:HD12	1:164:A:ILE:HA	5	0.17
(2,1796)	1:164:A:ILE:HD12	1:164:A:ILE:HA	10	0.17
(2,1788)	1:188:A:ARG:H	1:108:A:ALA:HB3	3	0.17
(2,1630)	1:164:A:ILE:H	1:164:A:ILE:HG21	5	0.17
(2,1169)	1:115:A:LEU:HD23	1:114:A:ARG:HA	9	0.17
(2,1168)	1:155:A:ALA:HA	1:155:A:ALA:HB3	7	0.17
(2,1168)	1:155:A:ALA:HA	1:155:A:ALA:HB3	8	0.17
(2,1067)	1:187:A:SER:HB2	1:187:A:SER:HA	8	0.17
(2,1021)	1:181:A:ILE:HG12	1:181:A:ILE:HD13	7	0.17
(2,996)	1:181:A:ILE:HD12	1:181:A:ILE:HB	4	0.17
(2,874)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	4	0.17
(2,874)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	6	0.17
(2,874)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	9	0.17
(2,790)	1:157:A:VAL:HG21	1:157:A:VAL:HA	4	0.17
(2,720)	1:148:A:GLN:HB2	1:148:A:GLN:HG2	1	0.17
(2,720)	1:148:A:GLN:HB2	1:148:A:GLN:HG2	6	0.17
(2,720)	1:148:A:GLN:HB2	1:148:A:GLN:HG2	8	0.17
(2,677)	1:144:A:PRO:HB2	1:144:A:PRO:HA	3	0.17
(2,677)	1:144:A:PRO:HB2	1:144:A:PRO:HA	5	0.17
(2,677)	1:144:A:PRO:HB2	1:144:A:PRO:HA	6	0.17
(2,595)	1:139:A:ASN:HA	1:140:A:GLY:HA3	2	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,521)	1:134:A:LEU:HD11	1:134:A:LEU:HA	4	0.17
(2,368)	1:116:A:ARG:HD2	1:117:A:GLY:H	6	0.17
(2,139)	1:102:A:PRO:HA	1:103:A:ASN:H	7	0.17
(2,54)	1:191:A:VAL:HG13	1:137:A:VAL:HG13	1	0.17
(2,18)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	5	0.17
(2,18)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	9	0.17
(2,18)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	10	0.17
(2,16)	1:113:A:VAL:HG13	1:113:A:VAL:HB	3	0.17
(2,16)	1:113:A:VAL:HG13	1:113:A:VAL:HB	4	0.17
(2,16)	1:113:A:VAL:HG13	1:113:A:VAL:HB	5	0.17
(1,2992)	1:146:A:ASP:H	1:143:A:LEU:HD21	3	0.17
(1,2829)	1:174:A:GLU:HB2	1:181:A:ILE:HD13	7	0.17
(1,2777)	1:97:A:LEU:HG	1:97:A:LEU:HD13	3	0.17
(1,2746)	1:93:A:MET:HB2	1:93:A:MET:HG2	2	0.17
(1,2706)	1:143:A:LEU:HA	1:122:A:CYS:HB2	5	0.17
(1,2636)	1:169:A:LEU:HA	1:169:A:LEU:HD11	2	0.17
(1,2635)	1:169:A:LEU:HB2	1:169:A:LEU:HA	10	0.17
(1,2576)	1:141:A:ILE:HG12	1:158:A:GLN:H	3	0.17
(1,2553)	1:119:A:PRO:HB3	1:119:A:PRO:HA	2	0.17
(1,2553)	1:119:A:PRO:HB3	1:119:A:PRO:HA	3	0.17
(1,2553)	1:119:A:PRO:HB3	1:119:A:PRO:HA	6	0.17
(1,2527)	1:163:A:GLU:HB2	1:96:A:VAL:HG13	7	0.17
(1,2163)	1:98:A:LYS:HB3	1:100:A:THR:HG23	9	0.17
(1,2097)	1:143:A:LEU:HA	1:143:A:LEU:HB2	1	0.17
(1,2069)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	1	0.17
(1,2069)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	5	0.17
(1,2030)	1:169:A:LEU:HB2	1:169:A:LEU:HA	8	0.17
(1,1956)	1:181:A:ILE:HB	1:181:A:ILE:HA	5	0.17
(1,1948)	1:119:A:PRO:HB3	1:119:A:PRO:HA	4	0.17
(1,1759)	1:146:A:ASP:H	1:143:A:LEU:HD21	2	0.17
(1,1759)	1:146:A:ASP:H	1:143:A:LEU:HD21	6	0.17
(1,1700)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	1	0.17
(1,1658)	1:143:A:LEU:HD23	1:123:A:SER:HA	9	0.17
(1,1638)	1:164:A:ILE:HD13	1:93:A:MET:HA	3	0.17
(1,1638)	1:164:A:ILE:HD13	1:135:A:GLU:HA	4	0.17
(1,1638)	1:164:A:ILE:HD13	1:93:A:MET:HA	9	0.17
(1,1552)	1:97:A:LEU:HG	1:97:A:LEU:HD13	2	0.17
(1,1552)	1:97:A:LEU:HG	1:97:A:LEU:HD13	9	0.17
(1,1537)	1:150:A:ARG:HB2	1:150:A:ARG:HA	4	0.17
(1,1537)	1:150:A:ARG:HB2	1:150:A:ARG:HA	6	0.17
(1,1528)	1:166:A:GLU:HB2	1:167:A:LYS:H	1	0.17
(1,1520)	1:141:A:ILE:HG21	1:143:A:LEU:HG	9	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1477)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	4	0.17
(1,1363)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	2	0.17
(1,1363)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	5	0.17
(1,1363)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.17
(1,1363)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	8	0.17
(1,1363)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	9	0.17
(1,1349)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.17
(1,1349)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	2	0.17
(1,1349)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.17
(1,1349)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	4	0.17
(1,1349)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	5	0.17
(1,1349)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.17
(1,1349)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.17
(1,1349)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	8	0.17
(1,1349)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	9	0.17
(1,1349)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.17
(1,1339)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	5	0.17
(1,1339)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	10	0.17
(1,1315)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	5	0.17
(1,1286)	1:134:A:LEU:HD13	1:133:A:GLY:H	4	0.17
(1,1260)	1:183:A:ILE:HG21	1:184:A:PHE:HA	8	0.17
(1,1148)	1:146:A:ASP:H	1:143:A:LEU:HD21	1	0.17
(1,1087)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	10	0.17
(1,868)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	5	0.17
(1,756)	1:144:A:PRO:HB2	1:144:A:PRO:HB3	4	0.17
(1,756)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	8	0.17
(1,756)	1:144:A:PRO:HB2	1:144:A:PRO:HB3	10	0.17
(1,743)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.17
(1,743)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	2	0.17
(1,743)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.17
(1,743)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	4	0.17
(1,743)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	5	0.17
(1,743)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.17
(1,743)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	8	0.17
(1,743)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	9	0.17
(1,743)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.17
(1,668)	1:141:A:ILE:HG21	1:141:A:ILE:HB	8	0.17
(1,304)	1:150:A:ARG:HB2	1:150:A:ARG:HA	9	0.17
(1,297)	1:164:A:ILE:HD13	1:93:A:MET:HG3	2	0.17
(1,297)	1:164:A:ILE:HD13	1:93:A:MET:HG3	5	0.17
(1,288)	1:141:A:ILE:HG21	1:143:A:LEU:HG	2	0.17
(1,247)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	1	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.17
(1,106)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.17
(1,106)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	5	0.17
(1,106)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.17
(1,106)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	8	0.17
(1,106)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	9	0.17
(1,106)	1:135:A:GLU:HG2	1:135:A:GLU:HG3	10	0.17
(1,94)	1:119:A:PRO:HB3	1:119:A:PRO:HA	1	0.17
(1,94)	1:119:A:PRO:HB3	1:119:A:PRO:HA	2	0.17
(1,94)	1:119:A:PRO:HB3	1:119:A:PRO:HA	6	0.17
(1,94)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.17
(1,84)	1:115:A:LEU:HG	1:115:A:LEU:HB2	7	0.17
(1,54)	1:166:A:GLU:HB2	1:168:A:ALA:H	5	0.17
(1,43)	1:134:A:LEU:HD13	1:133:A:GLY:H	9	0.17
(1,31)	1:181:A:ILE:HG21	1:181:A:ILE:HB	1	0.17
(1,31)	1:181:A:ILE:HG21	1:181:A:ILE:HB	7	0.17
(4,50)	1:183:A:ILE:H	1:181:A:ILE:O	3	0.16
(4,48)	1:183:A:ILE:H	1:171:A:LYS:O	3	0.16
(4,43)	1:169:A:LEU:N	1:165:A:ALA:O	5	0.16
(4,34)	1:159:A:PHE:H	1:111:A:GLY:O	8	0.16
(4,11)	1:118:A:LEU:H	1:152:A:THR:O	1	0.16
(4,11)	1:118:A:LEU:H	1:152:A:THR:O	9	0.16
(4,10)	1:117:A:GLY:N	1:153:A:GLY:O	3	0.16
(3,627)	1:108:A:ALA:H	1:189:A:ALA:H	9	0.16
(3,625)	1:139:A:ASN:H	1:128:A:VAL:HA	6	0.16
(3,499)	1:139:A:ASN:H	1:128:A:VAL:HA	6	0.16
(2,9104)	1:122:A:CYS:H	1:151:A:SER:HB2	6	0.16
(2,8951)	1:164:A:ILE:H	1:164:A:ILE:HG21	4	0.16
(2,8951)	1:164:A:ILE:H	1:164:A:ILE:HG21	7	0.16
(2,8895)	1:154:A:GLU:H	1:154:A:GLU:HB3	6	0.16
(2,8796)	1:132:A:SER:HB2	1:133:A:GLY:H	9	0.16
(2,8697)	1:110:A:ASP:HA	1:110:A:ASP:H	8	0.16
(2,8566)	1:139:A:ASN:H	1:141:A:ILE:HD12	10	0.16
(2,8461)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	6	0.16
(2,8461)	1:149:A:GLY:HA3	1:146:A:ASP:HB3	8	0.16
(2,8414)	1:191:A:VAL:HG13	1:192:A:ARG:HA	1	0.16
(2,8405)	1:191:A:VAL:HG22	1:191:A:VAL:HB	2	0.16
(2,8352)	1:183:A:ILE:HG21	1:184:A:PHE:HA	4	0.16
(2,8182)	1:167:A:LYS:HB2	1:167:A:LYS:HE2	3	0.16
(2,8120)	1:163:A:GLU:HB3	1:163:A:GLU:HA	9	0.16
(2,8105)	1:160:A:ALA:HB3	1:161:A:SER:H	1	0.16
(2,8105)	1:160:A:ALA:HB3	1:161:A:SER:H	5	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7946)	1:144:A:PRO:HD3	1:143:A:LEU:HA	9	0.16
(2,7693)	1:122:A:CYS:HA	1:121:A:GLY:H	8	0.16
(2,7693)	1:122:A:CYS:HA	1:121:A:GLY:H	9	0.16
(2,7394)	1:142:A:THR:HG23	1:141:A:ILE:HG21	1	0.16
(2,7394)	1:142:A:THR:HG21	1:141:A:ILE:HG21	3	0.16
(2,7394)	1:142:A:THR:HG22	1:141:A:ILE:HG21	9	0.16
(2,7388)	1:150:A:ARG:HB2	1:150:A:ARG:HA	1	0.16
(2,7388)	1:150:A:ARG:HB2	1:150:A:ARG:HA	7	0.16
(2,7360)	1:187:A:SER:HB3	1:189:A:ALA:H	1	0.16
(2,7360)	1:187:A:SER:HB3	1:189:A:ALA:H	2	0.16
(2,7322)	1:191:A:VAL:HG13	1:190:A:GLU:H	3	0.16
(2,7271)	1:164:A:ILE:HD13	1:91:A:ASN:HA	5	0.16
(2,7230)	1:150:A:ARG:HG2	1:151:A:SER:H	3	0.16
(2,7193)	1:190:A:GLU:HB3	1:190:A:GLU:H	2	0.16
(2,7180)	1:187:A:SER:HB3	1:188:A:ARG:H	2	0.16
(2,7105)	1:166:A:GLU:HB3	1:167:A:LYS:H	3	0.16
(2,7104)	1:166:A:GLU:HB3	1:166:A:GLU:H	3	0.16
(2,7104)	1:166:A:GLU:HB3	1:166:A:GLU:H	8	0.16
(2,6714)	1:108:A:ALA:H	1:189:A:ALA:H	7	0.16
(2,6699)	1:168:A:ALA:H	1:167:A:LYS:HB3	5	0.16
(2,6621)	1:166:A:GLU:HA	1:169:A:LEU:HD11	3	0.16
(2,6599)	1:155:A:ALA:HA	1:155:A:ALA:HB3	4	0.16
(2,6599)	1:155:A:ALA:HA	1:155:A:ALA:HB3	10	0.16
(2,6533)	1:191:A:VAL:HG22	1:191:A:VAL:HB	1	0.16
(2,6519)	1:189:A:ALA:HB1	1:190:A:GLU:H	3	0.16
(2,6519)	1:189:A:ALA:HB1	1:190:A:GLU:H	6	0.16
(2,6519)	1:189:A:ALA:HB1	1:190:A:GLU:H	9	0.16
(2,6258)	1:163:A:GLU:HG3	1:163:A:GLU:H	7	0.16
(2,6226)	1:157:A:VAL:HG22	1:158:A:GLN:H	4	0.16
(2,6036)	1:141:A:ILE:HG13	1:141:A:ILE:H	8	0.16
(2,5866)	1:127:A:ILE:HG23	1:127:A:ILE:HG12	9	0.16
(2,5866)	1:127:A:ILE:HG23	1:127:A:ILE:HG12	10	0.16
(2,5829)	1:124:A:LYS:HA	1:124:A:LYS:HB2	9	0.16
(2,5821)	1:122:A:CYS:HA	1:121:A:GLY:H	10	0.16
(2,5537)	1:155:A:ALA:HB2	1:154:A:GLU:H	5	0.16
(2,5537)	1:155:A:ALA:HB2	1:154:A:GLU:H	9	0.16
(2,5502)	1:156:A:PHE:HB2	1:191:A:VAL:H	10	0.16
(2,5444)	1:191:A:VAL:HG13	1:193:A:THR:H	10	0.16
(2,5413)	1:160:A:ALA:HB3	1:159:A:PHE:HB2	3	0.16
(2,5328)	1:190:A:GLU:HB3	1:191:A:VAL:H	10	0.16
(2,5244)	1:166:A:GLU:HB3	1:167:A:LYS:H	2	0.16
(2,4907)	1:151:A:SER:H	1:151:A:SER:HB2	4	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4869)	1:108:A:ALA:H	1:188:A:ARG:HG2	1	0.16
(2,4869)	1:108:A:ALA:H	1:188:A:ARG:HG2	4	0.16
(2,4657)	1:183:A:ILE:HA	1:183:A:ILE:HD11	5	0.16
(2,4657)	1:183:A:ILE:HA	1:183:A:ILE:HD11	8	0.16
(2,4650)	1:183:A:ILE:HG21	1:184:A:PHE:HA	1	0.16
(2,4650)	1:183:A:ILE:HG21	1:184:A:PHE:HA	7	0.16
(2,4496)	1:169:A:LEU:HD22	1:169:A:LEU:HA	10	0.16
(2,4481)	1:167:A:LYS:HB2	1:167:A:LYS:HA	3	0.16
(2,4481)	1:167:A:LYS:HB2	1:167:A:LYS:HA	4	0.16
(2,4433)	1:163:A:GLU:HB3	1:164:A:ILE:H	7	0.16
(2,4390)	1:157:A:VAL:HG21	1:157:A:VAL:HA	1	0.16
(2,4390)	1:157:A:VAL:HG21	1:157:A:VAL:HA	3	0.16
(2,4269)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	1	0.16
(2,3731)	1:135:A:GLU:HA	1:164:A:ILE:HA	3	0.16
(2,3728)	1:123:A:SER:HB3	1:181:A:ILE:HD11	5	0.16
(2,3728)	1:123:A:SER:HB3	1:181:A:ILE:HD11	9	0.16
(2,3668)	1:154:A:GLU:HG2	1:118:A:LEU:H	3	0.16
(2,3606)	1:164:A:ILE:HD12	1:164:A:ILE:HA	6	0.16
(2,3606)	1:164:A:ILE:HD12	1:164:A:ILE:HA	9	0.16
(2,3568)	1:188:A:ARG:HG2	1:188:A:ARG:H	7	0.16
(2,3532)	1:190:A:GLU:HB3	1:190:A:GLU:H	5	0.16
(2,3532)	1:190:A:GLU:HB3	1:190:A:GLU:H	8	0.16
(2,3104)	1:151:A:SER:H	1:151:A:SER:HB2	4	0.16
(2,3091)	1:181:A:ILE:H	1:116:A:ARG:H	5	0.16
(2,3091)	1:181:A:ILE:H	1:116:A:ARG:H	7	0.16
(2,2985)	1:188:A:ARG:HG2	1:188:A:ARG:HD2	1	0.16
(2,2985)	1:188:A:ARG:HG2	1:188:A:ARG:HD2	5	0.16
(2,2861)	1:187:A:SER:HB3	1:188:A:ARG:H	1	0.16
(2,2841)	1:183:A:ILE:HG21	1:184:A:PHE:HA	4	0.16
(2,2670)	1:167:A:LYS:HB2	1:167:A:LYS:HA	2	0.16
(2,2670)	1:167:A:LYS:HB2	1:167:A:LYS:HA	6	0.16
(2,2670)	1:167:A:LYS:HB2	1:167:A:LYS:HA	8	0.16
(2,2670)	1:167:A:LYS:HB2	1:167:A:LYS:HA	10	0.16
(2,2660)	1:166:A:GLU:HG3	1:166:A:GLU:HA	6	0.16
(2,2625)	1:163:A:GLU:HG3	1:163:A:GLU:H	2	0.16
(2,2619)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	2	0.16
(2,2619)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	5	0.16
(2,2619)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	6	0.16
(2,2578)	1:157:A:VAL:HG21	1:157:A:VAL:HA	8	0.16
(2,2510)	1:148:A:GLN:HB2	1:148:A:GLN:HG2	1	0.16
(2,2510)	1:148:A:GLN:HB2	1:148:A:GLN:HG2	2	0.16
(2,2510)	1:148:A:GLN:HB2	1:148:A:GLN:HG2	5	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2510)	1:148:A:GLN:HB2	1:148:A:GLN:HG2	6	0.16
(2,2510)	1:148:A:GLN:HB2	1:148:A:GLN:HG2	8	0.16
(2,2510)	1:148:A:GLN:HB2	1:148:A:GLN:HG2	10	0.16
(2,2459)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	5	0.16
(2,2459)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	6	0.16
(2,2459)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	10	0.16
(2,2172)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	3	0.16
(2,2172)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	9	0.16
(2,2172)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	10	0.16
(2,2097)	1:111:A:GLY:HA3	1:112:A:PHE:H	2	0.16
(2,2079)	1:107:A:THR:HG23	1:107:A:THR:H	9	0.16
(2,2051)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	4	0.16
(2,2051)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	5	0.16
(2,1853)	1:95:A:TRP:HB3	1:91:A:ASN:HB3	1	0.16
(2,1853)	1:95:A:TRP:HB3	1:91:A:ASN:HB3	3	0.16
(2,1853)	1:95:A:TRP:HB3	1:91:A:ASN:HB3	5	0.16
(2,1853)	1:95:A:TRP:HB3	1:91:A:ASN:HB3	7	0.16
(2,1849)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	3	0.16
(2,1838)	1:191:A:VAL:HG13	1:193:A:THR:H	10	0.16
(2,1796)	1:164:A:ILE:HD12	1:164:A:ILE:HA	1	0.16
(2,1796)	1:164:A:ILE:HD12	1:164:A:ILE:HA	3	0.16
(2,1777)	1:166:A:GLU:H	1:169:A:LEU:HB2	4	0.16
(2,1630)	1:164:A:ILE:H	1:164:A:ILE:HG21	10	0.16
(2,1292)	1:111:A:GLY:HA3	1:159:A:PHE:H	8	0.16
(2,1236)	1:130:A:PHE:H	1:136:A:ILE:HG22	5	0.16
(2,1186)	1:188:A:ARG:HG2	1:188:A:ARG:HD2	1	0.16
(2,1186)	1:188:A:ARG:HG2	1:188:A:ARG:HD2	5	0.16
(2,1171)	1:190:A:GLU:HB2	1:187:A:SER:H	8	0.16
(2,1168)	1:155:A:ALA:HA	1:155:A:ALA:HB3	1	0.16
(2,1067)	1:187:A:SER:HB2	1:187:A:SER:HA	5	0.16
(2,996)	1:181:A:ILE:HD12	1:181:A:ILE:HB	5	0.16
(2,996)	1:181:A:ILE:HD12	1:181:A:ILE:HB	10	0.16
(2,790)	1:157:A:VAL:HG21	1:157:A:VAL:HA	5	0.16
(2,139)	1:102:A:PRO:HA	1:103:A:ASN:H	9	0.16
(2,126)	1:115:A:LEU:HA	1:115:A:LEU:HD21	6	0.16
(2,126)	1:115:A:LEU:HA	1:115:A:LEU:HD21	9	0.16
(2,98)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	7	0.16
(2,80)	1:156:A:PHE:HA	1:141:A:ILE:HA	3	0.16
(2,25)	1:96:A:VAL:HG22	1:161:A:SER:H	10	0.16
(2,18)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	8	0.16
(2,9)	1:181:A:ILE:HG12	1:175:A:ARG:HD2	5	0.16
(1,3003)	1:108:A:ALA:H	1:109:A:ASN:HA	5	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2777)	1:97:A:LEU:HG	1:97:A:LEU:HD13	1	0.16
(1,2777)	1:97:A:LEU:HG	1:97:A:LEU:HD13	6	0.16
(1,2777)	1:97:A:LEU:HG	1:97:A:LEU:HD11	7	0.16
(1,2746)	1:93:A:MET:HB2	1:135:A:GLU:HB3	9	0.16
(1,2739)	1:143:A:LEU:HG	1:141:A:ILE:HG21	3	0.16
(1,2702)	1:169:A:LEU:HB2	1:166:A:GLU:HA	10	0.16
(1,2635)	1:169:A:LEU:HB2	1:169:A:LEU:HA	7	0.16
(1,2585)	1:179:A:ARG:HB3	1:119:A:PRO:HD2	3	0.16
(1,2472)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	2	0.16
(1,2410)	1:166:A:GLU:HB2	1:167:A:LYS:H	1	0.16
(1,2133)	1:143:A:LEU:HG	1:141:A:ILE:HG21	5	0.16
(1,2076)	1:150:A:ARG:HD3	1:149:A:GLY:H	10	0.16
(1,2072)	1:175:A:ARG:HD2	1:178:A:HIS:HA	10	0.16
(1,2030)	1:169:A:LEU:HB2	1:169:A:LEU:HA	10	0.16
(1,2003)	1:130:A:PHE:HB3	1:132:A:SER:H	5	0.16
(1,2003)	1:130:A:PHE:HB3	1:132:A:SER:H	7	0.16
(1,1976)	1:179:A:ARG:HB3	1:119:A:PRO:HD2	8	0.16
(1,1956)	1:181:A:ILE:HB	1:181:A:ILE:HA	4	0.16
(1,1956)	1:181:A:ILE:HB	1:181:A:ILE:HA	10	0.16
(1,1917)	1:166:A:GLU:HB3	1:168:A:ALA:H	1	0.16
(1,1908)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	8	0.16
(1,1868)	1:183:A:ILE:HG22	1:113:A:VAL:HB	2	0.16
(1,1859)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	10	0.16
(1,1826)	1:184:A:PHE:H	1:186:A:SER:HB3	3	0.16
(1,1826)	1:184:A:PHE:H	1:186:A:SER:HB3	4	0.16
(1,1805)	1:158:A:GLN:H	1:141:A:ILE:HG23	3	0.16
(1,1770)	1:108:A:ALA:H	1:109:A:ASN:HA	8	0.16
(1,1598)	1:169:A:LEU:HD21	1:167:A:LYS:H	5	0.16
(1,1598)	1:169:A:LEU:HD21	1:167:A:LYS:H	6	0.16
(1,1537)	1:150:A:ARG:HB2	1:150:A:ARG:HA	10	0.16
(1,1432)	1:137:A:VAL:HA	1:140:A:GLY:H	10	0.16
(1,1363)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.16
(1,1363)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.16
(1,1363)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.16
(1,1350)	1:144:A:PRO:HB3	1:144:A:PRO:HA	1	0.16
(1,1350)	1:144:A:PRO:HB3	1:144:A:PRO:HA	2	0.16
(1,1350)	1:144:A:PRO:HB3	1:144:A:PRO:HA	3	0.16
(1,1350)	1:144:A:PRO:HB3	1:144:A:PRO:HA	4	0.16
(1,1350)	1:144:A:PRO:HB3	1:144:A:PRO:HA	5	0.16
(1,1350)	1:144:A:PRO:HB3	1:144:A:PRO:HA	6	0.16
(1,1350)	1:144:A:PRO:HB3	1:144:A:PRO:HA	7	0.16
(1,1350)	1:144:A:PRO:HB3	1:144:A:PRO:HA	8	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1341)	1:119:A:PRO:HB3	1:119:A:PRO:HA	7	0.16
(1,1341)	1:119:A:PRO:HB3	1:119:A:PRO:HA	8	0.16
(1,1329)	1:115:A:LEU:HG	1:115:A:LEU:HB2	8	0.16
(1,1304)	1:166:A:GLU:HB2	1:169:A:LEU:HD13	7	0.16
(1,1286)	1:134:A:LEU:HD13	1:133:A:GLY:H	5	0.16
(1,1269)	1:137:A:VAL:HG22	1:140:A:GLY:H	6	0.16
(1,1087)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	1	0.16
(1,1046)	1:115:A:LEU:HD23	1:114:A:ARG:HA	4	0.16
(1,1014)	1:135:A:GLU:HA	1:136:A:ILE:HB	9	0.16
(1,937)	1:98:A:LYS:HB3	1:100:A:THR:HG22	3	0.16
(1,869)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	4	0.16
(1,858)	1:159:A:PHE:HB2	1:159:A:PHE:HA	1	0.16
(1,858)	1:159:A:PHE:HB2	1:159:A:PHE:HA	3	0.16
(1,858)	1:159:A:PHE:HB2	1:159:A:PHE:HA	4	0.16
(1,845)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	6	0.16
(1,841)	1:111:A:GLY:HA3	1:188:A:ARG:HG3	4	0.16
(1,756)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.16
(1,756)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	2	0.16
(1,756)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.16
(1,756)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	5	0.16
(1,756)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.16
(1,756)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	9	0.16
(1,743)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.16
(1,684)	1:167:A:LYS:HG2	1:134:A:LEU:HD12	6	0.16
(1,545)	1:168:A:ALA:H	1:169:A:LEU:HB2	1	0.16
(1,447)	1:154:A:GLU:HG2	1:118:A:LEU:HD23	5	0.16
(1,413)	1:162:A:GLN:HG3	1:110:A:ASP:HA	7	0.16
(1,248)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	1	0.16
(1,233)	1:116:A:ARG:HD2	1:116:A:ARG:HA	6	0.16
(1,165)	1:109:A:ASN:HA	1:108:A:ALA:HB3	2	0.16
(1,124)	1:144:A:PRO:HB2	1:144:A:PRO:HB3	4	0.16
(1,124)	1:144:A:PRO:HB2	1:144:A:PRO:HB3	10	0.16
(1,94)	1:119:A:PRO:HB3	1:119:A:PRO:HA	3	0.16
(1,84)	1:115:A:LEU:HG	1:115:A:LEU:HB2	2	0.16
(4,50)	1:183:A:ILE:H	1:181:A:ILE:O	1	0.15
(4,48)	1:183:A:ILE:H	1:171:A:LYS:O	9	0.15
(4,41)	1:168:A:ALA:N	1:164:A:ILE:O	9	0.15
(4,36)	1:160:A:ALA:H	1:135:A:GLU:O	4	0.15
(4,36)	1:160:A:ALA:H	1:135:A:GLU:O	10	0.15
(4,4)	1:114:A:ARG:N	1:184:A:PHE:O	5	0.15
(4,1)	1:113:A:VAL:H	1:157:A:VAL:O	8	0.15
(2,9104)	1:122:A:CYS:H	1:151:A:SER:HB2	8	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9054)	1:192:A:ARG:HG2	1:192:A:ARG:H	6	0.15
(2,9034)	1:187:A:SER:HB3	1:188:A:ARG:H	10	0.15
(2,8951)	1:164:A:ILE:H	1:164:A:ILE:HG21	2	0.15
(2,8951)	1:164:A:ILE:H	1:164:A:ILE:HG21	6	0.15
(2,8781)	1:127:A:ILE:H	1:127:A:ILE:HG13	1	0.15
(2,8697)	1:110:A:ASP:HA	1:110:A:ASP:H	9	0.15
(2,8688)	1:107:A:THR:HB	1:107:A:THR:H	2	0.15
(2,8688)	1:107:A:THR:HB	1:107:A:THR:H	4	0.15
(2,8608)	1:151:A:SER:H	1:151:A:SER:HB2	6	0.15
(2,8578)	1:143:A:LEU:H	1:141:A:ILE:HB	9	0.15
(2,8566)	1:139:A:ASN:H	1:141:A:ILE:HD12	4	0.15
(2,8566)	1:139:A:ASN:H	1:141:A:ILE:HD12	7	0.15
(2,8412)	1:191:A:VAL:HG13	1:191:A:VAL:HB	4	0.15
(2,8405)	1:191:A:VAL:HG22	1:191:A:VAL:HB	6	0.15
(2,8405)	1:191:A:VAL:HG22	1:191:A:VAL:HB	7	0.15
(2,8405)	1:191:A:VAL:HG22	1:191:A:VAL:HB	9	0.15
(2,8282)	1:179:A:ARG:HG3	1:179:A:ARG:HB3	5	0.15
(2,8105)	1:160:A:ALA:HB3	1:161:A:SER:H	3	0.15
(2,8105)	1:160:A:ALA:HB3	1:161:A:SER:H	8	0.15
(2,8032)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	1	0.15
(2,8032)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	5	0.15
(2,7713)	1:126:A:GLU:HG3	1:127:A:ILE:H	8	0.15
(2,7498)	1:96:A:VAL:HG22	1:97:A:LEU:H	8	0.15
(2,7433)	1:92:A:ALA:HB3	1:93:A:MET:H	7	0.15
(2,7413)	1:181:A:ILE:HD12	1:183:A:ILE:H	10	0.15
(2,7388)	1:150:A:ARG:HB2	1:150:A:ARG:HA	4	0.15
(2,7388)	1:150:A:ARG:HB2	1:150:A:ARG:HA	6	0.15
(2,7377)	1:181:A:ILE:HG21	1:174:A:GLU:HA	4	0.15
(2,7322)	1:191:A:VAL:HG13	1:190:A:GLU:H	10	0.15
(2,7290)	1:96:A:VAL:HG22	1:97:A:LEU:H	4	0.15
(2,7271)	1:164:A:ILE:HD13	1:91:A:ASN:HA	2	0.15
(2,7271)	1:164:A:ILE:HD13	1:91:A:ASN:HA	7	0.15
(2,7271)	1:164:A:ILE:HD13	1:91:A:ASN:HA	10	0.15
(2,7270)	1:164:A:ILE:HD12	1:164:A:ILE:HA	5	0.15
(2,7230)	1:150:A:ARG:HG2	1:151:A:SER:H	5	0.15
(2,7200)	1:192:A:ARG:HG2	1:192:A:ARG:H	6	0.15
(2,7180)	1:187:A:SER:HB3	1:188:A:ARG:H	8	0.15
(2,7104)	1:166:A:GLU:HB3	1:166:A:GLU:H	10	0.15
(2,7096)	1:164:A:ILE:H	1:164:A:ILE:HG21	8	0.15
(2,6845)	1:110:A:ASP:HB3	1:110:A:ASP:H	6	0.15
(2,6845)	1:110:A:ASP:HB3	1:110:A:ASP:H	7	0.15
(2,6599)	1:155:A:ALA:HA	1:155:A:ALA:HB3	2	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6599)	1:155:A:ALA:HA	1:155:A:ALA:HB3	7	0.15
(2,6599)	1:155:A:ALA:HA	1:155:A:ALA:HB3	8	0.15
(2,6558)	1:192:A:ARG:HD2	1:192:A:ARG:HB2	1	0.15
(2,6533)	1:191:A:VAL:HG22	1:191:A:VAL:HB	8	0.15
(2,6519)	1:189:A:ALA:HB1	1:190:A:GLU:H	8	0.15
(2,6519)	1:189:A:ALA:HB1	1:190:A:GLU:H	10	0.15
(2,6258)	1:163:A:GLU:HG3	1:163:A:GLU:H	4	0.15
(2,6233)	1:161:A:SER:HB2	1:161:A:SER:HA	9	0.15
(2,6073)	1:144:A:PRO:HD3	1:143:A:LEU:HA	9	0.15
(2,6036)	1:141:A:ILE:HG13	1:141:A:ILE:H	1	0.15
(2,5915)	1:130:A:PHE:HB2	1:131:A:PHE:H	4	0.15
(2,5866)	1:127:A:ILE:HG23	1:127:A:ILE:HG12	3	0.15
(2,5721)	1:111:A:GLY:HA3	1:112:A:PHE:H	3	0.15
(2,5676)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	6	0.15
(2,5643)	1:100:A:THR:HA	1:99:A:HIS:HB2	7	0.15
(2,5643)	1:100:A:THR:HA	1:99:A:HIS:HB2	8	0.15
(2,5454)	1:183:A:ILE:HG12	1:115:A:LEU:HD21	6	0.15
(2,5444)	1:191:A:VAL:HG13	1:193:A:THR:H	6	0.15
(2,5382)	1:164:A:ILE:HG13	1:167:A:LYS:H	5	0.15
(2,5278)	1:179:A:ARG:HG3	1:179:A:ARG:H	4	0.15
(2,5001)	1:112:A:PHE:H	1:111:A:GLY:H	7	0.15
(2,4907)	1:151:A:SER:H	1:151:A:SER:HB2	10	0.15
(2,4869)	1:108:A:ALA:H	1:188:A:ARG:HG2	2	0.15
(2,4869)	1:108:A:ALA:H	1:188:A:ARG:HG2	5	0.15
(2,4846)	1:130:A:PHE:H	1:136:A:ILE:HG22	9	0.15
(2,4765)	1:119:A:PRO:HB2	1:120:A:PHE:H	1	0.15
(2,4496)	1:169:A:LEU:HD22	1:169:A:LEU:HA	9	0.15
(2,4481)	1:167:A:LYS:HB2	1:167:A:LYS:HA	9	0.15
(2,4433)	1:163:A:GLU:HB3	1:164:A:ILE:H	8	0.15
(2,4330)	1:150:A:ARG:HG2	1:150:A:ARG:HA	9	0.15
(2,4321)	1:148:A:GLN:HB2	1:149:A:GLY:H	4	0.15
(2,4269)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	2	0.15
(2,4269)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	4	0.15
(2,4269)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	7	0.15
(2,4269)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	9	0.15
(2,3821)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	8	0.15
(2,3793)	1:97:A:LEU:HD12	1:97:A:LEU:H	5	0.15
(2,3735)	1:102:A:PRO:HA	1:103:A:ASN:H	2	0.15
(2,3695)	1:181:A:ILE:HG21	1:174:A:GLU:HA	3	0.15
(2,3635)	1:191:A:VAL:HG21	1:156:A:PHE:HB2	9	0.15
(2,3615)	1:160:A:ALA:HB2	1:162:A:GLN:H	1	0.15
(2,3608)	1:164:A:ILE:HD11	1:161:A:SER:H	6	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3606)	1:164:A:ILE:HD12	1:164:A:ILE:HA	2	0.15
(2,3606)	1:164:A:ILE:HD12	1:164:A:ILE:HA	7	0.15
(2,3572)	1:184:A:PHE:H	1:182:A:GLU:HG2	1	0.15
(2,3532)	1:190:A:GLU:HB3	1:190:A:GLU:H	2	0.15
(2,3532)	1:190:A:GLU:HB3	1:190:A:GLU:H	6	0.15
(2,3532)	1:190:A:GLU:HB3	1:190:A:GLU:H	9	0.15
(2,3439)	1:165:A:ALA:HB1	1:166:A:GLU:H	1	0.15
(2,3182)	1:107:A:THR:HA	1:108:A:ALA:H	9	0.15
(2,3104)	1:151:A:SER:H	1:151:A:SER:HB2	10	0.15
(2,3091)	1:181:A:ILE:H	1:116:A:ARG:H	1	0.15
(2,2987)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	4	0.15
(2,2987)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	10	0.15
(2,2969)	1:116:A:ARG:HG2	1:154:A:GLU:HG2	1	0.15
(2,2969)	1:116:A:ARG:HG2	1:154:A:GLU:HG2	9	0.15
(2,2954)	1:110:A:ASP:HB2	1:107:A:THR:HB	4	0.15
(2,2848)	1:183:A:ILE:HA	1:183:A:ILE:HD11	9	0.15
(2,2670)	1:167:A:LYS:HB2	1:167:A:LYS:HA	3	0.15
(2,2670)	1:167:A:LYS:HB2	1:167:A:LYS:HA	4	0.15
(2,2619)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	1	0.15
(2,2619)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	4	0.15
(2,2619)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	7	0.15
(2,2607)	1:162:A:GLN:HG3	1:162:A:GLN:HA	1	0.15
(2,2520)	1:150:A:ARG:HG2	1:150:A:ARG:HA	9	0.15
(2,2180)	1:119:A:PRO:HA	1:119:A:PRO:HG3	5	0.15
(2,2180)	1:119:A:PRO:HA	1:119:A:PRO:HG3	8	0.15
(2,2180)	1:119:A:PRO:HA	1:119:A:PRO:HG3	9	0.15
(2,2172)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	1	0.15
(2,2051)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	1	0.15
(2,1853)	1:95:A:TRP:HB3	1:91:A:ASN:HB3	4	0.15
(2,1849)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	4	0.15
(2,1849)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	5	0.15
(2,1849)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	10	0.15
(2,1838)	1:191:A:VAL:HG13	1:193:A:THR:H	6	0.15
(2,1796)	1:164:A:ILE:HD12	1:164:A:ILE:HA	4	0.15
(2,1796)	1:164:A:ILE:HD12	1:164:A:ILE:HA	6	0.15
(2,1729)	1:191:A:VAL:HG12	1:191:A:VAL:H	2	0.15
(2,1600)	1:159:A:PHE:H	1:158:A:GLN:HG3	1	0.15
(2,1553)	1:150:A:ARG:H	1:149:A:GLY:H	5	0.15
(2,1243)	1:127:A:ILE:H	1:115:A:LEU:HD22	6	0.15
(2,1231)	1:169:A:LEU:H	1:169:A:LEU:HG	10	0.15
(2,1168)	1:155:A:ALA:HA	1:155:A:ALA:HB3	9	0.15
(2,1106)	1:191:A:VAL:HG11	1:191:A:VAL:HA	2	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1067)	1:187:A:SER:HB2	1:187:A:SER:HA	10	0.15
(2,996)	1:181:A:ILE:HD12	1:181:A:ILE:HB	9	0.15
(2,829)	1:163:A:GLU:HB2	1:163:A:GLU:HG2	4	0.15
(2,829)	1:163:A:GLU:HB2	1:163:A:GLU:HG2	5	0.15
(2,315)	1:113:A:VAL:HG13	1:113:A:VAL:HB	1	0.15
(2,264)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	4	0.15
(2,264)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	5	0.15
(2,125)	1:115:A:LEU:HD23	1:115:A:LEU:H	7	0.15
(2,125)	1:115:A:LEU:HD23	1:115:A:LEU:H	8	0.15
(2,100)	1:181:A:ILE:HG21	1:174:A:GLU:HA	5	0.15
(2,92)	1:183:A:ILE:HG12	1:116:A:ARG:HD2	6	0.15
(2,27)	1:181:A:ILE:HG21	1:174:A:GLU:H	5	0.15
(2,16)	1:113:A:VAL:HG13	1:113:A:VAL:HB	2	0.15
(2,16)	1:113:A:VAL:HG13	1:113:A:VAL:HB	7	0.15
(2,16)	1:113:A:VAL:HG13	1:113:A:VAL:HB	9	0.15
(2,6)	1:164:A:ILE:HD11	1:161:A:SER:H	10	0.15
(1,3018)	1:97:A:LEU:H	1:99:A:HIS:H	1	0.15
(1,2926)	1:179:A:ARG:HD2	1:179:A:ARG:HA	5	0.15
(1,2777)	1:97:A:LEU:HG	1:97:A:LEU:HD11	4	0.15
(1,2772)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	3	0.15
(1,2772)	1:110:A:ASP:HB2	1:188:A:ARG:HG2	6	0.15
(1,2553)	1:119:A:PRO:HB3	1:119:A:PRO:HA	4	0.15
(1,2403)	1:96:A:VAL:HB	1:97:A:LEU:H	5	0.15
(1,2316)	1:156:A:PHE:HB2	1:141:A:ILE:HG23	4	0.15
(1,2315)	1:114:A:ARG:HG3	1:114:A:ARG:HD2	5	0.15
(1,2134)	1:143:A:LEU:HG	1:141:A:ILE:HG21	10	0.15
(1,2133)	1:97:A:LEU:HD12	1:163:A:GLU:HB3	2	0.15
(1,2069)	1:150:A:ARG:HG2	1:150:A:ARG:HD2	3	0.15
(1,2030)	1:169:A:LEU:HB2	1:169:A:LEU:HA	7	0.15
(1,1976)	1:179:A:ARG:HB3	1:119:A:PRO:HD2	3	0.15
(1,1869)	1:183:A:ILE:HG23	1:183:A:ILE:HG12	8	0.15
(1,1859)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	3	0.15
(1,1798)	1:165:A:ALA:H	1:110:A:ASP:HB3	10	0.15
(1,1793)	1:166:A:GLU:HB2	1:167:A:LYS:H	1	0.15
(1,1759)	1:146:A:ASP:H	1:143:A:LEU:HD21	1	0.15
(1,1700)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	7	0.15
(1,1670)	1:133:A:GLY:HA3	1:134:A:LEU:HG	3	0.15
(1,1625)	1:135:A:GLU:HA	1:136:A:ILE:HB	2	0.15
(1,1537)	1:150:A:ARG:HB2	1:150:A:ARG:HA	2	0.15
(1,1537)	1:150:A:ARG:HB2	1:150:A:ARG:HA	8	0.15
(1,1466)	1:159:A:PHE:HB2	1:159:A:PHE:HA	1	0.15
(1,1466)	1:159:A:PHE:HB2	1:159:A:PHE:HA	3	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1466)	1:159:A:PHE:HB2	1:159:A:PHE:HA	4	0.15
(1,1466)	1:159:A:PHE:HB2	1:159:A:PHE:HA	7	0.15
(1,1442)	1:144:A:PRO:HD2	1:118:A:LEU:HD11	4	0.15
(1,1432)	1:141:A:ILE:HA	1:140:A:GLY:H	5	0.15
(1,1350)	1:144:A:PRO:HB3	1:144:A:PRO:HA	10	0.15
(1,1341)	1:119:A:PRO:HB3	1:119:A:PRO:HA	5	0.15
(1,1341)	1:119:A:PRO:HB3	1:119:A:PRO:HA	9	0.15
(1,1329)	1:115:A:LEU:HG	1:115:A:LEU:HB2	7	0.15
(1,1289)	1:167:A:LYS:HG2	1:134:A:LEU:HD11	7	0.15
(1,1286)	1:134:A:LEU:HD13	1:133:A:GLY:H	2	0.15
(1,1272)	1:181:A:ILE:HG21	1:181:A:ILE:HB	1	0.15
(1,1269)	1:137:A:VAL:HG22	1:140:A:GLY:H	3	0.15
(1,1260)	1:183:A:ILE:HG21	1:184:A:PHE:HA	2	0.15
(1,1209)	1:126:A:GLU:H	1:126:A:GLU:HB3	6	0.15
(1,1196)	1:158:A:GLN:H	1:141:A:ILE:HG23	4	0.15
(1,1173)	1:189:A:ALA:H	1:186:A:SER:HA	6	0.15
(1,1148)	1:146:A:ASP:H	1:143:A:LEU:HD21	4	0.15
(1,1148)	1:146:A:ASP:H	1:143:A:LEU:HD21	9	0.15
(1,1087)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	7	0.15
(1,1080)	1:174:A:GLU:HB2	1:181:A:ILE:HD13	7	0.15
(1,1046)	1:115:A:LEU:HD23	1:114:A:ARG:HA	3	0.15
(1,1034)	1:156:A:PHE:HB3	1:155:A:ALA:HB3	2	0.15
(1,1027)	1:164:A:ILE:HD13	1:93:A:MET:HA	2	0.15
(1,995)	1:123:A:SER:HB3	1:181:A:ILE:HD11	4	0.15
(1,993)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	9	0.15
(1,919)	1:164:A:ILE:HD13	1:93:A:MET:HG3	6	0.15
(1,868)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	4	0.15
(1,858)	1:159:A:PHE:HB2	1:159:A:PHE:HA	2	0.15
(1,858)	1:159:A:PHE:HB2	1:159:A:PHE:HA	5	0.15
(1,858)	1:159:A:PHE:HB2	1:159:A:PHE:HA	7	0.15
(1,858)	1:159:A:PHE:HB2	1:159:A:PHE:HA	8	0.15
(1,858)	1:159:A:PHE:HB2	1:159:A:PHE:HA	9	0.15
(1,810)	1:169:A:LEU:HA	1:169:A:LEU:HD11	2	0.15
(1,756)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.15
(1,735)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	6	0.15
(1,734)	1:119:A:PRO:HB3	1:119:A:PRO:HA	8	0.15
(1,684)	1:167:A:LYS:HG2	1:134:A:LEU:HD11	1	0.15
(1,667)	1:181:A:ILE:HG21	1:181:A:ILE:HB	1	0.15
(1,667)	1:181:A:ILE:HG21	1:181:A:ILE:HB	7	0.15
(1,598)	1:116:A:ARG:H	1:181:A:ILE:HD12	8	0.15
(1,504)	1:166:A:GLU:H	1:169:A:LEU:HD13	4	0.15
(1,297)	1:164:A:ILE:HD13	1:93:A:MET:HG3	10	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	1:141:A:ILE:HG21	1:143:A:LEU:HG	3	0.15
(1,247)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	5	0.15
(1,124)	1:119:A:PRO:HB3	1:119:A:PRO:HB2	1	0.15
(1,124)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	2	0.15
(1,124)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	5	0.15
(1,124)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	6	0.15
(1,124)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	8	0.15
(1,124)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	9	0.15
(1,107)	1:144:A:PRO:HB3	1:144:A:PRO:HA	2	0.15
(1,107)	1:144:A:PRO:HB3	1:144:A:PRO:HA	5	0.15
(1,94)	1:119:A:PRO:HB3	1:119:A:PRO:HA	4	0.15
(1,84)	1:115:A:LEU:HG	1:115:A:LEU:HB2	1	0.15
(1,31)	1:181:A:ILE:HG21	1:181:A:ILE:HB	3	0.15
(1,31)	1:181:A:ILE:HG21	1:181:A:ILE:HB	5	0.15
(1,31)	1:181:A:ILE:HG21	1:181:A:ILE:HB	8	0.15
(1,31)	1:181:A:ILE:HG21	1:181:A:ILE:HB	9	0.15
(1,15)	1:160:A:ALA:HB1	1:160:A:ALA:HA	2	0.15
(1,15)	1:160:A:ALA:HB1	1:160:A:ALA:HA	3	0.15
(1,15)	1:160:A:ALA:HB1	1:160:A:ALA:HA	4	0.15
(1,15)	1:160:A:ALA:HB1	1:160:A:ALA:HA	6	0.15
(1,15)	1:160:A:ALA:HB1	1:160:A:ALA:HA	7	0.15
(1,15)	1:160:A:ALA:HB1	1:160:A:ALA:HA	8	0.15
(1,15)	1:160:A:ALA:HB1	1:160:A:ALA:HA	10	0.15
(1,13)	1:181:A:ILE:HG12	1:175:A:ARG:HA	1	0.15
(4,51)	1:183:A:ILE:N	1:181:A:ILE:O	6	0.14
(4,50)	1:183:A:ILE:H	1:181:A:ILE:O	5	0.14
(4,50)	1:183:A:ILE:H	1:181:A:ILE:O	8	0.14
(4,50)	1:183:A:ILE:H	1:181:A:ILE:O	9	0.14
(4,48)	1:183:A:ILE:H	1:171:A:LYS:O	5	0.14
(4,48)	1:183:A:ILE:H	1:171:A:LYS:O	7	0.14
(4,46)	1:182:A:GLU:H	1:180:A:TYR:O	6	0.14
(4,32)	1:158:A:GLN:H	1:140:A:GLY:O	7	0.14
(4,15)	1:129:A:GLN:H	1:125:A:GLU:O	10	0.14
(4,10)	1:117:A:GLY:N	1:153:A:GLY:O	10	0.14
(4,1)	1:113:A:VAL:H	1:157:A:VAL:O	2	0.14
(4,1)	1:113:A:VAL:H	1:157:A:VAL:O	4	0.14
(3,625)	1:139:A:ASN:H	1:128:A:VAL:HA	1	0.14
(3,625)	1:139:A:ASN:H	1:128:A:VAL:HA	4	0.14
(3,499)	1:139:A:ASN:H	1:128:A:VAL:HA	1	0.14
(3,499)	1:139:A:ASN:H	1:128:A:VAL:HA	4	0.14
(3,281)	1:188:A:ARG:HG2	1:190:A:GLU:H	4	0.14
(3,281)	1:188:A:ARG:HG2	1:190:A:GLU:H	7	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,150)	1:188:A:ARG:HG2	1:190:A:GLU:H	4	0.14
(3,150)	1:188:A:ARG:HG2	1:190:A:GLU:H	7	0.14
(3,6)	1:188:A:ARG:HG2	1:190:A:GLU:H	4	0.14
(3,6)	1:188:A:ARG:HG2	1:190:A:GLU:H	7	0.14
(2,9034)	1:187:A:SER:HB3	1:188:A:ARG:H	4	0.14
(2,8968)	1:171:A:LYS:H	1:170:A:LYS:HB2	4	0.14
(2,8951)	1:164:A:ILE:H	1:164:A:ILE:HG21	1	0.14
(2,8951)	1:164:A:ILE:H	1:164:A:ILE:HG21	3	0.14
(2,8781)	1:127:A:ILE:H	1:127:A:ILE:HG13	7	0.14
(2,8779)	1:127:A:ILE:H	1:127:A:ILE:HG12	4	0.14
(2,8697)	1:110:A:ASP:HA	1:110:A:ASP:H	6	0.14
(2,8566)	1:139:A:ASN:H	1:141:A:ILE:HD12	3	0.14
(2,8560)	1:168:A:ALA:H	1:167:A:LYS:HB3	3	0.14
(2,8414)	1:191:A:VAL:HG13	1:192:A:ARG:HA	3	0.14
(2,8412)	1:191:A:VAL:HG13	1:191:A:VAL:HB	10	0.14
(2,8352)	1:183:A:ILE:HG21	1:184:A:PHE:HA	3	0.14
(2,8352)	1:183:A:ILE:HG21	1:184:A:PHE:HA	5	0.14
(2,8352)	1:183:A:ILE:HG21	1:184:A:PHE:HA	9	0.14
(2,8120)	1:163:A:GLU:HB3	1:163:A:GLU:HA	1	0.14
(2,8120)	1:163:A:GLU:HB3	1:163:A:GLU:HA	7	0.14
(2,7498)	1:96:A:VAL:HG22	1:97:A:LEU:H	9	0.14
(2,7433)	1:92:A:ALA:HB3	1:93:A:MET:H	2	0.14
(2,7433)	1:92:A:ALA:HB3	1:93:A:MET:H	5	0.14
(2,7413)	1:181:A:ILE:HD12	1:183:A:ILE:H	9	0.14
(2,7399)	1:166:A:GLU:HG2	1:168:A:ALA:H	2	0.14
(2,7394)	1:142:A:THR:HG21	1:141:A:ILE:HG21	4	0.14
(2,7388)	1:150:A:ARG:HB2	1:150:A:ARG:HA	10	0.14
(2,7379)	1:126:A:GLU:HA	1:136:A:ILE:HB	6	0.14
(2,7372)	1:156:A:PHE:HB2	1:191:A:VAL:H	5	0.14
(2,7270)	1:164:A:ILE:HD12	1:164:A:ILE:HA	1	0.14
(2,7270)	1:164:A:ILE:HD12	1:164:A:ILE:HA	3	0.14
(2,7270)	1:164:A:ILE:HD12	1:164:A:ILE:HA	10	0.14
(2,7105)	1:166:A:GLU:HB3	1:167:A:LYS:H	10	0.14
(2,7100)	1:165:A:ALA:HB1	1:166:A:GLU:H	1	0.14
(2,6858)	1:114:A:ARG:H	1:113:A:VAL:HG13	10	0.14
(2,6845)	1:110:A:ASP:HB3	1:110:A:ASP:H	3	0.14
(2,6638)	1:187:A:SER:H	1:184:A:PHE:HB2	7	0.14
(2,6621)	1:166:A:GLU:HA	1:169:A:LEU:HD11	7	0.14
(2,6599)	1:155:A:ALA:HA	1:155:A:ALA:HB3	1	0.14
(2,6558)	1:192:A:ARG:HD2	1:192:A:ARG:HB2	8	0.14
(2,6558)	1:192:A:ARG:HD2	1:192:A:ARG:HB2	10	0.14
(2,6533)	1:191:A:VAL:HG22	1:191:A:VAL:HB	2	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6533)	1:191:A:VAL:HG22	1:191:A:VAL:HB	6	0.14
(2,6533)	1:191:A:VAL:HG22	1:191:A:VAL:HB	7	0.14
(2,6533)	1:191:A:VAL:HG22	1:191:A:VAL:HB	9	0.14
(2,6519)	1:189:A:ALA:HB1	1:190:A:GLU:H	1	0.14
(2,6519)	1:189:A:ALA:HB1	1:190:A:GLU:H	2	0.14
(2,6519)	1:189:A:ALA:HB1	1:190:A:GLU:H	4	0.14
(2,6519)	1:189:A:ALA:HB1	1:190:A:GLU:H	5	0.14
(2,6321)	1:169:A:LEU:HD22	1:169:A:LEU:HA	2	0.14
(2,6298)	1:166:A:GLU:HA	1:167:A:LYS:H	5	0.14
(2,6233)	1:161:A:SER:HB2	1:161:A:SER:HA	4	0.14
(2,6233)	1:161:A:SER:HB2	1:161:A:SER:HA	5	0.14
(2,6233)	1:161:A:SER:HB2	1:161:A:SER:HA	6	0.14
(2,6233)	1:161:A:SER:HB2	1:161:A:SER:HA	8	0.14
(2,6233)	1:161:A:SER:HB2	1:161:A:SER:HA	10	0.14
(2,6226)	1:157:A:VAL:HG22	1:158:A:GLN:H	1	0.14
(2,6226)	1:157:A:VAL:HG22	1:158:A:GLN:H	2	0.14
(2,5866)	1:127:A:ILE:HG23	1:127:A:ILE:HG12	2	0.14
(2,5840)	1:126:A:GLU:HG3	1:127:A:ILE:H	3	0.14
(2,5741)	1:115:A:LEU:HA	1:115:A:LEU:HB2	2	0.14
(2,5741)	1:115:A:LEU:HA	1:115:A:LEU:HB2	3	0.14
(2,5741)	1:115:A:LEU:HA	1:115:A:LEU:HB2	4	0.14
(2,5741)	1:115:A:LEU:HA	1:115:A:LEU:HB2	5	0.14
(2,5741)	1:115:A:LEU:HA	1:115:A:LEU:HB2	6	0.14
(2,5741)	1:115:A:LEU:HA	1:115:A:LEU:HB2	8	0.14
(2,5741)	1:115:A:LEU:HA	1:115:A:LEU:HB2	9	0.14
(2,5741)	1:115:A:LEU:HA	1:115:A:LEU:HB2	10	0.14
(2,5643)	1:100:A:THR:HA	1:99:A:HIS:HB2	5	0.14
(2,5542)	1:181:A:ILE:HD12	1:183:A:ILE:H	7	0.14
(2,5542)	1:181:A:ILE:HD12	1:183:A:ILE:H	8	0.14
(2,5526)	1:97:A:LEU:HD13	1:97:A:LEU:HA	5	0.14
(2,5473)	1:109:A:ASN:HA	1:108:A:ALA:HB1	10	0.14
(2,5424)	1:96:A:VAL:HG22	1:97:A:LEU:H	6	0.14
(2,5402)	1:164:A:ILE:HD13	1:91:A:ASN:HA	6	0.14
(2,5355)	1:158:A:GLN:H	1:141:A:ILE:HB	9	0.14
(2,5103)	1:135:A:GLU:HB3	1:135:A:GLU:H	3	0.14
(2,4907)	1:151:A:SER:H	1:151:A:SER:HB2	3	0.14
(2,4907)	1:151:A:SER:H	1:151:A:SER:HB2	5	0.14
(2,4907)	1:151:A:SER:H	1:151:A:SER:HB2	9	0.14
(2,4785)	1:185:A:LYS:HB3	1:185:A:LYS:H	8	0.14
(2,4777)	1:111:A:GLY:HA3	1:109:A:ASN:H	5	0.14
(2,4657)	1:183:A:ILE:HA	1:183:A:ILE:HD11	10	0.14
(2,4496)	1:169:A:LEU:HD22	1:169:A:LEU:HA	5	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4481)	1:167:A:LYS:HB2	1:167:A:LYS:HA	1	0.14
(2,4481)	1:167:A:LYS:HB2	1:167:A:LYS:HA	7	0.14
(2,4474)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	4	0.14
(2,4474)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	6	0.14
(2,4474)	1:166:A:GLU:HB2	1:166:A:GLU:HG3	9	0.14
(2,4471)	1:166:A:GLU:HG3	1:166:A:GLU:HA	3	0.14
(2,4390)	1:157:A:VAL:HG21	1:157:A:VAL:HA	2	0.14
(2,4318)	1:148:A:GLN:HA	1:149:A:GLY:H	6	0.14
(2,4318)	1:148:A:GLN:HA	1:149:A:GLY:H	7	0.14
(2,4269)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	8	0.14
(2,3821)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	1	0.14
(2,3821)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	4	0.14
(2,3821)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	5	0.14
(2,3821)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	10	0.14
(2,3668)	1:154:A:GLU:HG2	1:118:A:LEU:H	2	0.14
(2,3668)	1:154:A:GLU:HG2	1:118:A:LEU:H	8	0.14
(2,3668)	1:154:A:GLU:HG2	1:118:A:LEU:H	9	0.14
(2,3657)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	3	0.14
(2,3615)	1:160:A:ALA:HB2	1:162:A:GLN:H	7	0.14
(2,3611)	1:181:A:ILE:HG12	1:175:A:ARG:HD2	1	0.14
(2,3608)	1:164:A:ILE:HD11	1:161:A:SER:H	1	0.14
(2,3581)	1:108:A:ALA:H	1:188:A:ARG:HG3	9	0.14
(2,3104)	1:151:A:SER:H	1:151:A:SER:HB2	3	0.14
(2,3104)	1:151:A:SER:H	1:151:A:SER:HB2	5	0.14
(2,3104)	1:151:A:SER:H	1:151:A:SER:HB2	9	0.14
(2,3096)	1:111:A:GLY:HA3	1:159:A:PHE:H	8	0.14
(2,3091)	1:181:A:ILE:H	1:116:A:ARG:H	3	0.14
(2,2997)	1:145:A:VAL:H	1:155:A:ALA:HA	9	0.14
(2,2987)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	5	0.14
(2,2969)	1:116:A:ARG:HG2	1:154:A:GLU:HG2	2	0.14
(2,2969)	1:116:A:ARG:HG2	1:154:A:GLU:HG2	4	0.14
(2,2860)	1:187:A:SER:HB3	1:187:A:SER:HA	4	0.14
(2,2841)	1:183:A:ILE:HG21	1:184:A:PHE:HA	3	0.14
(2,2841)	1:183:A:ILE:HG21	1:184:A:PHE:HA	5	0.14
(2,2841)	1:183:A:ILE:HG21	1:184:A:PHE:HA	9	0.14
(2,2670)	1:167:A:LYS:HB2	1:167:A:LYS:HA	9	0.14
(2,2622)	1:163:A:GLU:HB3	1:164:A:ILE:H	5	0.14
(2,2619)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	3	0.14
(2,2619)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	9	0.14
(2,2619)	1:163:A:GLU:HB3	1:163:A:GLU:HG2	10	0.14
(2,2180)	1:119:A:PRO:HA	1:119:A:PRO:HG3	7	0.14
(2,2154)	1:116:A:ARG:HB2	1:117:A:GLY:H	2	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2051)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	7	0.14
(2,2012)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	9	0.14
(2,1920)	1:115:A:LEU:HB3	1:118:A:LEU:HD12	6	0.14
(2,1870)	1:175:A:ARG:HA	1:179:A:ARG:H	6	0.14
(2,1870)	1:175:A:ARG:HA	1:179:A:ARG:H	9	0.14
(2,1867)	1:161:A:SER:HA	1:106:A:ASP:HB3	6	0.14
(2,1849)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	6	0.14
(2,1849)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	7	0.14
(2,1849)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	8	0.14
(2,1849)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	9	0.14
(2,1813)	1:113:A:VAL:HG12	1:112:A:PHE:H	5	0.14
(2,1796)	1:164:A:ILE:HD12	1:164:A:ILE:HA	2	0.14
(2,1796)	1:164:A:ILE:HD12	1:164:A:ILE:HA	7	0.14
(2,1796)	1:164:A:ILE:HD12	1:164:A:ILE:HA	9	0.14
(2,1729)	1:191:A:VAL:HG13	1:191:A:VAL:H	10	0.14
(2,1634)	1:165:A:ALA:HB1	1:166:A:GLU:H	1	0.14
(2,1630)	1:164:A:ILE:H	1:164:A:ILE:HG21	7	0.14
(2,1613)	1:162:A:GLN:HB2	1:163:A:GLU:H	8	0.14
(2,1562)	1:150:A:ARG:H	1:151:A:SER:H	10	0.14
(2,1231)	1:169:A:LEU:H	1:169:A:LEU:HG	6	0.14
(2,1171)	1:190:A:GLU:HB2	1:187:A:SER:H	5	0.14
(2,1168)	1:155:A:ALA:HA	1:155:A:ALA:HB3	6	0.14
(2,1133)	1:192:A:ARG:HB2	1:193:A:THR:HA	4	0.14
(2,1068)	1:187:A:SER:HB3	1:187:A:SER:HA	4	0.14
(2,1067)	1:187:A:SER:HB2	1:187:A:SER:HA	1	0.14
(2,829)	1:163:A:GLU:HB2	1:163:A:GLU:HG2	7	0.14
(2,790)	1:157:A:VAL:HG21	1:157:A:VAL:HA	1	0.14
(2,790)	1:157:A:VAL:HG21	1:157:A:VAL:HA	3	0.14
(2,521)	1:134:A:LEU:HD11	1:134:A:LEU:HA	2	0.14
(2,264)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	1	0.14
(2,125)	1:115:A:LEU:HD23	1:115:A:LEU:H	5	0.14
(2,121)	1:97:A:LEU:HD13	1:97:A:LEU:HA	5	0.14
(2,111)	1:188:A:ARG:HB2	1:189:A:ALA:H	5	0.14
(2,91)	1:155:A:ALA:HA	1:144:A:PRO:HD2	1	0.14
(2,16)	1:113:A:VAL:HG13	1:113:A:VAL:HB	10	0.14
(2,5)	1:164:A:ILE:HD13	1:91:A:ASN:HA	9	0.14
(1,3038)	1:158:A:GLN:H	1:141:A:ILE:HG23	4	0.14
(1,3018)	1:97:A:LEU:H	1:99:A:HIS:H	2	0.14
(1,3017)	1:96:A:VAL:HB	1:97:A:LEU:H	8	0.14
(1,3017)	1:96:A:VAL:HB	1:97:A:LEU:H	10	0.14
(1,3003)	1:108:A:ALA:H	1:109:A:ASN:HA	4	0.14
(1,2927)	1:114:A:ARG:HG3	1:114:A:ARG:HD2	5	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2791)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	7	0.14
(1,2777)	1:97:A:LEU:HG	1:97:A:LEU:HD11	10	0.14
(1,2746)	1:93:A:MET:HB2	1:93:A:MET:HG2	6	0.14
(1,2746)	1:93:A:MET:HB2	1:93:A:MET:HG2	10	0.14
(1,2739)	1:143:A:LEU:HG	1:141:A:ILE:HG21	5	0.14
(1,2694)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	8	0.14
(1,2609)	1:130:A:PHE:HB3	1:132:A:SER:H	9	0.14
(1,2563)	1:181:A:ILE:HB	1:181:A:ILE:HA	2	0.14
(1,2563)	1:181:A:ILE:HB	1:181:A:ILE:HA	8	0.14
(1,2405)	1:132:A:SER:H	1:136:A:ILE:HB	10	0.14
(1,2376)	1:145:A:VAL:HB	1:146:A:ASP:H	5	0.14
(1,2315)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	2	0.14
(1,2315)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	10	0.14
(1,2097)	1:143:A:LEU:HA	1:143:A:LEU:HB2	3	0.14
(1,2087)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	7	0.14
(1,2072)	1:175:A:ARG:HD2	1:178:A:HIS:HA	7	0.14
(1,2003)	1:130:A:PHE:HB3	1:132:A:SER:H	6	0.14
(1,2003)	1:130:A:PHE:HB3	1:132:A:SER:H	10	0.14
(1,1859)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	4	0.14
(1,1859)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	9	0.14
(1,1841)	1:134:A:LEU:HD12	1:167:A:LYS:H	1	0.14
(1,1826)	1:184:A:PHE:H	1:186:A:SER:HB3	6	0.14
(1,1826)	1:184:A:PHE:H	1:186:A:SER:HB3	9	0.14
(1,1700)	1:114:A:ARG:HG3	1:114:A:ARG:HD2	9	0.14
(1,1658)	1:143:A:LEU:HD23	1:123:A:SER:HA	6	0.14
(1,1647)	1:111:A:GLY:HA3	1:112:A:PHE:H	10	0.14
(1,1537)	1:150:A:ARG:HB2	1:150:A:ARG:HA	9	0.14
(1,1466)	1:159:A:PHE:HB2	1:159:A:PHE:HA	2	0.14
(1,1466)	1:159:A:PHE:HB2	1:159:A:PHE:HA	5	0.14
(1,1466)	1:159:A:PHE:HB2	1:159:A:PHE:HA	6	0.14
(1,1466)	1:159:A:PHE:HB2	1:159:A:PHE:HA	8	0.14
(1,1466)	1:159:A:PHE:HB2	1:159:A:PHE:HA	9	0.14
(1,1442)	1:144:A:PRO:HD2	1:118:A:LEU:HD11	10	0.14
(1,1350)	1:144:A:PRO:HB3	1:144:A:PRO:HA	9	0.14
(1,1341)	1:119:A:PRO:HB3	1:119:A:PRO:HA	1	0.14
(1,1341)	1:119:A:PRO:HB3	1:119:A:PRO:HA	2	0.14
(1,1341)	1:119:A:PRO:HB3	1:119:A:PRO:HA	6	0.14
(1,1341)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.14
(1,1329)	1:115:A:LEU:HG	1:115:A:LEU:HB2	2	0.14
(1,1289)	1:167:A:LYS:HG2	1:134:A:LEU:HD12	10	0.14
(1,1269)	1:137:A:VAL:HG22	1:140:A:GLY:H	1	0.14
(1,1269)	1:137:A:VAL:HG22	1:140:A:GLY:H	2	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1269)	1:137:A:VAL:HG22	1:140:A:GLY:H	9	0.14
(1,1259)	1:113:A:VAL:HG11	1:168:A:ALA:HB2	9	0.14
(1,1255)	1:164:A:ILE:HD13	1:95:A:TRP:HA	6	0.14
(1,1255)	1:164:A:ILE:HD12	1:95:A:TRP:HA	8	0.14
(1,1178)	1:132:A:SER:H	1:136:A:ILE:HB	5	0.14
(1,1178)	1:132:A:SER:H	1:136:A:ILE:HB	10	0.14
(1,1090)	1:166:A:GLU:HB2	1:166:A:GLU:HA	3	0.14
(1,993)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	3	0.14
(1,985)	1:169:A:LEU:HD21	1:167:A:LYS:H	7	0.14
(1,927)	1:164:A:ILE:HA	1:91:A:ASN:HB3	8	0.14
(1,858)	1:159:A:PHE:HB2	1:159:A:PHE:HA	6	0.14
(1,764)	1:166:A:GLU:HG3	1:168:A:ALA:H	10	0.14
(1,744)	1:144:A:PRO:HB3	1:144:A:PRO:HA	1	0.14
(1,744)	1:144:A:PRO:HB3	1:144:A:PRO:HA	3	0.14
(1,744)	1:144:A:PRO:HB3	1:144:A:PRO:HA	5	0.14
(1,735)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	9	0.14
(1,734)	1:119:A:PRO:HB3	1:119:A:PRO:HA	5	0.14
(1,734)	1:119:A:PRO:HB3	1:119:A:PRO:HA	7	0.14
(1,722)	1:148:A:GLN:HB3	1:147:A:PHE:H	6	0.14
(1,647)	1:164:A:ILE:HD13	1:95:A:TRP:HA	6	0.14
(1,647)	1:164:A:ILE:HD12	1:95:A:TRP:HA	8	0.14
(1,641)	1:141:A:ILE:HD12	1:125:A:GLU:H	3	0.14
(1,592)	1:97:A:LEU:HB2	1:97:A:LEU:H	5	0.14
(1,504)	1:166:A:GLU:H	1:169:A:LEU:HD13	6	0.14
(1,297)	1:164:A:ILE:HD13	1:93:A:MET:HG3	4	0.14
(1,248)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	5	0.14
(1,179)	1:169:A:LEU:HA	1:169:A:LEU:HD11	2	0.14
(1,124)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	3	0.14
(1,124)	1:126:A:GLU:HB2	1:126:A:GLU:HB3	7	0.14
(1,107)	1:144:A:PRO:HB3	1:144:A:PRO:HA	7	0.14
(1,84)	1:115:A:LEU:HG	1:115:A:LEU:HB2	3	0.14
(1,84)	1:115:A:LEU:HG	1:115:A:LEU:HB2	4	0.14
(1,84)	1:115:A:LEU:HG	1:115:A:LEU:HB2	5	0.14
(1,84)	1:115:A:LEU:HG	1:115:A:LEU:HB2	6	0.14
(1,84)	1:115:A:LEU:HG	1:115:A:LEU:HB2	10	0.14
(1,41)	1:134:A:LEU:HD11	1:134:A:LEU:HA	9	0.14
(1,31)	1:181:A:ILE:HG21	1:181:A:ILE:HB	2	0.14
(1,31)	1:181:A:ILE:HG21	1:181:A:ILE:HB	10	0.14
(1,15)	1:160:A:ALA:HB1	1:160:A:ALA:HA	1	0.14
(1,15)	1:160:A:ALA:HB1	1:160:A:ALA:HA	5	0.14
(1,15)	1:160:A:ALA:HB1	1:160:A:ALA:HA	9	0.14
(4,37)	1:160:A:ALA:N	1:135:A:GLU:O	4	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,34)	1:159:A:PHE:H	1:111:A:GLY:O	9	0.13
(4,32)	1:158:A:GLN:H	1:140:A:GLY:O	1	0.13
(4,32)	1:158:A:GLN:H	1:140:A:GLY:O	4	0.13
(4,32)	1:158:A:GLN:H	1:140:A:GLY:O	6	0.13
(4,30)	1:157:A:VAL:H	1:113:A:VAL:O	2	0.13
(4,10)	1:117:A:GLY:N	1:153:A:GLY:O	2	0.13
(4,10)	1:117:A:GLY:N	1:153:A:GLY:O	4	0.13
(4,1)	1:113:A:VAL:H	1:157:A:VAL:O	1	0.13
(3,625)	1:139:A:ASN:H	1:128:A:VAL:HA	2	0.13
(3,625)	1:139:A:ASN:H	1:128:A:VAL:HA	7	0.13
(3,541)	1:116:A:ARG:HD2	1:183:A:ILE:H	6	0.13
(3,499)	1:139:A:ASN:H	1:128:A:VAL:HA	2	0.13
(3,499)	1:139:A:ASN:H	1:128:A:VAL:HA	7	0.13
(3,417)	1:116:A:ARG:HD2	1:183:A:ILE:H	6	0.13
(3,281)	1:188:A:ARG:HG2	1:190:A:GLU:H	9	0.13
(3,278)	1:116:A:ARG:HD2	1:183:A:ILE:H	6	0.13
(3,150)	1:188:A:ARG:HG2	1:190:A:GLU:H	9	0.13
(3,146)	1:116:A:ARG:HD2	1:183:A:ILE:H	6	0.13
(3,6)	1:188:A:ARG:HG2	1:190:A:GLU:H	9	0.13
(3,2)	1:116:A:ARG:HD2	1:183:A:ILE:H	6	0.13
(2,8724)	1:114:A:ARG:HG3	1:115:A:LEU:H	5	0.13
(2,8637)	1:96:A:VAL:HG13	1:97:A:LEU:H	9	0.13
(2,8578)	1:143:A:LEU:H	1:141:A:ILE:HB	7	0.13
(2,8566)	1:139:A:ASN:H	1:141:A:ILE:HD12	1	0.13
(2,8566)	1:139:A:ASN:H	1:141:A:ILE:HD12	2	0.13
(2,8563)	1:168:A:ALA:H	1:95:A:TRP:HB2	6	0.13
(2,8464)	1:123:A:SER:HB3	1:126:A:GLU:HB2	4	0.13
(2,8414)	1:191:A:VAL:HG13	1:192:A:ARG:HA	2	0.13
(2,8414)	1:191:A:VAL:HG13	1:192:A:ARG:HA	5	0.13
(2,8412)	1:191:A:VAL:HG13	1:191:A:VAL:HB	3	0.13
(2,8120)	1:163:A:GLU:HB3	1:163:A:GLU:HA	4	0.13
(2,8120)	1:163:A:GLU:HB3	1:163:A:GLU:HA	5	0.13
(2,8120)	1:163:A:GLU:HB3	1:163:A:GLU:HA	10	0.13
(2,8105)	1:160:A:ALA:HB3	1:161:A:SER:H	4	0.13
(2,7711)	1:126:A:GLU:HG2	1:126:A:GLU:H	10	0.13
(2,7693)	1:122:A:CYS:HA	1:121:A:GLY:H	1	0.13
(2,7498)	1:96:A:VAL:HG22	1:97:A:LEU:H	2	0.13
(2,7413)	1:181:A:ILE:HD12	1:183:A:ILE:H	5	0.13
(2,7388)	1:150:A:ARG:HB2	1:150:A:ARG:HA	2	0.13
(2,7388)	1:150:A:ARG:HB2	1:150:A:ARG:HA	8	0.13
(2,7385)	1:188:A:ARG:HB2	1:187:A:SER:H	5	0.13
(2,7358)	1:141:A:ILE:HA	1:140:A:GLY:H	10	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7352)	1:150:A:ARG:HA	1:151:A:SER:H	4	0.13
(2,7344)	1:109:A:ASN:HA	1:108:A:ALA:HB1	10	0.13
(2,7290)	1:96:A:VAL:HG22	1:97:A:LEU:H	7	0.13
(2,7270)	1:164:A:ILE:HD12	1:164:A:ILE:HA	4	0.13
(2,7246)	1:166:A:GLU:H	1:95:A:TRP:HB2	3	0.13
(2,7180)	1:187:A:SER:HB3	1:188:A:ARG:H	6	0.13
(2,7105)	1:166:A:GLU:HB3	1:167:A:LYS:H	8	0.13
(2,6728)	1:93:A:MET:H	1:91:A:ASN:HA	3	0.13
(2,6728)	1:93:A:MET:H	1:91:A:ASN:HA	9	0.13
(2,6714)	1:108:A:ALA:H	1:189:A:ALA:H	5	0.13
(2,6633)	1:101:A:GLY:H	1:110:A:ASP:HA	7	0.13
(2,6599)	1:155:A:ALA:HA	1:155:A:ALA:HB3	9	0.13
(2,6321)	1:169:A:LEU:HD22	1:169:A:LEU:HA	1	0.13
(2,6233)	1:161:A:SER:HB2	1:161:A:SER:HA	1	0.13
(2,6233)	1:161:A:SER:HB2	1:161:A:SER:HA	2	0.13
(2,6226)	1:157:A:VAL:HG22	1:158:A:GLN:H	5	0.13
(2,6036)	1:141:A:ILE:HG13	1:141:A:ILE:H	5	0.13
(2,6036)	1:141:A:ILE:HG13	1:141:A:ILE:H	6	0.13
(2,6036)	1:141:A:ILE:HG13	1:141:A:ILE:H	7	0.13
(2,5866)	1:127:A:ILE:HG23	1:127:A:ILE:HG12	8	0.13
(2,5741)	1:115:A:LEU:HA	1:115:A:LEU:HB2	1	0.13
(2,5741)	1:115:A:LEU:HA	1:115:A:LEU:HB2	7	0.13
(2,5676)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	8	0.13
(2,5526)	1:97:A:LEU:HD13	1:97:A:LEU:HA	1	0.13
(2,5525)	1:142:A:THR:HG21	1:141:A:ILE:HG21	2	0.13
(2,5497)	1:116:A:ARG:HD2	1:116:A:ARG:H	6	0.13
(2,5444)	1:191:A:VAL:HG13	1:193:A:THR:H	8	0.13
(2,5418)	1:113:A:VAL:HG12	1:112:A:PHE:H	7	0.13
(2,5376)	1:166:A:GLU:H	1:95:A:TRP:HB2	3	0.13
(2,5364)	1:188:A:ARG:HG2	1:188:A:ARG:H	9	0.13
(2,5249)	1:167:A:LYS:HG2	1:168:A:ALA:H	8	0.13
(2,5249)	1:167:A:LYS:HG2	1:168:A:ALA:H	10	0.13
(2,5027)	1:116:A:ARG:H	1:116:A:ARG:HB3	6	0.13
(2,4963)	1:101:A:GLY:H	1:100:A:THR:H	3	0.13
(2,4963)	1:101:A:GLY:H	1:100:A:THR:H	9	0.13
(2,4963)	1:101:A:GLY:H	1:100:A:THR:H	10	0.13
(2,4899)	1:111:A:GLY:HA3	1:159:A:PHE:H	8	0.13
(2,4891)	1:105:A:PRO:HA	1:106:A:ASP:H	6	0.13
(2,4785)	1:185:A:LYS:HB3	1:185:A:LYS:H	2	0.13
(2,4761)	1:107:A:THR:HB	1:110:A:ASP:HB3	3	0.13
(2,4761)	1:107:A:THR:HB	1:110:A:ASP:HB3	10	0.13
(2,4496)	1:169:A:LEU:HD22	1:169:A:LEU:HA	4	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4496)	1:169:A:LEU:HD22	1:169:A:LEU:HA	6	0.13
(2,4477)	1:166:A:GLU:HG2	1:166:A:GLU:H	5	0.13
(2,4433)	1:163:A:GLU:HB3	1:164:A:ILE:H	1	0.13
(2,4433)	1:163:A:GLU:HB3	1:164:A:ILE:H	3	0.13
(2,4433)	1:163:A:GLU:HB3	1:164:A:ILE:H	4	0.13
(2,4433)	1:163:A:GLU:HB3	1:164:A:ILE:H	9	0.13
(2,4390)	1:157:A:VAL:HG21	1:157:A:VAL:HA	7	0.13
(2,4390)	1:157:A:VAL:HG21	1:157:A:VAL:HA	10	0.13
(2,4269)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	5	0.13
(2,4269)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	6	0.13
(2,4269)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	10	0.13
(2,4133)	1:135:A:GLU:HG3	1:135:A:GLU:HA	2	0.13
(2,4133)	1:135:A:GLU:HG3	1:135:A:GLU:HA	3	0.13
(2,4037)	1:127:A:ILE:HD12	1:127:A:ILE:HB	1	0.13
(2,4037)	1:127:A:ILE:HD12	1:127:A:ILE:HB	5	0.13
(2,3981)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	6	0.13
(2,3963)	1:116:A:ARG:HB2	1:117:A:GLY:H	2	0.13
(2,3728)	1:123:A:SER:HB3	1:181:A:ILE:HD11	4	0.13
(2,3657)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	4	0.13
(2,3657)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	5	0.13
(2,3657)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	10	0.13
(2,3607)	1:164:A:ILE:HD13	1:91:A:ASN:HA	1	0.13
(2,3606)	1:164:A:ILE:HD12	1:164:A:ILE:HA	8	0.13
(2,3559)	1:158:A:GLN:H	1:141:A:ILE:HB	8	0.13
(2,3533)	1:190:A:GLU:HB3	1:191:A:VAL:H	7	0.13
(2,3526)	1:189:A:ALA:HA	1:190:A:GLU:H	4	0.13
(2,3066)	1:108:A:ALA:H	1:188:A:ARG:HG2	4	0.13
(2,3019)	1:110:A:ASP:H	1:188:A:ARG:HG2	9	0.13
(2,2992)	1:161:A:SER:H	1:159:A:PHE:HB2	7	0.13
(2,2987)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	7	0.13
(2,2987)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	8	0.13
(2,2970)	1:111:A:GLY:HA3	1:109:A:ASN:H	1	0.13
(2,2969)	1:116:A:ARG:HG2	1:154:A:GLU:HG2	8	0.13
(2,2927)	1:192:A:ARG:HB2	1:193:A:THR:HA	4	0.13
(2,2861)	1:187:A:SER:HB3	1:188:A:ARG:H	2	0.13
(2,2861)	1:187:A:SER:HB3	1:188:A:ARG:H	8	0.13
(2,2860)	1:187:A:SER:HB3	1:187:A:SER:HA	10	0.13
(2,2848)	1:183:A:ILE:HA	1:183:A:ILE:HD11	5	0.13
(2,2848)	1:183:A:ILE:HA	1:183:A:ILE:HD11	8	0.13
(2,2790)	1:181:A:ILE:HG22	1:181:A:ILE:HG12	1	0.13
(2,2790)	1:181:A:ILE:HG22	1:181:A:ILE:HG12	7	0.13
(2,2693)	1:169:A:LEU:HB2	1:169:A:LEU:HD13	2	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2670)	1:167:A:LYS:HB2	1:167:A:LYS:HA	1	0.13
(2,2670)	1:167:A:LYS:HB2	1:167:A:LYS:HA	7	0.13
(2,2666)	1:166:A:GLU:HG2	1:166:A:GLU:H	5	0.13
(2,2660)	1:166:A:GLU:HG3	1:166:A:GLU:HA	2	0.13
(2,2660)	1:166:A:GLU:HG3	1:166:A:GLU:HA	9	0.13
(2,2520)	1:150:A:ARG:HG2	1:150:A:ARG:HA	2	0.13
(2,2459)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	3	0.13
(2,2455)	1:143:A:LEU:HG	1:143:A:LEU:HD13	4	0.13
(2,2333)	1:137:A:VAL:HA	1:136:A:ILE:HA	7	0.13
(2,2180)	1:119:A:PRO:HA	1:119:A:PRO:HG3	1	0.13
(2,2180)	1:119:A:PRO:HA	1:119:A:PRO:HG3	6	0.13
(2,2180)	1:119:A:PRO:HA	1:119:A:PRO:HG3	10	0.13
(2,2031)	1:101:A:GLY:HA3	1:101:A:GLY:H	1	0.13
(2,2031)	1:101:A:GLY:HA3	1:101:A:GLY:H	2	0.13
(2,2031)	1:101:A:GLY:HA3	1:101:A:GLY:H	4	0.13
(2,2031)	1:101:A:GLY:HA3	1:101:A:GLY:H	7	0.13
(2,1921)	1:143:A:LEU:HG	1:123:A:SER:HA	9	0.13
(2,1852)	1:95:A:TRP:HB2	1:96:A:VAL:HG21	4	0.13
(2,1849)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	1	0.13
(2,1849)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	2	0.13
(2,1844)	1:191:A:VAL:HG12	1:156:A:PHE:HB2	7	0.13
(2,1838)	1:191:A:VAL:HG13	1:193:A:THR:H	8	0.13
(2,1798)	1:164:A:ILE:HD11	1:161:A:SER:H	5	0.13
(2,1797)	1:164:A:ILE:HD13	1:91:A:ASN:HA	4	0.13
(2,1729)	1:191:A:VAL:HG12	1:191:A:VAL:H	9	0.13
(2,1639)	1:166:A:GLU:HB3	1:167:A:LYS:H	3	0.13
(2,1630)	1:164:A:ILE:H	1:164:A:ILE:HG21	2	0.13
(2,1630)	1:164:A:ILE:H	1:164:A:ILE:HG21	4	0.13
(2,1630)	1:164:A:ILE:H	1:164:A:ILE:HG21	6	0.13
(2,1613)	1:162:A:GLN:HB2	1:163:A:GLU:H	2	0.13
(2,1613)	1:162:A:GLN:HB2	1:163:A:GLU:H	4	0.13
(2,1600)	1:159:A:PHE:H	1:158:A:GLN:HG3	3	0.13
(2,1553)	1:150:A:ARG:H	1:149:A:GLY:H	4	0.13
(2,1553)	1:150:A:ARG:H	1:149:A:GLY:H	8	0.13
(2,1386)	1:110:A:ASP:H	1:109:A:ASN:H	6	0.13
(2,1231)	1:169:A:LEU:H	1:169:A:LEU:HG	5	0.13
(2,1231)	1:169:A:LEU:H	1:169:A:LEU:HG	8	0.13
(2,1231)	1:169:A:LEU:H	1:169:A:LEU:HG	9	0.13
(2,1180)	1:188:A:ARG:HB2	1:188:A:ARG:HG2	9	0.13
(2,1133)	1:192:A:ARG:HB2	1:193:A:THR:HA	5	0.13
(2,1133)	1:192:A:ARG:HB2	1:193:A:THR:HA	10	0.13
(2,1106)	1:191:A:VAL:HG11	1:191:A:VAL:HA	6	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1071)	1:188:A:ARG:HG3	1:188:A:ARG:HA	1	0.13
(2,1071)	1:188:A:ARG:HG3	1:188:A:ARG:HA	3	0.13
(2,1071)	1:188:A:ARG:HG3	1:188:A:ARG:HA	5	0.13
(2,1068)	1:187:A:SER:HB3	1:187:A:SER:HA	10	0.13
(2,1067)	1:187:A:SER:HB2	1:187:A:SER:HA	3	0.13
(2,1067)	1:187:A:SER:HB2	1:187:A:SER:HA	7	0.13
(2,1067)	1:187:A:SER:HB2	1:187:A:SER:HA	9	0.13
(2,829)	1:163:A:GLU:HB2	1:163:A:GLU:HG2	2	0.13
(2,521)	1:134:A:LEU:HD11	1:134:A:LEU:HA	1	0.13
(2,431)	1:126:A:GLU:HG3	1:127:A:ILE:H	4	0.13
(2,352)	1:115:A:LEU:HA	1:115:A:LEU:HD21	5	0.13
(2,352)	1:115:A:LEU:HA	1:115:A:LEU:HD21	8	0.13
(2,348)	1:115:A:LEU:HB3	1:115:A:LEU:HD13	7	0.13
(2,348)	1:115:A:LEU:HB3	1:115:A:LEU:HD13	8	0.13
(2,175)	1:96:A:VAL:HG13	1:96:A:VAL:HA	1	0.13
(2,175)	1:96:A:VAL:HG13	1:96:A:VAL:HA	4	0.13
(2,121)	1:97:A:LEU:HD13	1:97:A:LEU:HA	1	0.13
(2,36)	1:191:A:VAL:HG23	1:191:A:VAL:H	3	0.13
(2,36)	1:191:A:VAL:HG23	1:191:A:VAL:H	4	0.13
(2,22)	1:113:A:VAL:HG12	1:112:A:PHE:H	10	0.13
(2,17)	1:113:A:VAL:HG12	1:113:A:VAL:H	10	0.13
(2,6)	1:164:A:ILE:HD11	1:161:A:SER:H	8	0.13
(1,3017)	1:96:A:VAL:HB	1:97:A:LEU:H	2	0.13
(1,3006)	1:117:A:GLY:H	1:118:A:LEU:HD12	2	0.13
(1,2974)	1:100:A:THR:HG23	1:98:A:LYS:H	9	0.13
(1,2930)	1:166:A:GLU:HB2	1:166:A:GLU:HA	2	0.13
(1,2927)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	2	0.13
(1,2927)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	10	0.13
(1,2863)	1:164:A:ILE:HD13	1:135:A:GLU:HA	1	0.13
(1,2777)	1:97:A:LEU:HG	1:97:A:LEU:HD13	5	0.13
(1,2777)	1:97:A:LEU:HG	1:97:A:LEU:HD13	9	0.13
(1,2694)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	7	0.13
(1,2563)	1:96:A:VAL:HB	1:96:A:VAL:HA	1	0.13
(1,2563)	1:96:A:VAL:HB	1:96:A:VAL:HA	7	0.13
(1,2515)	1:114:A:ARG:HG2	1:115:A:LEU:HD23	4	0.13
(1,2472)	1:164:A:ILE:HD12	1:163:A:GLU:HB2	10	0.13
(1,2409)	1:122:A:CYS:H	1:118:A:LEU:HD22	2	0.13
(1,2405)	1:132:A:SER:H	1:136:A:ILE:HB	5	0.13
(1,2405)	1:132:A:SER:H	1:136:A:ILE:HB	6	0.13
(1,2405)	1:132:A:SER:H	1:136:A:ILE:HB	7	0.13
(1,2376)	1:145:A:VAL:HB	1:146:A:ASP:H	10	0.13
(1,2355)	1:143:A:LEU:HG	1:122:A:CYS:H	9	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2315)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	1	0.13
(1,2242)	1:139:A:ASN:HB3	1:137:A:VAL:HG22	4	0.13
(1,2097)	1:169:A:LEU:HB2	1:166:A:GLU:HA	10	0.13
(1,2076)	1:159:A:PHE:HB2	1:166:A:GLU:H	7	0.13
(1,2003)	1:130:A:PHE:HB3	1:132:A:SER:H	8	0.13
(1,1873)	1:96:A:VAL:HG21	1:96:A:VAL:HB	1	0.13
(1,1869)	1:113:A:VAL:HG11	1:168:A:ALA:HB2	4	0.13
(1,1859)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	1	0.13
(1,1770)	1:108:A:ALA:H	1:109:A:ASN:HA	9	0.13
(1,1759)	1:146:A:ASP:H	1:143:A:LEU:HD21	4	0.13
(1,1759)	1:146:A:ASP:H	1:143:A:LEU:HD21	9	0.13
(1,1700)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	8	0.13
(1,1647)	1:111:A:GLY:HA3	1:112:A:PHE:H	6	0.13
(1,1638)	1:164:A:ILE:HD13	1:93:A:MET:HA	10	0.13
(1,1625)	1:135:A:GLU:HA	1:136:A:ILE:HB	5	0.13
(1,1607)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	9	0.13
(1,1563)	1:166:A:GLU:HG3	1:168:A:ALA:H	10	0.13
(1,1552)	1:97:A:LEU:HG	1:97:A:LEU:HD13	8	0.13
(1,1451)	1:116:A:ARG:HG2	1:116:A:ARG:HD2	6	0.13
(1,1432)	1:141:A:ILE:HA	1:140:A:GLY:H	3	0.13
(1,1365)	1:150:A:ARG:HB2	1:150:A:ARG:HA	3	0.13
(1,1362)	1:144:A:PRO:HB3	1:144:A:PRO:HA	1	0.13
(1,1362)	1:144:A:PRO:HB3	1:144:A:PRO:HA	2	0.13
(1,1362)	1:144:A:PRO:HB3	1:144:A:PRO:HA	3	0.13
(1,1362)	1:144:A:PRO:HB3	1:144:A:PRO:HA	4	0.13
(1,1362)	1:144:A:PRO:HB3	1:144:A:PRO:HA	5	0.13
(1,1362)	1:144:A:PRO:HB3	1:144:A:PRO:HA	6	0.13
(1,1362)	1:144:A:PRO:HB3	1:144:A:PRO:HA	8	0.13
(1,1342)	1:119:A:PRO:HB2	1:177:A:GLY:HA3	3	0.13
(1,1341)	1:119:A:PRO:HB3	1:119:A:PRO:HA	3	0.13
(1,1329)	1:115:A:LEU:HG	1:115:A:LEU:HB2	1	0.13
(1,1329)	1:115:A:LEU:HG	1:115:A:LEU:HB2	10	0.13
(1,1272)	1:181:A:ILE:HG21	1:181:A:ILE:HB	3	0.13
(1,1272)	1:181:A:ILE:HG21	1:181:A:ILE:HB	8	0.13
(1,1272)	1:181:A:ILE:HG21	1:181:A:ILE:HB	9	0.13
(1,1269)	1:137:A:VAL:HG22	1:140:A:GLY:H	4	0.13
(1,1260)	1:183:A:ILE:HG21	1:184:A:PHE:HA	6	0.13
(1,1249)	1:141:A:ILE:HD12	1:125:A:GLU:H	8	0.13
(1,1178)	1:132:A:SER:H	1:136:A:ILE:HB	6	0.13
(1,1178)	1:132:A:SER:H	1:136:A:ILE:HB	7	0.13
(1,1087)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	8	0.13
(1,1087)	1:114:A:ARG:HG3	1:114:A:ARG:HD2	9	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1014)	1:135:A:GLU:HA	1:136:A:ILE:HB	1	0.13
(1,993)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	1	0.13
(1,993)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	2	0.13
(1,993)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	4	0.13
(1,993)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	5	0.13
(1,993)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	6	0.13
(1,910)	1:97:A:LEU:HD11	1:163:A:GLU:HB3	1	0.13
(1,834)	1:144:A:PRO:HD2	1:118:A:LEU:HD11	2	0.13
(1,834)	1:144:A:PRO:HD2	1:118:A:LEU:HD11	5	0.13
(1,744)	1:144:A:PRO:HB3	1:144:A:PRO:HA	2	0.13
(1,744)	1:144:A:PRO:HB3	1:144:A:PRO:HA	4	0.13
(1,744)	1:144:A:PRO:HB3	1:144:A:PRO:HA	6	0.13
(1,744)	1:144:A:PRO:HB3	1:144:A:PRO:HA	7	0.13
(1,744)	1:144:A:PRO:HB3	1:144:A:PRO:HA	8	0.13
(1,744)	1:144:A:PRO:HB3	1:144:A:PRO:HA	10	0.13
(1,735)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	5	0.13
(1,734)	1:119:A:PRO:HB3	1:119:A:PRO:HA	1	0.13
(1,734)	1:119:A:PRO:HB3	1:119:A:PRO:HA	6	0.13
(1,734)	1:119:A:PRO:HB3	1:119:A:PRO:HA	9	0.13
(1,734)	1:119:A:PRO:HB3	1:119:A:PRO:HA	10	0.13
(1,667)	1:181:A:ILE:HG21	1:181:A:ILE:HB	3	0.13
(1,667)	1:181:A:ILE:HG21	1:181:A:ILE:HB	9	0.13
(1,653)	1:113:A:VAL:HG11	1:168:A:ALA:HB2	9	0.13
(1,592)	1:97:A:LEU:HB2	1:97:A:LEU:H	4	0.13
(1,545)	1:168:A:ALA:H	1:169:A:LEU:HB2	2	0.13
(1,504)	1:166:A:GLU:H	1:169:A:LEU:HD13	9	0.13
(1,445)	1:116:A:ARG:HG2	1:154:A:GLU:HG2	6	0.13
(1,377)	1:123:A:SER:HB3	1:181:A:ILE:HD11	7	0.13
(1,288)	1:141:A:ILE:HG21	1:143:A:LEU:HG	5	0.13
(1,247)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	4	0.13
(1,195)	1:141:A:ILE:HA	1:140:A:GLY:H	10	0.13
(1,152)	1:130:A:PHE:HB2	1:131:A:PHE:H	7	0.13
(1,107)	1:126:A:GLU:HB3	1:126:A:GLU:HA	1	0.13
(1,107)	1:126:A:GLU:HB3	1:126:A:GLU:HA	3	0.13
(1,84)	1:115:A:LEU:HG	1:115:A:LEU:HB2	9	0.13
(1,43)	1:134:A:LEU:HD13	1:133:A:GLY:H	8	0.13
(1,31)	1:181:A:ILE:HG21	1:181:A:ILE:HB	4	0.13
(4,48)	1:183:A:ILE:H	1:171:A:LYS:O	4	0.12
(4,48)	1:183:A:ILE:H	1:171:A:LYS:O	10	0.12
(4,41)	1:168:A:ALA:N	1:164:A:ILE:O	3	0.12
(4,36)	1:160:A:ALA:H	1:135:A:GLU:O	3	0.12
(4,32)	1:158:A:GLN:H	1:140:A:GLY:O	10	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,4)	1:114:A:ARG:N	1:184:A:PHE:O	7	0.12
(4,2)	1:113:A:VAL:N	1:157:A:VAL:O	7	0.12
(4,1)	1:113:A:VAL:H	1:157:A:VAL:O	3	0.12
(3,620)	1:101:A:GLY:H	1:110:A:ASP:HA	7	0.12
(3,281)	1:188:A:ARG:HG2	1:190:A:GLU:H	8	0.12
(3,281)	1:188:A:ARG:HG2	1:190:A:GLU:H	10	0.12
(3,276)	1:136:A:ILE:HD13	1:164:A:ILE:HA	6	0.12
(3,150)	1:188:A:ARG:HG2	1:190:A:GLU:H	8	0.12
(3,150)	1:188:A:ARG:HG2	1:190:A:GLU:H	10	0.12
(3,145)	1:136:A:ILE:HD13	1:164:A:ILE:HA	6	0.12
(3,104)	1:101:A:GLY:H	1:110:A:ASP:HA	7	0.12
(3,6)	1:188:A:ARG:HG2	1:190:A:GLU:H	8	0.12
(3,6)	1:188:A:ARG:HG2	1:190:A:GLU:H	10	0.12
(2,8697)	1:110:A:ASP:HA	1:110:A:ASP:H	3	0.12
(2,8637)	1:96:A:VAL:HG13	1:97:A:LEU:H	8	0.12
(2,8578)	1:143:A:LEU:H	1:141:A:ILE:HB	2	0.12
(2,8566)	1:139:A:ASN:H	1:141:A:ILE:HD12	5	0.12
(2,8412)	1:191:A:VAL:HG13	1:191:A:VAL:HB	1	0.12
(2,8166)	1:166:A:GLU:HB2	1:166:A:GLU:HA	6	0.12
(2,8166)	1:166:A:GLU:HB2	1:166:A:GLU:HA	9	0.12
(2,8106)	1:161:A:SER:HB2	1:161:A:SER:HA	6	0.12
(2,8106)	1:161:A:SER:HB2	1:161:A:SER:HA	8	0.12
(2,8106)	1:161:A:SER:HB2	1:161:A:SER:HA	9	0.12
(2,8105)	1:160:A:ALA:HB3	1:161:A:SER:H	10	0.12
(2,8099)	1:157:A:VAL:HG22	1:158:A:GLN:H	4	0.12
(2,7721)	1:127:A:ILE:HD12	1:127:A:ILE:HB	3	0.12
(2,7498)	1:96:A:VAL:HG22	1:97:A:LEU:H	3	0.12
(2,7433)	1:92:A:ALA:HB3	1:93:A:MET:H	1	0.12
(2,7399)	1:166:A:GLU:HG2	1:168:A:ALA:H	5	0.12
(2,7388)	1:150:A:ARG:HB2	1:150:A:ARG:HA	9	0.12
(2,7385)	1:188:A:ARG:HB2	1:187:A:SER:H	4	0.12
(2,7377)	1:181:A:ILE:HG21	1:174:A:GLU:HA	9	0.12
(2,7270)	1:164:A:ILE:HD12	1:164:A:ILE:HA	6	0.12
(2,7270)	1:164:A:ILE:HD12	1:164:A:ILE:HA	7	0.12
(2,7270)	1:164:A:ILE:HD12	1:164:A:ILE:HA	9	0.12
(2,6796)	1:98:A:LYS:HG3	1:98:A:LYS:H	4	0.12
(2,6776)	1:96:A:VAL:H	1:95:A:TRP:H	3	0.12
(2,6776)	1:96:A:VAL:H	1:95:A:TRP:H	9	0.12
(2,6728)	1:93:A:MET:H	1:91:A:ASN:HA	8	0.12
(2,6710)	1:142:A:THR:H	1:155:A:ALA:HA	4	0.12
(2,6710)	1:142:A:THR:H	1:155:A:ALA:HA	10	0.12
(2,6707)	1:139:A:ASN:H	1:141:A:ILE:HA	9	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6633)	1:101:A:GLY:H	1:110:A:ASP:HA	2	0.12
(2,6633)	1:101:A:GLY:H	1:110:A:ASP:HA	4	0.12
(2,6599)	1:155:A:ALA:HA	1:155:A:ALA:HB3	6	0.12
(2,6558)	1:192:A:ARG:HD2	1:192:A:ARG:HB2	9	0.12
(2,6415)	1:179:A:ARG:HG3	1:179:A:ARG:HD2	5	0.12
(2,6216)	1:157:A:VAL:HG23	1:157:A:VAL:HG12	7	0.12
(2,6216)	1:157:A:VAL:HG23	1:157:A:VAL:HG12	8	0.12
(2,6205)	1:157:A:VAL:HG22	1:157:A:VAL:HG11	7	0.12
(2,6205)	1:157:A:VAL:HG22	1:157:A:VAL:HG11	8	0.12
(2,6205)	1:157:A:VAL:HG22	1:157:A:VAL:HG11	9	0.12
(2,6036)	1:141:A:ILE:HG13	1:141:A:ILE:H	3	0.12
(2,6036)	1:141:A:ILE:HG13	1:141:A:ILE:H	9	0.12
(2,6036)	1:141:A:ILE:HG13	1:141:A:ILE:H	10	0.12
(2,5840)	1:126:A:GLU:HG3	1:127:A:ILE:H	5	0.12
(2,5829)	1:124:A:LYS:HA	1:124:A:LYS:HB2	3	0.12
(2,5721)	1:111:A:GLY:HA3	1:112:A:PHE:H	1	0.12
(2,5721)	1:111:A:GLY:HA3	1:112:A:PHE:H	5	0.12
(2,5699)	1:107:A:THR:HB	1:107:A:THR:HG22	9	0.12
(2,5676)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	9	0.12
(2,5542)	1:181:A:ILE:HD12	1:183:A:ILE:H	1	0.12
(2,5542)	1:181:A:ILE:HD12	1:183:A:ILE:H	6	0.12
(2,5526)	1:97:A:LEU:HD13	1:97:A:LEU:HA	3	0.12
(2,5526)	1:97:A:LEU:HD13	1:97:A:LEU:HA	6	0.12
(2,5526)	1:97:A:LEU:HD13	1:97:A:LEU:HA	8	0.12
(2,5526)	1:97:A:LEU:HD13	1:97:A:LEU:HA	9	0.12
(2,5444)	1:191:A:VAL:HG13	1:193:A:THR:H	9	0.12
(2,5424)	1:96:A:VAL:HG22	1:97:A:LEU:H	8	0.12
(2,5364)	1:188:A:ARG:HG2	1:188:A:ARG:H	8	0.12
(2,5355)	1:158:A:GLN:H	1:141:A:ILE:HB	10	0.12
(2,5278)	1:179:A:ARG:HG3	1:179:A:ARG:H	1	0.12
(2,5009)	1:114:A:ARG:H	1:113:A:VAL:HG13	10	0.12
(2,4898)	1:159:A:PHE:H	1:110:A:ASP:HA	6	0.12
(2,4894)	1:181:A:ILE:H	1:116:A:ARG:H	4	0.12
(2,4894)	1:181:A:ILE:H	1:116:A:ARG:H	10	0.12
(2,4797)	1:161:A:SER:H	1:159:A:PHE:HB2	7	0.12
(2,4791)	1:188:A:ARG:HD2	1:108:A:ALA:H	8	0.12
(2,4660)	1:183:A:ILE:HG22	1:183:A:ILE:HD13	8	0.12
(2,4660)	1:183:A:ILE:HG22	1:183:A:ILE:HD13	9	0.12
(2,4496)	1:169:A:LEU:HD22	1:169:A:LEU:HA	8	0.12
(2,4437)	1:164:A:ILE:HD12	1:164:A:ILE:HA	5	0.12
(2,4390)	1:157:A:VAL:HG21	1:157:A:VAL:HA	8	0.12
(2,4390)	1:157:A:VAL:HG21	1:157:A:VAL:HA	9	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4330)	1:150:A:ARG:HG2	1:150:A:ARG:HA	2	0.12
(2,4330)	1:150:A:ARG:HG2	1:150:A:ARG:HA	6	0.12
(2,4318)	1:148:A:GLN:HA	1:149:A:GLY:H	3	0.12
(2,4133)	1:135:A:GLU:HG3	1:135:A:GLU:HA	1	0.12
(2,4133)	1:135:A:GLU:HG3	1:135:A:GLU:HA	5	0.12
(2,4088)	1:129:A:GLN:HG3	1:129:A:GLN:HB2	9	0.12
(2,3981)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	2	0.12
(2,3981)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	4	0.12
(2,3981)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	5	0.12
(2,3793)	1:97:A:LEU:HD12	1:97:A:LEU:H	2	0.12
(2,3793)	1:97:A:LEU:HD12	1:97:A:LEU:H	9	0.12
(2,3768)	1:96:A:VAL:HG11	1:96:A:VAL:H	7	0.12
(2,3695)	1:181:A:ILE:HG21	1:174:A:GLU:HA	1	0.12
(2,3695)	1:181:A:ILE:HG21	1:174:A:GLU:HA	8	0.12
(2,3657)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	6	0.12
(2,3657)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	7	0.12
(2,3657)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	8	0.12
(2,3657)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	9	0.12
(2,3615)	1:160:A:ALA:HB2	1:162:A:GLN:H	9	0.12
(2,3568)	1:188:A:ARG:HG2	1:188:A:ARG:H	5	0.12
(2,3470)	1:175:A:ARG:HB3	1:176:A:ILE:H	6	0.12
(2,3444)	1:166:A:GLU:HB3	1:167:A:LYS:H	5	0.12
(2,3182)	1:107:A:THR:HA	1:108:A:ALA:H	2	0.12
(2,3066)	1:108:A:ALA:H	1:188:A:ARG:HG2	1	0.12
(2,3045)	1:146:A:ASP:H	1:150:A:ARG:H	4	0.12
(2,2984)	1:188:A:ARG:HD2	1:108:A:ALA:H	8	0.12
(2,2969)	1:116:A:ARG:HG2	1:154:A:GLU:HG2	5	0.12
(2,2841)	1:183:A:ILE:HG21	1:184:A:PHE:HA	8	0.12
(2,2660)	1:166:A:GLU:HG3	1:166:A:GLU:HA	4	0.12
(2,2660)	1:166:A:GLU:HG3	1:166:A:GLU:HA	7	0.12
(2,2622)	1:163:A:GLU:HB3	1:164:A:ILE:H	2	0.12
(2,2607)	1:162:A:GLN:HG3	1:162:A:GLN:HA	10	0.12
(2,2585)	1:159:A:PHE:HA	1:158:A:GLN:HA	2	0.12
(2,2585)	1:159:A:PHE:HA	1:158:A:GLN:HA	3	0.12
(2,2585)	1:159:A:PHE:HA	1:158:A:GLN:HA	4	0.12
(2,2585)	1:159:A:PHE:HA	1:158:A:GLN:HA	6	0.12
(2,2585)	1:159:A:PHE:HA	1:158:A:GLN:HA	8	0.12
(2,2585)	1:159:A:PHE:HA	1:158:A:GLN:HA	9	0.12
(2,2585)	1:159:A:PHE:HA	1:158:A:GLN:HA	10	0.12
(2,2520)	1:150:A:ARG:HG2	1:150:A:ARG:HA	6	0.12
(2,2520)	1:150:A:ARG:HG2	1:150:A:ARG:HA	8	0.12
(2,2511)	1:148:A:GLN:HB2	1:149:A:GLY:H	4	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2334)	1:136:A:ILE:HG12	1:136:A:ILE:HB	1	0.12
(2,2334)	1:136:A:ILE:HG12	1:136:A:ILE:HB	2	0.12
(2,2334)	1:136:A:ILE:HG12	1:136:A:ILE:HB	4	0.12
(2,2333)	1:137:A:VAL:HA	1:136:A:ILE:HA	2	0.12
(2,2333)	1:137:A:VAL:HA	1:136:A:ILE:HA	6	0.12
(2,2333)	1:137:A:VAL:HA	1:136:A:ILE:HA	9	0.12
(2,2176)	1:118:A:LEU:HD12	1:118:A:LEU:HD23	6	0.12
(2,2154)	1:116:A:ARG:HB2	1:117:A:GLY:H	5	0.12
(2,2154)	1:116:A:ARG:HB2	1:117:A:GLY:H	10	0.12
(2,2097)	1:111:A:GLY:HA3	1:112:A:PHE:H	4	0.12
(2,2087)	1:108:A:ALA:HB3	1:109:A:ASN:H	8	0.12
(2,2031)	1:101:A:GLY:HA3	1:101:A:GLY:H	5	0.12
(2,2012)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	6	0.12
(2,1962)	1:96:A:VAL:HG13	1:96:A:VAL:HA	1	0.12
(2,1892)	1:92:A:ALA:HA	1:92:A:ALA:HB1	1	0.12
(2,1892)	1:92:A:ALA:HA	1:92:A:ALA:HB1	3	0.12
(2,1892)	1:92:A:ALA:HA	1:92:A:ALA:HB1	4	0.12
(2,1892)	1:92:A:ALA:HA	1:92:A:ALA:HB1	6	0.12
(2,1892)	1:92:A:ALA:HA	1:92:A:ALA:HB1	8	0.12
(2,1892)	1:92:A:ALA:HA	1:92:A:ALA:HB1	9	0.12
(2,1892)	1:92:A:ALA:HA	1:92:A:ALA:HB1	10	0.12
(2,1891)	1:181:A:ILE:HG21	1:174:A:GLU:HA	7	0.12
(2,1873)	1:187:A:SER:HB3	1:189:A:ALA:H	6	0.12
(2,1873)	1:187:A:SER:HB3	1:189:A:ALA:H	7	0.12
(2,1796)	1:164:A:ILE:HD12	1:164:A:ILE:HA	8	0.12
(2,1777)	1:166:A:GLU:H	1:169:A:LEU:HB2	9	0.12
(2,1729)	1:191:A:VAL:HG12	1:191:A:VAL:H	6	0.12
(2,1718)	1:190:A:GLU:H	1:189:A:ALA:H	8	0.12
(2,1685)	1:183:A:ILE:H	1:182:A:GLU:HG3	3	0.12
(2,1685)	1:183:A:ILE:H	1:182:A:GLU:HG3	8	0.12
(2,1639)	1:166:A:GLU:HB3	1:167:A:LYS:H	10	0.12
(2,1630)	1:164:A:ILE:H	1:164:A:ILE:HG21	1	0.12
(2,1630)	1:164:A:ILE:H	1:164:A:ILE:HG21	3	0.12
(2,1613)	1:162:A:GLN:HB2	1:163:A:GLU:H	7	0.12
(2,1583)	1:156:A:PHE:HB2	1:157:A:VAL:H	4	0.12
(2,1553)	1:150:A:ARG:H	1:149:A:GLY:H	1	0.12
(2,1374)	1:106:A:ASP:H	1:105:A:PRO:HD2	4	0.12
(2,1262)	1:142:A:THR:H	1:156:A:PHE:HB3	2	0.12
(2,1231)	1:169:A:LEU:H	1:169:A:LEU:HG	7	0.12
(2,1180)	1:188:A:ARG:HB2	1:188:A:ARG:HG2	8	0.12
(2,1162)	1:119:A:PRO:HB2	1:120:A:PHE:H	1	0.12
(2,1133)	1:192:A:ARG:HB2	1:193:A:THR:HA	1	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1133)	1:192:A:ARG:HB2	1:193:A:THR:HA	7	0.12
(2,1106)	1:191:A:VAL:HG11	1:191:A:VAL:HA	9	0.12
(2,1071)	1:188:A:ARG:HG3	1:188:A:ARG:HA	4	0.12
(2,1071)	1:188:A:ARG:HG3	1:188:A:ARG:HA	10	0.12
(2,996)	1:181:A:ILE:HD12	1:181:A:ILE:HB	2	0.12
(2,925)	1:173:A:LYS:HG2	1:174:A:GLU:H	7	0.12
(2,899)	1:169:A:LEU:HD22	1:169:A:LEU:HD12	2	0.12
(2,819)	1:162:A:GLN:HG3	1:162:A:GLN:HA	1	0.12
(2,790)	1:157:A:VAL:HG21	1:157:A:VAL:HA	2	0.12
(2,746)	1:152:A:THR:HA	1:151:A:SER:HA	9	0.12
(2,738)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	3	0.12
(2,649)	1:144:A:PRO:HD3	1:143:A:LEU:HA	9	0.12
(2,551)	1:136:A:ILE:HG12	1:136:A:ILE:HG22	2	0.12
(2,551)	1:136:A:ILE:HG12	1:136:A:ILE:HG22	4	0.12
(2,551)	1:136:A:ILE:HG12	1:136:A:ILE:HG22	7	0.12
(2,390)	1:119:A:PRO:HA	1:119:A:PRO:HG3	5	0.12
(2,352)	1:115:A:LEU:HA	1:115:A:LEU:HD21	2	0.12
(2,352)	1:115:A:LEU:HA	1:115:A:LEU:HD21	4	0.12
(2,352)	1:115:A:LEU:HA	1:115:A:LEU:HD21	10	0.12
(2,264)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	7	0.12
(2,175)	1:96:A:VAL:HG13	1:96:A:VAL:HA	5	0.12
(2,175)	1:96:A:VAL:HG13	1:96:A:VAL:HA	7	0.12
(2,139)	1:102:A:PRO:HA	1:103:A:ASN:H	10	0.12
(2,121)	1:97:A:LEU:HD13	1:97:A:LEU:HA	3	0.12
(2,121)	1:97:A:LEU:HD13	1:97:A:LEU:HA	6	0.12
(2,121)	1:97:A:LEU:HD13	1:97:A:LEU:HA	8	0.12
(2,121)	1:97:A:LEU:HD13	1:97:A:LEU:HA	9	0.12
(2,119)	1:142:A:THR:HG21	1:123:A:SER:HB2	3	0.12
(2,111)	1:188:A:ARG:HB2	1:189:A:ALA:H	1	0.12
(2,72)	1:91:A:ASN:HB3	1:96:A:VAL:H	6	0.12
(2,63)	1:95:A:TRP:HB2	1:96:A:VAL:HG21	6	0.12
(2,25)	1:96:A:VAL:HG22	1:161:A:SER:H	3	0.12
(2,6)	1:164:A:ILE:HD11	1:161:A:SER:H	2	0.12
(2,6)	1:164:A:ILE:HD11	1:161:A:SER:H	9	0.12
(2,5)	1:164:A:ILE:HD13	1:91:A:ASN:HA	3	0.12
(1,3017)	1:96:A:VAL:HB	1:97:A:LEU:H	9	0.12
(1,3003)	1:108:A:ALA:H	1:109:A:ASN:HA	1	0.12
(1,2928)	1:156:A:PHE:HB2	1:141:A:ILE:HG23	4	0.12
(1,2927)	1:192:A:ARG:HD3	1:192:A:ARG:HB3	1	0.12
(1,2863)	1:164:A:ILE:HD13	1:93:A:MET:HA	9	0.12
(1,2777)	1:97:A:LEU:HG	1:97:A:LEU:HD13	2	0.12
(1,2773)	1:98:A:LYS:HB3	1:100:A:THR:HG22	3	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2702)	1:169:A:LEU:HB2	1:166:A:GLU:HA	5	0.12
(1,2702)	1:169:A:LEU:HB2	1:166:A:GLU:HA	8	0.12
(1,2563)	1:181:A:ILE:HB	1:181:A:ILE:HA	3	0.12
(1,2563)	1:181:A:ILE:HB	1:181:A:ILE:HA	9	0.12
(1,2526)	1:166:A:GLU:HB3	1:168:A:ALA:H	1	0.12
(1,2487)	1:96:A:VAL:HG21	1:96:A:VAL:HB	1	0.12
(1,2483)	1:183:A:ILE:HG22	1:113:A:VAL:HB	2	0.12
(1,2472)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	3	0.12
(1,2376)	1:145:A:VAL:HB	1:146:A:ASP:H	7	0.12
(1,2376)	1:145:A:VAL:HB	1:146:A:ASP:H	8	0.12
(1,2181)	1:119:A:PRO:HB2	1:119:A:PRO:HD3	4	0.12
(1,2133)	1:143:A:LEU:HG	1:141:A:ILE:HG21	9	0.12
(1,2113)	1:96:A:VAL:HA	1:97:A:LEU:HA	6	0.12
(1,2113)	1:96:A:VAL:HA	1:97:A:LEU:HA	8	0.12
(1,2113)	1:96:A:VAL:HA	1:97:A:LEU:HA	10	0.12
(1,2101)	1:143:A:LEU:HA	1:122:A:CYS:HB2	5	0.12
(1,2087)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	6	0.12
(1,2003)	1:130:A:PHE:HB3	1:132:A:SER:H	2	0.12
(1,1885)	1:137:A:VAL:HG22	1:140:A:GLY:H	10	0.12
(1,1876)	1:127:A:ILE:HG21	1:127:A:ILE:HB	1	0.12
(1,1876)	1:127:A:ILE:HG21	1:127:A:ILE:HB	5	0.12
(1,1873)	1:96:A:VAL:HG21	1:96:A:VAL:HB	5	0.12
(1,1826)	1:184:A:PHE:H	1:186:A:SER:HB3	2	0.12
(1,1805)	1:158:A:GLN:H	1:141:A:ILE:HG23	1	0.12
(1,1701)	1:188:A:ARG:HG2	1:188:A:ARG:HD2	1	0.12
(1,1701)	1:188:A:ARG:HG2	1:188:A:ARG:HD2	5	0.12
(1,1640)	1:162:A:GLN:HB3	1:162:A:GLN:HG2	9	0.12
(1,1638)	1:164:A:ILE:HD13	1:135:A:GLU:HA	5	0.12
(1,1624)	1:144:A:PRO:HB3	1:144:A:PRO:HA	1	0.12
(1,1624)	1:144:A:PRO:HB3	1:144:A:PRO:HA	3	0.12
(1,1624)	1:144:A:PRO:HB3	1:144:A:PRO:HA	4	0.12
(1,1624)	1:144:A:PRO:HB3	1:144:A:PRO:HA	5	0.12
(1,1624)	1:144:A:PRO:HB3	1:144:A:PRO:HA	6	0.12
(1,1607)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	3	0.12
(1,1598)	1:169:A:LEU:HD21	1:167:A:LYS:H	7	0.12
(1,1520)	1:141:A:ILE:HG21	1:143:A:LEU:HG	1	0.12
(1,1466)	1:159:A:PHE:HB2	1:159:A:PHE:HA	10	0.12
(1,1432)	1:137:A:VAL:HA	1:140:A:GLY:H	9	0.12
(1,1396)	1:95:A:TRP:HA	1:96:A:VAL:H	5	0.12
(1,1370)	1:166:A:GLU:HG3	1:169:A:LEU:HD13	5	0.12
(1,1365)	1:150:A:ARG:HB2	1:150:A:ARG:HA	5	0.12
(1,1365)	1:150:A:ARG:HB2	1:150:A:ARG:HA	7	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1362)	1:144:A:PRO:HB3	1:144:A:PRO:HA	7	0.12
(1,1362)	1:144:A:PRO:HB3	1:144:A:PRO:HA	10	0.12
(1,1346)	1:144:A:PRO:HB3	1:144:A:PRO:HA	1	0.12
(1,1346)	1:144:A:PRO:HB3	1:144:A:PRO:HA	2	0.12
(1,1346)	1:144:A:PRO:HB3	1:144:A:PRO:HA	3	0.12
(1,1346)	1:144:A:PRO:HB3	1:144:A:PRO:HA	4	0.12
(1,1346)	1:144:A:PRO:HB3	1:144:A:PRO:HA	5	0.12
(1,1346)	1:144:A:PRO:HB3	1:144:A:PRO:HA	6	0.12
(1,1346)	1:144:A:PRO:HB3	1:144:A:PRO:HA	8	0.12
(1,1341)	1:119:A:PRO:HB3	1:119:A:PRO:HA	4	0.12
(1,1329)	1:115:A:LEU:HG	1:115:A:LEU:HB2	3	0.12
(1,1329)	1:115:A:LEU:HG	1:115:A:LEU:HB2	4	0.12
(1,1329)	1:115:A:LEU:HG	1:115:A:LEU:HB2	5	0.12
(1,1329)	1:115:A:LEU:HG	1:115:A:LEU:HB2	6	0.12
(1,1327)	1:148:A:GLN:HB3	1:147:A:PHE:H	10	0.12
(1,1289)	1:167:A:LYS:HG2	1:134:A:LEU:HD12	6	0.12
(1,1272)	1:181:A:ILE:HG21	1:181:A:ILE:HB	5	0.12
(1,1272)	1:181:A:ILE:HG21	1:181:A:ILE:HB	10	0.12
(1,1260)	1:183:A:ILE:HG21	1:184:A:PHE:HA	1	0.12
(1,1260)	1:183:A:ILE:HG21	1:184:A:PHE:HA	7	0.12
(1,1148)	1:146:A:ASP:H	1:143:A:LEU:HD21	3	0.12
(1,1046)	1:115:A:LEU:HD23	1:114:A:ARG:HA	1	0.12
(1,985)	1:169:A:LEU:HD21	1:167:A:LYS:H	10	0.12
(1,858)	1:159:A:PHE:HB2	1:159:A:PHE:HA	10	0.12
(1,758)	1:150:A:ARG:HB2	1:150:A:ARG:HA	3	0.12
(1,758)	1:150:A:ARG:HB2	1:150:A:ARG:HA	5	0.12
(1,744)	1:144:A:PRO:HB3	1:144:A:PRO:HA	9	0.12
(1,735)	1:119:A:PRO:HB3	1:119:A:PRO:HD2	10	0.12
(1,734)	1:119:A:PRO:HB3	1:119:A:PRO:HA	2	0.12
(1,734)	1:119:A:PRO:HB3	1:119:A:PRO:HA	3	0.12
(1,722)	1:148:A:GLN:HB3	1:147:A:PHE:H	8	0.12
(1,684)	1:167:A:LYS:HG2	1:134:A:LEU:HD11	2	0.12
(1,667)	1:181:A:ILE:HG21	1:181:A:ILE:HB	5	0.12
(1,667)	1:181:A:ILE:HG21	1:181:A:ILE:HB	8	0.12
(1,667)	1:181:A:ILE:HG21	1:181:A:ILE:HB	10	0.12
(1,665)	1:137:A:VAL:HG22	1:140:A:GLY:H	10	0.12
(1,654)	1:183:A:ILE:HG21	1:184:A:PHE:HA	10	0.12
(1,645)	1:164:A:ILE:HD13	1:91:A:ASN:HB2	10	0.12
(1,592)	1:97:A:LEU:HB2	1:97:A:LEU:H	1	0.12
(1,297)	1:164:A:ILE:HD13	1:93:A:MET:HG3	6	0.12
(1,248)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	4	0.12
(1,195)	1:141:A:ILE:HA	1:140:A:GLY:H	6	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,195)	1:141:A:ILE:HA	1:140:A:GLY:H	7	0.12
(1,165)	1:109:A:ASN:HA	1:108:A:ALA:HB3	5	0.12
(1,140)	1:190:A:GLU:HG2	1:190:A:GLU:HA	5	0.12
(1,107)	1:126:A:GLU:HB3	1:126:A:GLU:HA	6	0.12
(1,107)	1:126:A:GLU:HB3	1:126:A:GLU:HA	8	0.12
(1,107)	1:126:A:GLU:HB3	1:126:A:GLU:HA	9	0.12
(1,31)	1:181:A:ILE:HG21	1:181:A:ILE:HB	6	0.12
(4,50)	1:183:A:ILE:H	1:181:A:ILE:O	10	0.11
(4,41)	1:168:A:ALA:N	1:164:A:ILE:O	10	0.11
(4,36)	1:160:A:ALA:H	1:135:A:GLU:O	1	0.11
(4,36)	1:160:A:ALA:H	1:135:A:GLU:O	2	0.11
(4,36)	1:160:A:ALA:H	1:135:A:GLU:O	8	0.11
(4,32)	1:158:A:GLN:H	1:140:A:GLY:O	9	0.11
(4,15)	1:129:A:GLN:H	1:125:A:GLU:O	5	0.11
(4,15)	1:129:A:GLN:H	1:125:A:GLU:O	7	0.11
(4,12)	1:118:A:LEU:N	1:152:A:THR:O	10	0.11
(4,8)	1:116:A:ARG:N	1:182:A:GLU:O	6	0.11
(4,1)	1:113:A:VAL:H	1:157:A:VAL:O	9	0.11
(4,1)	1:113:A:VAL:H	1:157:A:VAL:O	10	0.11
(3,625)	1:139:A:ASN:H	1:128:A:VAL:HA	10	0.11
(3,620)	1:101:A:GLY:H	1:110:A:ASP:HA	2	0.11
(3,620)	1:101:A:GLY:H	1:110:A:ASP:HA	4	0.11
(3,499)	1:139:A:ASN:H	1:128:A:VAL:HA	10	0.11
(3,281)	1:188:A:ARG:HG2	1:190:A:GLU:H	3	0.11
(3,276)	1:136:A:ILE:HD13	1:164:A:ILE:HA	8	0.11
(3,276)	1:136:A:ILE:HD13	1:164:A:ILE:HA	10	0.11
(3,150)	1:188:A:ARG:HG2	1:190:A:GLU:H	3	0.11
(3,145)	1:136:A:ILE:HD13	1:164:A:ILE:HA	8	0.11
(3,145)	1:136:A:ILE:HD13	1:164:A:ILE:HA	10	0.11
(3,104)	1:101:A:GLY:H	1:110:A:ASP:HA	2	0.11
(3,104)	1:101:A:GLY:H	1:110:A:ASP:HA	4	0.11
(3,6)	1:188:A:ARG:HG2	1:190:A:GLU:H	3	0.11
(2,8632)	1:96:A:VAL:H	1:95:A:TRP:H	3	0.11
(2,8632)	1:96:A:VAL:H	1:95:A:TRP:H	9	0.11
(2,8566)	1:139:A:ASN:H	1:141:A:ILE:HD12	8	0.11
(2,8563)	1:168:A:ALA:H	1:95:A:TRP:HB2	1	0.11
(2,8352)	1:183:A:ILE:HG21	1:184:A:PHE:HA	8	0.11
(2,8334)	1:182:A:GLU:HB2	1:182:A:GLU:HG3	1	0.11
(2,8334)	1:182:A:GLU:HB2	1:182:A:GLU:HG3	2	0.11
(2,8334)	1:182:A:GLU:HB2	1:182:A:GLU:HG3	5	0.11
(2,8216)	1:171:A:LYS:HB3	1:171:A:LYS:HA	7	0.11
(2,8166)	1:166:A:GLU:HB2	1:166:A:GLU:HA	4	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,8125)	1:163:A:GLU:HG2	1:163:A:GLU:HB3	2	0.11
(2,8125)	1:163:A:GLU:HG2	1:163:A:GLU:HB3	5	0.11
(2,8125)	1:163:A:GLU:HG2	1:163:A:GLU:HB3	6	0.11
(2,8120)	1:163:A:GLU:HB3	1:163:A:GLU:HA	2	0.11
(2,8106)	1:161:A:SER:HB2	1:161:A:SER:HA	4	0.11
(2,8106)	1:161:A:SER:HB2	1:161:A:SER:HA	5	0.11
(2,8106)	1:161:A:SER:HB2	1:161:A:SER:HA	10	0.11
(2,8105)	1:160:A:ALA:HB3	1:161:A:SER:H	2	0.11
(2,8105)	1:160:A:ALA:HB3	1:161:A:SER:H	9	0.11
(2,7721)	1:127:A:ILE:HD12	1:127:A:ILE:HB	4	0.11
(2,7721)	1:127:A:ILE:HD12	1:127:A:ILE:HB	6	0.11
(2,7721)	1:127:A:ILE:HD12	1:127:A:ILE:HB	10	0.11
(2,7693)	1:122:A:CYS:HA	1:121:A:GLY:H	3	0.11
(2,7693)	1:122:A:CYS:HA	1:121:A:GLY:H	7	0.11
(2,7433)	1:92:A:ALA:HB3	1:93:A:MET:H	4	0.11
(2,7433)	1:92:A:ALA:HB3	1:93:A:MET:H	8	0.11
(2,7394)	1:142:A:THR:HG22	1:141:A:ILE:HG21	5	0.11
(2,7385)	1:188:A:ARG:HB2	1:187:A:SER:H	2	0.11
(2,7385)	1:188:A:ARG:HB2	1:187:A:SER:H	3	0.11
(2,7358)	1:141:A:ILE:HA	1:140:A:GLY:H	4	0.11
(2,7358)	1:141:A:ILE:HA	1:140:A:GLY:H	6	0.11
(2,7358)	1:141:A:ILE:HA	1:140:A:GLY:H	7	0.11
(2,7349)	1:156:A:PHE:HA	1:141:A:ILE:HA	6	0.11
(2,7270)	1:164:A:ILE:HD12	1:164:A:ILE:HA	2	0.11
(2,7246)	1:166:A:GLU:H	1:95:A:TRP:HB2	7	0.11
(2,7246)	1:166:A:GLU:H	1:95:A:TRP:HB2	10	0.11
(2,6959)	1:135:A:GLU:HB3	1:135:A:GLU:H	3	0.11
(2,6796)	1:98:A:LYS:HG3	1:98:A:LYS:H	1	0.11
(2,6796)	1:98:A:LYS:HG3	1:98:A:LYS:H	6	0.11
(2,6796)	1:98:A:LYS:HG3	1:98:A:LYS:H	10	0.11
(2,6776)	1:96:A:VAL:H	1:95:A:TRP:H	2	0.11
(2,6776)	1:96:A:VAL:H	1:95:A:TRP:H	8	0.11
(2,6728)	1:93:A:MET:H	1:91:A:ASN:HA	5	0.11
(2,6710)	1:142:A:THR:H	1:155:A:ALA:HA	3	0.11
(2,6415)	1:179:A:ARG:HG3	1:179:A:ARG:HD2	4	0.11
(2,6298)	1:166:A:GLU:HA	1:167:A:LYS:H	2	0.11
(2,6293)	1:166:A:GLU:HB2	1:166:A:GLU:HA	6	0.11
(2,6293)	1:166:A:GLU:HB2	1:166:A:GLU:HA	9	0.11
(2,6271)	1:164:A:ILE:HG13	1:164:A:ILE:HG22	3	0.11
(2,6232)	1:160:A:ALA:HB3	1:161:A:SER:H	5	0.11
(2,6226)	1:157:A:VAL:HG22	1:158:A:GLN:H	3	0.11
(2,6216)	1:157:A:VAL:HG23	1:157:A:VAL:HG12	9	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6205)	1:157:A:VAL:HG22	1:157:A:VAL:HG11	6	0.11
(2,6063)	1:141:A:ILE:HD13	1:141:A:ILE:HG12	1	0.11
(2,6063)	1:141:A:ILE:HD13	1:141:A:ILE:HG12	5	0.11
(2,6063)	1:141:A:ILE:HD13	1:141:A:ILE:HG12	7	0.11
(2,6036)	1:141:A:ILE:HG13	1:141:A:ILE:H	2	0.11
(2,5866)	1:127:A:ILE:HG23	1:127:A:ILE:HG12	7	0.11
(2,5848)	1:127:A:ILE:HD12	1:127:A:ILE:HB	5	0.11
(2,5840)	1:126:A:GLU:HG3	1:127:A:ILE:H	6	0.11
(2,5729)	1:113:A:VAL:HG13	1:113:A:VAL:HB	1	0.11
(2,5721)	1:111:A:GLY:HA3	1:112:A:PHE:H	2	0.11
(2,5676)	1:102:A:PRO:HG2	1:102:A:PRO:HD3	3	0.11
(2,5552)	1:91:A:ASN:HB2	1:92:A:ALA:HA	3	0.11
(2,5552)	1:91:A:ASN:HB2	1:92:A:ALA:HA	5	0.11
(2,5552)	1:91:A:ASN:HB2	1:92:A:ALA:HA	8	0.11
(2,5537)	1:155:A:ALA:HB2	1:154:A:GLU:H	1	0.11
(2,5534)	1:115:A:LEU:HD23	1:115:A:LEU:H	7	0.11
(2,5487)	1:187:A:SER:HB3	1:189:A:ALA:H	5	0.11
(2,5478)	1:156:A:PHE:HA	1:141:A:ILE:HA	6	0.11
(2,5466)	1:166:A:GLU:HG2	1:166:A:GLU:H	3	0.11
(2,5424)	1:96:A:VAL:HG22	1:97:A:LEU:H	9	0.11
(2,5422)	1:96:A:VAL:HG22	1:96:A:VAL:HA	4	0.11
(2,5422)	1:96:A:VAL:HG22	1:96:A:VAL:HA	5	0.11
(2,5422)	1:96:A:VAL:HG22	1:96:A:VAL:HA	7	0.11
(2,5403)	1:164:A:ILE:HD11	1:161:A:SER:H	5	0.11
(2,5382)	1:164:A:ILE:HG13	1:167:A:LYS:H	10	0.11
(2,5376)	1:166:A:GLU:H	1:95:A:TRP:HB2	7	0.11
(2,5355)	1:158:A:GLN:H	1:141:A:ILE:HB	1	0.11
(2,5355)	1:158:A:GLN:H	1:141:A:ILE:HB	2	0.11
(2,5328)	1:190:A:GLU:HB3	1:191:A:VAL:H	3	0.11
(2,5103)	1:135:A:GLU:HB3	1:135:A:GLU:H	8	0.11
(2,4979)	1:106:A:ASP:H	1:106:A:ASP:HB2	8	0.11
(2,4894)	1:181:A:ILE:H	1:116:A:ARG:H	2	0.11
(2,4894)	1:181:A:ILE:H	1:116:A:ARG:H	6	0.11
(2,4894)	1:181:A:ILE:H	1:116:A:ARG:H	8	0.11
(2,4894)	1:181:A:ILE:H	1:116:A:ARG:H	9	0.11
(2,4869)	1:108:A:ALA:H	1:188:A:ARG:HG2	7	0.11
(2,4785)	1:185:A:LYS:HB3	1:185:A:LYS:H	5	0.11
(2,4660)	1:183:A:ILE:HG22	1:183:A:ILE:HD13	5	0.11
(2,4657)	1:183:A:ILE:HA	1:183:A:ILE:HD11	2	0.11
(2,4657)	1:183:A:ILE:HA	1:183:A:ILE:HD11	3	0.11
(2,4657)	1:183:A:ILE:HA	1:183:A:ILE:HD11	4	0.11
(2,4600)	1:181:A:ILE:HG22	1:181:A:ILE:HG12	7	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4500)	1:169:A:LEU:HD22	1:169:A:LEU:HD12	2	0.11
(2,4471)	1:166:A:GLU:HG3	1:166:A:GLU:HA	5	0.11
(2,4437)	1:164:A:ILE:HD12	1:164:A:ILE:HA	1	0.11
(2,4437)	1:164:A:ILE:HD12	1:164:A:ILE:HA	3	0.11
(2,4437)	1:164:A:ILE:HD12	1:164:A:ILE:HA	10	0.11
(2,4420)	1:162:A:GLN:HB2	1:162:A:GLN:HG2	8	0.11
(2,4420)	1:162:A:GLN:HB2	1:162:A:GLN:HG2	9	0.11
(2,4330)	1:150:A:ARG:HG2	1:150:A:ARG:HA	8	0.11
(2,4143)	1:137:A:VAL:HA	1:136:A:ILE:HA	7	0.11
(2,4133)	1:135:A:GLU:HG3	1:135:A:GLU:HA	7	0.11
(2,4133)	1:135:A:GLU:HG3	1:135:A:GLU:HA	8	0.11
(2,4133)	1:135:A:GLU:HG3	1:135:A:GLU:HA	9	0.11
(2,4133)	1:135:A:GLU:HG3	1:135:A:GLU:HA	10	0.11
(2,4057)	1:127:A:ILE:HD11	1:127:A:ILE:HB	1	0.11
(2,4020)	1:126:A:GLU:HB2	1:126:A:GLU:HA	1	0.11
(2,4020)	1:126:A:GLU:HB2	1:126:A:GLU:HA	3	0.11
(2,4020)	1:126:A:GLU:HB2	1:126:A:GLU:HA	8	0.11
(2,4020)	1:126:A:GLU:HB2	1:126:A:GLU:HA	9	0.11
(2,3981)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	3	0.11
(2,3981)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	9	0.11
(2,3981)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	10	0.11
(2,3963)	1:116:A:ARG:HB2	1:117:A:GLY:H	5	0.11
(2,3963)	1:116:A:ARG:HB2	1:117:A:GLY:H	10	0.11
(2,3821)	1:98:A:LYS:HD2	1:98:A:LYS:HG2	9	0.11
(2,3793)	1:97:A:LEU:HD12	1:97:A:LEU:H	1	0.11
(2,3768)	1:96:A:VAL:HG11	1:96:A:VAL:H	5	0.11
(2,3735)	1:102:A:PRO:HA	1:103:A:ASN:H	1	0.11
(2,3735)	1:102:A:PRO:HA	1:103:A:ASN:H	3	0.11
(2,3735)	1:102:A:PRO:HA	1:103:A:ASN:H	4	0.11
(2,3735)	1:102:A:PRO:HA	1:103:A:ASN:H	5	0.11
(2,3697)	1:92:A:ALA:HA	1:92:A:ALA:HB1	1	0.11
(2,3697)	1:92:A:ALA:HA	1:92:A:ALA:HB1	3	0.11
(2,3697)	1:92:A:ALA:HA	1:92:A:ALA:HB1	4	0.11
(2,3697)	1:92:A:ALA:HA	1:92:A:ALA:HB1	6	0.11
(2,3697)	1:92:A:ALA:HA	1:92:A:ALA:HB1	8	0.11
(2,3697)	1:92:A:ALA:HA	1:92:A:ALA:HB1	9	0.11
(2,3697)	1:92:A:ALA:HA	1:92:A:ALA:HB1	10	0.11
(2,3685)	1:155:A:ALA:HA	1:144:A:PRO:HD2	1	0.11
(2,3668)	1:154:A:GLU:HG2	1:118:A:LEU:H	1	0.11
(2,3661)	1:95:A:TRP:HB3	1:91:A:ASN:HB3	2	0.11
(2,3661)	1:95:A:TRP:HB3	1:91:A:ASN:HB3	8	0.11
(2,3657)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	1	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3657)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	2	0.11
(2,3559)	1:158:A:GLN:H	1:141:A:ILE:HB	3	0.11
(2,3538)	1:192:A:ARG:HG2	1:192:A:ARG:H	3	0.11
(2,3533)	1:190:A:GLU:HB3	1:191:A:VAL:H	9	0.11
(2,3104)	1:151:A:SER:H	1:151:A:SER:HB2	1	0.11
(2,3066)	1:108:A:ALA:H	1:188:A:ARG:HG2	2	0.11
(2,3066)	1:108:A:ALA:H	1:188:A:ARG:HG2	5	0.11
(2,3052)	1:185:A:LYS:H	1:169:A:LEU:HB2	6	0.11
(2,2987)	1:177:A:GLY:HA3	1:119:A:PRO:HD2	6	0.11
(2,2985)	1:188:A:ARG:HG2	1:188:A:ARG:HD2	2	0.11
(2,2985)	1:188:A:ARG:HG2	1:188:A:ARG:HD2	6	0.11
(2,2927)	1:192:A:ARG:HB2	1:193:A:THR:HA	5	0.11
(2,2927)	1:192:A:ARG:HB2	1:193:A:THR:HA	10	0.11
(2,2848)	1:183:A:ILE:HA	1:183:A:ILE:HD11	10	0.11
(2,2790)	1:181:A:ILE:HG22	1:181:A:ILE:HG12	2	0.11
(2,2790)	1:181:A:ILE:HG22	1:181:A:ILE:HG12	8	0.11
(2,2710)	1:173:A:LYS:HG2	1:173:A:LYS:HA	4	0.11
(2,2626)	1:164:A:ILE:HD12	1:164:A:ILE:HA	5	0.11
(2,2615)	1:163:A:GLU:HB3	1:163:A:GLU:HA	3	0.11
(2,2585)	1:159:A:PHE:HA	1:158:A:GLN:HA	1	0.11
(2,2585)	1:159:A:PHE:HA	1:158:A:GLN:HA	5	0.11
(2,2585)	1:159:A:PHE:HA	1:158:A:GLN:HA	7	0.11
(2,2398)	1:141:A:ILE:HD12	1:141:A:ILE:HG12	8	0.11
(2,2334)	1:136:A:ILE:HG12	1:136:A:ILE:HB	7	0.11
(2,2334)	1:136:A:ILE:HG12	1:136:A:ILE:HB	10	0.11
(2,2333)	1:137:A:VAL:HA	1:136:A:ILE:HA	5	0.11
(2,2333)	1:137:A:VAL:HA	1:136:A:ILE:HA	8	0.11
(2,2180)	1:119:A:PRO:HA	1:119:A:PRO:HG3	2	0.11
(2,2154)	1:116:A:ARG:HB2	1:117:A:GLY:H	3	0.11
(2,2154)	1:116:A:ARG:HB2	1:117:A:GLY:H	4	0.11
(2,2154)	1:116:A:ARG:HB2	1:117:A:GLY:H	6	0.11
(2,1962)	1:96:A:VAL:HG13	1:96:A:VAL:HA	4	0.11
(2,1962)	1:96:A:VAL:HG13	1:96:A:VAL:HA	7	0.11
(2,1926)	1:102:A:PRO:HA	1:103:A:ASN:H	2	0.11
(2,1892)	1:92:A:ALA:HA	1:92:A:ALA:HB1	2	0.11
(2,1892)	1:92:A:ALA:HA	1:92:A:ALA:HB1	5	0.11
(2,1892)	1:92:A:ALA:HA	1:92:A:ALA:HB1	7	0.11
(2,1870)	1:175:A:ARG:HA	1:179:A:ARG:H	5	0.11
(2,1870)	1:175:A:ARG:HA	1:179:A:ARG:H	7	0.11
(2,1838)	1:191:A:VAL:HG13	1:193:A:THR:H	9	0.11
(2,1729)	1:191:A:VAL:HG13	1:191:A:VAL:H	3	0.11
(2,1729)	1:191:A:VAL:HG13	1:191:A:VAL:H	4	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1710)	1:187:A:SER:HB2	1:187:A:SER:H	3	0.11
(2,1647)	1:171:A:LYS:H	1:170:A:LYS:HB2	1	0.11
(2,1647)	1:171:A:LYS:H	1:170:A:LYS:HB2	5	0.11
(2,1647)	1:171:A:LYS:H	1:170:A:LYS:HB2	7	0.11
(2,1613)	1:162:A:GLN:HB2	1:163:A:GLU:H	9	0.11
(2,1553)	1:150:A:ARG:H	1:149:A:GLY:H	3	0.11
(2,1403)	1:113:A:VAL:HB	1:114:A:ARG:H	1	0.11
(2,1231)	1:169:A:LEU:H	1:169:A:LEU:HG	4	0.11
(2,1207)	1:172:A:HIS:H	1:171:A:LYS:H	3	0.11
(2,1207)	1:172:A:HIS:H	1:171:A:LYS:H	7	0.11
(2,1186)	1:188:A:ARG:HG2	1:188:A:ARG:HD2	2	0.11
(2,1186)	1:188:A:ARG:HG2	1:188:A:ARG:HD2	6	0.11
(2,1133)	1:192:A:ARG:HB2	1:193:A:THR:HA	2	0.11
(2,1106)	1:191:A:VAL:HG11	1:191:A:VAL:HA	7	0.11
(2,996)	1:181:A:ILE:HD12	1:181:A:ILE:HB	1	0.11
(2,995)	1:181:A:ILE:HG12	1:181:A:ILE:HB	3	0.11
(2,808)	1:160:A:ALA:HB2	1:161:A:SER:H	3	0.11
(2,666)	1:143:A:LEU:HG	1:143:A:LEU:HD13	4	0.11
(2,551)	1:136:A:ILE:HG12	1:136:A:ILE:HG22	1	0.11
(2,551)	1:136:A:ILE:HG12	1:136:A:ILE:HG22	8	0.11
(2,551)	1:136:A:ILE:HG12	1:136:A:ILE:HG22	10	0.11
(2,526)	1:134:A:LEU:HD21	1:134:A:LEU:HA	9	0.11
(2,408)	1:120:A:PHE:HB3	1:120:A:PHE:H	9	0.11
(2,405)	1:120:A:PHE:HA	1:120:A:PHE:HB3	3	0.11
(2,405)	1:120:A:PHE:HA	1:120:A:PHE:HB3	5	0.11
(2,405)	1:120:A:PHE:HA	1:120:A:PHE:HB3	7	0.11
(2,405)	1:120:A:PHE:HA	1:120:A:PHE:HB3	8	0.11
(2,390)	1:119:A:PRO:HA	1:119:A:PRO:HG3	7	0.11
(2,390)	1:119:A:PRO:HA	1:119:A:PRO:HG3	8	0.11
(2,390)	1:119:A:PRO:HA	1:119:A:PRO:HG3	9	0.11
(2,352)	1:115:A:LEU:HA	1:115:A:LEU:HD21	1	0.11
(2,352)	1:115:A:LEU:HA	1:115:A:LEU:HD21	3	0.11
(2,352)	1:115:A:LEU:HA	1:115:A:LEU:HD21	7	0.11
(2,311)	1:113:A:VAL:HG12	1:113:A:VAL:HB	6	0.11
(2,175)	1:96:A:VAL:HG13	1:96:A:VAL:HA	10	0.11
(2,125)	1:115:A:LEU:HD23	1:115:A:LEU:H	6	0.11
(2,91)	1:155:A:ALA:HA	1:144:A:PRO:HD2	2	0.11
(2,91)	1:155:A:ALA:HA	1:144:A:PRO:HD2	7	0.11
(2,76)	1:107:A:THR:HB	1:110:A:ASP:HA	7	0.11
(2,41)	1:191:A:VAL:HG22	1:188:A:ARG:HA	3	0.11
(2,36)	1:191:A:VAL:HG23	1:191:A:VAL:H	10	0.11
(2,25)	1:96:A:VAL:HG22	1:161:A:SER:H	6	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,17)	1:113:A:VAL:HG12	1:113:A:VAL:H	4	0.11
(2,13)	1:160:A:ALA:HB2	1:162:A:GLN:H	1	0.11
(1,3030)	1:165:A:ALA:H	1:110:A:ASP:HB3	10	0.11
(1,3017)	1:96:A:VAL:HB	1:97:A:LEU:H	3	0.11
(1,3017)	1:96:A:VAL:HB	1:97:A:LEU:H	6	0.11
(1,3003)	1:108:A:ALA:H	1:109:A:ASN:HA	2	0.11
(1,2908)	1:165:A:ALA:HA	1:113:A:VAL:HG23	7	0.11
(1,2863)	1:164:A:ILE:HD13	1:93:A:MET:HA	3	0.11
(1,2863)	1:164:A:ILE:HD13	1:135:A:GLU:HA	4	0.11
(1,2739)	1:143:A:LEU:HG	1:141:A:ILE:HG21	8	0.11
(1,2694)	1:188:A:ARG:HD3	1:188:A:ARG:HG2	6	0.11
(1,2563)	1:181:A:ILE:HB	1:181:A:ILE:HA	5	0.11
(1,2513)	1:134:A:LEU:HD13	1:133:A:GLY:H	3	0.11
(1,2511)	1:134:A:LEU:HD11	1:134:A:LEU:HA	3	0.11
(1,2487)	1:96:A:VAL:HG21	1:96:A:VAL:HB	5	0.11
(1,2472)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	1	0.11
(1,2472)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	4	0.11
(1,2472)	1:164:A:ILE:HD12	1:163:A:GLU:HB3	9	0.11
(1,2422)	1:158:A:GLN:H	1:141:A:ILE:HG23	4	0.11
(1,2376)	1:145:A:VAL:HB	1:146:A:ASP:H	1	0.11
(1,2355)	1:143:A:LEU:HG	1:122:A:CYS:H	4	0.11
(1,2315)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	7	0.11
(1,2167)	1:97:A:LEU:HG	1:97:A:LEU:HD13	1	0.11
(1,2167)	1:97:A:LEU:HG	1:97:A:LEU:HD13	3	0.11
(1,2167)	1:97:A:LEU:HG	1:97:A:LEU:HD11	7	0.11
(1,2140)	1:93:A:MET:HB2	1:93:A:MET:HG2	3	0.11
(1,2134)	1:143:A:LEU:HG	1:141:A:ILE:HG21	4	0.11
(1,2133)	1:97:A:LEU:HD11	1:163:A:GLU:HB3	7	0.11
(1,2113)	1:96:A:VAL:HA	1:97:A:LEU:HA	2	0.11
(1,2087)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	9	0.11
(1,2003)	1:130:A:PHE:HB3	1:132:A:SER:H	1	0.11
(1,2003)	1:130:A:PHE:HB3	1:132:A:SER:H	4	0.11
(1,1992)	1:158:A:GLN:HG2	1:161:A:SER:H	4	0.11
(1,1960)	1:144:A:PRO:HB3	1:144:A:PRO:HA	1	0.11
(1,1960)	1:144:A:PRO:HB3	1:144:A:PRO:HA	3	0.11
(1,1960)	1:144:A:PRO:HB3	1:144:A:PRO:HA	4	0.11
(1,1960)	1:144:A:PRO:HB3	1:144:A:PRO:HA	5	0.11
(1,1960)	1:144:A:PRO:HB3	1:144:A:PRO:HA	6	0.11
(1,1818)	1:126:A:GLU:H	1:126:A:GLU:HB3	6	0.11
(1,1814)	1:97:A:LEU:HB2	1:97:A:LEU:H	5	0.11
(1,1784)	1:189:A:ALA:H	1:186:A:SER:HA	4	0.11
(1,1706)	1:174:A:GLU:HA	1:181:A:ILE:H	4	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1647)	1:111:A:GLY:HA3	1:112:A:PHE:H	8	0.11
(1,1647)	1:111:A:GLY:HA3	1:112:A:PHE:H	9	0.11
(1,1640)	1:162:A:GLN:HB2	1:162:A:GLN:HG3	3	0.11
(1,1640)	1:162:A:GLN:HB2	1:162:A:GLN:HG3	8	0.11
(1,1638)	1:164:A:ILE:HD13	1:93:A:MET:HA	7	0.11
(1,1625)	1:135:A:GLU:HA	1:136:A:ILE:HB	9	0.11
(1,1624)	1:144:A:PRO:HB3	1:144:A:PRO:HA	2	0.11
(1,1624)	1:144:A:PRO:HB3	1:144:A:PRO:HA	7	0.11
(1,1624)	1:144:A:PRO:HB3	1:144:A:PRO:HA	8	0.11
(1,1624)	1:144:A:PRO:HB3	1:144:A:PRO:HA	10	0.11
(1,1607)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	1	0.11
(1,1607)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	4	0.11
(1,1607)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	5	0.11
(1,1607)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	6	0.11
(1,1598)	1:169:A:LEU:HD21	1:167:A:LYS:H	10	0.11
(1,1467)	1:159:A:PHE:HB2	1:166:A:GLU:H	1	0.11
(1,1463)	1:159:A:PHE:HB2	1:159:A:PHE:HA	1	0.11
(1,1463)	1:159:A:PHE:HB2	1:159:A:PHE:HA	3	0.11
(1,1463)	1:159:A:PHE:HB2	1:159:A:PHE:HA	4	0.11
(1,1429)	1:98:A:LYS:HA	1:100:A:THR:HG23	2	0.11
(1,1365)	1:150:A:ARG:HB2	1:150:A:ARG:HA	1	0.11
(1,1362)	1:144:A:PRO:HB3	1:144:A:PRO:HA	9	0.11
(1,1346)	1:144:A:PRO:HB3	1:144:A:PRO:HA	7	0.11
(1,1346)	1:144:A:PRO:HB3	1:144:A:PRO:HA	10	0.11
(1,1329)	1:115:A:LEU:HG	1:115:A:LEU:HB2	9	0.11
(1,1326)	1:154:A:GLU:HB2	1:154:A:GLU:HG3	6	0.11
(1,1289)	1:167:A:LYS:HG2	1:134:A:LEU:HD11	1	0.11
(1,1272)	1:181:A:ILE:HG21	1:181:A:ILE:HB	2	0.11
(1,1255)	1:164:A:ILE:HD12	1:95:A:TRP:HA	10	0.11
(1,1253)	1:164:A:ILE:HD13	1:91:A:ASN:HB2	10	0.11
(1,1234)	1:97:A:LEU:H	1:99:A:HIS:HA	4	0.11
(1,1196)	1:158:A:GLN:H	1:141:A:ILE:HG23	3	0.11
(1,1046)	1:115:A:LEU:HD23	1:114:A:ARG:HA	5	0.11
(1,1046)	1:115:A:LEU:HD23	1:114:A:ARG:HA	10	0.11
(1,1037)	1:111:A:GLY:HA3	1:112:A:PHE:H	10	0.11
(1,1014)	1:135:A:GLU:HA	1:136:A:ILE:HB	3	0.11
(1,993)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	8	0.11
(1,993)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	10	0.11
(1,854)	1:179:A:ARG:HD2	1:179:A:ARG:HA	10	0.11
(1,834)	1:144:A:PRO:HD2	1:118:A:LEU:HD11	6	0.11
(1,758)	1:150:A:ARG:HB2	1:150:A:ARG:HA	7	0.11
(1,734)	1:119:A:PRO:HB3	1:119:A:PRO:HA	4	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,684)	1:167:A:LYS:HG2	1:134:A:LEU:HD12	8	0.11
(1,667)	1:181:A:ILE:HG21	1:181:A:ILE:HB	2	0.11
(1,667)	1:181:A:ILE:HG21	1:181:A:ILE:HB	4	0.11
(1,647)	1:164:A:ILE:HD12	1:95:A:TRP:HA	10	0.11
(1,593)	1:135:A:GLU:H	1:164:A:ILE:HG12	3	0.11
(1,549)	1:108:A:ALA:H	1:109:A:ASN:HA	3	0.11
(1,504)	1:166:A:GLU:H	1:169:A:LEU:HD13	2	0.11
(1,482)	1:174:A:GLU:HA	1:181:A:ILE:H	3	0.11
(1,165)	1:109:A:ASN:HA	1:108:A:ALA:HB3	4	0.11
(1,152)	1:130:A:PHE:HB2	1:131:A:PHE:H	8	0.11
(1,126)	1:150:A:ARG:HB2	1:150:A:ARG:HA	5	0.11
(1,10)	1:164:A:ILE:HD13	1:91:A:ASN:HB2	10	0.11
(4,54)	1:186:A:SER:H	1:184:A:PHE:O	3	0.1
(4,49)	1:183:A:ILE:N	1:171:A:LYS:O	7	0.1
(4,12)	1:118:A:LEU:N	1:152:A:THR:O	5	0.1
(4,4)	1:114:A:ARG:N	1:184:A:PHE:O	8	0.1
(4,4)	1:114:A:ARG:N	1:184:A:PHE:O	9	0.1
(4,2)	1:113:A:VAL:N	1:157:A:VAL:O	5	0.1
(3,281)	1:188:A:ARG:HG2	1:190:A:GLU:H	6	0.1
(3,150)	1:188:A:ARG:HG2	1:190:A:GLU:H	6	0.1
(3,6)	1:188:A:ARG:HG2	1:190:A:GLU:H	6	0.1
(2,8697)	1:110:A:ASP:HA	1:110:A:ASP:H	10	0.1
(2,8637)	1:96:A:VAL:HG13	1:97:A:LEU:H	6	0.1
(2,8632)	1:96:A:VAL:H	1:95:A:TRP:H	8	0.1
(2,8414)	1:191:A:VAL:HG13	1:192:A:ARG:HA	10	0.1
(2,8352)	1:183:A:ILE:HG21	1:184:A:PHE:HA	2	0.1
(2,8302)	1:181:A:ILE:HG22	1:181:A:ILE:HG12	7	0.1
(2,8216)	1:171:A:LYS:HB3	1:171:A:LYS:HA	4	0.1
(2,8144)	1:164:A:ILE:HG13	1:164:A:ILE:HG22	3	0.1
(2,8125)	1:163:A:GLU:HG2	1:163:A:GLU:HB3	1	0.1
(2,8125)	1:163:A:GLU:HG2	1:163:A:GLU:HB3	4	0.1
(2,8106)	1:161:A:SER:HB2	1:161:A:SER:HA	1	0.1
(2,8106)	1:161:A:SER:HB2	1:161:A:SER:HA	2	0.1
(2,8099)	1:157:A:VAL:HG22	1:158:A:GLN:H	1	0.1
(2,8099)	1:157:A:VAL:HG22	1:158:A:GLN:H	2	0.1
(2,7721)	1:127:A:ILE:HD12	1:127:A:ILE:HB	2	0.1
(2,7721)	1:127:A:ILE:HD12	1:127:A:ILE:HB	9	0.1
(2,7570)	1:107:A:THR:HB	1:107:A:THR:HG22	9	0.1
(2,7524)	1:100:A:THR:HG23	1:100:A:THR:HB	1	0.1
(2,7498)	1:96:A:VAL:HG22	1:97:A:LEU:H	10	0.1
(2,7413)	1:181:A:ILE:HD12	1:183:A:ILE:H	4	0.1
(2,7358)	1:141:A:ILE:HA	1:140:A:GLY:H	5	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7288)	1:96:A:VAL:HG22	1:96:A:VAL:HA	4	0.1
(2,7288)	1:96:A:VAL:HG22	1:96:A:VAL:HA	5	0.1
(2,7288)	1:96:A:VAL:HG22	1:96:A:VAL:HA	7	0.1
(2,6850)	1:112:A:PHE:H	1:111:A:GLY:H	7	0.1
(2,6796)	1:98:A:LYS:HG3	1:98:A:LYS:H	7	0.1
(2,6776)	1:96:A:VAL:H	1:95:A:TRP:H	6	0.1
(2,6733)	1:150:A:ARG:HB2	1:147:A:PHE:H	2	0.1
(2,6728)	1:93:A:MET:H	1:91:A:ASN:HA	10	0.1
(2,6710)	1:142:A:THR:H	1:155:A:ALA:HA	5	0.1
(2,6558)	1:192:A:ARG:HD2	1:192:A:ARG:HB2	2	0.1
(2,6558)	1:192:A:ARG:HD2	1:192:A:ARG:HB2	7	0.1
(2,6415)	1:179:A:ARG:HG3	1:179:A:ARG:HD2	8	0.1
(2,6293)	1:166:A:GLU:HB2	1:166:A:GLU:HA	4	0.1
(2,6232)	1:160:A:ALA:HB3	1:161:A:SER:H	1	0.1
(2,6226)	1:157:A:VAL:HG22	1:158:A:GLN:H	7	0.1
(2,6226)	1:157:A:VAL:HG22	1:158:A:GLN:H	10	0.1
(2,6216)	1:157:A:VAL:HG23	1:157:A:VAL:HG12	6	0.1
(2,6205)	1:157:A:VAL:HG22	1:157:A:VAL:HG11	2	0.1
(2,6205)	1:157:A:VAL:HG22	1:157:A:VAL:HG11	3	0.1
(2,6205)	1:157:A:VAL:HG22	1:157:A:VAL:HG11	10	0.1
(2,6063)	1:141:A:ILE:HD13	1:141:A:ILE:HG12	2	0.1
(2,6063)	1:141:A:ILE:HD13	1:141:A:ILE:HG12	10	0.1
(2,5848)	1:127:A:ILE:HD12	1:127:A:ILE:HB	1	0.1
(2,5829)	1:124:A:LYS:HA	1:124:A:LYS:HB2	10	0.1
(2,5542)	1:181:A:ILE:HD12	1:183:A:ILE:H	2	0.1
(2,5534)	1:115:A:LEU:HD23	1:115:A:LEU:H	8	0.1
(2,5526)	1:97:A:LEU:HD13	1:97:A:LEU:HA	2	0.1
(2,5526)	1:97:A:LEU:HD13	1:97:A:LEU:HA	7	0.1
(2,5502)	1:156:A:PHE:HB2	1:191:A:VAL:H	3	0.1
(2,5466)	1:166:A:GLU:HG2	1:166:A:GLU:H	2	0.1
(2,5466)	1:166:A:GLU:HG2	1:166:A:GLU:H	8	0.1
(2,5422)	1:96:A:VAL:HG22	1:96:A:VAL:HA	6	0.1
(2,5422)	1:96:A:VAL:HG22	1:96:A:VAL:HA	8	0.1
(2,5402)	1:164:A:ILE:HD13	1:91:A:ASN:HA	9	0.1
(2,5382)	1:164:A:ILE:HG13	1:167:A:LYS:H	3	0.1
(2,5376)	1:166:A:GLU:H	1:95:A:TRP:HB2	10	0.1
(2,5244)	1:166:A:GLU:HB3	1:167:A:LYS:H	5	0.1
(2,5103)	1:135:A:GLU:HB3	1:135:A:GLU:H	10	0.1
(2,4907)	1:151:A:SER:H	1:151:A:SER:HB2	1	0.1
(2,4891)	1:105:A:PRO:HA	1:106:A:ASP:H	10	0.1
(2,4791)	1:188:A:ARG:HD2	1:108:A:ALA:H	1	0.1
(2,4785)	1:185:A:LYS:HB3	1:185:A:LYS:H	6	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4660)	1:183:A:ILE:HG22	1:183:A:ILE:HD13	4	0.1
(2,4600)	1:181:A:ILE:HG22	1:181:A:ILE:HG12	1	0.1
(2,4471)	1:166:A:GLU:HG3	1:166:A:GLU:HA	8	0.1
(2,4462)	1:165:A:ALA:HB3	1:165:A:ALA:HA	2	0.1
(2,4437)	1:164:A:ILE:HD12	1:164:A:ILE:HA	4	0.1
(2,4420)	1:162:A:GLN:HB2	1:162:A:GLN:HG2	1	0.1
(2,4420)	1:162:A:GLN:HB2	1:162:A:GLN:HG2	2	0.1
(2,4420)	1:162:A:GLN:HB2	1:162:A:GLN:HG2	7	0.1
(2,4269)	1:143:A:LEU:HD21	1:143:A:LEU:HB2	3	0.1
(2,4133)	1:135:A:GLU:HG3	1:135:A:GLU:HA	4	0.1
(2,4133)	1:135:A:GLU:HG3	1:135:A:GLU:HA	6	0.1
(2,3989)	1:119:A:PRO:HA	1:119:A:PRO:HG3	5	0.1
(2,3981)	1:118:A:LEU:HD13	1:118:A:LEU:HD22	1	0.1
(2,3963)	1:116:A:ARG:HB2	1:117:A:GLY:H	3	0.1
(2,3697)	1:92:A:ALA:HA	1:92:A:ALA:HB1	2	0.1
(2,3697)	1:92:A:ALA:HA	1:92:A:ALA:HB1	5	0.1
(2,3661)	1:95:A:TRP:HB3	1:91:A:ASN:HB3	6	0.1
(2,3628)	1:181:A:ILE:HG21	1:174:A:GLU:H	3	0.1
(2,3227)	1:116:A:ARG:H	1:116:A:ARG:HB3	6	0.1
(2,3182)	1:107:A:THR:HA	1:108:A:ALA:H	7	0.1
(2,3179)	1:106:A:ASP:H	1:105:A:PRO:HD2	10	0.1
(2,3019)	1:110:A:ASP:H	1:188:A:ARG:HG2	8	0.1
(2,2861)	1:187:A:SER:HB3	1:188:A:ARG:H	6	0.1
(2,2841)	1:183:A:ILE:HG21	1:184:A:PHE:HA	2	0.1
(2,2689)	1:169:A:LEU:HD22	1:169:A:LEU:HD12	2	0.1
(2,2626)	1:164:A:ILE:HD12	1:164:A:ILE:HA	10	0.1
(2,2622)	1:163:A:GLU:HB3	1:164:A:ILE:H	10	0.1
(2,2615)	1:163:A:GLU:HB3	1:163:A:GLU:HA	9	0.1
(2,2334)	1:136:A:ILE:HG12	1:136:A:ILE:HB	3	0.1
(2,2226)	1:127:A:ILE:HD12	1:127:A:ILE:HB	1	0.1
(2,2226)	1:127:A:ILE:HD12	1:127:A:ILE:HB	5	0.1
(2,2213)	1:126:A:GLU:HG2	1:126:A:GLU:HB2	7	0.1
(2,2180)	1:119:A:PRO:HA	1:119:A:PRO:HG3	3	0.1
(2,2031)	1:101:A:GLY:HA3	1:101:A:GLY:H	6	0.1
(2,2031)	1:101:A:GLY:HA3	1:101:A:GLY:H	10	0.1
(2,2015)	1:98:A:LYS:HG3	1:98:A:LYS:HE3	2	0.1
(2,1962)	1:96:A:VAL:HG13	1:96:A:VAL:HA	5	0.1
(2,1878)	1:136:A:ILE:HD13	1:134:A:LEU:HA	7	0.1
(2,1798)	1:164:A:ILE:HD11	1:161:A:SER:H	10	0.1
(2,1639)	1:166:A:GLU:HB3	1:167:A:LYS:H	8	0.1
(2,1583)	1:156:A:PHE:HB2	1:157:A:VAL:H	1	0.1
(2,1562)	1:150:A:ARG:H	1:151:A:SER:H	2	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1250)	1:167:A:LYS:HB3	1:168:A:ALA:H	7	0.1
(2,1133)	1:192:A:ARG:HB2	1:193:A:THR:HA	3	0.1
(2,1120)	1:191:A:VAL:HG23	1:191:A:VAL:H	4	0.1
(2,899)	1:169:A:LEU:HD22	1:169:A:LEU:HD12	1	0.1
(2,790)	1:157:A:VAL:HG21	1:157:A:VAL:HA	10	0.1
(2,738)	1:150:A:ARG:HD3	1:150:A:ARG:HB3	1	0.1
(2,599)	1:141:A:ILE:HG12	1:141:A:ILE:HA	6	0.1
(2,551)	1:136:A:ILE:HG12	1:136:A:ILE:HG22	6	0.1
(2,526)	1:134:A:LEU:HD21	1:134:A:LEU:HA	3	0.1
(2,526)	1:134:A:LEU:HD21	1:134:A:LEU:HA	8	0.1
(2,526)	1:134:A:LEU:HD21	1:134:A:LEU:HA	10	0.1
(2,405)	1:120:A:PHE:HA	1:120:A:PHE:HB3	6	0.1
(2,175)	1:96:A:VAL:HG13	1:96:A:VAL:HA	2	0.1
(2,125)	1:115:A:LEU:HD23	1:115:A:LEU:H	1	0.1
(2,121)	1:97:A:LEU:HD13	1:97:A:LEU:HA	7	0.1
(2,74)	1:169:A:LEU:HB2	1:166:A:GLU:HA	2	0.1
(2,69)	1:166:A:GLU:HG2	1:166:A:GLU:H	3	0.1
(2,60)	1:164:A:ILE:HG13	1:94:A:ASP:HB2	3	0.1
(2,27)	1:181:A:ILE:HG21	1:174:A:GLU:H	9	0.1
(2,17)	1:113:A:VAL:HG12	1:113:A:VAL:H	5	0.1
(2,6)	1:164:A:ILE:HD11	1:161:A:SER:H	3	0.1
(2,6)	1:164:A:ILE:HD11	1:161:A:SER:H	4	0.1
(2,1)	1:141:A:ILE:HD12	1:125:A:GLU:H	8	0.1
(1,3081)	1:118:A:LEU:H	1:118:A:LEU:HD11	7	0.1
(1,3081)	1:118:A:LEU:H	1:118:A:LEU:HD11	8	0.1
(1,2927)	1:175:A:ARG:HD2	1:175:A:ARG:HB3	7	0.1
(1,2492)	1:127:A:ILE:HG21	1:127:A:ILE:HB	1	0.1
(1,2433)	1:126:A:GLU:H	1:126:A:GLU:HB3	6	0.1
(1,2314)	1:179:A:ARG:HD2	1:179:A:ARG:HA	5	0.1
(1,2167)	1:97:A:LEU:HG	1:97:A:LEU:HD13	6	0.1
(1,2113)	1:96:A:VAL:HA	1:97:A:LEU:HA	5	0.1
(1,1960)	1:144:A:PRO:HB3	1:144:A:PRO:HA	2	0.1
(1,1960)	1:144:A:PRO:HB3	1:144:A:PRO:HA	8	0.1
(1,1814)	1:97:A:LEU:HB2	1:97:A:LEU:H	4	0.1
(1,1784)	1:189:A:ALA:H	1:186:A:SER:HA	7	0.1
(1,1784)	1:189:A:ALA:H	1:186:A:SER:HA	10	0.1
(1,1704)	1:169:A:LEU:HB2	1:166:A:GLU:HA	10	0.1
(1,1657)	1:115:A:LEU:HD23	1:114:A:ARG:HA	4	0.1
(1,1607)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	2	0.1
(1,1486)	1:169:A:LEU:HB2	1:166:A:GLU:HA	7	0.1
(1,1463)	1:159:A:PHE:HB2	1:159:A:PHE:HA	5	0.1
(1,1463)	1:159:A:PHE:HB2	1:159:A:PHE:HA	8	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1432)	1:141:A:ILE:HA	1:140:A:GLY:H	2	0.1
(1,1365)	1:150:A:ARG:HB2	1:150:A:ARG:HA	4	0.1
(1,1365)	1:150:A:ARG:HB2	1:150:A:ARG:HA	6	0.1
(1,1346)	1:144:A:PRO:HB3	1:144:A:PRO:HA	9	0.1
(1,1297)	1:166:A:GLU:HB2	1:168:A:ALA:H	5	0.1
(1,1046)	1:115:A:LEU:HD23	1:114:A:ARG:HA	8	0.1
(1,1029)	1:162:A:GLN:HB3	1:162:A:GLN:HG2	9	0.1
(1,993)	1:136:A:ILE:HG12	1:136:A:ILE:HD11	7	0.1
(1,861)	1:150:A:ARG:HG3	1:150:A:ARG:HD2	6	0.1
(1,764)	1:166:A:GLU:HG3	1:168:A:ALA:H	3	0.1
(1,758)	1:150:A:ARG:HB2	1:150:A:ARG:HA	1	0.1
(1,654)	1:183:A:ILE:HG21	1:184:A:PHE:HA	4	0.1
(1,598)	1:116:A:ARG:H	1:181:A:ILE:HD12	3	0.1
(1,549)	1:108:A:ALA:H	1:109:A:ASN:HA	10	0.1
(1,518)	1:110:A:ASP:HB3	1:110:A:ASP:H	7	0.1
(1,456)	1:165:A:ALA:HA	1:113:A:VAL:HG21	5	0.1
(1,288)	1:141:A:ILE:HG21	1:143:A:LEU:HG	8	0.1
(1,126)	1:150:A:ARG:HB2	1:150:A:ARG:HA	7	0.1
(1,107)	1:126:A:GLU:HB3	1:126:A:GLU:HA	4	0.1
(1,107)	1:126:A:GLU:HB3	1:126:A:GLU:HA	10	0.1
(1,41)	1:134:A:LEU:HD11	1:134:A:LEU:HA	6	0.1
(1,41)	1:134:A:LEU:HD11	1:134:A:LEU:HA	8	0.1
(1,20)	1:96:A:VAL:HG22	1:96:A:VAL:HA	4	0.1
(1,20)	1:96:A:VAL:HG22	1:96:A:VAL:HA	5	0.1
(1,20)	1:96:A:VAL:HG22	1:96:A:VAL:HA	7	0.1

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

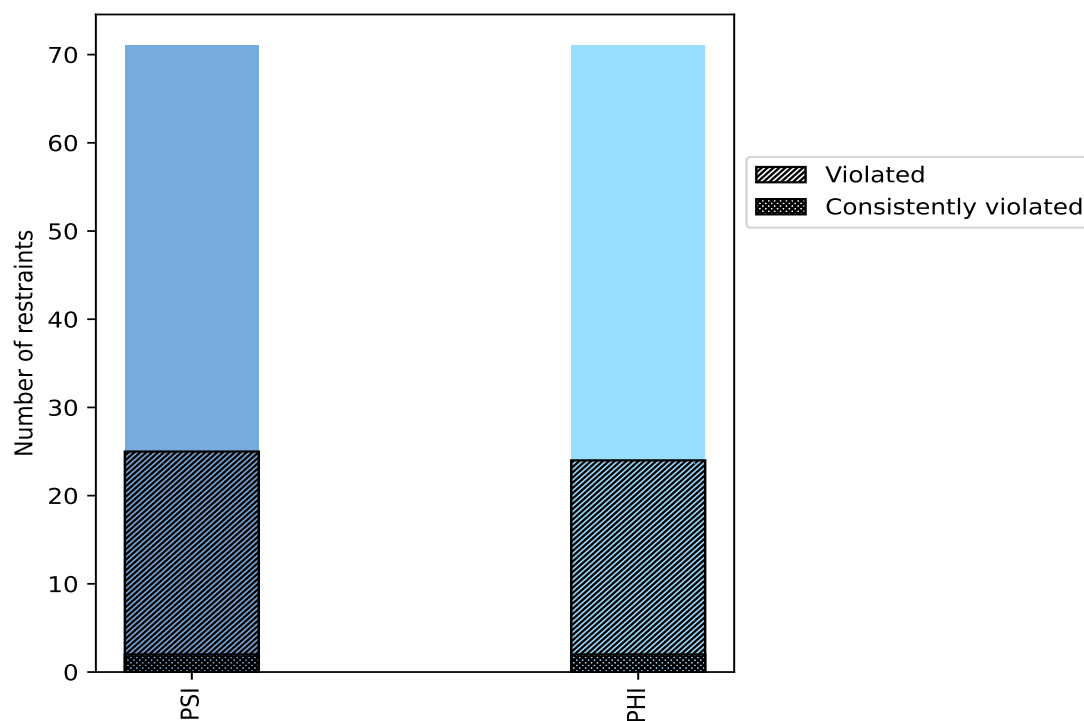
10.1 Summary of dihedral-angle violations [i](#)

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
PSI	71	50.0	25	35.2	17.6	2	2.8	1.4
PHI	71	50.0	24	33.8	16.9	2	2.8	1.4
Total	142	100.0	49	34.5	34.5	4	2.8	2.8

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](#)



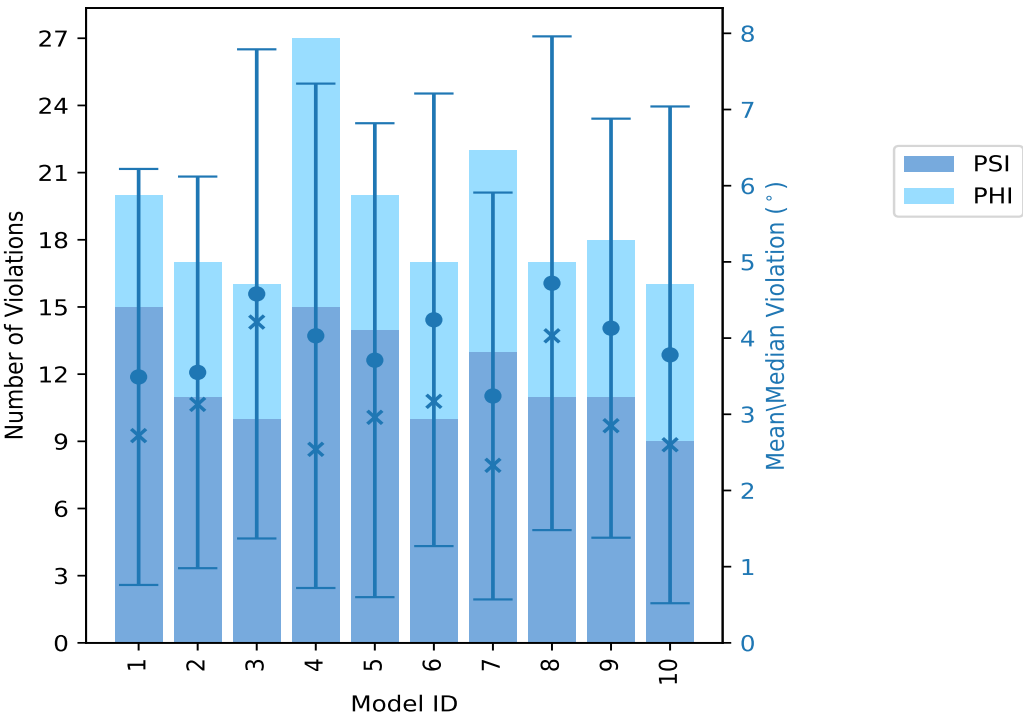
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PSI	PHI	Total				
1	15	5	20	3.49	12.91	2.73	2.72
2	11	6	17	3.55	10.87	2.57	3.13
3	10	6	16	4.58	14.3	3.21	4.21
4	15	12	27	4.03	13.83	3.31	2.54
5	14	6	20	3.71	14.78	3.11	2.96
6	10	7	17	4.24	12.19	2.97	3.17
7	13	9	22	3.24	11.99	2.67	2.33
8	11	6	17	4.72	15.22	3.24	4.03
9	11	7	18	4.13	12.56	2.75	2.85
10	9	7	16	3.78	12.71	3.26	2.6

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

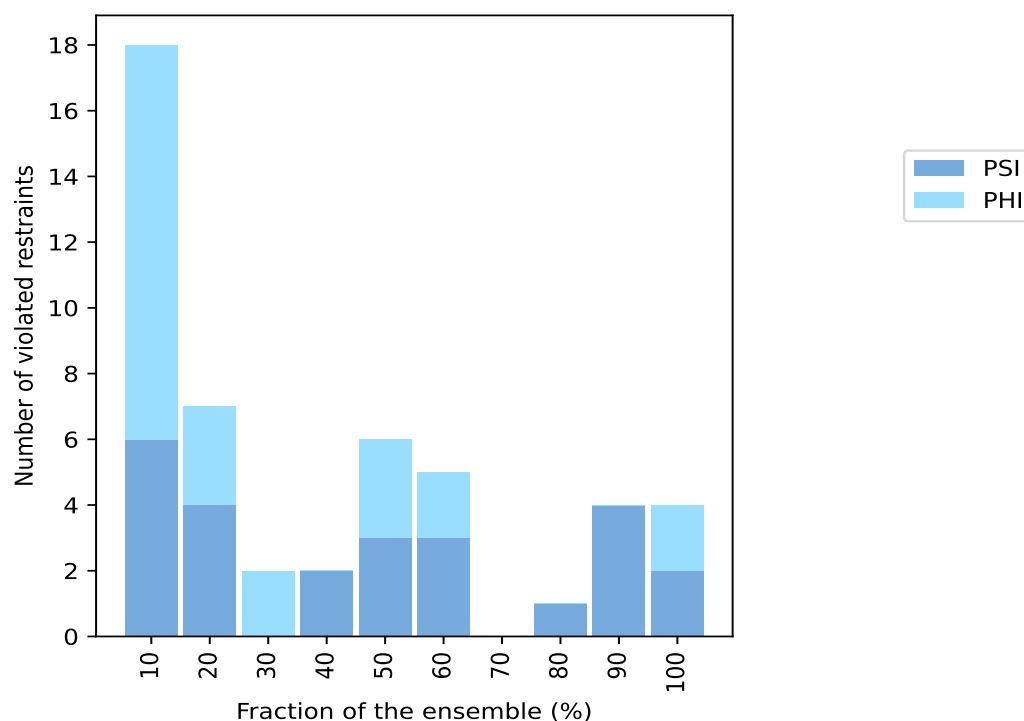
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	
PSI	PHI	Total	Count ¹	%
6	12	18	1	10.0
4	3	7	2	20.0
0	2	2	3	30.0
2	0	2	4	40.0
3	3	6	5	50.0
3	2	5	6	60.0
0	0	0	7	70.0
1	0	1	8	80.0
4	0	4	9	90.0
2	2	4	10	100.0

¹ Number of models with violations

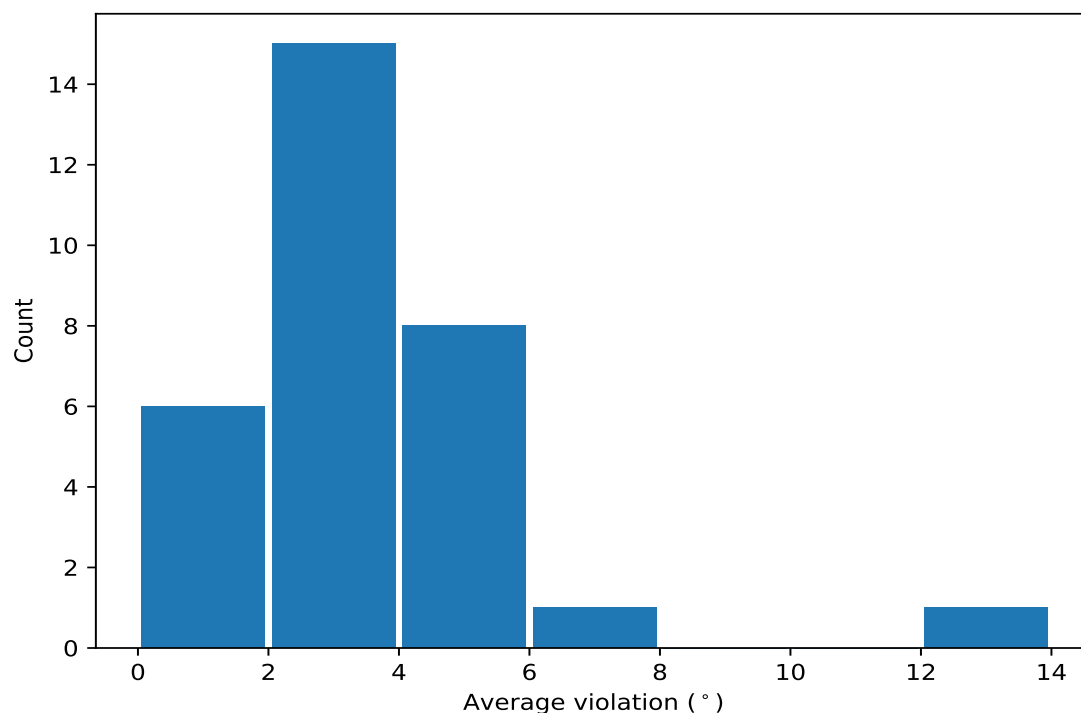
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,142)	1:191:A:VAL:N	1:191:A:VAL:CA	1:191:A:VAL:C	1:192:A:ARG:N	10	12.44	2.25	12.81
(1,79)	1:158:A:GLN:C	1:159:A:PHE:N	1:159:A:PHE:CA	1:159:A:PHE:C	10	6.59	3.09	6.77
(1,45)	1:135:A:GLU:C	1:136:A:ILE:N	1:136:A:ILE:CA	1:136:A:ILE:C	10	5.87	0.97	6.06
(1,6)	1:107:A:THR:N	1:107:A:THR:CA	1:107:A:THR:C	1:108:A:ALA:N	10	4.17	1.88	3.48
(1,8)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	9	4.59	2.89	5.08
(1,116)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:HIS:N	9	4.08	2.0	3.64
(1,18)	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	1:121:A:GLY:N	9	3.83	1.7	4.03
(1,66)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:ARG:N	9	2.79	1.62	2.63
(1,124)	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	1:182:A:GLU:N	8	2.82	1.11	2.72
(1,134)	1:187:A:SER:N	1:187:A:SER:CA	1:187:A:SER:C	1:188:A:ARG:N	6	2.88	1.23	2.4
(1,130)	1:184:A:PHE:N	1:184:A:PHE:CA	1:184:A:PHE:C	1:185:A:LYS:N	6	2.78	0.93	2.8
(1,13)	1:114:A:ARG:C	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	6	2.35	0.57	2.12
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:HIS:N	6	2.05	1.08	1.44

Continued on next page...

Continued from previous page...

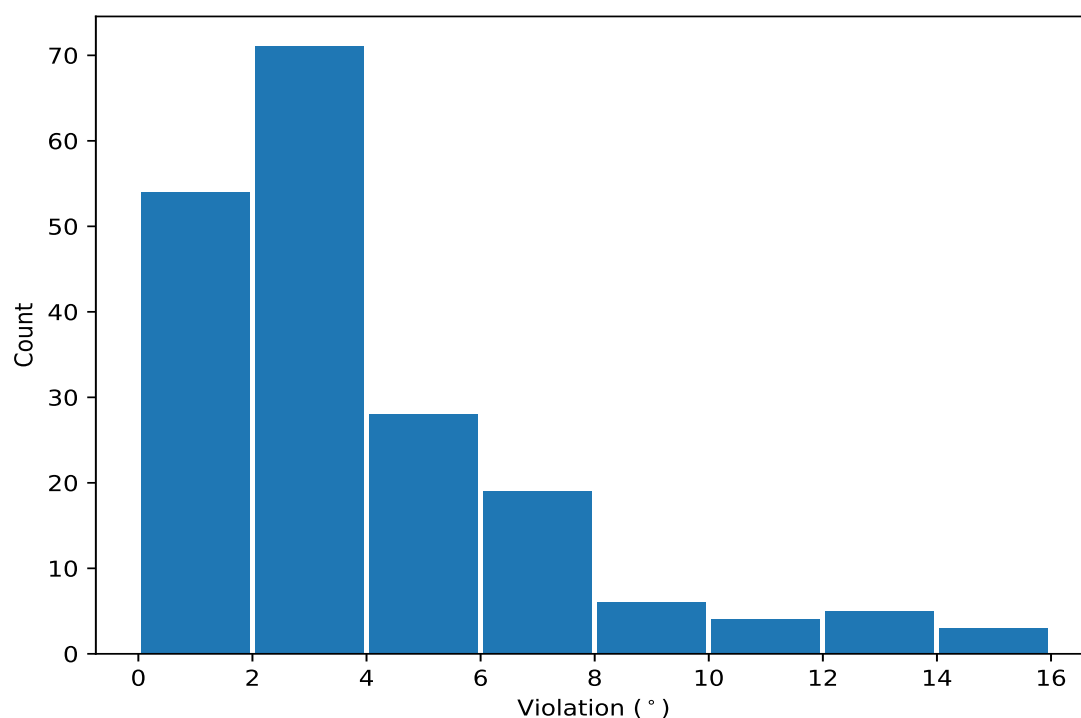
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,89)	1:163:A:GLU:C	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	6	1.28	0.26	1.14
(1,120)	1:179:A:ARG:N	1:179:A:ARG:CA	1:179:A:ARG:C	1:180:A:TYR:N	5	5.2	4.01	2.89
(1,4)	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	1:107:A:THR:N	5	3.52	0.49	3.49
(1,133)	1:186:A:SER:C	1:187:A:SER:N	1:187:A:SER:CA	1:187:A:SER:C	5	2.92	0.6	3.04
(1,41)	1:132:A:SER:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	5	2.54	0.89	2.23
(1,123)	1:180:A:TYR:C	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	5	2.39	0.25	2.54
(1,118)	1:178:A:HIS:N	1:178:A:HIS:CA	1:178:A:HIS:C	1:179:A:ARG:N	5	2.18	0.53	2.19
(1,42)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:LEU:N	4	2.05	0.58	2.25
(1,110)	1:174:A:GLU:N	1:174:A:GLU:CA	1:174:A:GLU:C	1:175:A:ARG:N	4	1.58	0.65	1.25
(1,17)	1:119:A:PRO:C	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	3	5.09	0.49	4.95
(1,71)	1:154:A:GLU:C	1:155:A:ALA:N	1:155:A:ALA:CA	1:155:A:ALA:C	3	3.81	1.37	4.73
(1,59)	1:145:A:VAL:C	1:146:A:ASP:N	1:146:A:ASP:CA	1:146:A:ASP:C	2	4.73	2.86	4.73
(1,114)	1:176:A:ILE:N	1:176:A:ILE:CA	1:176:A:ILE:C	1:177:A:GLY:N	2	4.14	2.06	4.14
(1,122)	1:180:A:TYR:N	1:180:A:TYR:CA	1:180:A:TYR:C	1:181:A:ILE:N	2	2.03	0.54	2.03
(1,109)	1:173:A:LYS:C	1:174:A:GLU:N	1:174:A:GLU:CA	1:174:A:GLU:C	2	1.98	0.9	1.98
(1,132)	1:185:A:LYS:N	1:185:A:LYS:CA	1:185:A:LYS:C	1:186:A:SER:N	2	1.93	0.56	1.93
(1,36)	1:130:A:PHE:N	1:130:A:PHE:CA	1:130:A:PHE:C	1:131:A:PHE:N	2	1.82	0.12	1.82
(1,5)	1:106:A:ASP:C	1:107:A:THR:N	1:107:A:THR:CA	1:107:A:THR:C	2	1.23	0.01	1.23

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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



10.5.2 Table: All violated dihedral-angle restraints [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 (°)
(1,142)	1:191:A:VAL:N	1:191:A:VAL:CA	1:191:A:VAL:C	1:192:A:ARG:N	8	15.22
(1,142)	1:191:A:VAL:N	1:191:A:VAL:CA	1:191:A:VAL:C	1:192:A:ARG:N	5	14.78
(1,142)	1:191:A:VAL:N	1:191:A:VAL:CA	1:191:A:VAL:C	1:192:A:ARG:N	3	14.3
(1,142)	1:191:A:VAL:N	1:191:A:VAL:CA	1:191:A:VAL:C	1:192:A:ARG:N	4	13.83
(1,142)	1:191:A:VAL:N	1:191:A:VAL:CA	1:191:A:VAL:C	1:192:A:ARG:N	1	12.91
(1,142)	1:191:A:VAL:N	1:191:A:VAL:CA	1:191:A:VAL:C	1:192:A:ARG:N	10	12.71
(1,142)	1:191:A:VAL:N	1:191:A:VAL:CA	1:191:A:VAL:C	1:192:A:ARG:N	9	12.56
(1,120)	1:179:A:ARG:N	1:179:A:ARG:CA	1:179:A:ARG:C	1:180:A:TYR:N	6	12.19
(1,79)	1:158:A:GLN:C	1:159:A:PHE:N	1:159:A:PHE:CA	1:159:A:PHE:C	7	11.99
(1,57)	1:144:A:PRO:C	1:145:A:VAL:N	1:145:A:VAL:CA	1:145:A:VAL:C	4	11.13
(1,142)	1:191:A:VAL:N	1:191:A:VAL:CA	1:191:A:VAL:C	1:192:A:ARG:N	2	10.87
(1,8)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	10	10.03
(1,79)	1:158:A:GLN:C	1:159:A:PHE:N	1:159:A:PHE:CA	1:159:A:PHE:C	4	9.69
(1,79)	1:158:A:GLN:C	1:159:A:PHE:N	1:159:A:PHE:CA	1:159:A:PHE:C	2	9.3
(1,6)	1:107:A:THR:N	1:107:A:THR:CA	1:107:A:THR:C	1:108:A:ALA:N	8	8.87
(1,142)	1:191:A:VAL:N	1:191:A:VAL:CA	1:191:A:VAL:C	1:192:A:ARG:N	7	8.63
(1,142)	1:191:A:VAL:N	1:191:A:VAL:CA	1:191:A:VAL:C	1:192:A:ARG:N	6	8.61
(1,79)	1:158:A:GLN:C	1:159:A:PHE:N	1:159:A:PHE:CA	1:159:A:PHE:C	1	8.19
(1,59)	1:145:A:VAL:C	1:146:A:ASP:N	1:146:A:ASP:CA	1:146:A:ASP:C	4	7.59
(1,79)	1:158:A:GLN:C	1:159:A:PHE:N	1:159:A:PHE:CA	1:159:A:PHE:C	5	7.31
(1,120)	1:179:A:ARG:N	1:179:A:ARG:CA	1:179:A:ARG:C	1:180:A:TYR:N	9	7.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,45)	1:135:A:GLU:C	1:136:A:ILE:N	1:136:A:ILE:CA	1:136:A:ILE:C	6	7.1
(1,45)	1:135:A:GLU:C	1:136:A:ILE:N	1:136:A:ILE:CA	1:136:A:ILE:C	9	7.07
(1,116)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:HIS:N	5	7.06
(1,65)	1:148:A:GLN:C	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	4	7.05
(1,66)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:ARG:N	4	6.87
(1,116)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:HIS:N	7	6.78
(1,8)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	9	6.66
(1,45)	1:135:A:GLU:C	1:136:A:ILE:N	1:136:A:ILE:CA	1:136:A:ILE:C	3	6.61
(1,8)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	3	6.6
(1,45)	1:135:A:GLU:C	1:136:A:ILE:N	1:136:A:ILE:CA	1:136:A:ILE:C	8	6.58
(1,45)	1:135:A:GLU:C	1:136:A:ILE:N	1:136:A:ILE:CA	1:136:A:ILE:C	10	6.46
(1,6)	1:107:A:THR:N	1:107:A:THR:CA	1:107:A:THR:C	1:108:A:ALA:N	3	6.41
(1,18)	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	1:121:A:GLY:N	6	6.35
(1,79)	1:158:A:GLN:C	1:159:A:PHE:N	1:159:A:PHE:CA	1:159:A:PHE:C	3	6.23
(1,114)	1:176:A:ILE:N	1:176:A:ILE:CA	1:176:A:ILE:C	1:177:A:GLY:N	8	6.2
(1,8)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	6	6.13
(1,116)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:HIS:N	10	5.81
(1,40)	1:132:A:SER:N	1:132:A:SER:CA	1:132:A:SER:C	1:133:A:GLY:N	3	5.78
(1,17)	1:119:A:PRO:C	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	6	5.75
(1,45)	1:135:A:GLU:C	1:136:A:ILE:N	1:136:A:ILE:CA	1:136:A:ILE:C	5	5.65
(1,18)	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	1:121:A:GLY:N	3	5.38
(1,45)	1:135:A:GLU:C	1:136:A:ILE:N	1:136:A:ILE:CA	1:136:A:ILE:C	7	5.26
(1,18)	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	1:121:A:GLY:N	4	5.15
(1,18)	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	1:121:A:GLY:N	9	5.08
(1,8)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	8	5.08
(1,67)	1:150:A:ARG:C	1:151:A:SER:N	1:151:A:SER:CA	1:151:A:SER:C	4	5.07
(1,45)	1:135:A:GLU:C	1:136:A:ILE:N	1:136:A:ILE:CA	1:136:A:ILE:C	4	5.02
(1,37)	1:130:A:PHE:C	1:131:A:PHE:N	1:131:A:PHE:CA	1:131:A:PHE:C	3	4.95
(1,17)	1:119:A:PRO:C	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	1	4.95
(1,71)	1:154:A:GLU:C	1:155:A:ALA:N	1:155:A:ALA:CA	1:155:A:ALA:C	1	4.83
(1,124)	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	1:182:A:GLU:N	8	4.82
(1,45)	1:135:A:GLU:C	1:136:A:ILE:N	1:136:A:ILE:CA	1:136:A:ILE:C	1	4.75
(1,71)	1:154:A:GLU:C	1:155:A:ALA:N	1:155:A:ALA:CA	1:155:A:ALA:C	9	4.73
(1,116)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:HIS:N	4	4.7
(1,134)	1:187:A:SER:N	1:187:A:SER:CA	1:187:A:SER:C	1:188:A:ARG:N	8	4.58
(1,17)	1:119:A:PRO:C	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	9	4.57
(1,134)	1:187:A:SER:N	1:187:A:SER:CA	1:187:A:SER:C	1:188:A:ARG:N	5	4.52
(1,79)	1:158:A:GLN:C	1:159:A:PHE:N	1:159:A:PHE:CA	1:159:A:PHE:C	9	4.45
(1,4)	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	1:107:A:THR:N	7	4.37
(1,6)	1:107:A:THR:N	1:107:A:THR:CA	1:107:A:THR:C	1:108:A:ALA:N	5	4.31
(1,45)	1:135:A:GLU:C	1:136:A:ILE:N	1:136:A:ILE:CA	1:136:A:ILE:C	2	4.21
(1,130)	1:184:A:PHE:N	1:184:A:PHE:CA	1:184:A:PHE:C	1:185:A:LYS:N	8	4.14
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:HIS:N	6	4.12
(1,18)	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	1:121:A:GLY:N	8	4.03
(1,41)	1:132:A:SER:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1	3.94
(1,133)	1:186:A:SER:C	1:187:A:SER:N	1:187:A:SER:CA	1:187:A:SER:C	8	3.86
(1,124)	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	1:182:A:GLU:N	2	3.76
(1,141)	1:190:A:GLU:C	1:191:A:VAL:N	1:191:A:VAL:CA	1:191:A:VAL:C	8	3.73
(1,116)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:HIS:N	2	3.64
(1,4)	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	1:107:A:THR:N	2	3.64
(1,79)	1:158:A:GLN:C	1:159:A:PHE:N	1:159:A:PHE:CA	1:159:A:PHE:C	8	3.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,6)	1:107:A:THR:N	1:107:A:THR:CA	1:107:A:THR:C	1:108:A:ALA:N	6	3.53
(1,6)	1:107:A:THR:N	1:107:A:THR:CA	1:107:A:THR:C	1:108:A:ALA:N	10	3.52
(1,124)	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	1:182:A:GLU:N	4	3.49
(1,4)	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	1:107:A:THR:N	1	3.49
(1,130)	1:184:A:PHE:N	1:184:A:PHE:CA	1:184:A:PHE:C	1:185:A:LYS:N	2	3.48
(1,66)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:ARG:N	3	3.47
(1,6)	1:107:A:THR:N	1:107:A:THR:CA	1:107:A:THR:C	1:108:A:ALA:N	2	3.43
(1,130)	1:184:A:PHE:N	1:184:A:PHE:CA	1:184:A:PHE:C	1:185:A:LYS:N	5	3.41
(1,13)	1:114:A:ARG:C	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	3	3.41
(1,18)	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	1:121:A:GLY:N	7	3.25
(1,6)	1:107:A:THR:N	1:107:A:THR:CA	1:107:A:THR:C	1:108:A:ALA:N	1	3.22
(1,6)	1:107:A:THR:N	1:107:A:THR:CA	1:107:A:THR:C	1:108:A:ALA:N	4	3.22
(1,4)	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	1:107:A:THR:N	5	3.2
(1,133)	1:186:A:SER:C	1:187:A:SER:N	1:187:A:SER:CA	1:187:A:SER:C	6	3.17
(1,41)	1:132:A:SER:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	2	3.13
(1,133)	1:186:A:SER:C	1:187:A:SER:N	1:187:A:SER:CA	1:187:A:SER:C	5	3.04
(1,66)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:ARG:N	5	3.03
(1,66)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:ARG:N	6	3.0
(1,6)	1:107:A:THR:N	1:107:A:THR:CA	1:107:A:THR:C	1:108:A:ALA:N	7	2.92
(1,4)	1:106:A:ASP:N	1:106:A:ASP:CA	1:106:A:ASP:C	1:107:A:THR:N	4	2.91
(1,120)	1:179:A:ARG:N	1:179:A:ARG:CA	1:179:A:ARG:C	1:180:A:TYR:N	5	2.89
(1,109)	1:173:A:LYS:C	1:174:A:GLU:N	1:174:A:GLU:CA	1:174:A:GLU:C	10	2.88
(1,135)	1:187:A:SER:C	1:188:A:ARG:N	1:188:A:ARG:CA	1:188:A:ARG:C	9	2.85
(1,118)	1:178:A:HIS:N	1:178:A:HIS:CA	1:178:A:HIS:C	1:179:A:ARG:N	7	2.85
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:HIS:N	9	2.85
(1,124)	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	1:182:A:GLU:N	1	2.84
(1,116)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:HIS:N	1	2.84
(1,13)	1:114:A:ARG:C	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	10	2.75
(1,110)	1:174:A:GLU:N	1:174:A:GLU:CA	1:174:A:GLU:C	1:175:A:ARG:N	3	2.69
(1,123)	1:180:A:TYR:C	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	5	2.65
(1,79)	1:158:A:GLN:C	1:159:A:PHE:N	1:159:A:PHE:CA	1:159:A:PHE:C	10	2.63
(1,66)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:ARG:N	7	2.63
(1,124)	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	1:182:A:GLU:N	7	2.6
(1,42)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:LEU:N	1	2.59
(1,122)	1:180:A:TYR:N	1:180:A:TYR:CA	1:180:A:TYR:C	1:181:A:ILE:N	9	2.57
(1,134)	1:187:A:SER:N	1:187:A:SER:CA	1:187:A:SER:C	1:188:A:ARG:N	1	2.56
(1,123)	1:180:A:TYR:C	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	10	2.56
(1,123)	1:180:A:TYR:C	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	4	2.54
(1,22)	1:122:A:CYS:N	1:122:A:CYS:CA	1:122:A:CYS:C	1:123:A:SER:N	8	2.54
(1,118)	1:178:A:HIS:N	1:178:A:HIS:CA	1:178:A:HIS:C	1:179:A:ARG:N	5	2.51
(1,79)	1:158:A:GLN:C	1:159:A:PHE:N	1:159:A:PHE:CA	1:159:A:PHE:C	6	2.51
(1,132)	1:185:A:LYS:N	1:185:A:LYS:CA	1:185:A:LYS:C	1:186:A:SER:N	1	2.49
(1,42)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:LEU:N	2	2.46
(1,8)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	7	2.42
(1,116)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:HIS:N	8	2.39
(1,116)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:HIS:N	9	2.35
(1,133)	1:186:A:SER:C	1:187:A:SER:N	1:187:A:SER:CA	1:187:A:SER:C	2	2.31
(1,6)	1:107:A:THR:N	1:107:A:THR:CA	1:107:A:THR:C	1:108:A:ALA:N	9	2.3
(1,124)	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	1:182:A:GLU:N	9	2.27
(1,18)	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	1:121:A:GLY:N	10	2.25
(1,134)	1:187:A:SER:N	1:187:A:SER:CA	1:187:A:SER:C	1:188:A:ARG:N	2	2.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,133)	1:186:A:SER:C	1:187:A:SER:N	1:187:A:SER:CA	1:187:A:SER:C	7	2.24
(1,41)	1:132:A:SER:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	4	2.23
(1,123)	1:180:A:TYR:C	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	6	2.22
(1,130)	1:184:A:PHE:N	1:184:A:PHE:CA	1:184:A:PHE:C	1:185:A:LYS:N	7	2.2
(1,120)	1:179:A:ARG:N	1:179:A:ARG:CA	1:179:A:ARG:C	1:180:A:TYR:N	10	2.19
(1,118)	1:178:A:HIS:N	1:178:A:HIS:CA	1:178:A:HIS:C	1:179:A:ARG:N	9	2.19
(1,13)	1:114:A:ARG:C	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	2	2.17
(1,118)	1:178:A:HIS:N	1:178:A:HIS:CA	1:178:A:HIS:C	1:179:A:ARG:N	1	2.08
(1,114)	1:176:A:ILE:N	1:176:A:ILE:CA	1:176:A:ILE:C	1:177:A:GLY:N	3	2.08
(1,13)	1:114:A:ARG:C	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	5	2.07
(1,42)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:LEU:N	4	2.04
(1,13)	1:114:A:ARG:C	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	4	2.04
(1,8)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	4	2.02
(1,134)	1:187:A:SER:N	1:187:A:SER:CA	1:187:A:SER:C	1:188:A:ARG:N	9	1.98
(1,123)	1:180:A:TYR:C	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	7	1.98
(1,36)	1:130:A:PHE:N	1:130:A:PHE:CA	1:130:A:PHE:C	1:131:A:PHE:N	2	1.94
(1,41)	1:132:A:SER:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	7	1.91
(1,71)	1:154:A:GLU:C	1:155:A:ALA:N	1:155:A:ALA:CA	1:155:A:ALA:C	4	1.87
(1,59)	1:145:A:VAL:C	1:146:A:ASP:N	1:146:A:ASP:CA	1:146:A:ASP:C	8	1.87
(1,130)	1:184:A:PHE:N	1:184:A:PHE:CA	1:184:A:PHE:C	1:185:A:LYS:N	6	1.8
(1,89)	1:163:A:GLU:C	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	6	1.76
(1,18)	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	1:121:A:GLY:N	5	1.76
(1,66)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:ARG:N	8	1.71
(1,36)	1:130:A:PHE:N	1:130:A:PHE:CA	1:130:A:PHE:C	1:131:A:PHE:N	4	1.71
(1,130)	1:184:A:PHE:N	1:184:A:PHE:CA	1:184:A:PHE:C	1:185:A:LYS:N	10	1.68
(1,127)	1:182:A:GLU:C	1:183:A:ILE:N	1:183:A:ILE:CA	1:183:A:ILE:C	7	1.67
(1,66)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:ARG:N	1	1.67
(1,13)	1:114:A:ARG:C	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	9	1.66
(1,111)	1:174:A:GLU:C	1:175:A:ARG:N	1:175:A:ARG:CA	1:175:A:ARG:C	3	1.58
(1,120)	1:179:A:ARG:N	1:179:A:ARG:CA	1:179:A:ARG:C	1:180:A:TYR:N	1	1.57
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:HIS:N	5	1.54
(1,124)	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	1:182:A:GLU:N	3	1.52
(1,89)	1:163:A:GLU:C	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	2	1.51
(1,122)	1:180:A:TYR:N	1:180:A:TYR:CA	1:180:A:TYR:C	1:181:A:ILE:N	7	1.49
(1,41)	1:132:A:SER:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	6	1.48
(1,66)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:ARG:N	10	1.47
(1,134)	1:187:A:SER:N	1:187:A:SER:CA	1:187:A:SER:C	1:188:A:ARG:N	7	1.39
(1,25)	1:124:A:LYS:C	1:125:A:GLU:N	1:125:A:GLU:CA	1:125:A:GLU:C	7	1.38
(1,8)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	1	1.38
(1,132)	1:185:A:LYS:N	1:185:A:LYS:CA	1:185:A:LYS:C	1:186:A:SER:N	4	1.37
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:HIS:N	4	1.35
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:HIS:N	10	1.33
(1,110)	1:174:A:GLU:N	1:174:A:GLU:CA	1:174:A:GLU:C	1:175:A:ARG:N	6	1.32
(1,80)	1:159:A:PHE:N	1:159:A:PHE:CA	1:159:A:PHE:C	1:160:A:ALA:N	7	1.29
(1,121)	1:179:A:ARG:C	1:180:A:TYR:N	1:180:A:TYR:CA	1:180:A:TYR:C	4	1.27
(1,24)	1:124:A:LYS:N	1:124:A:LYS:CA	1:124:A:LYS:C	1:125:A:GLU:N	4	1.27
(1,118)	1:178:A:HIS:N	1:178:A:HIS:CA	1:178:A:HIS:C	1:179:A:ARG:N	4	1.26
(1,66)	1:149:A:GLY:N	1:149:A:GLY:CA	1:149:A:GLY:C	1:150:A:ARG:N	2	1.26
(1,124)	1:181:A:ILE:N	1:181:A:ILE:CA	1:181:A:ILE:C	1:182:A:GLU:N	5	1.25
(1,18)	1:120:A:PHE:N	1:120:A:PHE:CA	1:120:A:PHE:C	1:121:A:GLY:N	1	1.25
(1,5)	1:106:A:ASP:C	1:107:A:THR:N	1:107:A:THR:CA	1:107:A:THR:C	10	1.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,5)	1:106:A:ASP:C	1:107:A:THR:N	1:107:A:THR:CA	1:107:A:THR:C	3	1.22
(1,110)	1:174:A:GLU:N	1:174:A:GLU:CA	1:174:A:GLU:C	1:175:A:ARG:N	1	1.19
(1,89)	1:163:A:GLU:C	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	4	1.14
(1,89)	1:163:A:GLU:C	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	5	1.14
(1,116)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:HIS:N	3	1.12
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:HIS:N	1	1.12
(1,42)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:LEU:N	5	1.11
(1,110)	1:174:A:GLU:N	1:174:A:GLU:CA	1:174:A:GLU:C	1:175:A:ARG:N	4	1.1
(1,89)	1:163:A:GLU:C	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	7	1.1
(1,109)	1:173:A:LYS:C	1:174:A:GLU:N	1:174:A:GLU:CA	1:174:A:GLU:C	9	1.08
(1,89)	1:163:A:GLU:C	1:164:A:ILE:N	1:164:A:ILE:CA	1:164:A:ILE:C	8	1.05
(1,81)	1:159:A:PHE:C	1:160:A:ALA:N	1:160:A:ALA:CA	1:160:A:ALA:C	10	1.03
(1,64)	1:148:A:GLN:N	1:148:A:GLN:CA	1:148:A:GLN:C	1:149:A:GLY:N	6	1.02
(1,34)	1:129:A:GLN:N	1:129:A:GLN:CA	1:129:A:GLN:C	1:130:A:PHE:N	2	1.02
(1,31)	1:127:A:ILE:C	1:128:A:VAL:N	1:128:A:VAL:CA	1:128:A:VAL:C	7	1.0
(1,8)	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1:113:A:VAL:N	5	1.0