Full wwPDB NMR Structure Validation Report (i)

Apr 29, 2024 – 05:31 PM EDT

PDB ID	:	8SG2
BMRB ID	:	31080
Title	:	BIVALENT INTERACTIONS OF PIN1 WITH THE C-TERMINAL TAIL OF PKC
Authors	:	Dixit, K.; Yang, Y.; Chen, X.R.; Igumenova, T.I.
Deposited on	:	2023-04-11

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

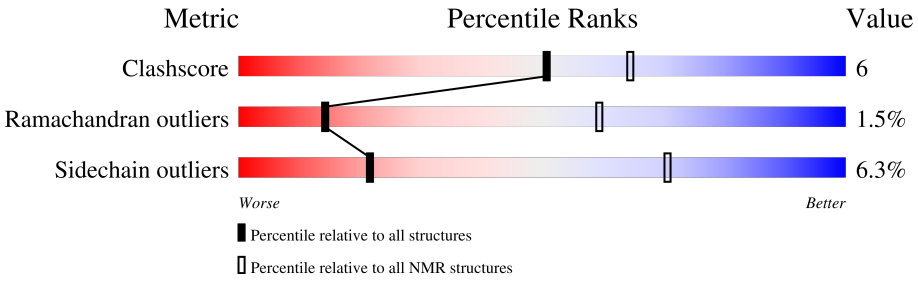
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 80%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	163	80% 8% 12%
2	B	25	40% 32% 28%

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 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:7-A:37, A:52-A:163, B:639-B:640, B:642-B:646, B:650-B:659, B:661-B:661 (161)	1.07	4

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

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

The models can be grouped into 1 clusters and 10 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2902 atoms, of which 1420 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	163	2526	786	1244	239	251	6	0

- Molecule 2 is a protein called Protein kinase C beta type.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	25	376	122	176	30	46	2	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	638	ACE	-	acetylation	UNP P05771
B	662	NH2	-	amidation	UNP P05771

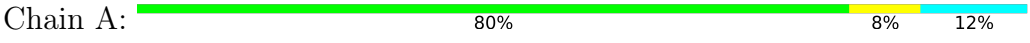
4 Residue-property plots (i)

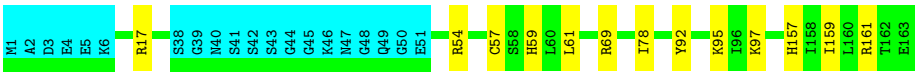
4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

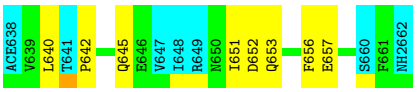
Chain A:





• Molecule 2: Protein kinase C beta type

Chain B:



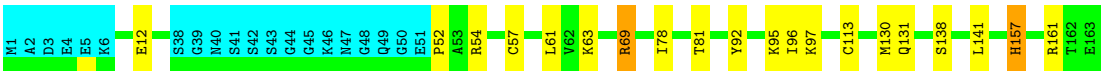
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

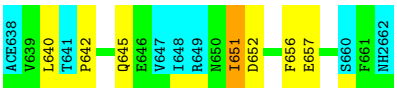
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

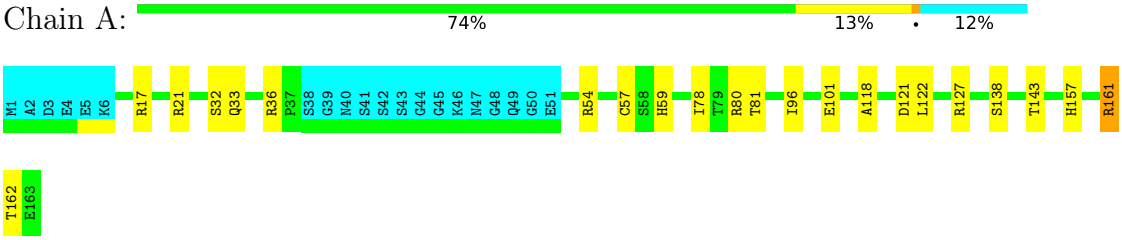
Chain B:



4.2.2 Score per residue for model 2

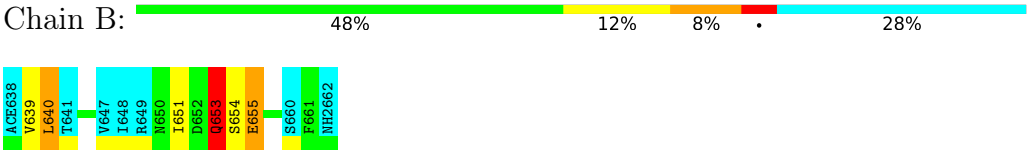
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

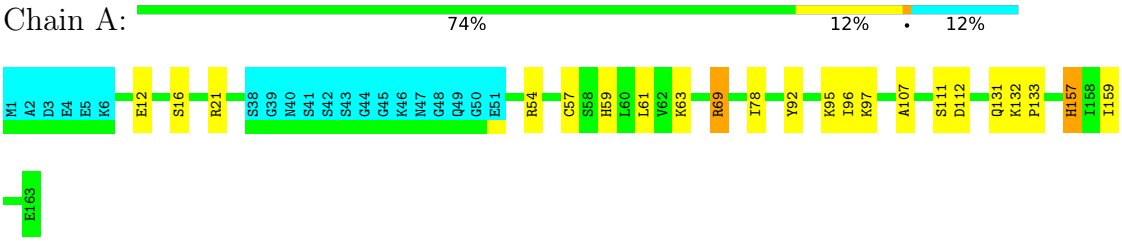
Chain B:



4.2.3 Score per residue for model 3

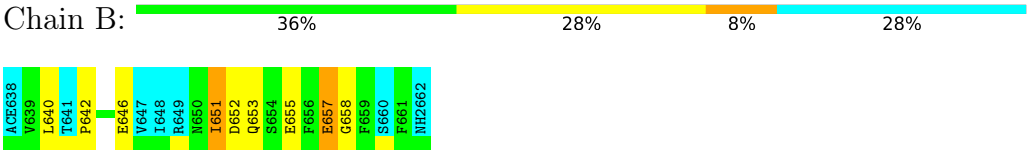
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

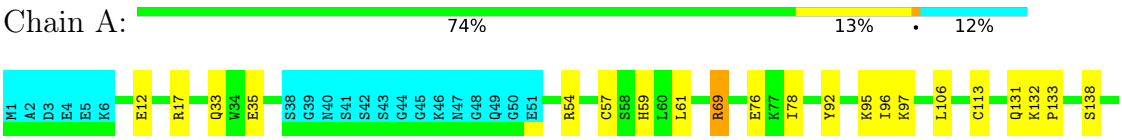
Chain B:



4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

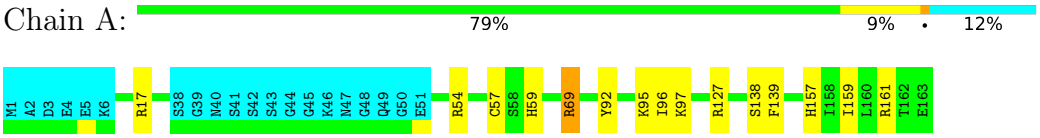
Chain A:



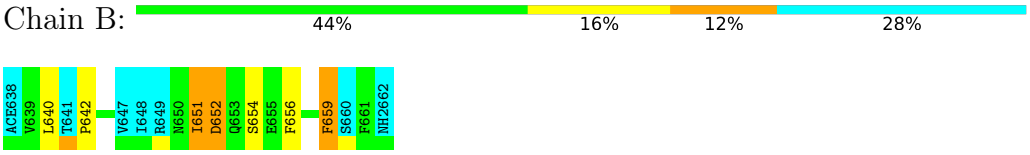
• Molecule 2: Protein kinase C beta type

4.2.5 Score per residue for model 5

• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

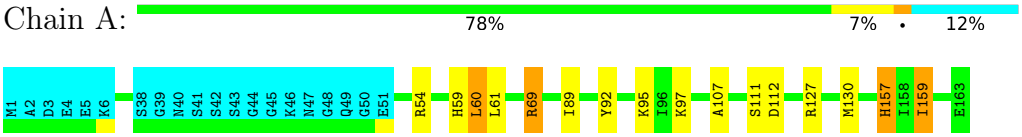


• Molecule 2: Protein kinase C beta type

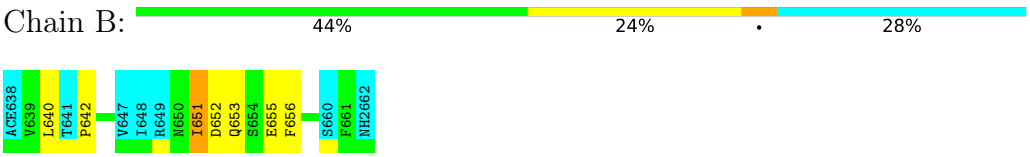


4.2.6 Score per residue for model 6

• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



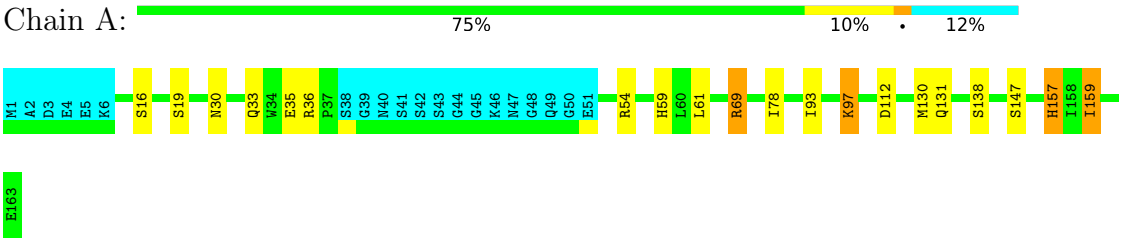
• Molecule 2: Protein kinase C beta type



4.2.7 Score per residue for model 7

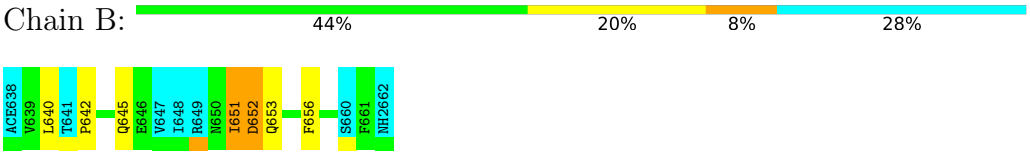
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

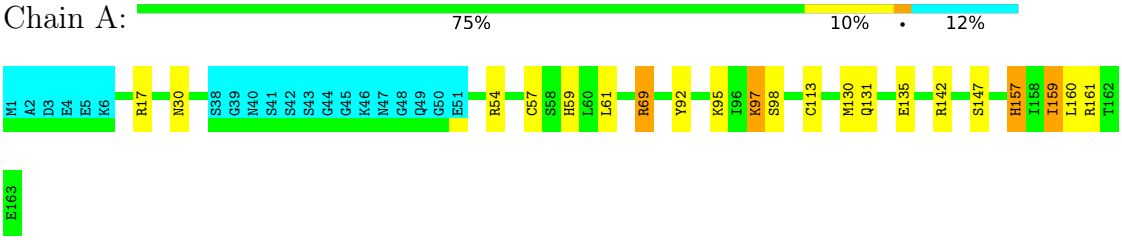
Chain B:



4.2.8 Score per residue for model 8

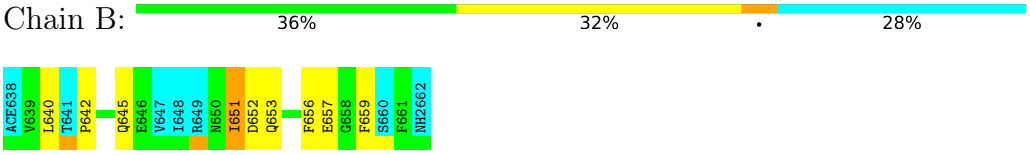
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

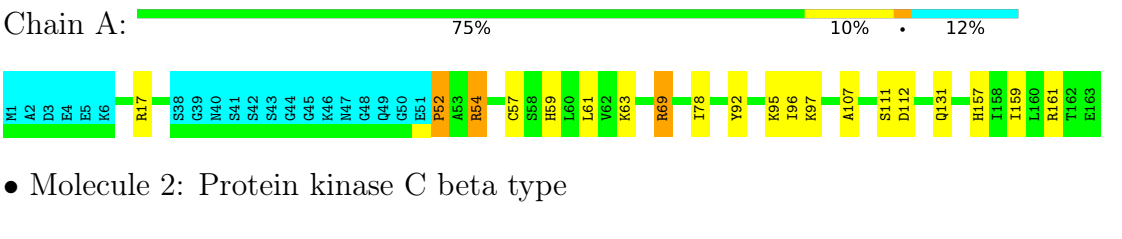
Chain B:



4.2.9 Score per residue for model 9

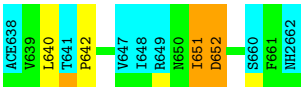
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

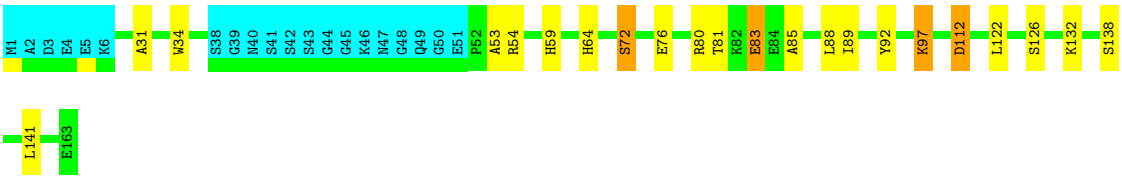
Chain B:



4.2.10 Score per residue for model 10

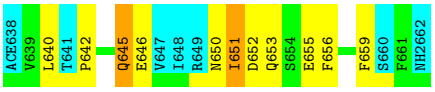
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

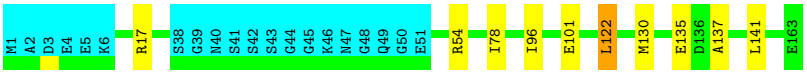
Chain B:



4.2.11 Score per residue for model 11

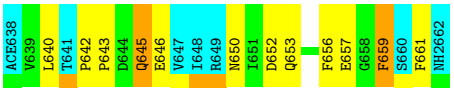
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

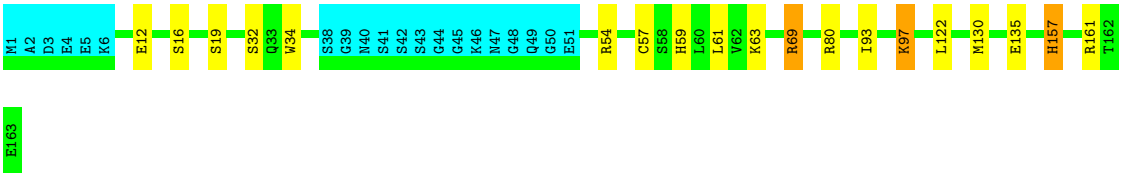
Chain B:



4.2.12 Score per residue for model 12

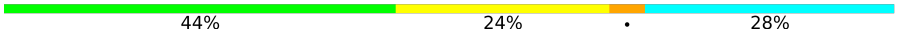
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

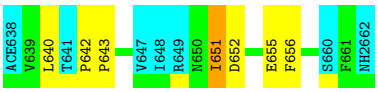
Chain A:



• Molecule 2: Protein kinase C beta type

Chain B:

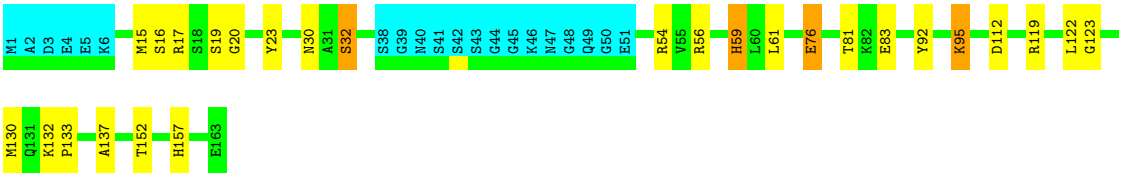




4.2.13 Score per residue for model 13

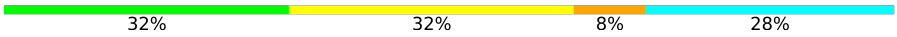
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

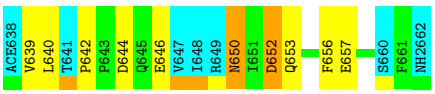
Chain A:



• Molecule 2: Protein kinase C beta type

Chain B:

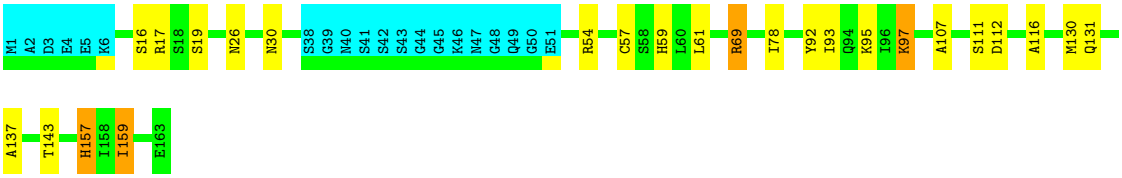




4.2.14 Score per residue for model 14

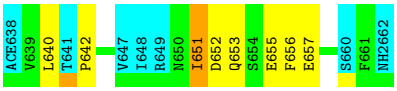
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



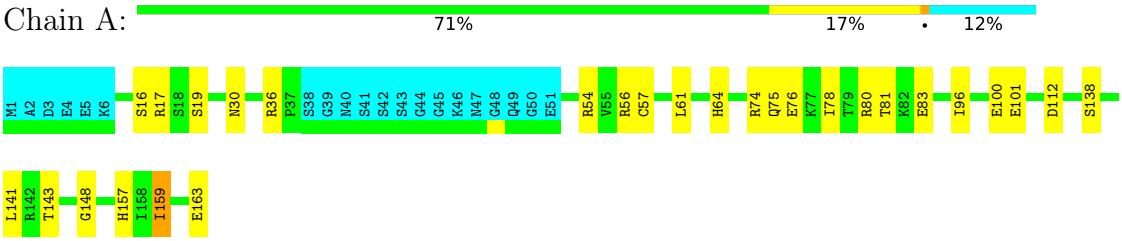
• Molecule 2: Protein kinase C beta type

Chain B:

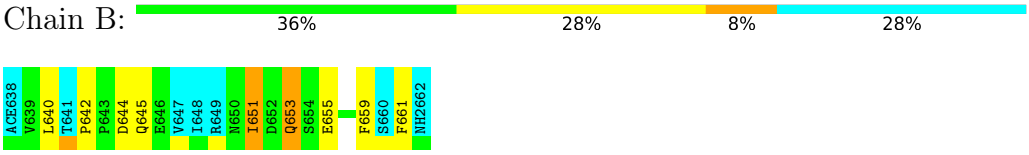


4.2.15 Score per residue for model 15

• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

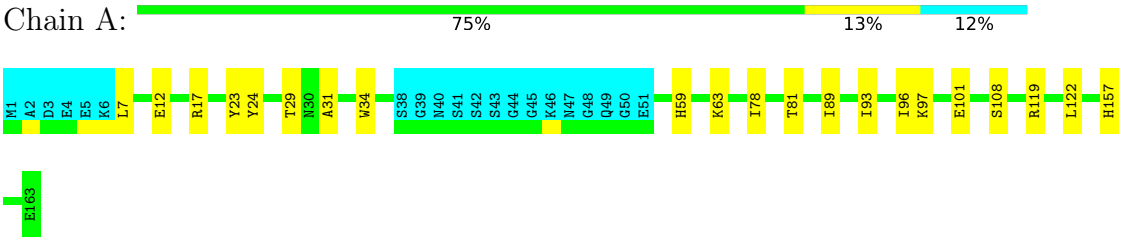


• Molecule 2: Protein kinase C beta type

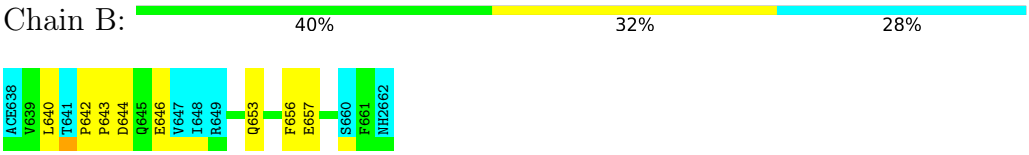


4.2.16 Score per residue for model 16

• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



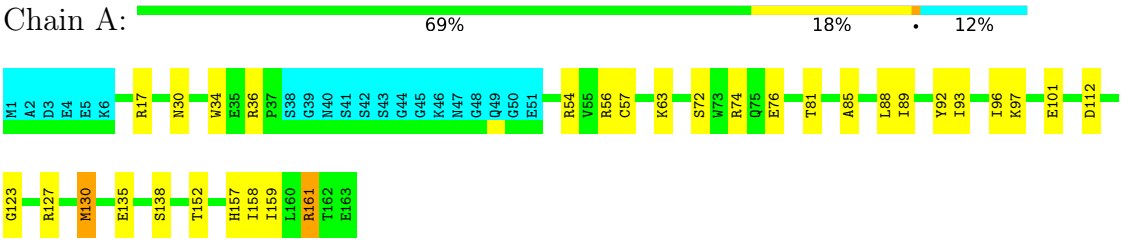
• Molecule 2: Protein kinase C beta type



4.2.17 Score per residue for model 17

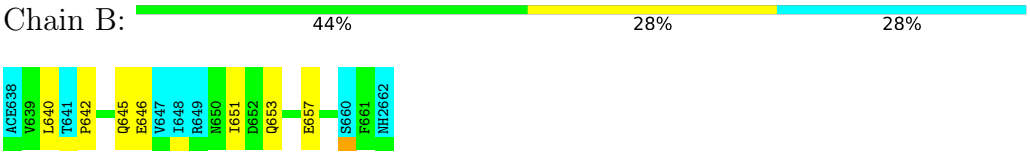
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

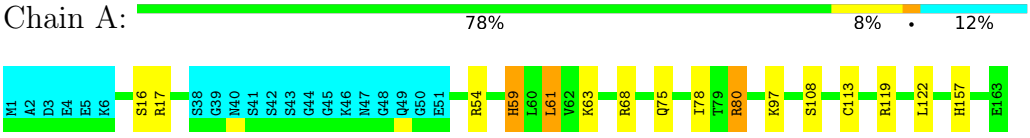
Chain B:



4.2.18 Score per residue for model 18

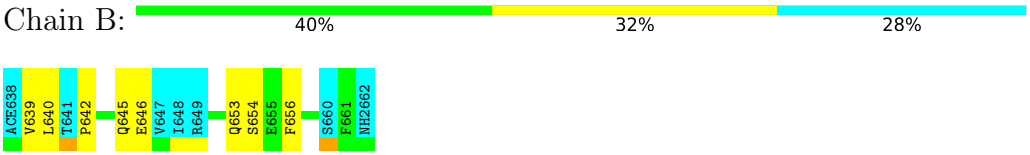
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

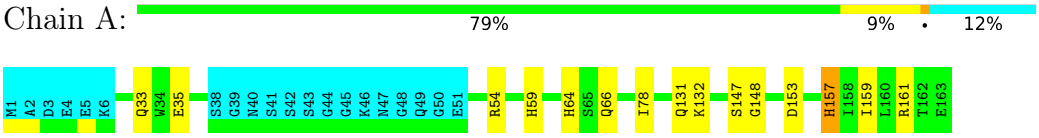
Chain B:



4.2.19 Score per residue for model 19

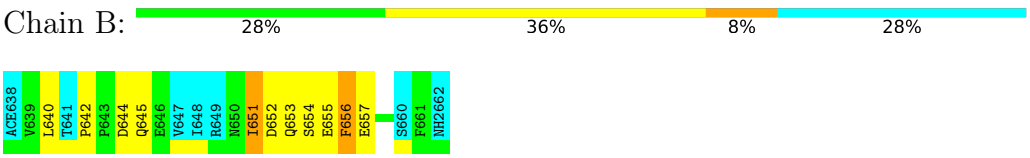
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



• Molecule 2: Protein kinase C beta type

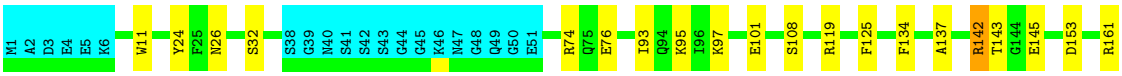
Chain B:



4.2.20 Score per residue for model 20

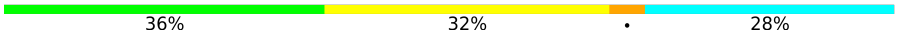
• Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

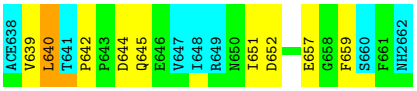
Chain A:



• Molecule 2: Protein kinase C beta type

Chain B:





5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
X-PLOR NIH	refinement	
CYANA	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	2
Total number of shifts	1960
Number of shifts mapped to atoms	1960
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, SEP, TPO, ACE

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1147	1125	1121	12±3
2	B	149	128	128	7±2
All	All	25920	25060	24980	298

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:640:LEU:O	2:B:642:PRO:HD2	0.70	1.85	11	14
2:B:653:GLN:H	2:B:653:GLN:NE2	0.68	1.86	15	1
1:A:61:LEU:HG	1:A:113:CYS:SG	0.65	2.31	18	1
1:A:63:LYS:O	1:A:80:ARG:HD3	0.64	1.93	18	1
1:A:107:ALA:O	1:A:111:SER:HB2	0.62	1.95	14	4
1:A:69:ARG:HD3	1:A:69:ARG:N	0.62	2.10	14	9
1:A:69:ARG:N	1:A:69:ARG:HD3	0.62	2.09	7	1
1:A:31:ALA:HA	2:B:645:GLN:NE2	0.61	2.10	10	1
1:A:92:TYR:HB3	1:A:106:LEU:HD21	0.60	1.71	4	1
1:A:64:HIS:CE1	1:A:66:GLN:HB2	0.60	2.32	19	1
1:A:72:SER:HB3	1:A:112:ASP:OD1	0.59	1.97	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:ILE:HG23	2:B:653:GLN:NE2	0.59	2.12	3	4
1:A:57:CYS:SG	2:B:652:ASP:HB2	0.59	2.38	9	8
2:B:654:SER:HB3	2:B:659:PHE:CE2	0.58	2.33	5	1
2:B:652:ASP:HB3	2:B:656:PHE:CG	0.57	2.34	5	1
1:A:141:LEU:HG	2:B:650:ASN:O	0.57	1.99	10	1
2:B:652:ASP:HA	2:B:656:PHE:CD2	0.57	2.34	19	1
1:A:57:CYS:SG	2:B:651:ILE:HG12	0.57	2.39	2	1
1:A:57:CYS:SG	2:B:651:ILE:HG13	0.56	2.40	15	2
1:A:148:GLY:HA3	2:B:644:ASP:OD2	0.55	2.01	19	1
2:B:652:ASP:HB3	2:B:656:PHE:CD2	0.54	2.36	5	1
1:A:130:MET:HB2	2:B:656:PHE:O	0.54	2.03	13	1
2:B:651:ILE:O	2:B:656:PHE:HB3	0.54	2.02	19	1
1:A:81:THR:HB	1:A:83:GLU:OE2	0.53	2.03	13	2
2:B:645:GLN:NE2	2:B:646:GLU:H	0.53	2.01	10	1
1:A:59:HIS:CG	1:A:122:LEU:HD21	0.53	2.37	16	1
1:A:134:PHE:CG	2:B:652:ASP:HB3	0.53	2.39	20	1
2:B:651:ILE:HG12	2:B:652:ASP:H	0.53	1.62	5	10
1:A:93:ILE:HG21	2:B:644:ASP:HB3	0.53	1.79	20	1
1:A:108:SER:OG	1:A:119:ARG:HA	0.53	2.04	18	2
2:B:640:LEU:C	2:B:642:PRO:HD2	0.53	2.24	15	10
1:A:69:ARG:H	1:A:69:ARG:HD3	0.53	1.63	12	2
1:A:63:LYS:HB2	1:A:78:ILE:HD13	0.52	1.80	16	1
1:A:130:MET:SD	1:A:135:GLU:HA	0.52	2.45	11	3
1:A:34:TRP:CZ2	1:A:97:LYS:HE2	0.52	2.40	12	1
1:A:69:ARG:HD3	1:A:69:ARG:H	0.51	1.64	3	7
1:A:130:MET:HG3	2:B:656:PHE:O	0.51	2.05	6	2
1:A:17:ARG:NH2	2:B:639:VAL:HG21	0.51	2.21	18	1
1:A:132:LYS:HA	1:A:132:LYS:HE2	0.51	1.83	19	1
1:A:92:TYR:O	1:A:95:LYS:HG2	0.51	2.07	9	8
1:A:59:HIS:CD2	1:A:122:LEU:HD21	0.51	2.40	13	1
1:A:127:ARG:HB2	1:A:135:GLU:OE2	0.51	2.06	17	1
1:A:138:SER:HA	2:B:651:ILE:HG13	0.50	1.84	2	1
1:A:74:ARG:HB2	1:A:112:ASP:OD2	0.50	2.06	17	1
1:A:54:ARG:O	1:A:54:ARG:HD2	0.50	2.05	4	2
2:B:651:ILE:HG23	2:B:652:ASP:N	0.50	2.22	12	9
1:A:138:SER:O	2:B:651:ILE:HG13	0.50	2.06	7	1
1:A:72:SER:HB2	1:A:112:ASP:OD1	0.50	2.06	17	1
1:A:143:THR:HG23	1:A:162:THR:O	0.50	2.06	20	2
1:A:131:GLN:CG	2:B:655:GLU:HB3	0.50	2.37	19	1
1:A:61:LEU:O	1:A:112:ASP:HB3	0.50	2.07	7	5
1:A:138:SER:HB3	2:B:651:ILE:HD13	0.50	1.83	17	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:655:GLU:H	2:B:655:GLU:CD	0.49	2.10	2	2
1:A:53:ALA:O	1:A:126:SER:HA	0.49	2.07	10	1
1:A:61:LEU:HD23	1:A:157:HIS:ND1	0.49	2.22	8	3
1:A:157:HIS:CE1	2:B:653:GLN:HG3	0.49	2.42	7	2
1:A:64:HIS:HB2	1:A:80:ARG:O	0.49	2.08	15	2
1:A:30:ASN:O	2:B:645:GLN:HB3	0.49	2.08	15	2
2:B:640:LEU:O	2:B:642:PRO:HD3	0.48	2.08	19	3
1:A:159:ILE:HD12	2:B:651:ILE:HG22	0.48	1.83	7	1
1:A:132:LYS:HA	1:A:132:LYS:CE	0.48	2.38	19	1
1:A:93:ILE:O	1:A:97:LYS:HG3	0.48	2.08	14	3
1:A:127:ARG:HA	1:A:130:MET:SD	0.48	2.49	6	1
2:B:643:PRO:HB2	2:B:645:GLN:OE1	0.47	2.08	11	1
1:A:118:ALA:HB3	1:A:121:ASP:O	0.47	2.09	2	1
1:A:63:LYS:O	1:A:80:ARG:HD2	0.47	2.10	12	1
1:A:61:LEU:HB3	1:A:113:CYS:SG	0.47	2.49	8	3
1:A:61:LEU:HA	1:A:157:HIS:HB3	0.47	1.85	7	4
1:A:127:ARG:HB3	1:A:139:PHE:CE1	0.47	2.44	5	1
1:A:137:ALA:O	2:B:650:ASN:HA	0.47	2.10	11	1
1:A:125:PHE:CZ	2:B:657:GLU:HG3	0.47	2.45	20	1
1:A:96:ILE:HA	1:A:101:GLU:O	0.46	2.09	11	5
1:A:85:ALA:O	1:A:88:LEU:HG	0.46	2.10	10	2
1:A:159:ILE:HG12	2:B:653:GLN:NE2	0.46	2.26	19	2
1:A:95:LYS:HD3	1:A:101:GLU:OE2	0.46	2.10	20	1
1:A:59:HIS:HB3	2:B:653:GLN:CD	0.46	2.31	18	1
1:A:92:TYR:O	1:A:96:ILE:HG13	0.46	2.11	3	5
1:A:130:MET:HA	2:B:656:PHE:O	0.46	2.10	7	4
1:A:33:GLN:HG3	1:A:35:GLU:O	0.46	2.10	19	3
1:A:56:ARG:HD3	1:A:163:GLU:OE2	0.46	2.11	15	1
1:A:23:TYR:HB3	1:A:34:TRP:CZ3	0.45	2.46	16	1
1:A:147:SER:CB	1:A:159:ILE:HG13	0.45	2.42	7	1
2:B:651:ILE:HG12	2:B:652:ASP:N	0.45	2.26	19	1
1:A:63:LYS:CD	1:A:69:ARG:HG2	0.45	2.42	9	1
1:A:57:CYS:SG	1:A:161:ARG:HG2	0.45	2.51	17	2
1:A:32:SER:O	2:B:643:PRO:HA	0.45	2.12	12	1
1:A:138:SER:HA	2:B:651:ILE:HA	0.45	1.89	1	5
1:A:16:SER:HB2	1:A:19:SER:OG	0.45	2.12	14	1
1:A:31:ALA:HA	2:B:644:ASP:O	0.45	2.12	16	1
1:A:132:LYS:N	1:A:133:PRO:HD2	0.44	2.27	3	3
2:B:640:LEU:HD11	2:B:644:ASP:HB2	0.44	1.89	16	1
1:A:60:LEU:HD23	1:A:61:LEU:H	0.44	1.72	6	1
1:A:89:ILE:CD1	1:A:157:HIS:HA	0.44	2.42	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:639:VAL:HG22	2:B:640:LEU:H	0.44	1.72	18	1
1:A:36:ARG:N	1:A:36:ARG:HD2	0.44	2.27	2	1
1:A:147:SER:HB3	1:A:159:ILE:HG13	0.44	1.88	7	1
1:A:24:TYR:O	1:A:32:SER:HA	0.44	2.13	20	1
1:A:34:TRP:CE3	1:A:97:LYS:HE2	0.44	2.48	10	1
1:A:122:LEU:HD22	2:B:656:PHE:CE2	0.44	2.48	12	1
1:A:16:SER:OG	1:A:19:SER:HB3	0.44	2.13	13	2
1:A:23:TYR:CE1	2:B:640:LEU:HB3	0.44	2.48	13	1
1:A:161:ARG:HB2	2:B:651:ILE:CD1	0.43	2.43	1	2
1:A:69:ARG:N	1:A:69:ARG:CD	0.43	2.81	9	2
1:A:122:LEU:HG	2:B:657:GLU:OE2	0.43	2.12	11	1
2:B:657:GLU:HG3	2:B:659:PHE:HB3	0.43	1.90	11	1
1:A:137:ALA:HB1	2:B:650:ASN:O	0.43	2.13	13	1
1:A:142:ARG:HA	1:A:161:ARG:NH1	0.43	2.29	8	1
2:B:657:GLU:CD	2:B:658:GLY:H	0.43	2.17	3	2
1:A:56:ARG:HA	1:A:123:GLY:O	0.43	2.13	13	2
1:A:148:GLY:HA3	2:B:644:ASP:CG	0.43	2.33	15	1
2:B:651:ILE:HG23	2:B:652:ASP:H	0.43	1.73	19	1
1:A:97:LYS:HD2	1:A:98:SER:N	0.43	2.29	8	1
1:A:83:GLU:H	1:A:83:GLU:CD	0.43	2.17	10	1
1:A:89:ILE:HA	1:A:92:TYR:CD1	0.43	2.49	10	2
1:A:132:LYS:C	1:A:132:LYS:HD3	0.43	2.34	13	1
1:A:159:ILE:HG12	2:B:653:GLN:HE21	0.43	1.74	7	1
1:A:57:CYS:CB	1:A:161:ARG:HA	0.43	2.44	9	1
1:A:111:SER:HB3	1:A:116:ALA:HB2	0.43	1.91	14	1
1:A:93:ILE:HD11	1:A:158:ILE:HG21	0.43	1.90	17	1
2:B:652:ASP:O	2:B:653:GLN:HB2	0.43	2.13	11	1
1:A:134:PHE:HA	1:A:137:ALA:HB3	0.43	1.90	20	1
1:A:32:SER:OG	2:B:640:LEU:HD21	0.43	2.14	2	1
1:A:138:SER:HA	2:B:652:ASP:N	0.42	2.28	5	1
1:A:17:ARG:O	1:A:17:ARG:HG3	0.42	2.13	5	1
1:A:159:ILE:CD1	2:B:651:ILE:HG22	0.42	2.44	7	1
1:A:157:HIS:NE2	2:B:652:ASP:OD2	0.42	2.52	13	1
1:A:159:ILE:HG12	2:B:651:ILE:O	0.42	2.14	15	1
1:A:157:HIS:NE2	2:B:653:GLN:HB3	0.42	2.29	19	1
1:A:16:SER:OG	1:A:21:ARG:HB2	0.42	2.14	3	1
1:A:159:ILE:HD13	2:B:651:ILE:HG22	0.42	1.92	19	1
1:A:142:ARG:HD2	1:A:145:GLU:OE2	0.42	2.14	20	1
1:A:32:SER:HB3	2:B:640:LEU:HD22	0.42	1.91	13	1
2:B:657:GLU:CG	2:B:659:PHE:HB3	0.42	2.44	11	1
1:A:158:ILE:C	1:A:159:ILE:HD12	0.42	2.35	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LYS:HD2	1:A:69:ARG:O	0.42	2.15	3	1
1:A:152:THR:OG1	1:A:157:HIS:HE1	0.42	1.97	17	2
1:A:59:HIS:CG	2:B:653:GLN:HE21	0.41	2.33	16	1
1:A:130:MET:N	1:A:130:MET:SD	0.41	2.93	17	1
1:A:157:HIS:N	1:A:157:HIS:CD2	0.41	2.87	12	3
1:A:15:MET:SD	1:A:20:GLY:HA2	0.41	2.55	13	1
1:A:26:ASN:O	1:A:30:ASN:HA	0.41	2.16	14	1
1:A:131:GLN:HG2	2:B:655:GLU:HB3	0.41	1.92	19	1
1:A:74:ARG:HD3	1:A:112:ASP:HA	0.41	1.91	15	1
1:A:89:ILE:O	1:A:93:ILE:HG13	0.41	2.16	16	1
1:A:34:TRP:CD2	1:A:97:LYS:HE2	0.41	2.50	17	1
1:A:108:SER:HB2	1:A:119:ARG:HA	0.41	1.93	20	1
1:A:138:SER:HA	2:B:651:ILE:C	0.41	2.36	1	1
1:A:76:GLU:H	1:A:76:GLU:CD	0.41	2.19	13	1
1:A:157:HIS:HE1	2:B:654:SER:OG	0.41	1.99	2	1
2:B:653:GLN:HA	2:B:656:PHE:CD2	0.41	2.51	13	1
1:A:157:HIS:CD2	2:B:653:GLN:HB2	0.41	2.51	18	1
1:A:63:LYS:HD3	1:A:69:ARG:NE	0.41	2.31	1	1
1:A:7:LEU:HD21	1:A:24:TYR:CD2	0.41	2.50	16	1
1:A:59:HIS:CD2	1:A:122:LEU:HD11	0.41	2.51	2	1
1:A:11:TRP:CD2	1:A:26:ASN:HB2	0.41	2.51	20	1
1:A:137:ALA:O	2:B:651:ILE:HA	0.41	2.16	14	1
1:A:16:SER:HB2	1:A:19:SER:HB3	0.40	1.93	7	1
1:A:54:ARG:C	1:A:54:ARG:HD2	0.40	2.37	9	1
1:A:16:SER:HB2	1:A:19:SER:HB2	0.40	1.93	12	1
1:A:147:SER:HB3	1:A:159:ILE:HD12	0.40	1.92	19	1
1:A:34:TRP:NE1	2:B:643:PRO:HG3	0.40	2.32	16	1
1:A:157:HIS:NE2	2:B:653:GLN:HB2	0.40	2.32	18	1
1:A:59:HIS:HB3	2:B:653:GLN:NE2	0.40	2.32	2	1
1:A:61:LEU:HD22	1:A:157:HIS:ND1	0.40	2.32	3	1
2:B:640:LEU:HD23	2:B:640:LEU:H	0.40	1.77	11	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	142/163 (87%)	135±2 (95±1%)	6±2 (4±1%)	1±1 (1±0%)	32 76
2	B	18/25 (72%)	11±2 (62±10%)	5±1 (29±8%)	2±1 (9±5%)	1 12
All	All	3200/3760 (85%)	2927 (91%)	226 (7%)	47 (1%)	14 59

All 14 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	651	ILE	14
1	A	78	ILE	11
2	B	652	ASP	4
2	B	639	VAL	3
1	A	52	PRO	2
1	A	17	ARG	2
2	B	640	LEU	2
2	B	653	GLN	2
2	B	661	PHE	2
2	B	644	ASP	1
2	B	655	GLU	1
2	B	657	GLU	1
2	B	645	GLN	1
2	B	654	SER	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	124/138 (90%)	117±2 (94±1%)	7±2 (6±1%)	24 73
2	B	17/20 (85%)	15±1 (89±7%)	2±1 (11±7%)	10 54
All	All	2820/3160 (89%)	2642 (94%)	178 (6%)	21 70

All 47 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	54	ARG	16
1	A	97	LYS	14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	157	HIS	13
1	A	59	HIS	13
1	A	69	ARG	10
2	B	657	GLU	8
1	A	131	GLN	7
1	A	159	ILE	7
2	B	655	GLU	6
1	A	76	GLU	6
2	B	659	PHE	6
1	A	12	GLU	5
1	A	81	THR	5
1	A	161	ARG	5
2	B	656	PHE	5
2	B	653	GLN	3
2	B	646	GLU	3
1	A	30	ASN	3
1	A	122	LEU	3
2	B	645	GLN	3
1	A	61	LEU	3
1	A	80	ARG	2
1	A	95	LYS	2
1	A	112	ASP	2
1	A	141	LEU	2
1	A	143	THR	2
1	A	36	ARG	2
1	A	75	GLN	2
1	A	153	ASP	2
1	A	21	ARG	1
1	A	33	GLN	1
1	A	127	ARG	1
1	A	60	LEU	1
1	A	160	LEU	1
1	A	72	SER	1
1	A	83	GLU	1
1	A	132	LYS	1
2	B	652	ASP	1
1	A	32	SER	1
1	A	119	ARG	1
2	B	650	ASN	1
1	A	100	GLU	1
1	A	17	ARG	1
1	A	130	MET	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	B	654	SER	1
1	A	74	ARG	1
1	A	142	ARG	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	TPO	B	641	2	8,10,11	1.57±0.08	1±0 (14±4%)
2	SEP	B	660	2	8,9,10	1.01±0.05	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	TPO	B	641	2	10,14,16	1.65±0.03	4±1 (39±6%)
2	SEP	B	660	2	8,12,14	2.04±0.09	2±0 (25±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	B	660	2	-	0±0,5,8,10	-
2	TPO	B	641	2	-	0±0,9,11,13	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	641	TPO	P-O1P	3.78	1.62	1.50	18	20
2	B	641	TPO	P-O3P	2.09	1.62	1.54	4	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	660	SEP	OG-P-O1P	4.08	117.92	106.47	7	20
2	B	660	SEP	OG-CB-CA	3.54	111.59	108.14	2	20
2	B	641	TPO	O-C-CA	2.60	117.98	124.78	13	20
2	B	641	TPO	O2P-P-OG1	2.59	117.60	105.99	19	20
2	B	641	TPO	O3P-P-O1P	2.45	101.08	110.68	16	20
2	B	641	TPO	O3P-P-O2P	2.31	116.47	107.64	2	15
2	B	641	TPO	OG1-P-O1P	2.05	101.48	109.39	11	3

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping

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

Total number of shifts	1776
Number of shifts mapped to atoms	1776
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	161	-0.27 ± 0.18	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	143	-0.13 ± 0.17	None needed (< 0.5 ppm)
$^{13}C'$	160	-0.05 ± 0.14	None needed (< 0.5 ppm)
^{15}N	153	0.09 ± 0.20	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 74%, i.e. 1623 atoms were assigned a chemical shift out of a possible 2206. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	701/798 (88%)	283/324 (87%)	283/322 (88%)	135/152 (89%)
Sidechain	817/1213 (67%)	534/778 (69%)	258/372 (69%)	25/63 (40%)

Continued on next page...

Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Aromatic	105/195 (54%)	59/96 (61%)	43/88 (49%)	3/11 (27%)
Overall	1623/2206 (74%)	876/1198 (73%)	584/782 (75%)	163/226 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 1776 atoms were assigned a chemical shift out of a possible 2468. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	794/918 (86%)	320/375 (85%)	321/368 (87%)	153/175 (87%)
Sidechain	877/1355 (65%)	570/867 (66%)	281/417 (67%)	26/71 (37%)
Aromatic	105/195 (54%)	59/96 (61%)	43/88 (49%)	3/11 (27%)
Overall	1776/2468 (72%)	949/1338 (71%)	645/873 (74%)	182/257 (71%)

7.1.4 Statistically unusual chemical shifts (i)

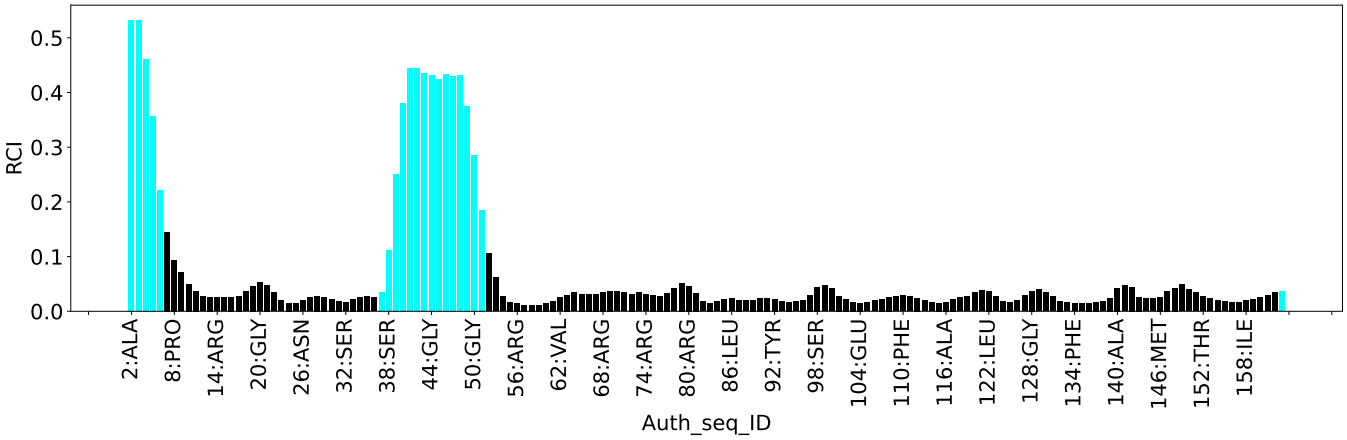
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	26	ASN	HB2	-0.66	1.27 – 4.34	-11.3
1	A	74	ARG	HG3	-0.55	0.15 – 2.94	-7.5
1	A	37	PRO	HG2	-0.03	0.41 – 3.45	-6.4
1	A	14	ARG	HB3	0.08	0.43 – 3.11	-6.3
1	A	26	ASN	HD22	4.24	4.69 – 9.61	-5.9
1	A	74	ARG	HG2	0.03	0.26 – 2.87	-5.9
1	A	109	GLN	HB2	0.77	0.80 – 3.29	-5.1
1	A	55	VAL	HG21	-0.58	-0.58 – 2.19	-5.0
1	A	55	VAL	HG22	-0.58	-0.58 – 2.19	-5.0
1	A	55	VAL	HG23	-0.58	-0.58 – 2.19	-5.0

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_2*

7.2.1 Bookkeeping

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

Total number of shifts	184
Number of shifts mapped to atoms	184
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.2.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.2.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 6%, i.e. 137 atoms were assigned a chemical shift out of a possible 2206. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	41/798 (5%)	33/324 (10%)	5/322 (2%)	3/152 (2%)

Continued on next page...

Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Sidechain	76/1213 (6%)	67/778 (9%)	9/372 (2%)	0/63 (0%)
Aromatic	20/195 (10%)	10/96 (10%)	10/88 (11%)	0/11 (0%)
Overall	137/2206 (6%)	110/1198 (9%)	24/782 (3%)	3/226 (1%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 7%, i.e. 176 atoms were assigned a chemical shift out of a possible 2468. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	51/918 (6%)	39/375 (10%)	7/368 (2%)	5/175 (3%)
Sidechain	105/1355 (8%)	89/867 (10%)	16/417 (4%)	0/71 (0%)
Aromatic	20/195 (10%)	10/96 (10%)	10/88 (11%)	0/11 (0%)
Overall	176/2468 (7%)	138/1338 (10%)	33/873 (4%)	5/257 (2%)

7.2.4 Statistically unusual chemical shifts (i)

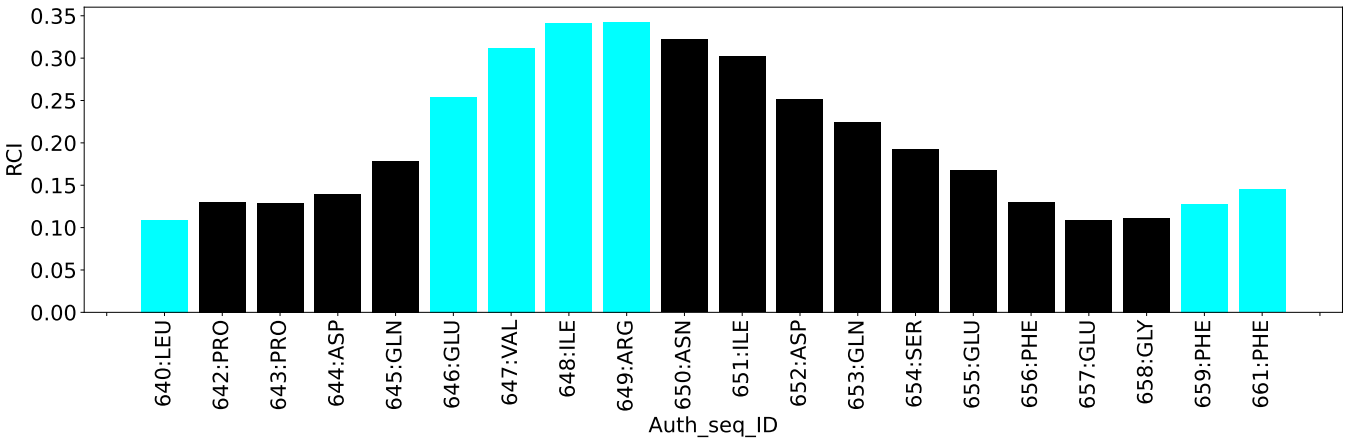
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
2	B	642	PRO	HG3	0.15	0.33 – 3.48	-5.6

7.2.5 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 B:


RCI
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
640:LEU
642:PRO
643:PRO
644:ASP
645:GLN
646:GLU
647:VAL
648:ILE
649:ARG
650:ASN
651:ILE
652:ASP
653:GLN
654:SER
655:GLU
656:PHE
657:GLU
658:GLY
659:PHE
661:PHE
Auth_seq_ID

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	5666
Intra-residue (|i-j|=0)	2179
Sequential (|i-j|=1)	1277
Medium range (|i-j|>1 and |i-j|<5)	732
Long range (|i-j|≥5)	1284
Inter-chain	111
Hydrogen bond restraints	83
Disulfide bond restraints	0
Total dihedral-angle restraints	244
Number of unmapped restraints	0
Number of restraints per residue	31.4
Number of long range restraints per residue[1]	7.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	58.7	0.2
0.2-0.5 (Medium)	130.8	0.5
>0.5 (Large)	75.0	12.07

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)	10.6	5.69
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

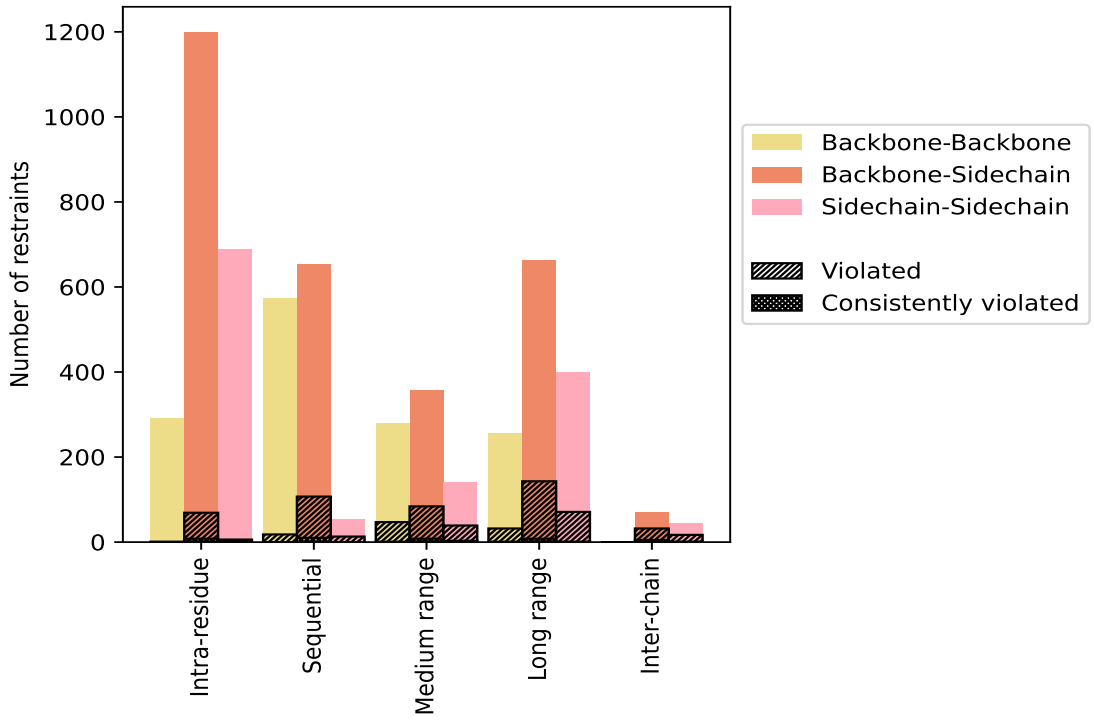
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	2179	38.5	76	3.5	1.3	10	0.5	0.2
Backbone-Backbone	292	5.2	1	0.3	0.0	0	0.0	0.0
Backbone-Sidechain	1199	21.2	69	5.8	1.2	8	0.7	0.1
Sidechain-Sidechain	688	12.1	6	0.9	0.1	2	0.3	0.0
Sequential (|i-j|=1)	1277	22.5	138	10.8	2.4	10	0.8	0.2
Backbone-Backbone	572	10.1	18	3.1	0.3	0	0.0	0.0
Backbone-Sidechain	652	11.5	107	16.4	1.9	10	1.5	0.2
Sidechain-Sidechain	53	0.9	13	24.5	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	732	12.9	154	21.0	2.7	11	1.5	0.2
Backbone-Backbone	280	4.9	47	16.8	0.8	1	0.4	0.0
Backbone-Sidechain	311	5.5	68	21.9	1.2	7	2.3	0.1
Sidechain-Sidechain	141	2.5	39	27.7	0.7	3	2.1	0.1
Long range (|i-j|≥5)	1284	22.7	238	18.5	4.2	10	0.8	0.2
Backbone-Backbone	256	4.5	32	12.5	0.6	1	0.4	0.0
Backbone-Sidechain	629	11.1	135	21.5	2.4	8	1.3	0.1
Sidechain-Sidechain	399	7.0	71	17.8	1.3	1	0.3	0.0
Inter-chain	111	2.0	49	44.1	0.9	6	5.4	0.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	69	1.2	32	46.4	0.6	5	7.2	0.1
Sidechain-Sidechain	42	0.7	17	40.5	0.3	1	2.4	0.0
Hydrogen bond	83	1.5	24	28.9	0.4	1	1.2	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	5666	100.0	679	12.0	12.0	48	0.8	0.8
Backbone-Backbone	1400	24.7	98	7.0	1.7	2	0.1	0.0
Backbone-Sidechain	2940	51.9	435	14.8	7.7	39	1.3	0.7
Sidechain-Sidechain	1326	23.4	146	11.0	2.6	7	0.5	0.1

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	37	52	69	93	24	275	0.47	10.81	0.92	0.37
2	34	52	64	85	23	258	0.46	9.46	0.78	0.38
3	30	56	60	103	26	275	0.47	11.07	0.93	0.37
4	34	49	65	89	24	261	0.47	11.49	0.98	0.37
5	32	61	68	94	25	280	0.46	10.54	0.89	0.37
6	32	50	70	95	28	275	0.47	9.95	0.89	0.4
7	31	59	68	85	20	263	0.46	10.86	0.94	0.36
8	31	58	57	93	24	263	0.47	11.25	0.94	0.36
9	30	53	55	92	27	257	0.49	11.6	0.97	0.37
10	32	47	62	95	26	262	0.47	8.4	0.74	0.4

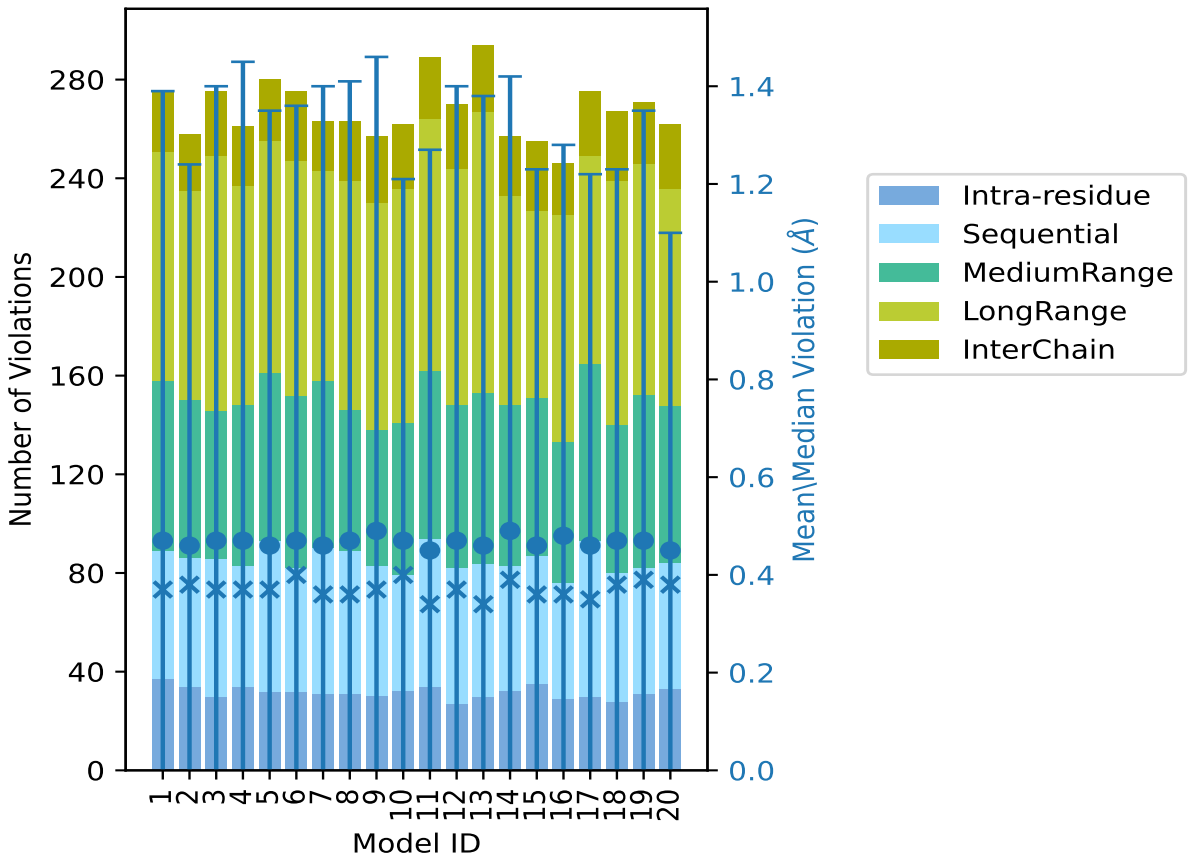
Continued on next page...

Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	34	60	68	102	25	289	0.45	9.85	0.82	0.34
12	27	55	66	96	26	270	0.47	11.26	0.93	0.37
13	30	54	69	114	27	294	0.46	12.07	0.92	0.34
14	32	51	65	85	24	257	0.49	10.51	0.93	0.39
15	35	52	64	76	28	255	0.46	8.88	0.77	0.36
16	29	47	57	92	21	246	0.48	9.24	0.8	0.36
17	30	63	72	84	26	275	0.46	8.86	0.76	0.35
18	28	52	60	99	28	267	0.47	8.25	0.76	0.38
19	31	51	70	94	25	271	0.47	10.5	0.88	0.39
20	33	51	64	88	26	262	0.45	7.35	0.65	0.38

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

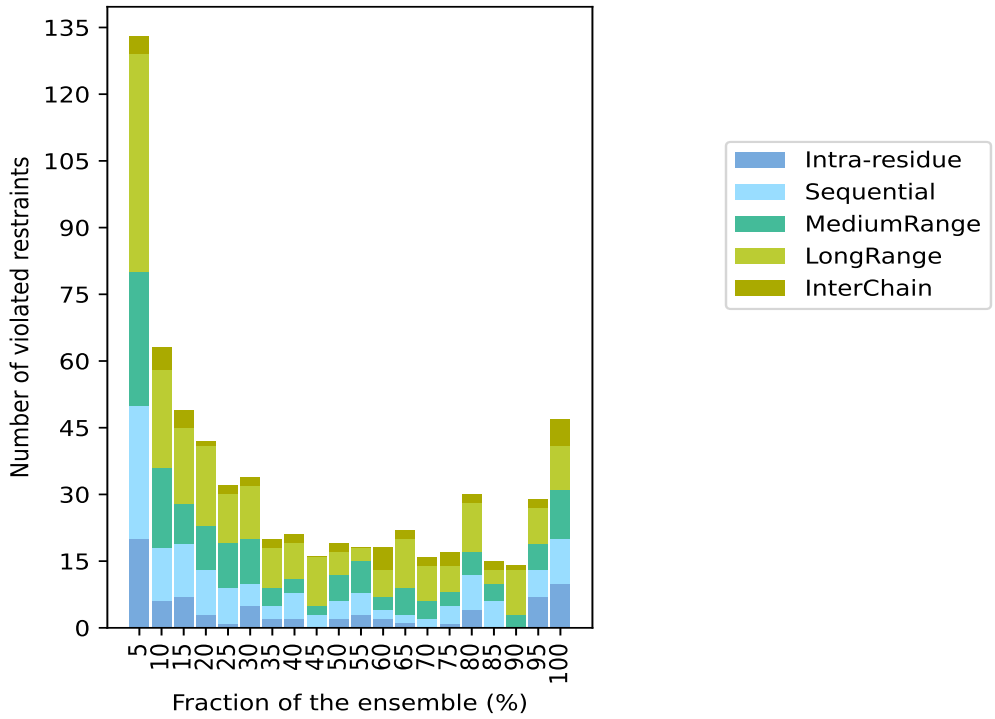
9.3 Distance violation statistics for the ensemble (i)

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, 4928(IR:2103, SQ:1139, MR:578, LR:1046, IC:62) 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]	%
20	30	30	49	4	133	1	5.0
6	12	18	22	5	63	2	10.0
7	12	9	17	4	49	3	15.0
3	10	10	18	1	42	4	20.0
1	8	10	11	2	32	5	25.0
5	5	10	12	2	34	6	30.0
2	3	4	9	2	20	7	35.0
2	6	3	8	2	21	8	40.0
0	3	2	11	0	16	9	45.0
2	4	6	5	2	19	10	50.0
3	5	7	3	0	18	11	55.0
2	2	3	6	5	18	12	60.0
1	2	6	11	2	22	13	65.0
0	2	4	8	2	16	14	70.0
1	4	3	6	3	17	15	75.0
4	8	5	11	2	30	16	80.0
0	6	4	3	2	15	17	85.0
0	0	3	10	1	14	18	90.0
7	6	6	8	2	29	19	95.0
10	10	11	10	6	47	20	100.0

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

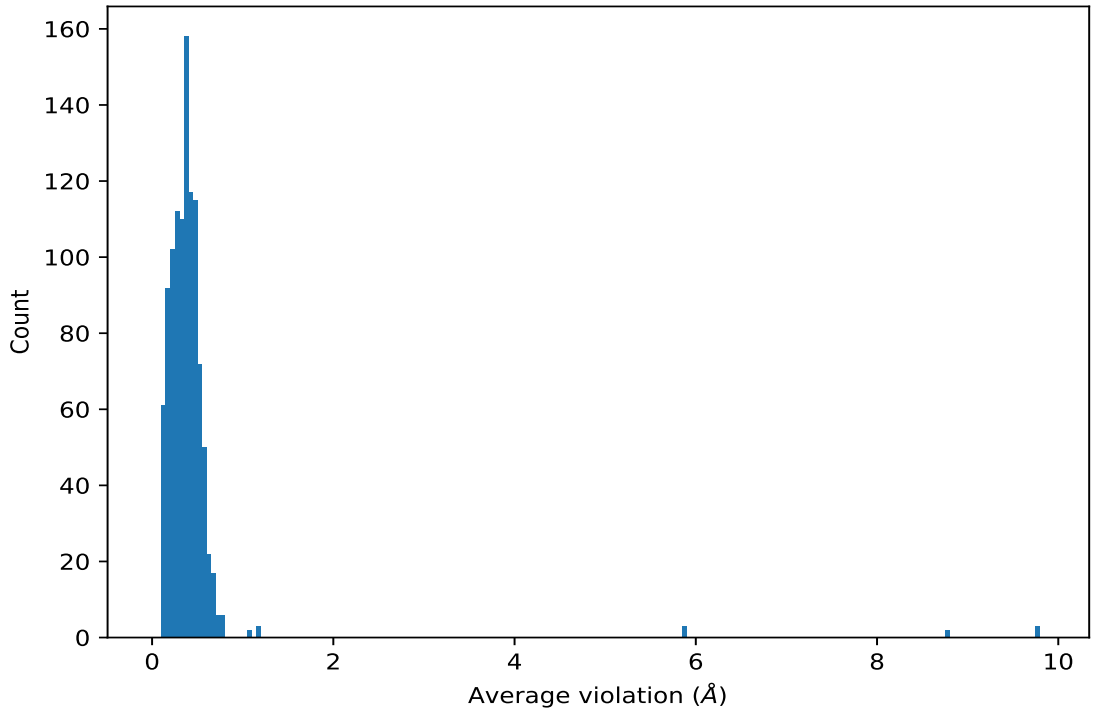
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of theviolation 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)
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	20	9.76	1.66	10.5
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	20	9.76	1.66	10.5
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	20	9.76	1.66	10.5
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	20	8.75	0.86	9.09
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	20	8.75	0.86	9.09
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	20	5.87	0.88	6.39
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	20	5.87	0.88	6.39
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	20	5.87	0.88	6.39
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	20	1.19	0.42	1.18
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	20	1.19	0.42	1.18
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	20	1.19	0.42	1.18
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	20	0.75	0.08	0.75
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	20	0.75	0.08	0.75
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	20	0.75	0.08	0.75
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	20	0.71	0.11	0.72
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	20	0.68	0.04	0.68

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	20	0.64	0.09	0.64
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	20	0.62	0.11	0.66
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	20	0.62	0.22	0.65
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	20	0.56	0.04	0.57
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	20	0.56	0.04	0.57
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	20	0.55	0.12	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	20	0.55	0.03	0.55
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	20	0.55	0.03	0.55
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	20	0.55	0.03	0.55
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	20	0.54	0.04	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	20	0.54	0.04	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	20	0.54	0.04	0.54
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	20	0.54	0.09	0.56
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	20	0.52	0.1	0.55
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	20	0.51	0.05	0.52
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	20	0.51	0.04	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	20	0.51	0.04	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	20	0.51	0.04	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	20	0.5	0.02	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	20	0.5	0.02	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	20	0.5	0.02	0.5
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	20	0.5	0.14	0.46
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	20	0.5	0.06	0.5
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	20	0.5	0.06	0.5
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	20	0.49	0.12	0.52
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	20	0.48	0.11	0.51
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	20	0.48	0.11	0.51
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	20	0.48	0.11	0.51
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	20	0.48	0.05	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	20	0.48	0.05	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	20	0.48	0.05	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	20	0.48	0.05	0.49
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	20	0.48	0.12	0.51
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	20	0.46	0.09	0.48
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	20	0.45	0.04	0.44
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	20	0.45	0.04	0.44
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	20	0.43	0.11	0.49
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	20	0.43	0.11	0.49
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	20	0.43	0.11	0.49
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	20	0.43	0.15	0.51
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	20	0.42	0.07	0.44
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	20	0.42	0.08	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	20	0.37	0.09	0.38
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	20	0.36	0.08	0.38
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	20	0.34	0.05	0.34
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	20	0.34	0.05	0.34
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	20	0.34	0.05	0.34
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	20	0.32	0.08	0.29
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	20	0.31	0.05	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	20	0.31	0.05	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	20	0.31	0.05	0.32
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	20	0.31	0.07	0.3
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	20	0.31	0.07	0.33
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	20	0.3	0.08	0.32
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	20	0.3	0.08	0.32
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	20	0.3	0.08	0.32
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	20	0.28	0.09	0.3
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	20	0.26	0.06	0.29
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	20	0.26	0.09	0.26
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	20	0.26	0.09	0.26
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	20	0.26	0.09	0.26
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	20	0.25	0.01	0.25
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	20	0.23	0.07	0.2
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	20	0.23	0.07	0.2
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	20	0.23	0.07	0.2
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	20	0.2	0.04	0.2
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	20	0.19	0.02	0.18
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	20	0.19	0.02	0.18
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	20	0.19	0.02	0.18
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	20	0.11	0.0	0.11
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	19	0.68	0.17	0.74
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	19	0.62	0.14	0.62
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	19	0.62	0.14	0.62
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	19	0.61	0.11	0.62
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	19	0.61	0.11	0.62
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	19	0.59	0.13	0.63
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	19	0.55	0.09	0.56
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	19	0.55	0.08	0.56
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	19	0.52	0.11	0.55
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	19	0.49	0.09	0.54
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	19	0.47	0.13	0.52
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	19	0.47	0.13	0.52
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	19	0.46	0.1	0.49
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	19	0.44	0.08	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	19	0.44	0.06	0.44
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	19	0.41	0.13	0.39
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	19	0.41	0.04	0.41
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	19	0.41	0.06	0.41
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	19	0.41	0.06	0.41
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	19	0.41	0.12	0.43
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	19	0.41	0.12	0.43
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	19	0.39	0.08	0.39
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	19	0.39	0.08	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	19	0.39	0.08	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	19	0.39	0.08	0.42
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	19	0.38	0.1	0.37
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	19	0.37	0.09	0.38
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	19	0.37	0.09	0.38
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	19	0.37	0.09	0.38
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	19	0.37	0.09	0.38
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	19	0.37	0.09	0.38
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	19	0.35	0.12	0.34
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	19	0.34	0.13	0.34
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	19	0.32	0.1	0.33
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	19	0.28	0.06	0.28
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	19	0.27	0.11	0.3
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	19	0.23	0.08	0.22
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	19	0.18	0.03	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	19	0.18	0.03	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	19	0.18	0.03	0.18
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	19	0.18	0.04	0.19
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	18	0.61	0.07	0.62
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	18	0.56	0.11	0.59
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	18	0.56	0.11	0.59
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	18	0.55	0.19	0.55
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	18	0.55	0.19	0.55
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	18	0.55	0.19	0.55
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	18	0.55	0.19	0.55
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	18	0.55	0.19	0.55
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	18	0.55	0.19	0.55
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	18	0.5	0.17	0.57
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	18	0.5	0.17	0.57
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	18	0.48	0.11	0.52
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	18	0.48	0.11	0.52
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	18	0.48	0.11	0.52
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	18	0.47	0.09	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	18	0.47	0.09	0.49
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	18	0.47	0.09	0.49
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	18	0.45	0.15	0.51
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	18	0.45	0.15	0.51
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	18	0.45	0.15	0.51
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	18	0.45	0.15	0.51
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	18	0.45	0.15	0.51
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	18	0.45	0.15	0.51
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	18	0.4	0.1	0.44
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	18	0.4	0.1	0.44
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	18	0.38	0.16	0.34
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	18	0.38	0.16	0.34
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	18	0.38	0.16	0.34
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	18	0.37	0.07	0.38
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	18	0.33	0.13	0.4
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	18	0.32	0.09	0.32
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	18	0.32	0.13	0.28
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	18	0.18	0.04	0.19
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	17	0.63	0.44	0.49
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	17	0.63	0.44	0.49
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	17	0.63	0.44	0.49
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	17	0.59	0.19	0.66
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	17	0.59	0.19	0.66
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	17	0.59	0.19	0.66
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	17	0.53	0.04	0.54
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	17	0.47	0.04	0.47
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	17	0.47	0.08	0.5
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	17	0.46	0.13	0.5
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	17	0.46	0.13	0.5
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	17	0.46	0.13	0.5
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	17	0.35	0.11	0.36
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	17	0.35	0.11	0.36
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	17	0.35	0.11	0.36
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	17	0.35	0.11	0.39
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	17	0.32	0.12	0.33
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	17	0.31	0.1	0.31
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	17	0.27	0.06	0.27
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	17	0.27	0.06	0.27
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	17	0.27	0.06	0.27
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	17	0.26	0.1	0.25
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	17	0.26	0.1	0.25
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	17	0.24	0.06	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	17	0.22	0.06	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	17	0.22	0.06	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	17	0.22	0.06	0.2
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	17	0.16	0.04	0.15
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	16	0.58	0.03	0.58
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	16	0.56	0.04	0.57
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	16	0.56	0.04	0.57
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	16	0.56	0.04	0.57
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	16	0.55	0.13	0.61
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	16	0.54	0.17	0.61
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	16	0.54	0.17	0.61
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	16	0.54	0.06	0.54
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	16	0.54	0.06	0.54
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	16	0.54	0.06	0.54
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	16	0.53	0.17	0.6
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	16	0.53	0.17	0.6
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	16	0.53	0.17	0.6
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	16	0.53	0.06	0.54
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	16	0.53	0.06	0.54
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	16	0.53	0.06	0.54
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	16	0.52	0.13	0.56
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	16	0.49	0.01	0.49
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	16	0.46	0.12	0.43
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	16	0.46	0.16	0.49
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	16	0.46	0.16	0.49
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	16	0.46	0.16	0.49
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	16	0.44	0.15	0.48
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	16	0.4	0.11	0.44
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	16	0.4	0.11	0.44
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	16	0.4	0.11	0.44
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	16	0.39	0.14	0.36
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	16	0.39	0.14	0.42
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	16	0.39	0.14	0.42
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	16	0.36	0.09	0.36
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	16	0.36	0.14	0.41
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	16	0.36	0.14	0.41
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	16	0.36	0.14	0.41
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	16	0.36	0.12	0.4
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	16	0.36	0.12	0.4
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	16	0.36	0.12	0.4
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	16	0.36	0.12	0.4
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	16	0.36	0.12	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	16	0.36	0.12	0.4
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	16	0.36	0.12	0.4
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	16	0.36	0.12	0.4
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	16	0.36	0.12	0.4
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	16	0.33	0.13	0.3
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	16	0.33	0.13	0.3
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	16	0.33	0.13	0.3
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	16	0.32	0.16	0.34
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	16	0.28	0.16	0.22
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	16	0.27	0.04	0.26
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	16	0.26	0.08	0.26
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	16	0.26	0.08	0.26
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	16	0.26	0.08	0.26
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	16	0.25	0.12	0.23
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	16	0.25	0.1	0.23
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	16	0.25	0.1	0.23
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	16	0.23	0.07	0.19
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	16	0.22	0.08	0.21
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	16	0.22	0.08	0.21
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	16	0.22	0.08	0.21
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	16	0.22	0.08	0.2
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	16	0.19	0.05	0.19
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	16	0.14	0.01	0.14
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	15	0.59	0.09	0.58
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	15	0.59	0.18	0.65
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	15	0.59	0.18	0.65
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	15	0.59	0.18	0.65
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	15	0.56	0.19	0.61
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	15	0.56	0.19	0.61
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	15	0.56	0.19	0.61
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	15	0.51	0.18	0.51
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	15	0.5	0.08	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	15	0.5	0.08	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	15	0.5	0.08	0.53
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	15	0.5	0.14	0.49
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	15	0.48	0.14	0.55
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	15	0.48	0.14	0.55
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	15	0.48	0.14	0.55
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	15	0.47	0.15	0.53
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	15	0.47	0.15	0.53
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	15	0.47	0.15	0.53
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	15	0.42	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)
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	15	0.42	0.17	0.42
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	15	0.41	0.14	0.37
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	15	0.41	0.14	0.37
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	15	0.41	0.14	0.37
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	15	0.36	0.21	0.5
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	15	0.33	0.08	0.34
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	15	0.33	0.15	0.33
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	15	0.33	0.15	0.33
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	15	0.28	0.11	0.29
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	15	0.28	0.11	0.29
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	15	0.28	0.11	0.29
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	15	0.25	0.09	0.24
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	15	0.25	0.09	0.24
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	15	0.25	0.09	0.24
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	15	0.22	0.08	0.19
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	15	0.2	0.08	0.17
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	15	0.16	0.05	0.15
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	14	0.69	0.37	0.64
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	14	0.69	0.37	0.64
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	14	0.69	0.37	0.64
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	14	0.69	0.37	0.64
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	14	0.69	0.37	0.64
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	14	0.69	0.37	0.64
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	14	0.6	0.13	0.6
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	14	0.51	0.16	0.58
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	14	0.45	0.18	0.44
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	14	0.45	0.18	0.44
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	14	0.44	0.13	0.5
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	14	0.41	0.1	0.46
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	14	0.41	0.15	0.45
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	14	0.41	0.15	0.45
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	14	0.41	0.15	0.45
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	14	0.37	0.15	0.32
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	14	0.36	0.17	0.36
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	14	0.36	0.17	0.36
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	14	0.36	0.17	0.36
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	14	0.36	0.13	0.32
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	14	0.36	0.13	0.32
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	14	0.36	0.13	0.32
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	14	0.36	0.13	0.32
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	14	0.36	0.13	0.32
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	14	0.36	0.13	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	14	0.36	0.13	0.32
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	14	0.36	0.13	0.32
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	14	0.36	0.13	0.32
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	14	0.34	0.11	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	14	0.34	0.11	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	14	0.34	0.11	0.38
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	14	0.34	0.11	0.32
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	14	0.3	0.1	0.3
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	14	0.27	0.13	0.22
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	14	0.24	0.12	0.22
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	14	0.21	0.12	0.16
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	13	0.52	0.14	0.57
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	13	0.52	0.14	0.57
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	13	0.49	0.2	0.47
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	13	0.49	0.2	0.47
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	13	0.49	0.2	0.47
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	13	0.47	0.15	0.46
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	13	0.47	0.15	0.46
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	13	0.47	0.15	0.46
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	13	0.43	0.14	0.51
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	13	0.42	0.13	0.49
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	13	0.42	0.13	0.49
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	13	0.42	0.13	0.49
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	13	0.42	0.13	0.49
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	13	0.42	0.13	0.49
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	13	0.42	0.13	0.49
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	13	0.38	0.13	0.42
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	13	0.38	0.22	0.37
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	13	0.36	0.11	0.34
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	13	0.36	0.08	0.38
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	13	0.34	0.12	0.34
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	13	0.34	0.07	0.35
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	13	0.34	0.07	0.35
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	13	0.34	0.07	0.35
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	13	0.33	0.08	0.35
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	13	0.33	0.14	0.34
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	13	0.33	0.14	0.34
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	13	0.33	0.14	0.34
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	13	0.33	0.14	0.34
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	13	0.33	0.14	0.34
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	13	0.33	0.14	0.34
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	13	0.33	0.11	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	13	0.33	0.11	0.32
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	13	0.32	0.18	0.34
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	13	0.32	0.18	0.34
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	13	0.32	0.18	0.34
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	13	0.32	0.15	0.3
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	13	0.31	0.14	0.28
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	13	0.31	0.12	0.33
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	13	0.22	0.07	0.22
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	13	0.19	0.06	0.2
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	13	0.19	0.07	0.16
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	13	0.19	0.07	0.16
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	13	0.19	0.07	0.16
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	13	0.19	0.07	0.16
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	13	0.19	0.07	0.16
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	13	0.19	0.07	0.16
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	13	0.19	0.07	0.16
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	13	0.19	0.07	0.16
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	13	0.19	0.07	0.16
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	13	0.15	0.04	0.14
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	12	0.69	0.12	0.68
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	12	0.69	0.12	0.68
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	12	0.69	0.12	0.68
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	12	0.52	0.09	0.56
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	12	0.48	0.1	0.5
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	12	0.48	0.1	0.5
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	12	0.47	0.11	0.49
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	12	0.47	0.11	0.49
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	12	0.46	0.16	0.42
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	12	0.46	0.16	0.42
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	12	0.45	0.11	0.44
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	12	0.44	0.15	0.46
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	12	0.44	0.12	0.5
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	12	0.44	0.12	0.5
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	12	0.39	0.08	0.43
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	12	0.39	0.08	0.43
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	12	0.39	0.08	0.43
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	12	0.39	0.08	0.43
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	12	0.39	0.08	0.43
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	12	0.39	0.08	0.43
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	12	0.37	0.2	0.32
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	12	0.37	0.2	0.32
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	12	0.37	0.2	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	12	0.36	0.15	0.38
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	12	0.36	0.15	0.38
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	12	0.35	0.14	0.32
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	12	0.35	0.14	0.32
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	12	0.35	0.14	0.32
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	12	0.35	0.11	0.38
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	12	0.35	0.11	0.38
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	12	0.35	0.11	0.38
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	12	0.33	0.07	0.34
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	12	0.26	0.15	0.25
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	12	0.26	0.02	0.26
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	12	0.21	0.07	0.2
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	12	0.18	0.05	0.18
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	12	0.11	0.01	0.11
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	11	0.52	0.06	0.52
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	11	0.46	0.2	0.52
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	11	0.46	0.2	0.52
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	11	0.46	0.2	0.52
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	11	0.46	0.2	0.52
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	11	0.45	0.1	0.46
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	11	0.45	0.1	0.46
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	11	0.45	0.1	0.46
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	11	0.41	0.05	0.41
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	11	0.39	0.21	0.38
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	11	0.38	0.19	0.29
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	11	0.36	0.13	0.38
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	11	0.36	0.13	0.38
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	11	0.36	0.13	0.38
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	11	0.35	0.08	0.38
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	11	0.35	0.14	0.33
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	11	0.35	0.14	0.33
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	11	0.35	0.14	0.33
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	11	0.34	0.11	0.37
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	11	0.32	0.17	0.26
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	11	0.32	0.17	0.26
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	11	0.32	0.17	0.26
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	11	0.3	0.07	0.27
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	11	0.23	0.12	0.22
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	11	0.2	0.05	0.18
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	11	0.18	0.11	0.14
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	11	0.17	0.07	0.13
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	11	0.17	0.05	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	11	0.11	0.01	0.11
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	10	1.08	0.31	1.21
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	10	0.76	0.37	0.62
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	10	0.76	0.37	0.62
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	10	0.73	0.17	0.78
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	10	0.73	0.17	0.78
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	10	0.73	0.17	0.78
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	10	0.73	0.17	0.78
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	10	0.62	0.06	0.64
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	10	0.62	0.06	0.64
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	10	0.62	0.06	0.64
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	10	0.57	0.05	0.58
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	10	0.49	0.19	0.49
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	10	0.48	0.17	0.55
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	10	0.46	0.12	0.5
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	10	0.41	0.13	0.42
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	10	0.41	0.13	0.42
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	10	0.4	0.15	0.45
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	10	0.4	0.15	0.45
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	10	0.4	0.15	0.45
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	10	0.37	0.1	0.38
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	10	0.37	0.1	0.38
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	10	0.37	0.1	0.38
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	10	0.37	0.1	0.38
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	10	0.37	0.1	0.38
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	10	0.37	0.1	0.38
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	10	0.33	0.17	0.28
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	10	0.33	0.17	0.28
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	10	0.28	0.09	0.26
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	10	0.27	0.08	0.29
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	10	0.25	0.07	0.22
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	10	0.25	0.07	0.22
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	10	0.25	0.07	0.22
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	10	0.22	0.1	0.18
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	10	0.2	0.05	0.19
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	10	0.13	0.04	0.12
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	10	0.12	0.02	0.12
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	10	0.12	0.02	0.12
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	9	0.49	0.23	0.59
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	9	0.49	0.23	0.59
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	9	0.49	0.23	0.59
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	9	0.49	0.23	0.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	9	0.49	0.23	0.59
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	9	0.49	0.23	0.59
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	9	0.41	0.16	0.41
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	9	0.41	0.16	0.41
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	9	0.41	0.16	0.41
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	9	0.4	0.15	0.51
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	9	0.39	0.16	0.48
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	9	0.39	0.09	0.38
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	9	0.39	0.09	0.38
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	9	0.35	0.15	0.38
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	9	0.35	0.15	0.38
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	9	0.35	0.15	0.38
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	9	0.35	0.15	0.38
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	9	0.35	0.15	0.38
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	9	0.35	0.15	0.38
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	9	0.35	0.15	0.38
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	9	0.35	0.15	0.38
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	9	0.35	0.15	0.38
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	9	0.35	0.09	0.33
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	9	0.34	0.16	0.3
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	9	0.34	0.16	0.3
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	9	0.34	0.16	0.3
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	9	0.34	0.16	0.3
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	9	0.34	0.16	0.3
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	9	0.34	0.16	0.3
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	9	0.34	0.11	0.38
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	9	0.33	0.14	0.3
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	9	0.33	0.16	0.28
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	9	0.33	0.08	0.33
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	9	0.31	0.16	0.25
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	9	0.31	0.16	0.25
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	9	0.31	0.16	0.25
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	9	0.31	0.06	0.33
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	9	0.22	0.07	0.24
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	9	0.22	0.08	0.19
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	9	0.21	0.07	0.19
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	8	0.63	0.18	0.64
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	8	0.63	0.18	0.64
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	8	0.63	0.18	0.64
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	8	0.56	0.15	0.58
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	8	0.56	0.15	0.58
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	8	0.56	0.15	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	8	0.55	0.02	0.55
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	8	0.55	0.14	0.52
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	8	0.55	0.14	0.52
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	8	0.52	0.16	0.58
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	8	0.48	0.14	0.51
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	8	0.48	0.14	0.51
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	8	0.43	0.12	0.42
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	8	0.43	0.12	0.42
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	8	0.43	0.12	0.42
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	8	0.43	0.15	0.45
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	8	0.43	0.15	0.45
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	8	0.43	0.15	0.45
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	8	0.38	0.13	0.33
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	8	0.37	0.13	0.42
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	8	0.35	0.14	0.38
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	8	0.35	0.14	0.38
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	8	0.32	0.14	0.26
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	8	0.31	0.13	0.26
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	8	0.26	0.14	0.2
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	8	0.24	0.11	0.22
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	8	0.21	0.08	0.19
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	8	0.19	0.06	0.2
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	8	0.19	0.06	0.2
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	8	0.19	0.06	0.2
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	8	0.17	0.04	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	8	0.17	0.04	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	8	0.17	0.04	0.18
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	8	0.15	0.03	0.15
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	8	0.14	0.03	0.13
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	8	0.14	0.03	0.13
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	8	0.14	0.03	0.13
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	8	0.12	0.02	0.12
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	8	0.12	0.02	0.12
(2,88)	1:34:A:TRP:HE1	2:641:B:TPO:H	7	1.05	0.76	0.68
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE1	7	0.58	0.16	0.63
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE2	7	0.58	0.16	0.63
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE1	7	0.58	0.16	0.63
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE2	7	0.58	0.16	0.63
(1,1057)	1:59:A:HIS:H	1:122:A:LEU:HG	7	0.53	0.04	0.54
(1,138)	1:21:A:ARG:HE	1:34:A:TRP:HH2	7	0.5	0.1	0.52
(1,1303)	1:156:A:ILE:HG21	1:157:A:HIS:HD2	7	0.49	0.12	0.54
(1,1303)	1:156:A:ILE:HG22	1:157:A:HIS:HD2	7	0.49	0.12	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1303)	1:156:A:ILE:HG23	1:157:A:HIS:HD2	7	0.49	0.12	0.54
(1,1560)	1:18:A:SER:H	1:18:A:SER:HB3	7	0.44	0.02	0.43
(2,102)	1:135:A:GLU:H	2:656:B:PHE:HB2	7	0.42	0.22	0.38
(1,571)	1:73:A:TRP:HE1	1:74:A:ARG:HB3	7	0.39	0.16	0.42
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE1	7	0.38	0.19	0.51
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE2	7	0.38	0.19	0.51
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE3	7	0.38	0.19	0.51
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE1	7	0.38	0.19	0.51
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE2	7	0.38	0.19	0.51
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE3	7	0.38	0.19	0.51
(2,34)	1:59:A:HIS:H	1:122:A:LEU:HB2	7	0.37	0.19	0.42
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD1	7	0.37	0.12	0.37
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD2	7	0.37	0.12	0.37
(1,1441)	1:162:A:THR:HG21	1:163:A:GLU:HG3	7	0.36	0.19	0.32
(1,1441)	1:162:A:THR:HG22	1:163:A:GLU:HG3	7	0.36	0.19	0.32
(1,1441)	1:162:A:THR:HG23	1:163:A:GLU:HG3	7	0.36	0.19	0.32
(3,9)	1:16:A:SER:O	1:19:A:SER:N	7	0.33	0.09	0.37
(1,129)	1:16:A:SER:HB2	1:21:A:ARG:H	7	0.32	0.12	0.36
(1,1402)	1:143:A:THR:HG21	1:161:A:ARG:HD2	7	0.29	0.16	0.26
(1,1402)	1:143:A:THR:HG22	1:161:A:ARG:HD2	7	0.29	0.16	0.26
(1,1402)	1:143:A:THR:HG23	1:161:A:ARG:HD2	7	0.29	0.16	0.26
(1,1346)	1:148:A:GLY:H	1:159:A:ILE:H	7	0.26	0.1	0.25
(1,28)	1:7:A:LEU:HD21	1:13:A:LYS:HG3	7	0.25	0.11	0.2
(1,28)	1:7:A:LEU:HD22	1:13:A:LYS:HG3	7	0.25	0.11	0.2
(1,28)	1:7:A:LEU:HD23	1:13:A:LYS:HG3	7	0.25	0.11	0.2
(1,654)	1:82:A:LYS:HG2	1:84:A:GLU:H	7	0.22	0.08	0.21
(1,654)	1:82:A:LYS:HG3	1:84:A:GLU:H	7	0.22	0.08	0.21
(1,1703)	1:36:A:ARG:H	1:36:A:ARG:HD2	7	0.19	0.06	0.18
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD1	7	0.19	0.06	0.18
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD2	7	0.19	0.06	0.18
(1,619)	1:78:A:ILE:HB	1:80:A:ARG:H	7	0.17	0.05	0.15
(2,94)	1:93:A:ILE:HG21	2:643:B:PRO:HB3	6	0.49	0.16	0.53
(2,94)	1:93:A:ILE:HG22	2:643:B:PRO:HB3	6	0.49	0.16	0.53
(2,94)	1:93:A:ILE:HG23	2:643:B:PRO:HB3	6	0.49	0.16	0.53
(1,2514)	2:646:B:GLU:HA	2:649:B:ARG:H	6	0.48	0.18	0.48
(1,1410)	1:161:A:ARG:HE	1:163:A:GLU:HG2	6	0.43	0.19	0.5
(1,44)	1:8:A:PRO:HB2	1:11:A:TRP:HE1	6	0.42	0.11	0.47
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB1	6	0.42	0.16	0.38
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB2	6	0.42	0.16	0.38
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB3	6	0.42	0.16	0.38
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD11	6	0.42	0.17	0.49
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD12	6	0.42	0.17	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD13	6	0.42	0.17	0.49
(1,1208)	1:103:A:PHE:HD1	1:146:A:MET:HB2	6	0.42	0.15	0.49
(1,1208)	1:103:A:PHE:HD2	1:146:A:MET:HB2	6	0.42	0.15	0.49
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG21	6	0.41	0.11	0.43
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG22	6	0.41	0.11	0.43
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG23	6	0.41	0.11	0.43
(1,123)	1:15:A:MET:HE1	1:20:A:GLY:H	6	0.4	0.1	0.45
(1,123)	1:15:A:MET:HE2	1:20:A:GLY:H	6	0.4	0.1	0.45
(1,123)	1:15:A:MET:HE3	1:20:A:GLY:H	6	0.4	0.1	0.45
(1,531)	1:64:A:HIS:HE1	1:67:A:SER:HB2	6	0.4	0.17	0.5
(1,401)	1:54:A:ARG:HD2	1:55:A:VAL:HA	6	0.38	0.15	0.32
(1,2209)	1:131:A:GLN:HA	1:131:A:GLN:HE22	6	0.35	0.06	0.34
(1,1276)	1:63:A:LYS:HA	1:155:A:GLY:HA2	6	0.34	0.14	0.3
(3,35)	1:62:A:VAL:N	1:156:A:ILE:O	6	0.33	0.03	0.34
(1,334)	1:27:A:HIS:HA	1:31:A:ALA:H	6	0.32	0.14	0.32
(1,178)	1:23:A:TYR:HE1	1:33:A:GLN:H	6	0.31	0.17	0.21
(1,178)	1:23:A:TYR:HE2	1:33:A:GLN:H	6	0.31	0.17	0.21
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB1	6	0.3	0.14	0.3
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB2	6	0.3	0.14	0.3
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB3	6	0.3	0.14	0.3
(1,695)	1:86:A:LEU:HD21	1:149:A:PRO:HD3	6	0.29	0.14	0.22
(1,695)	1:86:A:LEU:HD22	1:149:A:PRO:HD3	6	0.29	0.14	0.22
(1,695)	1:86:A:LEU:HD23	1:149:A:PRO:HD3	6	0.29	0.14	0.22
(1,1085)	1:56:A:ARG:HE	1:124:A:ALA:H	6	0.28	0.16	0.3
(1,748)	1:87:A:GLU:HA	1:91:A:GLY:H	6	0.27	0.08	0.26
(1,2597)	1:138:A:SER:H	2:656:B:PHE:HB2	6	0.27	0.12	0.25
(1,1456)	1:6:A:LYS:H	1:6:A:LYS:HE2	6	0.26	0.15	0.18
(1,333)	1:25:A:PHE:HA	1:31:A:ALA:H	6	0.24	0.11	0.21
(1,393)	1:53:A:ALA:HB1	1:54:A:ARG:H	6	0.24	0.07	0.23
(1,393)	1:53:A:ALA:HB2	1:54:A:ARG:H	6	0.24	0.07	0.23
(1,393)	1:53:A:ALA:HB3	1:54:A:ARG:H	6	0.24	0.07	0.23
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE1	6	0.22	0.05	0.2
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE2	6	0.22	0.05	0.2
(1,242)	1:10:A:GLY:H	1:26:A:ASN:HD21	6	0.22	0.08	0.2
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD11	6	0.22	0.09	0.23
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD12	6	0.22	0.09	0.23
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD13	6	0.22	0.09	0.23
(1,772)	1:92:A:TYR:H	1:93:A:ILE:HB	6	0.21	0.06	0.23
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG21	6	0.21	0.04	0.2
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG22	6	0.21	0.04	0.2
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG23	6	0.21	0.04	0.2
(1,649)	1:66:A:GLN:HE21	1:82:A:LYS:HB2	6	0.2	0.07	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,63)	1:90:A:ASN:O	1:94:A:GLN:N	6	0.2	0.07	0.19
(1,130)	1:16:A:SER:H	1:21:A:ARG:HA	6	0.19	0.05	0.19
(1,854)	1:98:A:SER:H	1:101:A:GLU:H	6	0.19	0.07	0.16
(1,1571)	1:21:A:ARG:H	1:21:A:ARG:HD2	6	0.18	0.1	0.11
(1,843)	1:97:A:LYS:HB2	1:98:A:SER:H	6	0.13	0.03	0.12
(1,469)	1:60:A:LEU:HB2	1:61:A:LEU:H	6	0.13	0.02	0.12
(1,2529)	2:648:B:ILE:HG21	2:649:B:ARG:HD2	5	0.62	0.08	0.61
(1,2529)	2:648:B:ILE:HG22	2:649:B:ARG:HD2	5	0.62	0.08	0.61
(1,2529)	2:648:B:ILE:HG23	2:649:B:ARG:HD2	5	0.62	0.08	0.61
(2,66)	2:645:B:GLN:H	2:648:B:ILE:H	5	0.6	0.17	0.56
(2,5)	1:23:A:TYR:H	1:34:A:TRP:HZ3	5	0.55	0.13	0.61
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG12	5	0.54	0.14	0.59
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG13	5	0.54	0.14	0.59
(1,1504)	1:13:A:LYS:H	1:13:A:LYS:HE2	5	0.51	0.03	0.52
(1,1313)	1:156:A:ILE:HA	1:157:A:HIS:HD2	5	0.51	0.06	0.51
(1,1054)	1:59:A:HIS:HD2	1:122:A:LEU:H	5	0.49	0.18	0.59
(1,2513)	2:646:B:GLU:HA	2:649:B:ARG:HD2	5	0.47	0.25	0.5
(1,1184)	1:140:A:ALA:H	1:141:A:LEU:HG	5	0.45	0.24	0.6
(1,1280)	1:64:A:HIS:HD2	1:156:A:ILE:HG12	5	0.43	0.12	0.45
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE1	5	0.4	0.16	0.43
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE2	5	0.4	0.16	0.43
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE1	5	0.4	0.16	0.43
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE2	5	0.4	0.16	0.43
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE1	5	0.4	0.16	0.43
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE2	5	0.4	0.16	0.43
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG21	5	0.35	0.14	0.3
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG22	5	0.35	0.14	0.3
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG23	5	0.35	0.14	0.3
(1,1399)	1:143:A:THR:H	1:161:A:ARG:HD2	5	0.35	0.09	0.37
(1,514)	1:63:A:LYS:HB2	1:70:A:PRO:HA	5	0.29	0.12	0.27
(1,1242)	1:150:A:VAL:HG11	1:157:A:HIS:H	5	0.27	0.11	0.23
(1,1242)	1:150:A:VAL:HG12	1:157:A:HIS:H	5	0.27	0.11	0.23
(1,1242)	1:150:A:VAL:HG13	1:157:A:HIS:H	5	0.27	0.11	0.23
(1,116)	1:16:A:SER:H	1:20:A:GLY:HA2	5	0.27	0.14	0.22
(1,2506)	2:644:B:ASP:H	2:645:B:GLN:HA	5	0.26	0.08	0.3
(1,1141)	1:130:A:MET:HB2	1:134:A:PHE:H	5	0.25	0.1	0.22
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD1	5	0.25	0.11	0.19
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD2	5	0.25	0.11	0.19
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE1	5	0.24	0.1	0.25
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE2	5	0.24	0.1	0.25
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE3	5	0.24	0.1	0.25
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG21	5	0.23	0.13	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG22	5	0.23	0.13	0.2
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG23	5	0.23	0.13	0.2
(1,2517)	2:646:B:GLU:HG2	2:647:B:VAL:H	5	0.21	0.06	0.17
(1,373)	1:34:A:TRP:HD1	1:35:A:GLU:H	5	0.21	0.1	0.16
(3,10)	1:16:A:SER:O	1:19:A:SER:H	5	0.2	0.08	0.21
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG21	5	0.2	0.06	0.18
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG22	5	0.2	0.06	0.18
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG23	5	0.2	0.06	0.18
(1,1178)	1:137:A:ALA:HA	1:141:A:LEU:H	5	0.19	0.05	0.18
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE1	5	0.19	0.06	0.16
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE2	5	0.19	0.06	0.16
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE3	5	0.19	0.06	0.16
(1,278)	1:26:A:ASN:HB2	1:30:A:ASN:H	5	0.19	0.08	0.18
(1,205)	1:24:A:TYR:H	1:33:A:GLN:HG2	5	0.17	0.04	0.15
(1,921)	1:106:A:LEU:H	1:109:A:GLN:H	5	0.17	0.05	0.16
(1,750)	1:88:A:LEU:H	1:91:A:GLY:H	5	0.16	0.03	0.17
(1,378)	1:33:A:GLN:H	1:35:A:GLU:H	5	0.13	0.03	0.13
(1,878)	1:102:A:ASP:H	1:103:A:PHE:H	5	0.12	0.01	0.12
(3,27)	1:56:A:ARG:N	1:163:A:GLU:O	4	0.78	0.42	0.77
(1,833)	1:94:A:GLN:HE21	1:97:A:LYS:HG2	4	0.66	0.02	0.65
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG21	4	0.56	0.13	0.62
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG22	4	0.56	0.13	0.62
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG23	4	0.56	0.13	0.62
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD11	4	0.55	0.05	0.54
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD12	4	0.55	0.05	0.54
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD13	4	0.55	0.05	0.54
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE1	4	0.54	0.01	0.54
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE2	4	0.54	0.01	0.54
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE3	4	0.54	0.01	0.54
(1,814)	1:94:A:GLN:HG2	1:95:A:LYS:H	4	0.53	0.04	0.53
(1,1328)	1:89:A:ILE:HG12	1:158:A:ILE:HB	4	0.52	0.01	0.52
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG21	4	0.51	0.22	0.58
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG22	4	0.51	0.22	0.58
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG23	4	0.51	0.22	0.58
(1,693)	1:86:A:LEU:HD21	1:149:A:PRO:HD2	4	0.47	0.02	0.48
(1,693)	1:86:A:LEU:HD22	1:149:A:PRO:HD2	4	0.47	0.02	0.48
(1,693)	1:86:A:LEU:HD23	1:149:A:PRO:HD2	4	0.47	0.02	0.48
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB2	4	0.46	0.16	0.5
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB3	4	0.46	0.16	0.5
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB2	4	0.46	0.16	0.5
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB3	4	0.46	0.16	0.5
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB2	4	0.46	0.16	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB3	4	0.46	0.16	0.5
(1,440)	1:59:A:HIS:H	1:115:A:SER:HB3	4	0.46	0.17	0.53
(1,640)	1:65:A:SER:HB3	1:81:A:THR:HA	4	0.45	0.14	0.43
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE1	4	0.42	0.19	0.49
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE2	4	0.42	0.19	0.49
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE1	4	0.42	0.21	0.44
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE2	4	0.42	0.21	0.44
(1,2022)	1:94:A:GLN:H	1:94:A:GLN:HG2	4	0.4	0.05	0.39
(1,1027)	1:118:A:ALA:HA	1:119:A:ARG:HG2	4	0.4	0.09	0.36
(1,1231)	1:149:A:PRO:HG2	1:150:A:VAL:H	4	0.39	0.16	0.48
(1,1429)	1:143:A:THR:HG21	1:163:A:GLU:HB2	4	0.38	0.09	0.36
(1,1429)	1:143:A:THR:HG22	1:163:A:GLU:HB2	4	0.38	0.09	0.36
(1,1429)	1:143:A:THR:HG23	1:163:A:GLU:HB2	4	0.38	0.09	0.36
(1,2532)	2:648:B:ILE:HG21	2:650:B:ASN:H	4	0.37	0.2	0.37
(1,2532)	2:648:B:ILE:HG22	2:650:B:ASN:H	4	0.37	0.2	0.37
(1,2532)	2:648:B:ILE:HG23	2:650:B:ASN:H	4	0.37	0.2	0.37
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG21	4	0.37	0.07	0.39
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG22	4	0.37	0.07	0.39
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG23	4	0.37	0.07	0.39
(1,181)	1:23:A:TYR:HB2	1:34:A:TRP:HE3	4	0.33	0.16	0.35
(1,1406)	1:147:A:SER:H	1:161:A:ARG:H	4	0.32	0.17	0.3
(1,549)	1:70:A:PRO:HG2	1:71:A:SER:H	4	0.32	0.13	0.32
(1,520)	1:64:A:HIS:HE1	1:66:A:GLN:HG2	4	0.31	0.16	0.28
(1,2510)	2:645:B:GLN:H	2:647:B:VAL:H	4	0.3	0.1	0.28
(1,1428)	1:143:A:THR:HG21	1:163:A:GLU:H	4	0.28	0.14	0.26
(1,1428)	1:143:A:THR:HG22	1:163:A:GLU:H	4	0.28	0.14	0.26
(1,1428)	1:143:A:THR:HG23	1:163:A:GLU:H	4	0.28	0.14	0.26
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD1	4	0.28	0.13	0.24
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD2	4	0.28	0.13	0.24
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD21	4	0.27	0.12	0.24
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD22	4	0.27	0.12	0.24
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD23	4	0.27	0.12	0.24
(3,65)	1:91:A:GLY:O	1:95:A:LYS:N	4	0.26	0.06	0.27
(1,103)	1:14:A:ARG:HG2	1:15:A:MET:H	4	0.26	0.03	0.26
(1,1078)	1:122:A:LEU:HG	1:123:A:GLY:H	4	0.25	0.12	0.18
(1,1031)	1:118:A:ALA:HB1	1:121:A:ASP:HB2	4	0.24	0.11	0.18
(1,1031)	1:118:A:ALA:HB2	1:121:A:ASP:HB2	4	0.24	0.11	0.18
(1,1031)	1:118:A:ALA:HB3	1:121:A:ASP:HB2	4	0.24	0.11	0.18
(1,1424)	1:55:A:VAL:HG21	1:163:A:GLU:H	4	0.24	0.04	0.23
(1,1424)	1:55:A:VAL:HG22	1:163:A:GLU:H	4	0.24	0.04	0.23
(1,1424)	1:55:A:VAL:HG23	1:163:A:GLU:H	4	0.24	0.04	0.23
(1,1424)	1:55:A:VAL:HG11	1:163:A:GLU:H	4	0.24	0.04	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1424)	1:55:A:VAL:HG12	1:163:A:GLU:H	4	0.24	0.04	0.23
(1,1424)	1:55:A:VAL:HG13	1:163:A:GLU:H	4	0.24	0.04	0.23
(1,740)	1:89:A:ILE:HG12	1:90:A:ASN:H	4	0.23	0.03	0.22
(3,45)	1:70:A:PRO:O	1:78:A:ILE:N	4	0.22	0.08	0.2
(3,47)	1:81:A:THR:O	1:85:A:ALA:N	4	0.2	0.04	0.2
(1,121)	1:17:A:ARG:HB2	1:18:A:SER:H	4	0.2	0.14	0.12
(1,978)	1:107:A:ALA:HB1	1:111:A:SER:HA	4	0.2	0.07	0.16
(1,978)	1:107:A:ALA:HB2	1:111:A:SER:HA	4	0.2	0.07	0.16
(1,978)	1:107:A:ALA:HB3	1:111:A:SER:HA	4	0.2	0.07	0.16
(1,737)	1:86:A:LEU:HB3	1:90:A:ASN:H	4	0.19	0.06	0.16
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE1	4	0.18	0.02	0.18
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE2	4	0.18	0.02	0.18
(1,510)	1:62:A:VAL:HG11	1:156:A:ILE:H	4	0.18	0.05	0.16
(1,510)	1:62:A:VAL:HG12	1:156:A:ILE:H	4	0.18	0.05	0.16
(1,510)	1:62:A:VAL:HG13	1:156:A:ILE:H	4	0.18	0.05	0.16
(1,2383)	1:163:A:GLU:H	1:163:A:GLU:HB2	4	0.15	0.02	0.15
(1,20)	1:7:A:LEU:HD11	1:11:A:TRP:H	4	0.14	0.02	0.13
(1,20)	1:7:A:LEU:HD12	1:11:A:TRP:H	4	0.14	0.02	0.13
(1,20)	1:7:A:LEU:HD13	1:11:A:TRP:H	4	0.14	0.02	0.13
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE1	4	0.12	0.03	0.11
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE2	4	0.12	0.03	0.11
(1,265)	1:26:A:ASN:H	1:27:A:HIS:H	4	0.12	0.02	0.12
(1,165)	1:22:A:VAL:H	1:23:A:TYR:H	4	0.12	0.02	0.11
(1,88)	1:12:A:GLU:HB2	1:14:A:ARG:HE	3	0.66	0.05	0.69
(1,88)	1:12:A:GLU:HB3	1:14:A:ARG:HE	3	0.66	0.05	0.69
(1,606)	1:75:A:GLN:HE22	1:78:A:ILE:HA	3	0.53	0.2	0.62
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG21	3	0.53	0.03	0.51
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG22	3	0.53	0.03	0.51
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG23	3	0.53	0.03	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG21	3	0.53	0.03	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG22	3	0.53	0.03	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG23	3	0.53	0.03	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG21	3	0.53	0.03	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG22	3	0.53	0.03	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG23	3	0.53	0.03	0.51
(1,2596)	1:137:A:ALA:HB1	2:651:B:ILE:HG12	3	0.5	0.18	0.54
(1,2596)	1:137:A:ALA:HB1	2:651:B:ILE:HG13	3	0.5	0.18	0.54
(1,2596)	1:137:A:ALA:HB2	2:651:B:ILE:HG12	3	0.5	0.18	0.54
(1,2596)	1:137:A:ALA:HB2	2:651:B:ILE:HG13	3	0.5	0.18	0.54
(1,2596)	1:137:A:ALA:HB3	2:651:B:ILE:HG12	3	0.5	0.18	0.54
(1,2596)	1:137:A:ALA:HB3	2:651:B:ILE:HG13	3	0.5	0.18	0.54
(3,28)	1:56:A:ARG:H	1:163:A:GLU:O	3	0.49	0.23	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,224)	1:14:A:ARG:HE	1:25:A:PHE:HB3	3	0.43	0.11	0.39
(1,480)	1:61:A:LEU:HD21	1:156:A:ILE:H	3	0.42	0.15	0.44
(1,480)	1:61:A:LEU:HD22	1:156:A:ILE:H	3	0.42	0.15	0.44
(1,480)	1:61:A:LEU:HD23	1:156:A:ILE:H	3	0.42	0.15	0.44
(1,384)	1:7:A:LEU:HD21	1:36:A:ARG:HA	3	0.41	0.21	0.55
(1,384)	1:7:A:LEU:HD22	1:36:A:ARG:HA	3	0.41	0.21	0.55
(1,384)	1:7:A:LEU:HD23	1:36:A:ARG:HA	3	0.41	0.21	0.55
(1,16)	1:6:A:LYS:HE2	1:7:A:LEU:H	3	0.41	0.14	0.45
(1,471)	1:61:A:LEU:HD21	1:63:A:LYS:HA	3	0.4	0.1	0.45
(1,471)	1:61:A:LEU:HD22	1:63:A:LYS:HA	3	0.4	0.1	0.45
(1,471)	1:61:A:LEU:HD23	1:63:A:LYS:HA	3	0.4	0.1	0.45
(1,479)	1:61:A:LEU:HD21	1:155:A:GLY:H	3	0.39	0.16	0.3
(1,479)	1:61:A:LEU:HD22	1:155:A:GLY:H	3	0.39	0.16	0.3
(1,479)	1:61:A:LEU:HD23	1:155:A:GLY:H	3	0.39	0.16	0.3
(2,55)	1:150:A:VAL:HG21	1:158:A:ILE:HA	3	0.38	0.17	0.31
(2,55)	1:150:A:VAL:HG22	1:158:A:ILE:HA	3	0.38	0.17	0.31
(2,55)	1:150:A:VAL:HG23	1:158:A:ILE:HA	3	0.38	0.17	0.31
(1,844)	1:97:A:LYS:HG2	1:98:A:SER:H	3	0.37	0.16	0.47
(2,68)	2:649:B:ARG:HD2	2:650:B:ASN:H	3	0.37	0.09	0.41
(2,108)	1:140:A:ALA:HB1	2:649:B:ARG:HA	3	0.36	0.2	0.3
(2,108)	1:140:A:ALA:HB2	2:649:B:ARG:HA	3	0.36	0.2	0.3
(2,108)	1:140:A:ALA:HB3	2:649:B:ARG:HA	3	0.36	0.2	0.3
(1,917)	1:105:A:SER:HB2	1:106:A:LEU:H	3	0.34	0.06	0.32
(1,385)	1:24:A:TYR:HD1	1:36:A:ARG:H	3	0.33	0.06	0.32
(1,385)	1:24:A:TYR:HD2	1:36:A:ARG:H	3	0.33	0.06	0.32
(1,1143)	1:130:A:MET:HB2	1:135:A:GLU:H	3	0.33	0.12	0.31
(2,107)	1:140:A:ALA:HB1	2:651:B:ILE:HA	3	0.32	0.24	0.2
(2,107)	1:140:A:ALA:HB2	2:651:B:ILE:HA	3	0.32	0.24	0.2
(2,107)	1:140:A:ALA:HB3	2:651:B:ILE:HA	3	0.32	0.24	0.2
(1,87)	1:13:A:LYS:HG3	1:14:A:ARG:H	3	0.32	0.21	0.21
(3,25)	1:55:A:VAL:N	1:125:A:PHE:O	3	0.3	0.05	0.31
(1,211)	1:24:A:TYR:HE1	1:36:A:ARG:HD2	3	0.29	0.09	0.32
(1,211)	1:24:A:TYR:HE2	1:36:A:ARG:HD2	3	0.29	0.09	0.32
(1,576)	1:73:A:TRP:HE1	1:115:A:SER:H	3	0.29	0.07	0.28
(1,1910)	1:82:A:LYS:H	1:82:A:LYS:HE2	3	0.27	0.12	0.2
(1,1152)	1:135:A:GLU:HG2	1:136:A:ASP:H	3	0.27	0.06	0.23
(1,2589)	1:122:A:LEU:HD21	2:656:B:PHE:HE1	3	0.27	0.11	0.29
(1,2589)	1:122:A:LEU:HD21	2:656:B:PHE:HE2	3	0.27	0.11	0.29
(1,2589)	1:122:A:LEU:HD22	2:656:B:PHE:HE1	3	0.27	0.11	0.29
(1,2589)	1:122:A:LEU:HD22	2:656:B:PHE:HE2	3	0.27	0.11	0.29
(1,2589)	1:122:A:LEU:HD23	2:656:B:PHE:HE1	3	0.27	0.11	0.29
(1,2589)	1:122:A:LEU:HD23	2:656:B:PHE:HE2	3	0.27	0.11	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,362)	1:11:A:TRP:HH2	1:33:A:GLN:HE21	3	0.27	0.1	0.22
(1,923)	1:106:A:LEU:HA	1:110:A:PHE:H	3	0.25	0.13	0.2
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG21	3	0.25	0.07	0.29
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG22	3	0.25	0.07	0.29
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG23	3	0.25	0.07	0.29
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG21	3	0.25	0.07	0.29
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG22	3	0.25	0.07	0.29
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG23	3	0.25	0.07	0.29
(1,2527)	2:646:B:GLU:H	2:648:B:ILE:H	3	0.24	0.12	0.21
(1,354)	1:24:A:TYR:H	1:32:A:SER:HB3	3	0.24	0.1	0.29
(1,634)	1:80:A:ARG:HB2	1:81:A:THR:H	3	0.23	0.07	0.21
(1,17)	1:6:A:LYS:HB3	1:7:A:LEU:H	3	0.23	0.05	0.2
(1,1700)	1:36:A:ARG:H	1:36:A:ARG:HG2	3	0.22	0.06	0.18
(1,751)	1:89:A:ILE:HG21	1:91:A:GLY:H	3	0.19	0.03	0.17
(1,751)	1:89:A:ILE:HG22	1:91:A:GLY:H	3	0.19	0.03	0.17
(1,751)	1:89:A:ILE:HG23	1:91:A:GLY:H	3	0.19	0.03	0.17
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB1	3	0.19	0.09	0.14
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB2	3	0.19	0.09	0.14
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB3	3	0.19	0.09	0.14
(1,692)	1:86:A:LEU:HG	1:90:A:ASN:HD22	3	0.18	0.04	0.16
(1,1384)	1:159:A:ILE:HD11	1:160:A:LEU:H	3	0.17	0.0	0.17
(1,1384)	1:159:A:ILE:HD12	1:160:A:LEU:H	3	0.17	0.0	0.17
(1,1384)	1:159:A:ILE:HD13	1:160:A:LEU:H	3	0.17	0.0	0.17
(1,143)	1:15:A:MET:HA	1:22:A:VAL:H	3	0.16	0.03	0.18
(1,523)	1:64:A:HIS:HE1	1:66:A:GLN:H	3	0.16	0.05	0.13
(1,2386)	1:163:A:GLU:H	1:163:A:GLU:HG2	3	0.16	0.05	0.15
(1,383)	1:34:A:TRP:H	1:35:A:GLU:HB3	3	0.16	0.02	0.16
(1,367)	1:24:A:TYR:HD1	1:34:A:TRP:H	3	0.15	0.03	0.16
(1,367)	1:24:A:TYR:HD2	1:34:A:TRP:H	3	0.15	0.03	0.16
(1,805)	1:93:A:ILE:HG21	1:94:A:GLN:H	3	0.14	0.03	0.15
(1,805)	1:93:A:ILE:HG22	1:94:A:GLN:H	3	0.14	0.03	0.15
(1,805)	1:93:A:ILE:HG23	1:94:A:GLN:H	3	0.14	0.03	0.15
(1,2074)	1:104:A:GLU:H	1:104:A:GLU:HG2	3	0.14	0.05	0.11
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG21	3	0.13	0.02	0.13
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG22	3	0.13	0.02	0.13
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG23	3	0.13	0.02	0.13
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD11	3	0.13	0.03	0.12
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD12	3	0.13	0.03	0.12
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD13	3	0.13	0.03	0.12
(1,926)	1:60:A:LEU:HD11	1:107:A:ALA:H	3	0.13	0.02	0.11
(1,926)	1:60:A:LEU:HD12	1:107:A:ALA:H	3	0.13	0.02	0.11
(1,926)	1:60:A:LEU:HD13	1:107:A:ALA:H	3	0.13	0.02	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1547)	1:15:A:MET:H	1:15:A:MET:HB2	3	0.12	0.02	0.12
(1,586)	1:73:A:TRP:HB3	1:74:A:ARG:H	3	0.12	0.01	0.11
(4,1958)	1:75:A:GLN:HB2	1:75:A:GLN:HE21	3	0.11	0.0	0.11
(4,1958)	1:75:A:GLN:HB2	1:75:A:GLN:HE22	3	0.11	0.0	0.11
(1,897)	1:104:A:GLU:HG2	1:108:A:SER:H	2	0.72	0.0	0.72
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG21	2	0.68	0.44	0.68
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG22	2	0.68	0.44	0.68
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG23	2	0.68	0.44	0.68
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD21	2	0.48	0.01	0.48
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD22	2	0.48	0.01	0.48
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD23	2	0.48	0.01	0.48
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD21	2	0.48	0.01	0.48
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD22	2	0.48	0.01	0.48
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD23	2	0.48	0.01	0.48
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD21	2	0.48	0.01	0.48
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD22	2	0.48	0.01	0.48
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD23	2	0.48	0.01	0.48
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD21	2	0.48	0.01	0.48
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD22	2	0.48	0.01	0.48
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD23	2	0.48	0.01	0.48
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD11	2	0.45	0.12	0.45
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD12	2	0.45	0.12	0.45
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD13	2	0.45	0.12	0.45
(1,612)	1:75:A:GLN:HE21	1:78:A:ILE:HA	2	0.45	0.14	0.45
(1,646)	1:81:A:THR:HG21	1:84:A:GLU:HB2	2	0.43	0.1	0.43
(1,646)	1:81:A:THR:HG22	1:84:A:GLU:HB2	2	0.43	0.1	0.43
(1,646)	1:81:A:THR:HG23	1:84:A:GLU:HB2	2	0.43	0.1	0.43
(1,2553)	2:651:B:ILE:HG21	2:653:B:GLN:HE21	2	0.43	0.15	0.43
(1,2553)	2:651:B:ILE:HG21	2:653:B:GLN:HE22	2	0.43	0.15	0.43
(1,2553)	2:651:B:ILE:HG22	2:653:B:GLN:HE21	2	0.43	0.15	0.43
(1,2553)	2:651:B:ILE:HG22	2:653:B:GLN:HE22	2	0.43	0.15	0.43
(1,2553)	2:651:B:ILE:HG23	2:653:B:GLN:HE21	2	0.43	0.15	0.43
(1,2553)	2:651:B:ILE:HG23	2:653:B:GLN:HE22	2	0.43	0.15	0.43
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB1	2	0.42	0.13	0.42
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB2	2	0.42	0.13	0.42
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB3	2	0.42	0.13	0.42
(1,2538)	2:649:B:ARG:H	2:650:B:ASN:HD21	2	0.41	0.19	0.41
(2,101)	1:129:A:GLN:HE21	2:657:B:GLU:HB2	2	0.4	0.24	0.4
(2,101)	1:129:A:GLN:HE21	2:657:B:GLU:HB3	2	0.4	0.24	0.4
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB1	2	0.4	0.04	0.4
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB2	2	0.4	0.04	0.4
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB3	2	0.4	0.04	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2590)	1:122:A:LEU:HD21	2:656:B:PHE:HD1	2	0.38	0.04	0.38
(1,2590)	1:122:A:LEU:HD21	2:656:B:PHE:HD2	2	0.38	0.04	0.38
(1,2590)	1:122:A:LEU:HD22	2:656:B:PHE:HD1	2	0.38	0.04	0.38
(1,2590)	1:122:A:LEU:HD22	2:656:B:PHE:HD2	2	0.38	0.04	0.38
(1,2590)	1:122:A:LEU:HD23	2:656:B:PHE:HD1	2	0.38	0.04	0.38
(1,2590)	1:122:A:LEU:HD23	2:656:B:PHE:HD2	2	0.38	0.04	0.38
(3,33)	1:60:A:LEU:N	1:158:A:ILE:O	2	0.38	0.01	0.38
(1,1378)	1:147:A:SER:H	1:160:A:LEU:H	2	0.38	0.19	0.38
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD11	2	0.36	0.12	0.36
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD12	2	0.36	0.12	0.36
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD13	2	0.36	0.12	0.36
(1,1355)	1:57:A:CYS:HB2	1:160:A:LEU:H	2	0.36	0.16	0.36
(2,91)	1:57:A:CYS:H	2:651:B:ILE:HG12	2	0.36	0.26	0.36
(2,91)	1:57:A:CYS:H	2:651:B:ILE:HG13	2	0.36	0.26	0.36
(1,125)	1:15:A:MET:HA	1:21:A:ARG:H	2	0.34	0.22	0.34
(1,2251)	1:141:A:LEU:H	1:141:A:LEU:HG	2	0.32	0.01	0.32
(1,188)	1:13:A:LYS:HG2	1:24:A:TYR:HE1	2	0.32	0.14	0.32
(1,188)	1:13:A:LYS:HG2	1:24:A:TYR:HE2	2	0.32	0.14	0.32
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG21	2	0.32	0.22	0.32
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG22	2	0.32	0.22	0.32
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG23	2	0.32	0.22	0.32
(1,901)	1:103:A:PHE:H	1:105:A:SER:H	2	0.3	0.01	0.3
(1,1435)	1:161:A:ARG:HG3	1:163:A:GLU:H	2	0.3	0.2	0.3
(1,1403)	1:144:A:GLY:H	1:161:A:ARG:HG2	2	0.3	0.1	0.3
(1,1525)	1:14:A:ARG:H	1:14:A:ARG:HE	2	0.3	0.1	0.3
(1,1309)	1:150:A:VAL:HB	1:157:A:HIS:H	2	0.3	0.15	0.3
(1,1000)	1:113:A:CYS:H	1:116:A:ALA:H	2	0.29	0.07	0.29
(1,475)	1:61:A:LEU:HD11	1:113:A:CYS:H	2	0.29	0.11	0.29
(1,475)	1:61:A:LEU:HD12	1:113:A:CYS:H	2	0.29	0.11	0.29
(1,475)	1:61:A:LEU:HD13	1:113:A:CYS:H	2	0.29	0.11	0.29
(1,475)	1:61:A:LEU:HD21	1:113:A:CYS:H	2	0.29	0.11	0.29
(1,475)	1:61:A:LEU:HD22	1:113:A:CYS:H	2	0.29	0.11	0.29
(1,475)	1:61:A:LEU:HD23	1:113:A:CYS:H	2	0.29	0.11	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD21	2	0.29	0.0	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD22	2	0.29	0.0	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD23	2	0.29	0.0	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD11	2	0.29	0.0	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD12	2	0.29	0.0	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD13	2	0.29	0.0	0.29
(2,105)	1:138:A:SER:H	2:656:B:PHE:HD1	2	0.28	0.08	0.28
(2,105)	1:138:A:SER:H	2:656:B:PHE:HD2	2	0.28	0.08	0.28
(1,81)	1:12:A:GLU:H	1:14:A:ARG:H	2	0.26	0.14	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,21)	1:73:A:TRP:HE1	1:74:A:ARG:HG3	2	0.26	0.05	0.26
(1,1066)	1:122:A:LEU:HD21	1:125:A:PHE:HD1	2	0.26	0.06	0.26
(1,1066)	1:122:A:LEU:HD21	1:125:A:PHE:HD2	2	0.26	0.06	0.26
(1,1066)	1:122:A:LEU:HD22	1:125:A:PHE:HD1	2	0.26	0.06	0.26
(1,1066)	1:122:A:LEU:HD22	1:125:A:PHE:HD2	2	0.26	0.06	0.26
(1,1066)	1:122:A:LEU:HD23	1:125:A:PHE:HD1	2	0.26	0.06	0.26
(1,1066)	1:122:A:LEU:HD23	1:125:A:PHE:HD2	2	0.26	0.06	0.26
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD21	2	0.24	0.06	0.24
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD22	2	0.24	0.06	0.24
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD23	2	0.24	0.06	0.24
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD21	2	0.24	0.06	0.24
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD22	2	0.24	0.06	0.24
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD23	2	0.24	0.06	0.24
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD21	2	0.24	0.06	0.24
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD22	2	0.24	0.06	0.24
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD23	2	0.24	0.06	0.24
(1,223)	1:14:A:ARG:HB2	1:25:A:PHE:H	2	0.24	0.12	0.24
(1,599)	1:70:A:PRO:HB2	1:78:A:ILE:H	2	0.24	0.12	0.24
(3,39)	1:64:A:HIS:O	1:67:A:SER:N	2	0.23	0.05	0.23
(1,540)	1:67:A:SER:HA	1:69:A:ARG:H	2	0.22	0.06	0.22
(3,49)	1:82:A:LYS:O	1:86:A:LEU:N	2	0.22	0.0	0.22
(1,825)	1:96:A:ILE:HD11	1:106:A:LEU:HG	2	0.22	0.04	0.22
(1,825)	1:96:A:ILE:HD12	1:106:A:LEU:HG	2	0.22	0.04	0.22
(1,825)	1:96:A:ILE:HD13	1:106:A:LEU:HG	2	0.22	0.04	0.22
(1,1500)	1:12:A:GLU:H	1:12:A:GLU:HB2	2	0.22	0.02	0.22
(1,2302)	1:151:A:PHE:H	1:151:A:PHE:HE1	2	0.2	0.03	0.2
(1,2302)	1:151:A:PHE:H	1:151:A:PHE:HE2	2	0.2	0.03	0.2
(1,84)	1:13:A:LYS:HG2	1:14:A:ARG:H	2	0.2	0.09	0.2
(1,1029)	1:118:A:ALA:H	1:121:A:ASP:H	2	0.2	0.04	0.2
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD11	2	0.19	0.07	0.19
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD12	2	0.19	0.07	0.19
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD13	2	0.19	0.07	0.19
(1,934)	1:104:A:GLU:HA	1:107:A:ALA:H	2	0.18	0.04	0.18
(3,34)	1:60:A:LEU:H	1:158:A:ILE:O	2	0.18	0.01	0.18
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG11	2	0.18	0.04	0.18
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG12	2	0.18	0.04	0.18
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG13	2	0.18	0.04	0.18
(1,170)	1:16:A:SER:H	1:23:A:TYR:H	2	0.18	0.03	0.18
(1,402)	1:55:A:VAL:HA	1:125:A:PHE:H	2	0.18	0.02	0.18
(1,1190)	1:141:A:LEU:HD21	1:142:A:ARG:HB2	2	0.18	0.03	0.18
(1,1190)	1:141:A:LEU:HD22	1:142:A:ARG:HB2	2	0.18	0.03	0.18
(1,1190)	1:141:A:LEU:HD23	1:142:A:ARG:HB2	2	0.18	0.03	0.18

Continued on next page...

Continued from previous page...

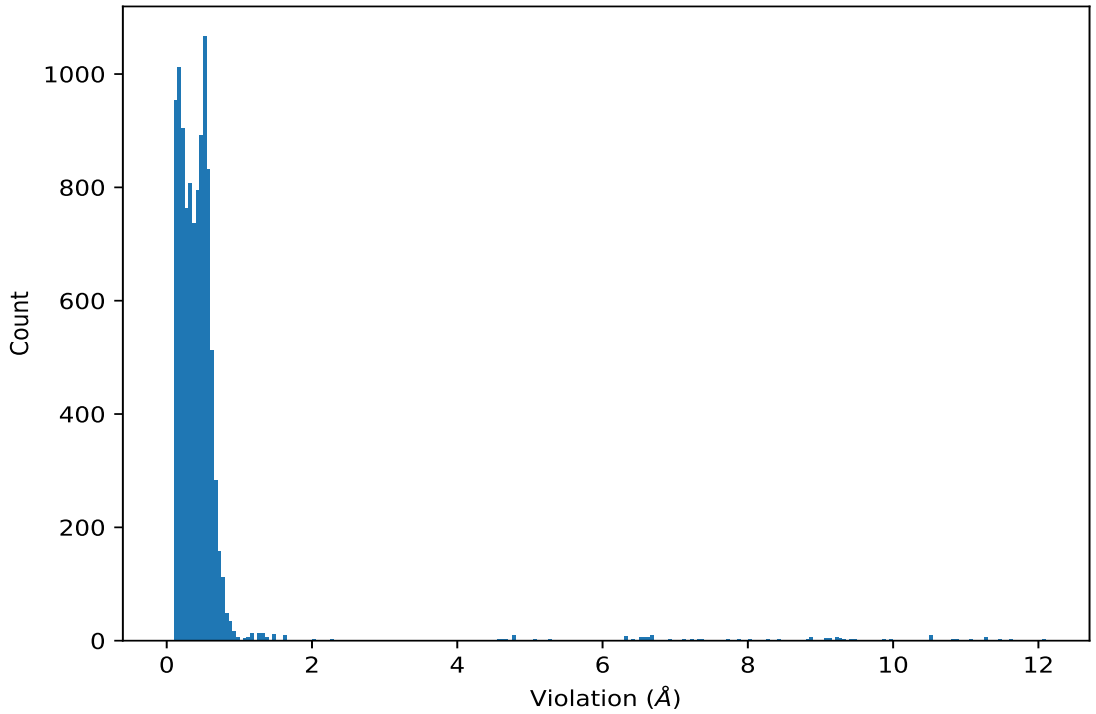
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1431)	1:161:A:ARG:HA	1:163:A:GLU:H	2	0.18	0.06	0.18
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD11	2	0.16	0.04	0.16
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD12	2	0.16	0.04	0.16
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD13	2	0.16	0.04	0.16
(3,46)	1:70:A:PRO:O	1:78:A:ILE:H	2	0.16	0.01	0.16
(1,698)	1:86:A:LEU:HD11	1:87:A:GLU:H	2	0.15	0.02	0.15
(1,698)	1:86:A:LEU:HD12	1:87:A:GLU:H	2	0.15	0.02	0.15
(1,698)	1:86:A:LEU:HD13	1:87:A:GLU:H	2	0.15	0.02	0.15
(3,80)	1:105:A:SER:O	1:109:A:GLN:H	2	0.14	0.0	0.14
(1,2)	1:2:A:ALA:HA	1:3:A:ASP:H	2	0.14	0.02	0.14
(4,2774)	1:26:A:ASN:H	1:31:A:ALA:O	2	0.14	0.02	0.14
(1,807)	1:93:A:ILE:HD11	1:94:A:GLN:H	2	0.13	0.01	0.13
(1,807)	1:93:A:ILE:HD12	1:94:A:GLN:H	2	0.13	0.01	0.13
(1,807)	1:93:A:ILE:HD13	1:94:A:GLN:H	2	0.13	0.01	0.13
(1,317)	1:28:A:ILE:HG12	1:29:A:THR:H	2	0.12	0.01	0.12
(1,1072)	1:121:A:ASP:HB2	1:123:A:GLY:H	2	0.12	0.01	0.12
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG21	2	0.12	0.02	0.12
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG22	2	0.12	0.02	0.12
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG23	2	0.12	0.02	0.12
(1,1026)	1:118:A:ALA:H	1:119:A:ARG:HA	2	0.12	0.0	0.12
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG11	2	0.11	0.0	0.11
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG12	2	0.11	0.0	0.11
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG13	2	0.11	0.0	0.11
(4,2798)	1:72:A:SER:H	1:75:A:GLN:O	2	0.11	0.0	0.11
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB1	2	0.11	0.0	0.11
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB2	2	0.11	0.0	0.11
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB3	2	0.11	0.0	0.11
(1,2083)	1:106:A:LEU:H	1:106:A:LEU:HG	2	0.1	0.0	0.1
(4,2764)	1:16:A:SER:H	1:21:A:ARG:O	2	0.1	0.0	0.1

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	13	12.07
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	13	12.07
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	13	12.07
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	9	11.6
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	9	11.6
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	9	11.6
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	4	11.49
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	4	11.49
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	4	11.49
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	12	11.26
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	12	11.26
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	12	11.26
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	8	11.25
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	8	11.25
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	8	11.25
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	3	11.07

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	3	11.07
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	3	11.07
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	7	10.86
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	7	10.86
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	7	10.86
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	1	10.81
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	1	10.81
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	1	10.81
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	5	10.54
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	5	10.54
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	5	10.54
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	14	10.51
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	14	10.51
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	14	10.51
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	19	10.5
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	19	10.5
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	19	10.5
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	6	9.95
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	6	9.95
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	6	9.95
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	11	9.85
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	11	9.85
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	2	9.46
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	2	9.46
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	13	9.42
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	13	9.42
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	3	9.33
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	3	9.33
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	4	9.26
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	4	9.26
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	6	9.25
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	6	9.25
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	1	9.24
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	1	9.24
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	16	9.24
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	16	9.24
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	11	9.2
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	11	9.2
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	11	9.2
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	9	9.14
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	9	9.14
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	7	9.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	7	9.1
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	14	9.07
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	14	9.07
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	5	9.05
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	5	9.05
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	15	8.88
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	15	8.88
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	12	8.87
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	12	8.87
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	17	8.86
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	17	8.86
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	17	8.86
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	8	8.84
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	8	8.84
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	10	8.4
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	10	8.4
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	10	8.4
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	18	8.25
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	18	8.25
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	18	8.25
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	19	8.0
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	19	8.0
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	17	7.85
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	17	7.85
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	10	7.74
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	10	7.74
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	20	7.35
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	20	7.35
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	20	7.35
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	2	7.34
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	2	7.34
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	2	7.34
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	15	7.21
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	15	7.21
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	15	7.21
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	18	7.12
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	18	7.12
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	4	6.92
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	4	6.92
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	4	6.92
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG21	16	6.69
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG22	16	6.69

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2592)	1:129:A:GLN:HE21	2:651:B:ILE:HG23	16	6.69
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	1	6.69
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	1	6.69
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	1	6.69
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	3	6.66
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	3	6.66
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	3	6.66
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	14	6.62
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	14	6.62
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	14	6.62
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	19	6.62
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	19	6.62
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	19	6.62
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	6	6.59
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	6	6.59
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	6	6.59
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	7	6.55
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	7	6.55
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	7	6.55
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	5	6.54
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	5	6.54
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	5	6.54
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	12	6.54
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	12	6.54
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	12	6.54
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	8	6.44
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	8	6.44
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	8	6.44
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	9	6.34
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	9	6.34
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	9	6.34
(1,2595)	1:131:A:GLN:HG2	2:652:B:ASP:HA	20	6.32
(1,2595)	1:131:A:GLN:HG3	2:652:B:ASP:HA	20	6.32
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	18	6.3
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	18	6.3
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	18	6.3
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	15	5.28
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	15	5.28
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	15	5.28
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	16	5.07
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	16	5.07
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	16	5.07

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	2	4.78
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	2	4.78
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	2	4.78
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	10	4.75
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	10	4.75
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	10	4.75
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	13	4.75
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	13	4.75
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	13	4.75
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	17	4.68
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	17	4.68
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	17	4.68
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	20	4.61
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	20	4.61
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	20	4.61
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD11	11	4.59
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD12	11	4.59
(1,1319)	1:157:A:HIS:H	1:159:A:ILE:HD13	11	4.59
(2,88)	1:34:A:TRP:HE1	2:641:B:TPO:H	16	2.68
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	18	2.26
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	18	2.26
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	18	2.26
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	16	2.0
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	16	2.0
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	16	2.0
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	19	1.63
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	19	1.63
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	19	1.63
(2,88)	1:34:A:TRP:HE1	2:641:B:TPO:H	12	1.61
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	16	1.61
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	16	1.61
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	16	1.61
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	18	1.61
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	18	1.61
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	18	1.61
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	9	1.48
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	9	1.48
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	9	1.48
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	9	1.48
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	9	1.48
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	9	1.48
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	17	1.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	17	1.45
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	17	1.45
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	17	1.45
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	17	1.45
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	17	1.45
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	15	1.39
(3,27)	1:56:A:ARG:N	1:163:A:GLU:O	13	1.38
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	15	1.38
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	15	1.38
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	17	1.36
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	13	1.35
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	6	1.33
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	6	1.33
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	6	1.33
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	18	1.33
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	3	1.32
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	3	1.32
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	3	1.32
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	14	1.32
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	14	1.32
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	14	1.32
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	19	1.3
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	19	1.3
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	19	1.3
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	10	1.27
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	10	1.27
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	10	1.27
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	17	1.27
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	17	1.27
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	17	1.27
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	20	1.27
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	20	1.27
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	15	1.25
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	15	1.25
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	15	1.25
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	17	1.25
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	17	1.25
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	16	1.24
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	8	1.19
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	8	1.19
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	8	1.19
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	4	1.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	4	1.18
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	4	1.18
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	11	1.18
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	11	1.18
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	11	1.18
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	10	1.18
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	5	1.15
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	5	1.15
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	5	1.15
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	7	1.13
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	7	1.13
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	7	1.13
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG21	16	1.13
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG22	16	1.13
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG23	16	1.13
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	20	1.09
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	2	1.07
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	2	1.07
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	2	1.07
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	13	0.98
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	13	0.98
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	13	0.98
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	13	0.96
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	13	0.96
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	13	0.96
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	12	0.94
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	12	0.94
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	12	0.94
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	12	0.94
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	12	0.94
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	12	0.94
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	5	0.94
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	5	0.94
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	5	0.94
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	5	0.94
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	2	0.91
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	17	0.91
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	10	0.9
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	10	0.9
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	14	0.9
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	14	0.9
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	14	0.9

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	9	0.89
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	9	0.89
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	9	0.89
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	15	0.89
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	15	0.89
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	15	0.89
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	13	0.88
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	13	0.88
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	13	0.88
(3,27)	1:56:A:ARG:N	1:163:A:GLU:O	17	0.87
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	15	0.87
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	17	0.87
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	17	0.87
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	17	0.87
(1,2513)	2:646:B:GLU:HA	2:649:B:ARG:HD2	20	0.87
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	20	0.86
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	10	0.86
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	10	0.86
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	10	0.86
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	3	0.86
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	3	0.86
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	3	0.86
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	18	0.86
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	18	0.86
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	18	0.86
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	18	0.86
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	18	0.86
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	18	0.86
(1,443)	1:59:A:HIS:HB2	1:158:A:ILE:H	16	0.86
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	8	0.85
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	8	0.85
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	8	0.85
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	1	0.85
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	7	0.85
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	11	0.84
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	5	0.84
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	5	0.84
(2,88)	1:34:A:TRP:HE1	2:641:B:TPO:H	18	0.84
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	20	0.84
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	20	0.84
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	20	0.84
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	20	0.84

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	20	0.84
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	20	0.84
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	16	0.84
(2,66)	2:645:B:GLN:H	2:648:B:ILE:H	20	0.83
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	16	0.83
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	5	0.82
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	5	0.82
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	5	0.82
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	8	0.82
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	14	0.82
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	8	0.82
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	7	0.82
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	17	0.82
(3,28)	1:56:A:ARG:H	1:163:A:GLU:O	13	0.81
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	19	0.81
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	2	0.81
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	2	0.81
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	2	0.81
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	4	0.81
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	4	0.81
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	4	0.81
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	4	0.81
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	1	0.81
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	1	0.81
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	12	0.81
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	10	0.8
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	1	0.8
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	1	0.8
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	1	0.8
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	7	0.8
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	7	0.8
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	7	0.8
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	18	0.8
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	18	0.8
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	3	0.8
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	3	0.8
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	3	0.8
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	3	0.8
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	17	0.8
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	16	0.8
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	2	0.79
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	2	0.79

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	2	0.79
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	6	0.79
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	6	0.79
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	6	0.79
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	1	0.79
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	1	0.79
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	1	0.79
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	1	0.79
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	6	0.79
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	6	0.79
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	6	0.79
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	6	0.79
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	7	0.79
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	7	0.79
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	7	0.79
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	13	0.79
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	13	0.79
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	13	0.79
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	13	0.79
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	13	0.79
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	13	0.79
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	3	0.79
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	19	0.79
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	19	0.78
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	19	0.78
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	4	0.78
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	4	0.78
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	4	0.78
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	17	0.78
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	17	0.78
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	17	0.78
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	8	0.78
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	8	0.78
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	8	0.78
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	8	0.78
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	9	0.78
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	9	0.78
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	9	0.78
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	6	0.78
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	18	0.78
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	3	0.77
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	3	0.77

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	3	0.77
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	3	0.77
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	3	0.77
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	3	0.77
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	10	0.77
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	13	0.77
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	13	0.77
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	13	0.77
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	9	0.77
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	11	0.77
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	3	0.77
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	5	0.77
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	11	0.76
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	11	0.76
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	11	0.76
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	9	0.76
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	9	0.76
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	9	0.76
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	9	0.76
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	9	0.76
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	9	0.76
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE1	15	0.76
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE2	15	0.76
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE1	15	0.76
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE2	15	0.76
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	19	0.76
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	19	0.76
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	19	0.76
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	19	0.76
(2,66)	2:645:B:GLN:H	2:648:B:ILE:H	13	0.76
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	16	0.76
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	16	0.76
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	16	0.76
(1,2516)	2:646:B:GLU:HA	2:647:B:VAL:HG21	13	0.76
(1,2516)	2:646:B:GLU:HA	2:647:B:VAL:HG22	13	0.76
(1,2516)	2:646:B:GLU:HA	2:647:B:VAL:HG23	13	0.76
(1,2514)	2:646:B:GLU:HA	2:649:B:ARG:H	17	0.76
(1,1426)	1:56:A:ARG:HA	1:163:A:GLU:H	11	0.76
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	12	0.76
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	4	0.75
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	4	0.75
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	4	0.75

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	4	0.75
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	4	0.75
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	4	0.75
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	8	0.75
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	8	0.75
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	20	0.75
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	20	0.75
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	20	0.75
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	17	0.75
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	17	0.75
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	11	0.75
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	11	0.75
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	11	0.75
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	18	0.75
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	18	0.75
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	18	0.75
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	13	0.75
(1,2529)	2:648:B:ILE:HG21	2:649:B:ARG:HD2	18	0.75
(1,2529)	2:648:B:ILE:HG22	2:649:B:ARG:HD2	18	0.75
(1,2529)	2:648:B:ILE:HG23	2:649:B:ARG:HD2	18	0.75
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	11	0.75
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	11	0.75
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	11	0.75
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	2	0.75
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	4	0.75
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	15	0.75
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	18	0.74
(2,102)	1:135:A:GLU:H	2:656:B:PHE:HB2	20	0.74
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	17	0.74
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	17	0.74
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	15	0.74
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	15	0.74
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	2	0.74
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	2	0.74
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	2	0.74
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE1	11	0.74
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE2	11	0.74
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE1	11	0.74
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE2	11	0.74
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	14	0.74
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	14	0.74
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	14	0.74

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	14	0.74
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	6	0.74
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	9	0.74
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	13	0.74
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	4	0.74
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	11	0.74
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	16	0.74
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	10	0.74
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	13	0.74
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	18	0.74
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	8	0.73
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	8	0.73
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	9	0.73
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	9	0.73
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	9	0.73
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	15	0.73
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	15	0.73
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	15	0.73
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	1	0.73
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	18	0.73
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	18	0.73
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	18	0.73
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	4	0.73
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	4	0.73
(1,2518)	2:646:B:GLU:H	2:647:B:VAL:HG21	13	0.73
(1,2518)	2:646:B:GLU:H	2:647:B:VAL:HG22	13	0.73
(1,2518)	2:646:B:GLU:H	2:647:B:VAL:HG23	13	0.73
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	17	0.73
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	18	0.73
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	18	0.73
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	15	0.73
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	15	0.73
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	15	0.73
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	15	0.73
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	18	0.72
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	18	0.72
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	18	0.72
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	18	0.72
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	18	0.72
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	18	0.72
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	1	0.72
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	1	0.72

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	1	0.72
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	9	0.72
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	9	0.72
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	9	0.72
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	20	0.72
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	20	0.72
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	20	0.72
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	1	0.72
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	1	0.72
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	1	0.72
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	1	0.72
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	1	0.72
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	1	0.72
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	7	0.72
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	7	0.72
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	7	0.72
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	7	0.72
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	17	0.72
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	8	0.72
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	8	0.72
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	8	0.72
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	11	0.72
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	4	0.72
(1,897)	1:104:A:GLU:HG2	1:108:A:SER:H	10	0.72
(1,897)	1:104:A:GLU:HG2	1:108:A:SER:H	18	0.72
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG21	20	0.72
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG22	20	0.72
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG23	20	0.72
(1,606)	1:75:A:GLN:HE22	1:78:A:ILE:HA	2	0.72
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	14	0.72
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	5	0.71
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	11	0.71
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	11	0.71
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	17	0.71
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	15	0.71
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	15	0.71
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	15	0.71
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	10	0.71
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	10	0.71
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	13	0.71
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	13	0.71
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	4	0.71

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	4	0.71
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	4	0.71
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	6	0.71
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	6	0.71
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	6	0.71
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	3	0.71
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	4	0.71
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	4	0.71
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	15	0.71
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	4	0.71
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	4	0.71
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	9	0.71
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	18	0.71
(1,1184)	1:140:A:ALA:H	1:141:A:LEU:HG	11	0.71
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	8	0.71
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	8	0.71
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	8	0.71
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	11	0.71
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	19	0.71
(1,88)	1:12:A:GLU:HB2	1:14:A:ARG:HE	10	0.71
(1,88)	1:12:A:GLU:HB3	1:14:A:ARG:HE	10	0.71
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	8	0.71
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	6	0.7
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	6	0.7
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	3	0.7
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	16	0.7
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	10	0.7
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	10	0.7
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	10	0.7
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	19	0.7
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	19	0.7
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	19	0.7
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE1	10	0.7
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE2	10	0.7
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE1	10	0.7
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE2	10	0.7
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	1	0.7
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	1	0.7
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	1	0.7
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	4	0.7
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	4	0.7
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	4	0.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	2	0.7
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	10	0.7
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	13	0.7
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	8	0.7
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	8	0.7
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	8	0.7
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	11	0.7
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	12	0.7
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	19	0.7
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	10	0.7
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	10	0.7
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	12	0.7
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	19	0.7
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	1	0.7
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	11	0.7
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	2	0.7
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	5	0.69
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	5	0.69
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	5	0.69
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	5	0.69
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	5	0.69
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	5	0.69
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	9	0.69
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	9	0.69
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	13	0.69
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	13	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	3	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	3	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	3	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	6	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	6	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	6	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	16	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	16	0.69
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	16	0.69
(2,94)	1:93:A:ILE:HG21	2:643:B:PRO:HB3	20	0.69
(2,94)	1:93:A:ILE:HG22	2:643:B:PRO:HB3	20	0.69
(2,94)	1:93:A:ILE:HG23	2:643:B:PRO:HB3	20	0.69
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	20	0.69
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	20	0.69
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	16	0.69
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	16	0.69

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	16	0.69
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	16	0.69
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	16	0.69
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	16	0.69
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	15	0.69
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	15	0.69
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	15	0.69
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	15	0.69
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	15	0.69
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	15	0.69
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	11	0.69
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	11	0.69
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	11	0.69
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	11	0.69
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	2	0.69
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	7	0.69
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	12	0.69
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	16	0.69
(1,2596)	1:137:A:ALA:HB1	2:651:B:ILE:HG12	17	0.69
(1,2596)	1:137:A:ALA:HB1	2:651:B:ILE:HG13	17	0.69
(1,2596)	1:137:A:ALA:HB2	2:651:B:ILE:HG12	17	0.69
(1,2596)	1:137:A:ALA:HB2	2:651:B:ILE:HG13	17	0.69
(1,2596)	1:137:A:ALA:HB3	2:651:B:ILE:HG12	17	0.69
(1,2596)	1:137:A:ALA:HB3	2:651:B:ILE:HG13	17	0.69
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	19	0.69
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	19	0.69
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	19	0.69
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	19	0.69
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	19	0.69
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	19	0.69
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	8	0.69
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	15	0.69
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	20	0.69
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	20	0.69
(1,1060)	1:121:A:ASP:H	1:122:A:LEU:HD11	9	0.69
(1,1060)	1:121:A:ASP:H	1:122:A:LEU:HD12	9	0.69
(1,1060)	1:121:A:ASP:H	1:122:A:LEU:HD13	9	0.69
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	18	0.69
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	19	0.69
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	2	0.69
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG21	1	0.69
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG22	1	0.69

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG23	1	0.69
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	9	0.69
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	20	0.69
(1,88)	1:12:A:GLU:HB2	1:14:A:ARG:HE	20	0.69
(1,88)	1:12:A:GLU:HB3	1:14:A:ARG:HE	20	0.69
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB1	11	0.69
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB2	11	0.69
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB3	11	0.69
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	17	0.69
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	5	0.68
(2,102)	1:135:A:GLU:H	2:656:B:PHE:HB2	16	0.68
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	20	0.68
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	20	0.68
(2,88)	1:34:A:TRP:HE1	2:641:B:TPO:H	7	0.68
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	8	0.68
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	12	0.68
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	2	0.68
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	2	0.68
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	2	0.68
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	1	0.68
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	7	0.68
(1,1054)	1:59:A:HIS:HD2	1:122:A:LEU:H	19	0.68
(1,833)	1:94:A:GLN:HE21	1:97:A:LYS:HG2	13	0.68
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	3	0.68
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	3	0.68
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	3	0.68
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	17	0.68
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	17	0.68
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	17	0.68
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	3	0.68
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	3	0.68
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	3	0.68
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	3	0.68
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	5	0.68
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	8	0.68
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	15	0.68
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	3	0.68
(3,27)	1:56:A:ARG:N	1:163:A:GLU:O	16	0.67
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	20	0.67
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	20	0.67
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	20	0.67
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG12	10	0.67

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG13	10	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	2	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	2	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	2	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	10	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	10	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	10	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	19	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	19	0.67
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	19	0.67
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	5	0.67
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	5	0.67
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	5	0.67
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	14	0.67
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	14	0.67
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	14	0.67
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	6	0.67
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	9	0.67
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	10	0.67
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	17	0.67
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	12	0.67
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	12	0.67
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	7	0.67
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	5	0.67
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	13	0.67
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	13	0.67
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	20	0.67
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	4	0.67
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	4	0.67
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	4	0.67
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	1	0.67
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	10	0.67
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	16	0.67
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	4	0.67
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	13	0.67
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	13	0.67
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	10	0.66
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	10	0.66
(2,107)	1:140:A:ALA:HB1	2:651:B:ILE:HA	17	0.66
(2,107)	1:140:A:ALA:HB2	2:651:B:ILE:HA	17	0.66
(2,107)	1:140:A:ALA:HB3	2:651:B:ILE:HA	17	0.66
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	18	0.66

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	18	0.66
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	12	0.66
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	12	0.66
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	12	0.66
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	6	0.66
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	6	0.66
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	5	0.66
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	5	0.66
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	5	0.66
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	14	0.66
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	14	0.66
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	14	0.66
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	9	0.66
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	9	0.66
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	12	0.66
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	12	0.66
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	12	0.66
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	12	0.66
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	1	0.66
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	1	0.66
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	1	0.66
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	1	0.66
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	1	0.66
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	1	0.66
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	13	0.66
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	1	0.66
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	8	0.66
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	9	0.66
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	6	0.66
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	6	0.66
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	6	0.66
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	14	0.66
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	14	0.66
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	14	0.66
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	10	0.66
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	15	0.66
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG21	19	0.66
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG22	19	0.66
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG23	19	0.66
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	10	0.66
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	10	0.66
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	15	0.66

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	15	0.66
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	15	0.66
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	18	0.66
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	18	0.66
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	18	0.66
(1,833)	1:94:A:GLN:HE21	1:97:A:LYS:HG2	15	0.66
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	14	0.66
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	14	0.66
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	14	0.66
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	8	0.66
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	8	0.66
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	12	0.66
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	9	0.66
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	17	0.66
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	5	0.66
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	9	0.65
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	9	0.65
(2,109)	1:150:A:VAL:HG21	2:649:B:ARG:HA	13	0.65
(2,109)	1:150:A:VAL:HG22	2:649:B:ARG:HA	13	0.65
(2,109)	1:150:A:VAL:HG23	2:649:B:ARG:HA	13	0.65
(2,101)	1:129:A:GLN:HE21	2:657:B:GLU:HB2	17	0.65
(2,101)	1:129:A:GLN:HE21	2:657:B:GLU:HB3	17	0.65
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	1	0.65
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	1	0.65
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	4	0.65
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	4	0.65
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	4	0.65
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	2	0.65
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	2	0.65
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	12	0.65
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	12	0.65
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	12	0.65
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	14	0.65
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	14	0.65
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	14	0.65
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	2	0.65
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	2	0.65
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	2	0.65
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	2	0.65
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	2	0.65
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	2	0.65
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	8	0.65

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	8	0.65
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	8	0.65
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	4	0.65
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	4	0.65
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	4	0.65
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	4	0.65
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	4	0.65
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	4	0.65
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	14	0.65
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	19	0.65
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	20	0.65
(2,34)	1:59:A:HIS:H	1:122:A:LEU:HB2	11	0.65
(2,5)	1:23:A:TYR:H	1:34:A:TRP:HZ3	19	0.65
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	6	0.65
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	16	0.65
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	11	0.65
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	11	0.65
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	18	0.65
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	18	0.65
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	13	0.65
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	13	0.65
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	17	0.65
(1,1410)	1:161:A:ARG:HE	1:163:A:GLU:HG2	2	0.65
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	16	0.65
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	16	0.65
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	16	0.65
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	4	0.65
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	4	0.65
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	4	0.65
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	9	0.65
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	20	0.65
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	20	0.65
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	2	0.65
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	2	0.65
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	9	0.65
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	15	0.65
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	18	0.65
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	7	0.65
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	7	0.65
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	7	0.65
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	2	0.65
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	13	0.65

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	11	0.65
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	7	0.65
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	12	0.65
(1,275)	1:26:A:ASN:H	1:29:A:THR:HG21	20	0.65
(1,275)	1:26:A:ASN:H	1:29:A:THR:HG22	20	0.65
(1,275)	1:26:A:ASN:H	1:29:A:THR:HG23	20	0.65
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	20	0.64
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	3	0.64
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	3	0.64
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	4	0.64
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	14	0.64
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	18	0.64
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	18	0.64
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	18	0.64
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG12	13	0.64
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG13	13	0.64
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	11	0.64
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	11	0.64
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	11	0.64
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	11	0.64
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	11	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	4	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	4	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	4	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	4	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	4	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	4	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	14	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	14	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	14	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	14	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	14	0.64
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	14	0.64
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	16	0.64
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	16	0.64
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	16	0.64
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	15	0.64
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	3	0.64
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	14	0.64
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	7	0.64
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	7	0.64
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	19	0.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5)	1:23:A:TYR:H	1:34:A:TRP:HZ3	15	0.64
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	8	0.64
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	8	0.64
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	8	0.64
(1,2529)	2:648:B:ILE:HG21	2:649:B:ARG:HD2	1	0.64
(1,2529)	2:648:B:ILE:HG22	2:649:B:ARG:HD2	1	0.64
(1,2529)	2:648:B:ILE:HG23	2:649:B:ARG:HD2	1	0.64
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG21	18	0.64
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG22	18	0.64
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG23	18	0.64
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	10	0.64
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	10	0.64
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	10	0.64
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	2	0.64
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	13	0.64
(1,1184)	1:140:A:ALA:H	1:141:A:LEU:HG	15	0.64
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	5	0.64
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	16	0.64
(1,833)	1:94:A:GLN:HE21	1:97:A:LYS:HG2	2	0.64
(1,833)	1:94:A:GLN:HE21	1:97:A:LYS:HG2	11	0.64
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	11	0.64
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	17	0.64
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	4	0.64
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	9	0.64
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	2	0.64
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	17	0.64
(1,138)	1:21:A:ARG:HE	1:34:A:TRP:HH2	17	0.64
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	17	0.64
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	16	0.64
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	11	0.63
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	5	0.63
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	5	0.63
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	5	0.63
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	8	0.63
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	8	0.63
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	13	0.63
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	13	0.63
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	1	0.63
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	1	0.63
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	1	0.63
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	12	0.63
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	12	0.63

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	12	0.63
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE1	2	0.63
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE2	2	0.63
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE1	2	0.63
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE2	2	0.63
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	12	0.63
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	12	0.63
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	12	0.63
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	2	0.63
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	2	0.63
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	2	0.63
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	5	0.63
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	4	0.63
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	18	0.63
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	18	0.63
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	14	0.63
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	14	0.63
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	10	0.63
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	10	0.63
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	10	0.63
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	2	0.63
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	10	0.63
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD11	18	0.63
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD12	18	0.63
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD13	18	0.63
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	3	0.63
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	3	0.63
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	3	0.63
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	8	0.63
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	8	0.63
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	8	0.63
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	6	0.63
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	16	0.63
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	16	0.63
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	16	0.63
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	20	0.63
(1,1441)	1:162:A:THR:HG21	1:163:A:GLU:HG3	11	0.63
(1,1441)	1:162:A:THR:HG22	1:163:A:GLU:HG3	11	0.63
(1,1441)	1:162:A:THR:HG23	1:163:A:GLU:HG3	11	0.63
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB2	11	0.63
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB3	11	0.63
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB2	11	0.63

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB3	11	0.63
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB2	11	0.63
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB3	11	0.63
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	6	0.63
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	7	0.63
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	14	0.63
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	20	0.63
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	19	0.63
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	19	0.63
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	19	0.63
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	14	0.63
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	14	0.63
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	14	0.63
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	18	0.63
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	11	0.63
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	9	0.63
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	9	0.63
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	9	0.63
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	1	0.63
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	20	0.63
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	3	0.63
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	4	0.63
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	8	0.63
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	9	0.63
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	14	0.63
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	18	0.63
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	2	0.63
(1,640)	1:65:A:SER:HB3	1:81:A:THR:HA	15	0.63
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	3	0.63
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	14	0.63
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	13	0.63
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	13	0.63
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	13	0.63
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	13	0.63
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	16	0.63
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	12	0.63
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	12	0.63
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	12	0.63
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	1	0.63
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	12	0.62
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	12	0.62
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	13	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	13	0.62
(2,108)	1:140:A:ALA:HB1	2:649:B:ARG:HA	20	0.62
(2,108)	1:140:A:ALA:HB2	2:649:B:ARG:HA	20	0.62
(2,108)	1:140:A:ALA:HB3	2:649:B:ARG:HA	20	0.62
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	12	0.62
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	12	0.62
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	2	0.62
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	3	0.62
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	3	0.62
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	12	0.62
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	12	0.62
(2,91)	1:57:A:CYS:H	2:651:B:ILE:HG12	10	0.62
(2,91)	1:57:A:CYS:H	2:651:B:ILE:HG13	10	0.62
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	19	0.62
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	19	0.62
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	3	0.62
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	3	0.62
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	3	0.62
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	15	0.62
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	15	0.62
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	15	0.62
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	9	0.62
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	9	0.62
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	9	0.62
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	9	0.62
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE1	1	0.62
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE2	1	0.62
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE1	4	0.62
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE2	4	0.62
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	3	0.62
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	3	0.62
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	3	0.62
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	8	0.62
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	8	0.62
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	8	0.62
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	9	0.62
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	9	0.62
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	9	0.62
(2,55)	1:150:A:VAL:HG21	1:158:A:ILE:HA	11	0.62
(2,55)	1:150:A:VAL:HG22	1:158:A:ILE:HA	11	0.62
(2,55)	1:150:A:VAL:HG23	1:158:A:ILE:HA	11	0.62
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	19	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	6	0.62
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	10	0.62
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	12	0.62
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	1	0.62
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	2	0.62
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	2	0.62
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	2	0.62
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	13	0.62
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	10	0.62
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	10	0.62
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	10	0.62
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	4	0.62
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	4	0.62
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	4	0.62
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	14	0.62
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	14	0.62
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	14	0.62
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	6	0.62
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	12	0.62
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	12	0.62
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	12	0.62
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	15	0.62
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	15	0.62
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	3	0.62
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	3	0.62
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	11	0.62
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	11	0.62
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	16	0.62
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	16	0.62
(1,1054)	1:59:A:HIS:HD2	1:122:A:LEU:H	16	0.62
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	6	0.62
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	14	0.62
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	19	0.62
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	17	0.62
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	17	0.62
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	6	0.62
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	7	0.62
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	19	0.62
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	5	0.62
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	7	0.62
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	13	0.62
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	19	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	19	0.62
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	19	0.62
(1,606)	1:75:A:GLN:HE22	1:78:A:ILE:HA	18	0.62
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	15	0.62
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	15	0.62
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	15	0.62
(1,479)	1:61:A:LEU:HD21	1:155:A:GLY:H	3	0.62
(1,479)	1:61:A:LEU:HD22	1:155:A:GLY:H	3	0.62
(1,479)	1:61:A:LEU:HD23	1:155:A:GLY:H	3	0.62
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	1	0.62
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	5	0.62
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	1	0.62
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	12	0.62
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	14	0.62
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	14	0.62
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	14	0.62
(1,87)	1:13:A:LYS:HG3	1:14:A:ARG:H	15	0.62
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	1	0.62
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	1	0.62
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	13	0.62
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	3	0.61
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	3	0.61
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	14	0.61
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	14	0.61
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	18	0.61
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	18	0.61
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	10	0.61
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	10	0.61
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	14	0.61
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	14	0.61
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	6	0.61
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	14	0.61
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	14	0.61
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	18	0.61
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	18	0.61
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG21	13	0.61
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG22	13	0.61
(2,84)	1:15:A:MET:H	2:641:B:TPO:HG23	13	0.61
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	2	0.61
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	2	0.61
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	2	0.61
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	2	0.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	7	0.61
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	7	0.61
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	7	0.61
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	7	0.61
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	7	0.61
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	7	0.61
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	4	0.61
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	4	0.61
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	4	0.61
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	2	0.61
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	18	0.61
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	12	0.61
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	3	0.61
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	7	0.61
(2,5)	1:23:A:TYR:H	1:34:A:TRP:HZ3	11	0.61
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	17	0.61
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	3	0.61
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	3	0.61
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	9	0.61
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	9	0.61
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	12	0.61
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	12	0.61
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	10	0.61
(1,2529)	2:648:B:ILE:HG21	2:649:B:ARG:HD2	11	0.61
(1,2529)	2:648:B:ILE:HG22	2:649:B:ARG:HD2	11	0.61
(1,2529)	2:648:B:ILE:HG23	2:649:B:ARG:HD2	11	0.61
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	6	0.61
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	6	0.61
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	6	0.61
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	14	0.61
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	14	0.61
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	14	0.61
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	16	0.61
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	16	0.61
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	16	0.61
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	8	0.61
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	14	0.61
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	2	0.61
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	3	0.61
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	20	0.61
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	18	0.61
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	18	0.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	18	0.61
(1,1303)	1:156:A:ILE:HG21	1:157:A:HIS:HD2	11	0.61
(1,1303)	1:156:A:ILE:HG22	1:157:A:HIS:HD2	11	0.61
(1,1303)	1:156:A:ILE:HG23	1:157:A:HIS:HD2	11	0.61
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD11	2	0.61
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD12	2	0.61
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD13	2	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	1	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	1	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	1	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	5	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	5	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	5	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	10	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	10	0.61
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	10	0.61
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	11	0.61
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	11	0.61
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	3	0.61
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	3	0.61
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	16	0.61
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	13	0.61
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	13	0.61
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	13	0.61
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	13	0.61
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	13	0.61
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	3	0.61
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	9	0.61
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	7	0.61
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	5	0.61
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	5	0.61
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	5	0.61
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	6	0.61
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	6	0.61
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	6	0.61
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	5	0.61
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	14	0.61
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	14	0.61
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	14	0.61
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	4	0.61
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	4	0.61
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	4	0.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	2	0.61
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	2	0.61
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	2	0.61
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	18	0.61
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	18	0.61
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	10	0.61
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	16	0.61
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	12	0.61
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	18	0.61
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	7	0.61
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	9	0.61
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	13	0.61
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	19	0.61
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	19	0.61
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	19	0.61
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	7	0.61
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	18	0.61
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	19	0.61
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	19	0.61
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	19	0.61
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	9	0.61
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	15	0.61
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	6	0.6
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	1	0.6
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	7	0.6
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	7	0.6
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	15	0.6
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	15	0.6
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	9	0.6
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	9	0.6
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	3	0.6
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	3	0.6
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	8	0.6
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	8	0.6
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	13	0.6
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	13	0.6
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	13	0.6
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	13	0.6
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	11	0.6
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	11	0.6
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	11	0.6
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	7	0.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE1	17	0.6
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE2	17	0.6
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	6	0.6
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	6	0.6
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	15	0.6
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	15	0.6
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	15	0.6
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	15	0.6
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	15	0.6
(1,2538)	2:649:B:ARG:H	2:650:B:ASN:HD21	19	0.6
(1,2514)	2:646:B:GLU:HA	2:649:B:ARG:H	2	0.6
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	12	0.6
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	3	0.6
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	3	0.6
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	3	0.6
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	5	0.6
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	5	0.6
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	5	0.6
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	5	0.6
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	5	0.6
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	5	0.6
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG21	16	0.6
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG22	16	0.6
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG23	16	0.6
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	10	0.6
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	10	0.6
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	10	0.6
(1,1303)	1:156:A:ILE:HG21	1:157:A:HIS:HD2	17	0.6
(1,1303)	1:156:A:ILE:HG22	1:157:A:HIS:HD2	17	0.6
(1,1303)	1:156:A:ILE:HG23	1:157:A:HIS:HD2	17	0.6
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	15	0.6
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	15	0.6
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	15	0.6
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	12	0.6
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	12	0.6
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	12	0.6
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	14	0.6
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	2	0.6
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	16	0.6
(1,1184)	1:140:A:ALA:H	1:141:A:LEU:HG	7	0.6
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	19	0.6
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	19	0.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	8	0.6
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	8	0.6
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	20	0.6
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	20	0.6
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	20	0.6
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	20	0.6
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	20	0.6
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	20	0.6
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	17	0.6
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	17	0.6
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	17	0.6
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	7	0.6
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	7	0.6
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	7	0.6
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	7	0.6
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	7	0.6
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	7	0.6
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	16	0.6
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	8	0.6
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	12	0.6
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	4	0.6
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	3	0.6
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	9	0.6
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	1	0.6
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	1	0.6
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	1	0.6
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	4	0.6
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	18	0.6
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	20	0.6
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	8	0.6
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	8	0.6
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	8	0.6
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	9	0.6
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	1	0.6
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	6	0.6
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	12	0.6
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	20	0.6
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	17	0.6
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	17	0.6
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	17	0.6
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	20	0.6
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	3	0.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	3	0.6
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	3	0.6
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	3	0.6
(1,440)	1:59:A:HIS:H	1:115:A:SER:HB3	19	0.6
(1,401)	1:54:A:ARG:HD2	1:55:A:VAL:HA	19	0.6
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	6	0.6
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	11	0.6
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	9	0.6
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	18	0.6
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	18	0.6
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	18	0.6
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	5	0.6
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	14	0.6
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	10	0.6
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	10	0.6
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	5	0.59
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	5	0.59
(2,94)	1:93:A:ILE:HG21	2:643:B:PRO:HB3	19	0.59
(2,94)	1:93:A:ILE:HG22	2:643:B:PRO:HB3	19	0.59
(2,94)	1:93:A:ILE:HG23	2:643:B:PRO:HB3	19	0.59
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	10	0.59
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	10	0.59
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	10	0.59
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG12	20	0.59
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG13	20	0.59
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	19	0.59
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	19	0.59
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	19	0.59
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	20	0.59
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	20	0.59
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	20	0.59
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	6	0.59
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	6	0.59
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	6	0.59
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	6	0.59
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	6	0.59
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	6	0.59
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	18	0.59
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	7	0.59
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	3	0.59
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	3	0.59
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	6	0.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	6	0.59
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	20	0.59
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	20	0.59
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	20	0.59
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	14	0.59
(1,2532)	2:648:B:ILE:HG21	2:650:B:ASN:H	15	0.59
(1,2532)	2:648:B:ILE:HG22	2:650:B:ASN:H	15	0.59
(1,2532)	2:648:B:ILE:HG23	2:650:B:ASN:H	15	0.59
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	1	0.59
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	20	0.59
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	20	0.59
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	20	0.59
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	2	0.59
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	2	0.59
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	2	0.59
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	2	0.59
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	2	0.59
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	2	0.59
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	11	0.59
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	11	0.59
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	11	0.59
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	6	0.59
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	6	0.59
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	6	0.59
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	12	0.59
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	12	0.59
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	12	0.59
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	13	0.59
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	13	0.59
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	13	0.59
(1,1227)	1:89:A:ILE:HG12	1:150:A:VAL:H	3	0.59
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	9	0.59
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	10	0.59
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	11	0.59
(1,1215)	1:141:A:LEU:HD21	1:147:A:SER:HB2	13	0.59
(1,1215)	1:141:A:LEU:HD22	1:147:A:SER:HB2	13	0.59
(1,1215)	1:141:A:LEU:HD23	1:147:A:SER:HB2	13	0.59
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	2	0.59
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	2	0.59
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	5	0.59
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	5	0.59
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	6	0.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	6	0.59
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	20	0.59
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	20	0.59
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	13	0.59
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	15	0.59
(1,1054)	1:59:A:HIS:HD2	1:122:A:LEU:H	18	0.59
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	10	0.59
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE1	19	0.59
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE2	19	0.59
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE3	19	0.59
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE1	19	0.59
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE2	19	0.59
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE3	19	0.59
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	14	0.59
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	14	0.59
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	1	0.59
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	12	0.59
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	17	0.59
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	15	0.59
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	15	0.59
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	15	0.59
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	8	0.59
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	8	0.59
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	8	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	1	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	1	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	2	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	2	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	3	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	3	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	10	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	10	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	11	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	11	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	15	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	15	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	19	0.59
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	19	0.59
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	2	0.59
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	9	0.59
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	14	0.59
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	16	0.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	18	0.59
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	4	0.59
(1,612)	1:75:A:GLN:HE21	1:78:A:ILE:HA	17	0.59
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	16	0.59
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	18	0.59
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	20	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	2	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	2	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	2	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	9	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	9	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	9	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	15	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	15	0.59
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	15	0.59
(1,480)	1:61:A:LEU:HD21	1:156:A:ILE:H	13	0.59
(1,480)	1:61:A:LEU:HD22	1:156:A:ILE:H	13	0.59
(1,480)	1:61:A:LEU:HD23	1:156:A:ILE:H	13	0.59
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	20	0.59
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	20	0.59
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	20	0.59
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	17	0.59
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	8	0.59
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	8	0.59
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	8	0.59
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	9	0.59
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	9	0.59
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	9	0.59
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	2	0.59
(1,88)	1:12:A:GLU:HB2	1:14:A:ARG:HE	13	0.59
(1,88)	1:12:A:GLU:HB3	1:14:A:ARG:HE	13	0.59
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	8	0.59
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	5	0.59
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	10	0.59
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	16	0.59
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	16	0.59
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB1	17	0.59
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB2	17	0.59
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB3	17	0.59
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	8	0.59
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	1	0.58
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	1	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	1	0.58
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	1	0.58
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	1	0.58
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	1	0.58
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	4	0.58
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	6	0.58
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	10	0.58
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	10	0.58
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	10	0.58
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	10	0.58
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	10	0.58
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	10	0.58
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	10	0.58
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	19	0.58
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	19	0.58
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	5	0.58
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	5	0.58
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	5	0.58
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	6	0.58
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	6	0.58
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	6	0.58
(1,2553)	2:651:B:ILE:HG21	2:653:B:GLN:HE21	17	0.58
(1,2553)	2:651:B:ILE:HG21	2:653:B:GLN:HE22	17	0.58
(1,2553)	2:651:B:ILE:HG22	2:653:B:GLN:HE21	17	0.58
(1,2553)	2:651:B:ILE:HG22	2:653:B:GLN:HE22	17	0.58
(1,2553)	2:651:B:ILE:HG23	2:653:B:GLN:HE21	17	0.58
(1,2553)	2:651:B:ILE:HG23	2:653:B:GLN:HE22	17	0.58
(1,2529)	2:648:B:ILE:HG21	2:649:B:ARG:HD2	14	0.58
(1,2529)	2:648:B:ILE:HG22	2:649:B:ARG:HD2	14	0.58
(1,2529)	2:648:B:ILE:HG23	2:649:B:ARG:HD2	14	0.58
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	6	0.58
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	7	0.58
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	12	0.58
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	14	0.58
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	14	0.58
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	14	0.58
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	7	0.58
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG21	8	0.58
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG22	8	0.58
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG23	8	0.58
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG21	8	0.58
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG22	8	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG23	8	0.58
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG21	8	0.58
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG22	8	0.58
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG23	8	0.58
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	12	0.58
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	12	0.58
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	12	0.58
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	12	0.58
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	12	0.58
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	12	0.58
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	12	0.58
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	12	0.58
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	12	0.58
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	4	0.58
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	4	0.58
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	4	0.58
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	6	0.58
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	6	0.58
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	6	0.58
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	16	0.58
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	16	0.58
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	16	0.58
(1,1313)	1:156:A:ILE:HA	1:157:A:HIS:HD2	17	0.58
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB2	16	0.58
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB3	16	0.58
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB2	16	0.58
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB3	16	0.58
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB2	16	0.58
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB3	16	0.58
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	6	0.58
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	6	0.58
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	6	0.58
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	9	0.58
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	9	0.58
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	9	0.58
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	5	0.58
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	1	0.58
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	1	0.58
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	1	0.58
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	17	0.58
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	17	0.58
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	17	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	11	0.58
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	11	0.58
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	11	0.58
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	10	0.58
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	10	0.58
(1,1122)	1:126:A:SER:H	1:129:A:GLN:HG2	17	0.58
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	1	0.58
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	12	0.58
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	12	0.58
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	18	0.58
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	18	0.58
(1,1057)	1:59:A:HIS:H	1:122:A:LEU:HG	2	0.58
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	6	0.58
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	4	0.58
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	2	0.58
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	2	0.58
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	2	0.58
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	17	0.58
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	17	0.58
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	17	0.58
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	7	0.58
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	4	0.58
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	3	0.58
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	3	0.58
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	3	0.58
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	3	0.58
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	3	0.58
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	3	0.58
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	4	0.58
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	9	0.58
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	14	0.58
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	15	0.58
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	5	0.58
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	5	0.58
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	2	0.58
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	7	0.58
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	17	0.58
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	19	0.58
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	1	0.58
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	6	0.58
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	5	0.58
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	5	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	5	0.58
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	11	0.58
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	11	0.58
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	11	0.58
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	4	0.58
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	5	0.58
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	14	0.58
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	13	0.58
(1,571)	1:73:A:TRP:HE1	1:74:A:ARG:HB3	15	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	3	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	3	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	3	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	4	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	4	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	4	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	16	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	16	0.58
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	16	0.58
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	3	0.58
(1,350)	1:23:A:TYR:HE1	1:32:A:SER:HB2	13	0.58
(1,350)	1:23:A:TYR:HE2	1:32:A:SER:HB2	13	0.58
(1,224)	1:14:A:ARG:HE	1:25:A:PHE:HB3	1	0.58
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	15	0.58
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	7	0.58
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	5	0.58
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	11	0.58
(1,138)	1:21:A:ARG:HE	1:34:A:TRP:HH2	18	0.58
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	18	0.58
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	18	0.58
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	6	0.58
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	6	0.58
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	13	0.58
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	14	0.57
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	3	0.57
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	9	0.57
(2,94)	1:93:A:ILE:HG21	2:643:B:PRO:HB3	2	0.57
(2,94)	1:93:A:ILE:HG22	2:643:B:PRO:HB3	2	0.57
(2,94)	1:93:A:ILE:HG23	2:643:B:PRO:HB3	2	0.57
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	2	0.57
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	2	0.57
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	11	0.57
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	11	0.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	8	0.57
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	8	0.57
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	8	0.57
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD1	8	0.57
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD2	8	0.57
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	14	0.57
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	7	0.57
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	7	0.57
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	8	0.57
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	8	0.57
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	9	0.57
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	9	0.57
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	9	0.57
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	14	0.57
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	14	0.57
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	12	0.57
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	5	0.57
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	5	0.57
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	5	0.57
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	12	0.57
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	12	0.57
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	12	0.57
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	2	0.57
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	8	0.57
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	9	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	3	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	3	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	3	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	10	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	10	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	10	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	15	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	15	0.57
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	15	0.57
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	8	0.57
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	13	0.57
(1,1410)	1:161:A:ARG:HE	1:163:A:GLU:HG2	11	0.57
(1,1410)	1:161:A:ARG:HE	1:163:A:GLU:HG2	18	0.57
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	18	0.57
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	18	0.57
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	18	0.57
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	8	0.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	8	0.57
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	8	0.57
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	15	0.57
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	15	0.57
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	15	0.57
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	3	0.57
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	3	0.57
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	13	0.57
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	13	0.57
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	17	0.57
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	17	0.57
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	6	0.57
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	8	0.57
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	8	0.57
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	8	0.57
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	17	0.57
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	19	0.57
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	20	0.57
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	20	0.57
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	20	0.57
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	1	0.57
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	6	0.57
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	8	0.57
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	19	0.57
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	11	0.57
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	11	0.57
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	11	0.57
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	1	0.57
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	1	0.57
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	1	0.57
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	1	0.57
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	1	0.57
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	1	0.57
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	7	0.57
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	14	0.57
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	20	0.57
(1,814)	1:94:A:GLN:HG2	1:95:A:LYS:H	2	0.57
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	20	0.57
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	20	0.57
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	20	0.57
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	9	0.57
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	9	0.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	9	0.57
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	20	0.57
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	20	0.57
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	20	0.57
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	20	0.57
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	20	0.57
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	20	0.57
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	10	0.57
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	15	0.57
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	1	0.57
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	20	0.57
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	20	0.57
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	20	0.57
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD11	20	0.57
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD12	20	0.57
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD13	20	0.57
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	1	0.57
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	16	0.57
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	10	0.57
(1,571)	1:73:A:TRP:HE1	1:74:A:ARG:HB3	10	0.57
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	17	0.57
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	1	0.57
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	1	0.57
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	1	0.57
(1,401)	1:54:A:ARG:HD2	1:55:A:VAL:HA	5	0.57
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	17	0.57
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	18	0.57
(1,384)	1:7:A:LEU:HD21	1:36:A:ARG:HA	13	0.57
(1,384)	1:7:A:LEU:HD22	1:36:A:ARG:HA	13	0.57
(1,384)	1:7:A:LEU:HD23	1:36:A:ARG:HA	13	0.57
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	5	0.57
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	5	0.57
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	12	0.57
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	10	0.57
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	10	0.57
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	15	0.57
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	15	0.57
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	4	0.57
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	6	0.57
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	6	0.57
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	1	0.57
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	14	0.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	1	0.57
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	1	0.57
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	1	0.57
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	2	0.57
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	2	0.57
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	2	0.57
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	5	0.57
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	5	0.57
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	5	0.57
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	6	0.57
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	11	0.57
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	14	0.57
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	5	0.57
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	5	0.57
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	7	0.56
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	8	0.56
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	12	0.56
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	6	0.56
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	6	0.56
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	1	0.56
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	1	0.56
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	1	0.56
(2,66)	2:645:B:GLN:H	2:648:B:ILE:H	17	0.56
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	11	0.56
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	19	0.56
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	5	0.56
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	12	0.56
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	12	0.56
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	9	0.56
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	9	0.56
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	4	0.56
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	4	0.56
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	4	0.56
(1,2514)	2:646:B:GLU:HA	2:649:B:ARG:H	14	0.56
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	14	0.56
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	18	0.56
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	2	0.56
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	2	0.56
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	2	0.56
(1,1406)	1:147:A:SER:H	1:161:A:ARG:H	3	0.56
(1,1378)	1:147:A:SER:H	1:160:A:LEU:H	3	0.56
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	19	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	19	0.56
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	19	0.56
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	17	0.56
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	17	0.56
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	17	0.56
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	11	0.56
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	11	0.56
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	11	0.56
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	17	0.56
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	17	0.56
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	17	0.56
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD11	10	0.56
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD12	10	0.56
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD13	10	0.56
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	8	0.56
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	7	0.56
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	7	0.56
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	14	0.56
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	14	0.56
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	19	0.56
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	5	0.56
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	5	0.56
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	5	0.56
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	9	0.56
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	9	0.56
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	9	0.56
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	11	0.56
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	13	0.56
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	7	0.56
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	7	0.56
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	7	0.56
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	7	0.56
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	9	0.56
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	11	0.56
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	3	0.56
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	3	0.56
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	3	0.56
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	2	0.56
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	18	0.56
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	14	0.56
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	14	0.56
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	6	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	6	0.56
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	6	0.56
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	6	0.56
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	6	0.56
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	6	0.56
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	17	0.56
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	17	0.56
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	17	0.56
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	17	0.56
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	17	0.56
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	17	0.56
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	2	0.56
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	18	0.56
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	6	0.56
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	16	0.56
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	18	0.56
(1,814)	1:94:A:GLN:HG2	1:95:A:LYS:H	11	0.56
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	19	0.56
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	19	0.56
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	19	0.56
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	20	0.56
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	20	0.56
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	20	0.56
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	4	0.56
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	4	0.56
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	7	0.56
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	7	0.56
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	8	0.56
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	8	0.56
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	3	0.56
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	15	0.56
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	5	0.56
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	5	0.56
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	5	0.56
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE1	13	0.56
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE2	13	0.56
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE1	13	0.56
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE2	13	0.56
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE1	13	0.56
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE2	13	0.56
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	18	0.56
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	8	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	2	0.56
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	4	0.56
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	4	0.56
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	4	0.56
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	6	0.56
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	19	0.56
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	19	0.56
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	19	0.56
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	20	0.56
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	20	0.56
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	20	0.56
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	11	0.56
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	13	0.56
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	3	0.56
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	8	0.56
(1,178)	1:23:A:TYR:HE1	1:33:A:GLN:H	13	0.56
(1,178)	1:23:A:TYR:HE2	1:33:A:GLN:H	13	0.56
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	4	0.56
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	4	0.56
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	20	0.56
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	20	0.56
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	4	0.56
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	4	0.56
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	4	0.56
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	6	0.56
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	6	0.56
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	6	0.56
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	7	0.56
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	7	0.56
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	7	0.56
(1,138)	1:21:A:ARG:HE	1:34:A:TRP:HH2	7	0.56
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	7	0.56
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	19	0.56
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	7	0.56
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	20	0.56
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	20	0.56
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	15	0.56
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	6	0.55
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	6	0.55
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	6	0.55
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	6	0.55
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	6	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	6	0.55
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	4	0.55
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	4	0.55
(2,34)	1:59:A:HIS:H	1:122:A:LEU:HB2	10	0.55
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	9	0.55
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	9	0.55
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	17	0.55
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	17	0.55
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	16	0.55
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	16	0.55
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	14	0.55
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	14	0.55
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	6	0.55
(1,2532)	2:648:B:ILE:HG21	2:650:B:ASN:H	18	0.55
(1,2532)	2:648:B:ILE:HG22	2:650:B:ASN:H	18	0.55
(1,2532)	2:648:B:ILE:HG23	2:650:B:ASN:H	18	0.55
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	4	0.55
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD11	10	0.55
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD12	10	0.55
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD13	10	0.55
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	7	0.55
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	7	0.55
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	7	0.55
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	3	0.55
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	1	0.55
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	3	0.55
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	5	0.55
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	6	0.55
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	7	0.55
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	20	0.55
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	5	0.55
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	5	0.55
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	5	0.55
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	16	0.55
(1,2045)	1:97:A:LYS:H	1:97:A:LYS:HD2	1	0.55
(1,1504)	1:13:A:LYS:H	1:13:A:LYS:HE2	11	0.55
(1,1456)	1:6:A:LYS:H	1:6:A:LYS:HE2	2	0.55
(1,1441)	1:162:A:THR:HG21	1:163:A:GLU:HG3	19	0.55
(1,1441)	1:162:A:THR:HG22	1:163:A:GLU:HG3	19	0.55
(1,1441)	1:162:A:THR:HG23	1:163:A:GLU:HG3	19	0.55
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	18	0.55
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	13	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	13	0.55
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	13	0.55
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	19	0.55
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	19	0.55
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	19	0.55
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	6	0.55
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	6	0.55
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	6	0.55
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	6	0.55
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	6	0.55
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	6	0.55
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	14	0.55
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	14	0.55
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	14	0.55
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	20	0.55
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	20	0.55
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	20	0.55
(1,1303)	1:156:A:ILE:HG21	1:157:A:HIS:HD2	18	0.55
(1,1303)	1:156:A:ILE:HG22	1:157:A:HIS:HD2	18	0.55
(1,1303)	1:156:A:ILE:HG23	1:157:A:HIS:HD2	18	0.55
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	13	0.55
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	13	0.55
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	13	0.55
(1,1280)	1:64:A:HIS:HD2	1:156:A:ILE:HG12	6	0.55
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	12	0.55
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	15	0.55
(1,1208)	1:103:A:PHE:HD1	1:146:A:MET:HB2	13	0.55
(1,1208)	1:103:A:PHE:HD2	1:146:A:MET:HB2	13	0.55
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	6	0.55
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	5	0.55
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	5	0.55
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	5	0.55
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	8	0.55
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	8	0.55
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	8	0.55
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	14	0.55
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	14	0.55
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	14	0.55
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	15	0.55
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	15	0.55
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	15	0.55
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	16	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	16	0.55
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB1	4	0.55
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB2	4	0.55
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB3	4	0.55
(1,1057)	1:59:A:HIS:H	1:122:A:LEU:HG	19	0.55
(1,1057)	1:59:A:HIS:H	1:122:A:LEU:HG	20	0.55
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	20	0.55
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	2	0.55
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	2	0.55
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	2	0.55
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	6	0.55
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	6	0.55
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	6	0.55
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	14	0.55
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	14	0.55
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	14	0.55
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	19	0.55
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	19	0.55
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	19	0.55
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	7	0.55
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	17	0.55
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	1	0.55
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	5	0.55
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	10	0.55
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	16	0.55
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	1	0.55
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	1	0.55
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	9	0.55
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	9	0.55
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	8	0.55
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	12	0.55
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	14	0.55
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	14	0.55
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	14	0.55
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	14	0.55
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	14	0.55
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	14	0.55
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	14	0.55
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE1	18	0.55
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE2	18	0.55
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE3	18	0.55
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	6	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	13	0.55
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	13	0.55
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	13	0.55
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	17	0.55
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	17	0.55
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	17	0.55
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	9	0.55
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	9	0.55
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	9	0.55
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	19	0.55
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	19	0.55
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	19	0.55
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	18	0.55
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	18	0.55
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	18	0.55
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	18	0.55
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	18	0.55
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	18	0.55
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	10	0.55
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	10	0.55
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	10	0.55
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	9	0.55
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	9	0.55
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	1	0.55
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	6	0.55
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	19	0.55
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	9	0.55
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	17	0.55
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	9	0.55
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	7	0.55
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	19	0.55
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	19	0.55
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	19	0.55
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	19	0.55
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	6	0.55
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	6	0.55
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	6	0.55
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	10	0.55
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	10	0.55
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	10	0.55
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	11	0.55
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	11	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	11	0.55
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	17	0.55
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	8	0.55
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	14	0.55
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	15	0.55
(1,384)	1:7:A:LEU:HD21	1:36:A:ARG:HA	8	0.55
(1,384)	1:7:A:LEU:HD22	1:36:A:ARG:HA	8	0.55
(1,384)	1:7:A:LEU:HD23	1:36:A:ARG:HA	8	0.55
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	18	0.55
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	15	0.55
(1,274)	1:26:A:ASN:HD21	1:29:A:THR:HG21	20	0.55
(1,274)	1:26:A:ASN:HD21	1:29:A:THR:HG22	20	0.55
(1,274)	1:26:A:ASN:HD21	1:29:A:THR:HG23	20	0.55
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	5	0.55
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	5	0.55
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	10	0.55
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	20	0.55
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	11	0.55
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	9	0.55
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	13	0.55
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	13	0.55
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	13	0.55
(1,178)	1:23:A:TYR:HE1	1:33:A:GLN:H	20	0.55
(1,178)	1:23:A:TYR:HE2	1:33:A:GLN:H	20	0.55
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	4	0.55
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	4	0.55
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	4	0.55
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	4	0.55
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	4	0.55
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	4	0.55
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	4	0.55
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	4	0.55
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	4	0.55
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	16	0.55
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	8	0.55
(1,125)	1:15:A:MET:HA	1:21:A:ARG:H	10	0.55
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	10	0.55
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	10	0.55
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	13	0.55
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	13	0.55
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	3	0.55
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	3	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	7	0.55
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	7	0.55
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	14	0.55
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	14	0.55
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	14	0.55
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	14	0.55
(1,16)	1:6:A:LYS:HE2	1:7:A:LEU:H	13	0.55
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	15	0.54
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	15	0.54
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	15	0.54
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG12	19	0.54
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG13	19	0.54
(2,88)	1:34:A:TRP:HE1	2:641:B:TPO:H	6	0.54
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	14	0.54
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	14	0.54
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	6	0.54
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	6	0.54
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	6	0.54
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	16	0.54
(1,2596)	1:137:A:ALA:HB1	2:651:B:ILE:HG12	15	0.54
(1,2596)	1:137:A:ALA:HB1	2:651:B:ILE:HG13	15	0.54
(1,2596)	1:137:A:ALA:HB2	2:651:B:ILE:HG12	15	0.54
(1,2596)	1:137:A:ALA:HB2	2:651:B:ILE:HG13	15	0.54
(1,2596)	1:137:A:ALA:HB3	2:651:B:ILE:HG12	15	0.54
(1,2596)	1:137:A:ALA:HB3	2:651:B:ILE:HG13	15	0.54
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE1	18	0.54
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE2	18	0.54
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	6	0.54
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	6	0.54
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	12	0.54
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	12	0.54
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	10	0.54
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	10	0.54
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	14	0.54
(1,2513)	2:646:B:GLU:HA	2:649:B:ARG:HD2	10	0.54
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	5	0.54
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	4	0.54
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	11	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	4	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	4	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	4	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	11	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	11	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	11	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	13	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	13	0.54
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	13	0.54
(1,1504)	1:13:A:LYS:H	1:13:A:LYS:HE2	13	0.54
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	18	0.54
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG21	20	0.54
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG22	20	0.54
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG23	20	0.54
(1,1402)	1:143:A:THR:HG21	1:161:A:ARG:HD2	5	0.54
(1,1402)	1:143:A:THR:HG22	1:161:A:ARG:HD2	5	0.54
(1,1402)	1:143:A:THR:HG23	1:161:A:ARG:HD2	5	0.54
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	2	0.54
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	2	0.54
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	2	0.54
(1,1328)	1:89:A:ILE:HG12	1:158:A:ILE:HB	5	0.54
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	15	0.54
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	15	0.54
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	15	0.54
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	9	0.54
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	9	0.54
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	9	0.54
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	11	0.54
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	11	0.54
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	11	0.54
(1,1303)	1:156:A:ILE:HG21	1:157:A:HIS:HD2	13	0.54
(1,1303)	1:156:A:ILE:HG22	1:157:A:HIS:HD2	13	0.54
(1,1303)	1:156:A:ILE:HG23	1:157:A:HIS:HD2	13	0.54
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG21	4	0.54
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG22	4	0.54
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG23	4	0.54
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	10	0.54
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	10	0.54
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	10	0.54
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	13	0.54
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	13	0.54
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	13	0.54
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	4	0.54
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	5	0.54
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	18	0.54
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	12	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1208)	1:103:A:PHE:HD1	1:146:A:MET:HB2	2	0.54
(1,1208)	1:103:A:PHE:HD2	1:146:A:MET:HB2	2	0.54
(1,1208)	1:103:A:PHE:HD1	1:146:A:MET:HB2	10	0.54
(1,1208)	1:103:A:PHE:HD2	1:146:A:MET:HB2	10	0.54
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	10	0.54
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	10	0.54
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	10	0.54
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	5	0.54
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	7	0.54
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	7	0.54
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	4	0.54
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	12	0.54
(1,1058)	1:59:A:HIS:HD2	1:122:A:LEU:HD11	16	0.54
(1,1058)	1:59:A:HIS:HD2	1:122:A:LEU:HD12	16	0.54
(1,1058)	1:59:A:HIS:HD2	1:122:A:LEU:HD13	16	0.54
(1,1057)	1:59:A:HIS:H	1:122:A:LEU:HG	11	0.54
(1,1027)	1:118:A:ALA:HA	1:119:A:ARG:HG2	15	0.54
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	12	0.54
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	8	0.54
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	10	0.54
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	10	0.54
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	10	0.54
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	20	0.54
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	6	0.54
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	9	0.54
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE1	10	0.54
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE2	10	0.54
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE3	10	0.54
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE1	10	0.54
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE2	10	0.54
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE3	10	0.54
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE1	18	0.54
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE2	18	0.54
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE3	18	0.54
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE1	18	0.54
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE2	18	0.54
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE3	18	0.54
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	7	0.54
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	7	0.54
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	5	0.54
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	4	0.54
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	4	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	4	0.54
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	4	0.54
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	4	0.54
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	4	0.54
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE1	13	0.54
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE2	13	0.54
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE3	13	0.54
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	3	0.54
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	8	0.54
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	8	0.54
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	13	0.54
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	18	0.54
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	18	0.54
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	18	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	1	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	1	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	1	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	7	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	7	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	7	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	12	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	12	0.54
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	12	0.54
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	2	0.54
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	2	0.54
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	2	0.54
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	11	0.54
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	11	0.54
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	11	0.54
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	16	0.54
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	16	0.54
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	16	0.54
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	20	0.54
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	20	0.54
(1,752)	1:89:A:ILE:HB	1:91:A:GLY:H	11	0.54
(1,695)	1:86:A:LEU:HD21	1:149:A:PRO:HD3	20	0.54
(1,695)	1:86:A:LEU:HD22	1:149:A:PRO:HD3	20	0.54
(1,695)	1:86:A:LEU:HD23	1:149:A:PRO:HD3	20	0.54
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	6	0.54
(1,640)	1:65:A:SER:HB3	1:81:A:THR:HA	13	0.54
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	5	0.54
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	1	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	9	0.54
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	15	0.54
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	1	0.54
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	1	0.54
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	1	0.54
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	8	0.54
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	10	0.54
(1,520)	1:64:A:HIS:HE1	1:66:A:GLN:HG2	19	0.54
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	7	0.54
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	7	0.54
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	7	0.54
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	11	0.54
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	11	0.54
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	11	0.54
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	6	0.54
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	6	0.54
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	6	0.54
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	6	0.54
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	8	0.54
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	11	0.54
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	9	0.54
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	20	0.54
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	2	0.54
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	7	0.54
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	20	0.54
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	3	0.54
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	3	0.54
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	10	0.54
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	18	0.54
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	18	0.54
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	20	0.54
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	6	0.54
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	20	0.54
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	2	0.54
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	9	0.54
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	20	0.54
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	20	0.54
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	20	0.54
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	9	0.53
(2,88)	1:34:A:TRP:HE1	2:641:B:TPO:H	5	0.53
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	9	0.53
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	9	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	9	0.53
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	12	0.53
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	12	0.53
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	12	0.53
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	12	0.53
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	12	0.53
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	12	0.53
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	19	0.53
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	19	0.53
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	19	0.53
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	14	0.53
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	14	0.53
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	14	0.53
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	14	0.53
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	14	0.53
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	14	0.53
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	18	0.53
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	14	0.53
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	14	0.53
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD11	19	0.53
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD12	19	0.53
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD13	19	0.53
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	7	0.53
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	15	0.53
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	15	0.53
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	15	0.53
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	16	0.53
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	19	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	8	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	8	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	8	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	9	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	9	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	9	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	19	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	19	0.53
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	19	0.53
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	8	0.53
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	9	0.53
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	14	0.53
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	16	0.53
(1,1429)	1:143:A:THR:HG21	1:163:A:GLU:HB2	20	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1429)	1:143:A:THR:HG22	1:163:A:GLU:HB2	20	0.53
(1,1429)	1:143:A:THR:HG23	1:163:A:GLU:HB2	20	0.53
(1,1402)	1:143:A:THR:HG21	1:161:A:ARG:HD2	6	0.53
(1,1402)	1:143:A:THR:HG22	1:161:A:ARG:HD2	6	0.53
(1,1402)	1:143:A:THR:HG23	1:161:A:ARG:HD2	6	0.53
(1,1328)	1:89:A:ILE:HG12	1:158:A:ILE:HB	8	0.53
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	1	0.53
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	1	0.53
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	1	0.53
(1,1313)	1:156:A:ILE:HA	1:157:A:HIS:HD2	20	0.53
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	5	0.53
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	5	0.53
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	5	0.53
(1,1276)	1:63:A:LYS:HA	1:155:A:GLY:HA2	3	0.53
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	19	0.53
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	17	0.53
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	17	0.53
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	17	0.53
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	19	0.53
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	16	0.53
(1,1057)	1:59:A:HIS:H	1:122:A:LEU:HG	13	0.53
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	3	0.53
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	14	0.53
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	8	0.53
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	8	0.53
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	13	0.53
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	13	0.53
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	6	0.53
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	15	0.53
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	15	0.53
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	15	0.53
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	15	0.53
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	15	0.53
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	15	0.53
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	15	0.53
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE1	16	0.53
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE2	16	0.53
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE3	16	0.53
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	12	0.53
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	12	0.53
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	12	0.53
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	2	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	2	0.53
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	2	0.53
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	14	0.53
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	14	0.53
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	14	0.53
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	6	0.53
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	6	0.53
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	6	0.53
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	10	0.53
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	10	0.53
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	10	0.53
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	8	0.53
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	8	0.53
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	8	0.53
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	6	0.53
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	6	0.53
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	13	0.53
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	13	0.53
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	11	0.53
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	12	0.53
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	12	0.53
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	12	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	3	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	3	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	3	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	6	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	6	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	6	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	12	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	12	0.53
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	12	0.53
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	10	0.53
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	5	0.53
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	7	0.53
(1,646)	1:81:A:THR:HG21	1:84:A:GLU:HB2	17	0.53
(1,646)	1:81:A:THR:HG22	1:84:A:GLU:HB2	17	0.53
(1,646)	1:81:A:THR:HG23	1:84:A:GLU:HB2	17	0.53
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG21	6	0.53
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG22	6	0.53
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG23	6	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	5	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	5	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	5	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	8	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	8	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	8	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	12	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	12	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	12	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	14	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	14	0.53
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	14	0.53
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	19	0.53
(1,531)	1:64:A:HIS:HE1	1:67:A:SER:HB2	10	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	8	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	8	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	8	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	13	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	13	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	13	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	18	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	18	0.53
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	18	0.53
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	5	0.53
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	5	0.53
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	5	0.53
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	2	0.53
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	2	0.53
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	2	0.53
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	18	0.53
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	18	0.53
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	18	0.53
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	10	0.53
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	10	0.53
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	10	0.53
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	10	0.53
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	10	0.53
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	10	0.53
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	10	0.53
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	10	0.53
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	10	0.53
(1,440)	1:59:A:HIS:H	1:115:A:SER:HB3	15	0.53
(1,440)	1:59:A:HIS:H	1:115:A:SER:HB3	17	0.53
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	15	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	15	0.53
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	16	0.53
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	17	0.53
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	3	0.53
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	7	0.53
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	2	0.53
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	19	0.53
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	1	0.53
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	8	0.53
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	14	0.53
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	14	0.53
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	17	0.53
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	17	0.53
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	17	0.53
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	2	0.53
(1,116)	1:16:A:SER:H	1:20:A:GLY:HA2	2	0.53
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	9	0.53
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	16	0.53
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	9	0.53
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	14	0.53
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	14	0.53
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	16	0.53
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	16	0.53
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	10	0.53
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	10	0.53
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	10	0.53
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	15	0.53
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	15	0.53
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	15	0.53
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	17	0.53
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	17	0.53
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	17	0.53
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	7	0.52
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	7	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	3	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	3	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	3	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	3	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	3	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	3	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	13	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	13	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	13	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	13	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	13	0.52
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	13	0.52
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	18	0.52
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	18	0.52
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	18	0.52
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	18	0.52
(2,71)	2:651:B:ILE:HG21	2:656:B:PHE:H	3	0.52
(2,71)	2:651:B:ILE:HG22	2:656:B:PHE:H	3	0.52
(2,71)	2:651:B:ILE:HG23	2:656:B:PHE:H	3	0.52
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	11	0.52
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	11	0.52
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	11	0.52
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	8	0.52
(2,5)	1:23:A:TYR:H	1:34:A:TRP:HZ3	3	0.52
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	8	0.52
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	8	0.52
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	7	0.52
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	7	0.52
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	6	0.52
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	6	0.52
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	7	0.52
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	7	0.52
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	6	0.52
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	12	0.52
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	17	0.52
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	17	0.52
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	17	0.52
(1,1504)	1:13:A:LYS:H	1:13:A:LYS:HE2	17	0.52
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	10	0.52
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	10	0.52
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	10	0.52
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	7	0.52
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	7	0.52
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	7	0.52
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	20	0.52
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	20	0.52
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	20	0.52
(1,1355)	1:57:A:CYS:HB2	1:160:A:LEU:H	19	0.52
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	19	0.52
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	4	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	4	0.52
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	4	0.52
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	1	0.52
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	1	0.52
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	1	0.52
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	4	0.52
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	4	0.52
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	4	0.52
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	8	0.52
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	8	0.52
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	8	0.52
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	19	0.52
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	19	0.52
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	19	0.52
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	9	0.52
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	16	0.52
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	4	0.52
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	4	0.52
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	4	0.52
(1,1125)	1:129:A:GLN:HG2	1:130:A:MET:H	17	0.52
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	4	0.52
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	14	0.52
(1,1057)	1:59:A:HIS:H	1:122:A:LEU:HG	10	0.52
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	15	0.52
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	14	0.52
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	5	0.52
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	5	0.52
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	5	0.52
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	12	0.52
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	12	0.52
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	12	0.52
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	3	0.52
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	8	0.52
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	11	0.52
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	12	0.52
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	20	0.52
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	17	0.52
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	17	0.52
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	10	0.52
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE1	20	0.52
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE2	20	0.52
(1,840)	1:97:A:LYS:HG2	1:146:A:MET:HE3	20	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	5	0.52
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	10	0.52
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	10	0.52
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	10	0.52
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	3	0.52
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	3	0.52
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	3	0.52
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	4	0.52
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	4	0.52
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	4	0.52
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	16	0.52
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	16	0.52
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	16	0.52
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	16	0.52
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	16	0.52
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	16	0.52
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	5	0.52
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	5	0.52
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	5	0.52
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	16	0.52
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	16	0.52
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	17	0.52
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE1	12	0.52
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE2	12	0.52
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE1	12	0.52
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE2	12	0.52
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE1	12	0.52
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE2	12	0.52
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	2	0.52
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	2	0.52
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	2	0.52
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	9	0.52
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	9	0.52
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	9	0.52
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	11	0.52
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	14	0.52
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	14	0.52
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	14	0.52
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	8	0.52
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	5	0.52
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	13	0.52
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	13	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	13	0.52
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	16	0.52
(1,531)	1:64:A:HIS:HE1	1:67:A:SER:HB2	15	0.52
(1,531)	1:64:A:HIS:HE1	1:67:A:SER:HB2	19	0.52
(1,530)	1:64:A:HIS:HE1	1:67:A:SER:HA	19	0.52
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	1	0.52
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	1	0.52
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	1	0.52
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	8	0.52
(1,514)	1:63:A:LYS:HB2	1:70:A:PRO:HA	18	0.52
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	14	0.52
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	14	0.52
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	14	0.52
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	17	0.52
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	17	0.52
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	17	0.52
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	18	0.52
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	18	0.52
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	18	0.52
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	11	0.52
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	11	0.52
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	11	0.52
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	11	0.52
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	11	0.52
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	11	0.52
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	11	0.52
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	11	0.52
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	11	0.52
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	4	0.52
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	13	0.52
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	13	0.52
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	12	0.52
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	17	0.52
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	2	0.52
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	15	0.52
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	10	0.52
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	1	0.52
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	1	0.52
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	1	0.52
(1,267)	1:26:A:ASN:HD21	1:28:A:ILE:HG12	20	0.52
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	1	0.52
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	1	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	5	0.52
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	5	0.52
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	20	0.52
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	1	0.52
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	1	0.52
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	1	0.52
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	1	0.52
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	1	0.52
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	1	0.52
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	1	0.52
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	1	0.52
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	1	0.52
(1,138)	1:21:A:ARG:HE	1:34:A:TRP:HH2	5	0.52
(1,138)	1:21:A:ARG:HE	1:34:A:TRP:HH2	12	0.52
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	17	0.52
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	16	0.52
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	16	0.52
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	20	0.52
(1,70)	1:12:A:GLU:HG2	1:13:A:LYS:H	8	0.52
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	9	0.52
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	9	0.52
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	18	0.52
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	18	0.52
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	12	0.52
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	17	0.52
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	12	0.51
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	12	0.51
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	16	0.51
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	5	0.51
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	19	0.51
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	19	0.51
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	19	0.51
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	5	0.51
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	20	0.51
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	19	0.51
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	19	0.51
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	20	0.51
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	20	0.51
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	12	0.51
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	12	0.51
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	14	0.51
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	14	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	14	0.51
(1,2529)	2:648:B:ILE:HG21	2:649:B:ARG:HD2	19	0.51
(1,2529)	2:648:B:ILE:HG22	2:649:B:ARG:HD2	19	0.51
(1,2529)	2:648:B:ILE:HG23	2:649:B:ARG:HD2	19	0.51
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	4	0.51
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	1	0.51
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	1	0.51
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	1	0.51
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	9	0.51
(1,1441)	1:162:A:THR:HG21	1:163:A:GLU:HG3	12	0.51
(1,1441)	1:162:A:THR:HG22	1:163:A:GLU:HG3	12	0.51
(1,1441)	1:162:A:THR:HG23	1:163:A:GLU:HG3	12	0.51
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	9	0.51
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG21	11	0.51
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG22	11	0.51
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG23	11	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG21	11	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG22	11	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG23	11	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG21	11	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG22	11	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG23	11	0.51
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG21	17	0.51
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG22	17	0.51
(1,1392)	1:160:A:LEU:HD11	1:162:A:THR:HG23	17	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG21	17	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG22	17	0.51
(1,1392)	1:160:A:LEU:HD12	1:162:A:THR:HG23	17	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG21	17	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG22	17	0.51
(1,1392)	1:160:A:LEU:HD13	1:162:A:THR:HG23	17	0.51
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	18	0.51
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	18	0.51
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	18	0.51
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	3	0.51
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	3	0.51
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	3	0.51
(1,1328)	1:89:A:ILE:HG12	1:158:A:ILE:HB	12	0.51
(1,1328)	1:89:A:ILE:HG12	1:158:A:ILE:HB	13	0.51
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	3	0.51
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	3	0.51
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	3	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	7	0.51
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	7	0.51
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	7	0.51
(1,1313)	1:156:A:ILE:HA	1:157:A:HIS:HD2	11	0.51
(1,1313)	1:156:A:ILE:HA	1:157:A:HIS:HD2	18	0.51
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	20	0.51
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	20	0.51
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	20	0.51
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG21	16	0.51
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG22	16	0.51
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG23	16	0.51
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	1	0.51
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	19	0.51
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	19	0.51
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	18	0.51
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	6	0.51
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	10	0.51
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	10	0.51
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	10	0.51
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	16	0.51
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	20	0.51
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	11	0.51
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	13	0.51
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	13	0.51
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	13	0.51
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	17	0.51
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	15	0.51
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE1	2	0.51
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE2	2	0.51
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE3	2	0.51
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE1	2	0.51
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE2	2	0.51
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE3	2	0.51
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	5	0.51
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	5	0.51
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	6	0.51
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	6	0.51
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	12	0.51
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	12	0.51
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	1	0.51
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	3	0.51
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	7	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	9	0.51
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	9	0.51
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	9	0.51
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	9	0.51
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	9	0.51
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	9	0.51
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	11	0.51
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	11	0.51
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	11	0.51
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	11	0.51
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	11	0.51
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	11	0.51
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	12	0.51
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	12	0.51
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	12	0.51
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	12	0.51
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	12	0.51
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	12	0.51
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	13	0.51
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	10	0.51
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	18	0.51
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	18	0.51
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	18	0.51
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	2	0.51
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	2	0.51
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	2	0.51
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	2	0.51
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	2	0.51
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	2	0.51
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	4	0.51
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	4	0.51
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	4	0.51
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	4	0.51
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	4	0.51
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	4	0.51
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	7	0.51
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	7	0.51
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	7	0.51
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	10	0.51
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	10	0.51
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	10	0.51
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	1	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	1	0.51
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	1	0.51
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	14	0.51
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	14	0.51
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	14	0.51
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	19	0.51
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	19	0.51
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	19	0.51
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	19	0.51
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	6	0.51
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	12	0.51
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	11	0.51
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	3	0.51
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	14	0.51
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	6	0.51
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	7	0.51
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	5	0.51
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	5	0.51
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	5	0.51
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD21	12	0.51
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD22	12	0.51
(1,498)	1:62:A:VAL:HA	1:88:A:LEU:HD23	12	0.51
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	3	0.51
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	3	0.51
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	3	0.51
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	3	0.51
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	3	0.51
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	3	0.51
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	3	0.51
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	3	0.51
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	3	0.51
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	13	0.51
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	12	0.51
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	19	0.51
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	7	0.51
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	7	0.51
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	20	0.51
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	20	0.51
(1,334)	1:27:A:HIS:HA	1:31:A:ALA:H	8	0.51
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	6	0.51
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	7	0.51
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	6	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	17	0.51
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	8	0.51
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	8	0.51
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	8	0.51
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	18	0.51
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	18	0.51
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	18	0.51
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	1	0.51
(1,181)	1:23:A:TYR:HB2	1:34:A:TRP:HE3	11	0.51
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	16	0.51
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	16	0.51
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	16	0.51
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	20	0.51
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	20	0.51
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	20	0.51
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	7	0.51
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	14	0.51
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	17	0.51
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	5	0.51
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	3	0.51
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	3	0.51
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	3	0.51
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	15	0.51
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	15	0.51
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	2	0.51
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	2	0.51
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	4	0.51
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	4	0.51
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	17	0.51
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	17	0.51
(1,44)	1:8:A:PRO:HB2	1:11:A:TRP:HE1	3	0.51
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	16	0.51
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	6	0.51
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	14	0.51
(2,102)	1:135:A:GLU:H	2:656:B:PHE:HB2	11	0.5
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	14	0.5
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	14	0.5
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	14	0.5
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	18	0.5
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	15	0.5
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	20	0.5
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	20	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	20	0.5
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	20	0.5
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	20	0.5
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	20	0.5
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	11	0.5
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	11	0.5
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	1	0.5
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	1	0.5
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	4	0.5
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	4	0.5
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	8	0.5
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	8	0.5
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	1	0.5
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	1	0.5
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	1	0.5
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	4	0.5
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	4	0.5
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	4	0.5
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	1	0.5
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	3	0.5
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD11	16	0.5
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD12	16	0.5
(1,2525)	2:645:B:GLN:HE22	2:648:B:ILE:HD13	16	0.5
(1,2513)	2:646:B:GLU:HA	2:649:B:ARG:HD2	13	0.5
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	9	0.5
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	10	0.5
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	7	0.5
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	7	0.5
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	7	0.5
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	12	0.5
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	12	0.5
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	12	0.5
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	11	0.5
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	16	0.5
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	20	0.5
(1,1435)	1:161:A:ARG:HG3	1:163:A:GLU:H	20	0.5
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	5	0.5
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	10	0.5
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	15	0.5
(1,1428)	1:143:A:THR:HG21	1:163:A:GLU:H	10	0.5
(1,1428)	1:143:A:THR:HG22	1:163:A:GLU:H	10	0.5
(1,1428)	1:143:A:THR:HG23	1:163:A:GLU:H	10	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	6	0.5
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	12	0.5
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	12	0.5
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	12	0.5
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	17	0.5
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	17	0.5
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	17	0.5
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	13	0.5
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	13	0.5
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	13	0.5
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG21	1	0.5
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG22	1	0.5
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG23	1	0.5
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	12	0.5
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	12	0.5
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	12	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	9	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	9	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	9	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	14	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	14	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	14	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	16	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	16	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	16	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	20	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	20	0.5
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	20	0.5
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD11	19	0.5
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD12	19	0.5
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD13	19	0.5
(1,1276)	1:63:A:LYS:HA	1:155:A:GLY:HA2	12	0.5
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	15	0.5
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	15	0.5
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	15	0.5
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	7	0.5
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	9	0.5
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	14	0.5
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	14	0.5
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	14	0.5
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	15	0.5
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	15	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	15	0.5
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	6	0.5
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	6	0.5
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	6	0.5
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	13	0.5
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	14	0.5
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	19	0.5
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	18	0.5
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	18	0.5
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	20	0.5
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	20	0.5
(1,844)	1:97:A:LYS:HG2	1:98:A:SER:H	2	0.5
(1,830)	1:93:A:ILE:HG21	1:97:A:LYS:HD2	1	0.5
(1,830)	1:93:A:ILE:HG22	1:97:A:LYS:HD2	1	0.5
(1,830)	1:93:A:ILE:HG23	1:97:A:LYS:HD2	1	0.5
(1,814)	1:94:A:GLN:HG2	1:95:A:LYS:H	17	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	6	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	6	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	6	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	7	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	7	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	7	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	8	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	8	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	8	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	16	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	16	0.5
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	16	0.5
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	7	0.5
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	7	0.5
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	7	0.5
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	14	0.5
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	14	0.5
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	14	0.5
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	1	0.5
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	1	0.5
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	1	0.5
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	1	0.5
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	1	0.5
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	1	0.5
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	13	0.5
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	13	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	13	0.5
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	14	0.5
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	14	0.5
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	2	0.5
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	2	0.5
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	2	0.5
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	3	0.5
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	3	0.5
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	3	0.5
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	4	0.5
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	4	0.5
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	4	0.5
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	6	0.5
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	6	0.5
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	6	0.5
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	11	0.5
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	11	0.5
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	11	0.5
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	15	0.5
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	15	0.5
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	15	0.5
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	16	0.5
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	16	0.5
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	16	0.5
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	18	0.5
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	18	0.5
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	18	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	4	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	4	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	4	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	5	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	5	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	5	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	8	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	8	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	8	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	16	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	16	0.5
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	16	0.5
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG21	4	0.5
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG22	4	0.5
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG23	4	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	3	0.5
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	17	0.5
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	6	0.5
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	6	0.5
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	6	0.5
(1,572)	1:73:A:TRP:HE1	1:111:A:SER:HB2	9	0.5
(1,571)	1:73:A:TRP:HE1	1:74:A:ARG:HB3	17	0.5
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	4	0.5
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	9	0.5
(1,471)	1:61:A:LEU:HD21	1:63:A:LYS:HA	18	0.5
(1,471)	1:61:A:LEU:HD22	1:63:A:LYS:HA	18	0.5
(1,471)	1:61:A:LEU:HD23	1:63:A:LYS:HA	18	0.5
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	5	0.5
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	9	0.5
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	9	0.5
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	9	0.5
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	18	0.5
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	16	0.5
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	16	0.5
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	6	0.5
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	17	0.5
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	17	0.5
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	9	0.5
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	10	0.5
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	4	0.5
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	14	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	4	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	4	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	4	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	5	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	5	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	5	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	10	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	10	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	10	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	14	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	14	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	14	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	19	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	19	0.5
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	19	0.5
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	3	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	5	0.5
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	1	0.5
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	8	0.5
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	12	0.5
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	19	0.5
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	19	0.5
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	4	0.5
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	4	0.5
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	4	0.5
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD1	12	0.5
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD2	12	0.5
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	8	0.5
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	8	0.5
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	20	0.5
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	6	0.5
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	6	0.5
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	6	0.5
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	7	0.5
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	7	0.5
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	7	0.5
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	9	0.5
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	9	0.5
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	9	0.5
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	5	0.49
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	5	0.49
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	13	0.49
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	13	0.49
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	13	0.49
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	13	0.49
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	13	0.49
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	13	0.49
(2,94)	1:93:A:ILE:HG21	2:643:B:PRO:HB3	13	0.49
(2,94)	1:93:A:ILE:HG22	2:643:B:PRO:HB3	13	0.49
(2,94)	1:93:A:ILE:HG23	2:643:B:PRO:HB3	13	0.49
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	12	0.49
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	12	0.49
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	13	0.49
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	13	0.49
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE1	18	0.49
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE2	18	0.49
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE1	18	0.49
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE2	18	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	17	0.49
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD1	7	0.49
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD2	7	0.49
(2,34)	1:59:A:HIS:H	1:122:A:LEU:HB2	18	0.49
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	5	0.49
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	15	0.49
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	15	0.49
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	3	0.49
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	3	0.49
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	3	0.49
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	17	0.49
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	17	0.49
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	17	0.49
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	14	0.49
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	5	0.49
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	6	0.49
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	6	0.49
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	6	0.49
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD21	18	0.49
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD22	18	0.49
(1,2084)	1:106:A:LEU:H	1:106:A:LEU:HD23	18	0.49
(1,2022)	1:94:A:GLN:H	1:94:A:GLN:HG2	20	0.49
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	1	0.49
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	4	0.49
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	6	0.49
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	7	0.49
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	15	0.49
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	18	0.49
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	19	0.49
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	9	0.49
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD21	11	0.49
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD22	11	0.49
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD23	11	0.49
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD21	11	0.49
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD22	11	0.49
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD23	11	0.49
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD21	11	0.49
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD22	11	0.49
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD23	11	0.49
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	1	0.49
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	1	0.49
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	1	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	5	0.49
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	5	0.49
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	5	0.49
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	5	0.49
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	5	0.49
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	5	0.49
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	5	0.49
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	5	0.49
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	5	0.49
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	5	0.49
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	5	0.49
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	5	0.49
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	6	0.49
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	6	0.49
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	6	0.49
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	6	0.49
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	6	0.49
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	6	0.49
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	6	0.49
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	6	0.49
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	6	0.49
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	5	0.49
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	3	0.49
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	3	0.49
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	3	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	8	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	8	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	8	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	18	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	18	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	18	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	20	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	20	0.49
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	20	0.49
(1,1280)	1:64:A:HIS:HD2	1:156:A:ILE:HG12	9	0.49
(1,1240)	1:150:A:VAL:H	1:157:A:HIS:HD2	10	0.49
(1,1231)	1:149:A:PRO:HG2	1:150:A:VAL:H	8	0.49
(1,1231)	1:149:A:PRO:HG2	1:150:A:VAL:H	12	0.49
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	1	0.49
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	1	0.49
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	2	0.49
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	2	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	2	0.49
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	3	0.49
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	3	0.49
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	3	0.49
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	4	0.49
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	5	0.49
(1,1143)	1:130:A:MET:HB2	1:135:A:GLU:H	13	0.49
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	10	0.49
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	17	0.49
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	11	0.49
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	11	0.49
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	11	0.49
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	14	0.49
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	6	0.49
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	6	0.49
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	6	0.49
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB1	11	0.49
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB2	11	0.49
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB3	11	0.49
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	16	0.49
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	12	0.49
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	15	0.49
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	3	0.49
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	3	0.49
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	4	0.49
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	4	0.49
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	16	0.49
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	16	0.49
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	9	0.49
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	12	0.49
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	12	0.49
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	12	0.49
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	6	0.49
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	6	0.49
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	6	0.49
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	6	0.49
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	6	0.49
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	6	0.49
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	4	0.49
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	4	0.49
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	4	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	7	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	7	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	7	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	11	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	11	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	11	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	13	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	13	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	13	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	15	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	15	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	15	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	20	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	20	0.49
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	20	0.49
(1,693)	1:86:A:LEU:HD21	1:149:A:PRO:HD2	9	0.49
(1,693)	1:86:A:LEU:HD22	1:149:A:PRO:HD2	9	0.49
(1,693)	1:86:A:LEU:HD23	1:149:A:PRO:HD2	9	0.49
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	7	0.49
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	7	0.49
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	7	0.49
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	11	0.49
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	11	0.49
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	11	0.49
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	6	0.49
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	6	0.49
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	6	0.49
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	6	0.49
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	2	0.49
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	2	0.49
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	2	0.49
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	2	0.49
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	2	0.49
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	2	0.49
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	2	0.49
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	2	0.49
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	2	0.49
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	16	0.49
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	16	0.49
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	16	0.49
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	16	0.49
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	16	0.49
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	16	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	16	0.49
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	16	0.49
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	16	0.49
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	8	0.49
(1,375)	1:33:A:GLN:HE21	1:35:A:GLU:H	11	0.49
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	12	0.49
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	13	0.49
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	6	0.49
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	6	0.49
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	12	0.49
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	12	0.49
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD11	18	0.49
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD12	18	0.49
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD13	18	0.49
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	1	0.49
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	3	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	11	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	11	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	11	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	16	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	16	0.49
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	16	0.49
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	14	0.49
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	14	0.49
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	3	0.49
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	18	0.49
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	18	0.49
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	4	0.49
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	5	0.49
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	7	0.49
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	12	0.49
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	1	0.49
(1,44)	1:8:A:PRO:HB2	1:11:A:TRP:HE1	11	0.49
(1,28)	1:7:A:LEU:HD21	1:13:A:LYS:HG3	4	0.49
(1,28)	1:7:A:LEU:HD22	1:13:A:LYS:HG3	4	0.49
(1,28)	1:7:A:LEU:HD23	1:13:A:LYS:HG3	4	0.49
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	1	0.49
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	1	0.49
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	1	0.49
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	5	0.49
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	5	0.49
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	5	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	1	0.48
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	13	0.48
(2,66)	2:645:B:GLN:H	2:648:B:ILE:H	16	0.48
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	1	0.48
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	1	0.48
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	10	0.48
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	10	0.48
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	10	0.48
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	10	0.48
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	10	0.48
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	10	0.48
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	19	0.48
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	19	0.48
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	6	0.48
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	6	0.48
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	7	0.48
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	16	0.48
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	9	0.48
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	10	0.48
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	14	0.48
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	14	0.48
(1,1504)	1:13:A:LYS:H	1:13:A:LYS:HE2	2	0.48
(1,1504)	1:13:A:LYS:H	1:13:A:LYS:HE2	10	0.48
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD21	10	0.48
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD22	10	0.48
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD23	10	0.48
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	10	0.48
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	18	0.48
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	18	0.48
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	18	0.48
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	1	0.48
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	1	0.48
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	1	0.48
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG21	15	0.48
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG22	15	0.48
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG23	15	0.48
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	19	0.48
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	19	0.48
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	19	0.48
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	2	0.48
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	2	0.48
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	2	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD11	13	0.48
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD12	13	0.48
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD13	13	0.48
(1,1242)	1:150:A:VAL:HG11	1:157:A:HIS:H	4	0.48
(1,1242)	1:150:A:VAL:HG12	1:157:A:HIS:H	4	0.48
(1,1242)	1:150:A:VAL:HG13	1:157:A:HIS:H	4	0.48
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	17	0.48
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	13	0.48
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	2	0.48
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	17	0.48
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	8	0.48
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	8	0.48
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	17	0.48
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	17	0.48
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	17	0.48
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	17	0.48
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	17	0.48
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	17	0.48
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	8	0.48
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	12	0.48
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	2	0.48
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	5	0.48
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	18	0.48
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	5	0.48
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	5	0.48
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	5	0.48
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	16	0.48
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	11	0.48
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	12	0.48
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	2	0.48
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	14	0.48
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	11	0.48
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	11	0.48
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	19	0.48
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	19	0.48
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	19	0.48
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	20	0.48
(1,814)	1:94:A:GLN:HG2	1:95:A:LYS:H	20	0.48
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	11	0.48
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	11	0.48
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	11	0.48
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	6	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	6	0.48
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	6	0.48
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	16	0.48
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	9	0.48
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	9	0.48
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	9	0.48
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	6	0.48
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	6	0.48
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	6	0.48
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	18	0.48
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	18	0.48
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	18	0.48
(1,693)	1:86:A:LEU:HD21	1:149:A:PRO:HD2	13	0.48
(1,693)	1:86:A:LEU:HD22	1:149:A:PRO:HD2	13	0.48
(1,693)	1:86:A:LEU:HD23	1:149:A:PRO:HD2	13	0.48
(1,693)	1:86:A:LEU:HD21	1:149:A:PRO:HD2	20	0.48
(1,693)	1:86:A:LEU:HD22	1:149:A:PRO:HD2	20	0.48
(1,693)	1:86:A:LEU:HD23	1:149:A:PRO:HD2	20	0.48
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG21	15	0.48
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG22	15	0.48
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG23	15	0.48
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	9	0.48
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	9	0.48
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	9	0.48
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	15	0.48
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	15	0.48
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	15	0.48
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	10	0.48
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	14	0.48
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	15	0.48
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	15	0.48
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	15	0.48
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	15	0.48
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	15	0.48
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	15	0.48
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	15	0.48
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	15	0.48
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	15	0.48
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	15	0.48
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	15	0.48
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	15	0.48
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	7	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	10	0.48
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	10	0.48
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	11	0.48
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	14	0.48
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	1	0.48
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	2	0.48
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	2	0.48
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	2	0.48
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	13	0.48
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	13	0.48
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	13	0.48
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	18	0.48
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	18	0.48
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	9	0.48
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	7	0.48
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	9	0.48
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	9	0.48
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	19	0.48
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	1	0.48
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	1	0.48
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	9	0.48
(1,123)	1:15:A:MET:HE1	1:20:A:GLY:H	10	0.48
(1,123)	1:15:A:MET:HE2	1:20:A:GLY:H	10	0.48
(1,123)	1:15:A:MET:HE3	1:20:A:GLY:H	10	0.48
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	2	0.48
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	2	0.48
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	12	0.48
(1,44)	1:8:A:PRO:HB2	1:11:A:TRP:HE1	4	0.48
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	12	0.48
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	12	0.48
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	12	0.48
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	16	0.48
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	16	0.48
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	16	0.48
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	1	0.48
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	20	0.47
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	4	0.47
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	4	0.47
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	16	0.47
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	16	0.47
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	11	0.47
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	6	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	18	0.47
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	11	0.47
(1,2597)	1:138:A:SER:H	2:656:B:PHE:HB2	20	0.47
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	9	0.47
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	9	0.47
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	17	0.47
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	17	0.47
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	17	0.47
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	3	0.47
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	3	0.47
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	7	0.47
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	5	0.47
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	14	0.47
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	14	0.47
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	14	0.47
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	19	0.47
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	19	0.47
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	19	0.47
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	19	0.47
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	2	0.47
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	17	0.47
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	1	0.47
(1,1560)	1:18:A:SER:H	1:18:A:SER:HB3	11	0.47
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	5	0.47
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	7	0.47
(1,1399)	1:143:A:THR:H	1:161:A:ARG:HD2	16	0.47
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD21	8	0.47
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD22	8	0.47
(1,1376)	1:146:A:MET:HE1	1:160:A:LEU:HD23	8	0.47
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD21	8	0.47
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD22	8	0.47
(1,1376)	1:146:A:MET:HE2	1:160:A:LEU:HD23	8	0.47
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD21	8	0.47
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD22	8	0.47
(1,1376)	1:146:A:MET:HE3	1:160:A:LEU:HD23	8	0.47
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD21	19	0.47
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD22	19	0.47
(1,1370)	1:144:A:GLY:H	1:160:A:LEU:HD23	19	0.47
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	16	0.47
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	16	0.47
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	16	0.47
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	5	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	5	0.47
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	5	0.47
(1,1303)	1:156:A:ILE:HG21	1:157:A:HIS:HD2	20	0.47
(1,1303)	1:156:A:ILE:HG22	1:157:A:HIS:HD2	20	0.47
(1,1303)	1:156:A:ILE:HG23	1:157:A:HIS:HD2	20	0.47
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	2	0.47
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	2	0.47
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	2	0.47
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	18	0.47
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	18	0.47
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	18	0.47
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	4	0.47
(1,1231)	1:149:A:PRO:HG2	1:150:A:VAL:H	7	0.47
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	13	0.47
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	13	0.47
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	13	0.47
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	19	0.47
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	19	0.47
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	19	0.47
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	14	0.47
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	14	0.47
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	14	0.47
(1,1085)	1:56:A:ARG:HE	1:124:A:ALA:H	20	0.47
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	7	0.47
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	12	0.47
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	12	0.47
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	12	0.47
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	2	0.47
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	7	0.47
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	7	0.47
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	7	0.47
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	19	0.47
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	19	0.47
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	19	0.47
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	13	0.47
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	20	0.47
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	7	0.47
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	4	0.47
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	2	0.47
(1,844)	1:97:A:LYS:HG2	1:98:A:SER:H	11	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	1	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	1	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	1	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	3	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	3	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	3	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	9	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	9	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	9	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	19	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	19	0.47
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	19	0.47
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	18	0.47
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	18	0.47
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	18	0.47
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	15	0.47
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	1	0.47
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	1	0.47
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	1	0.47
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	14	0.47
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	14	0.47
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	14	0.47
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	19	0.47
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	19	0.47
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	19	0.47
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	1	0.47
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	1	0.47
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	1	0.47
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	17	0.47
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	17	0.47
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	17	0.47
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	5	0.47
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	11	0.47
(1,531)	1:64:A:HIS:HE1	1:67:A:SER:HB2	17	0.47
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	16	0.47
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	16	0.47
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	16	0.47
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	14	0.47
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	8	0.47
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	13	0.47
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	13	0.47
(1,333)	1:25:A:PHE:HA	1:31:A:ALA:H	8	0.47
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	16	0.47
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	16	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	3	0.47
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	18	0.47
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	4	0.47
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	3	0.47
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	3	0.47
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	3	0.47
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	9	0.47
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	9	0.47
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	9	0.47
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	2	0.47
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	2	0.47
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	3	0.47
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	3	0.47
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	6	0.47
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	6	0.47
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	11	0.47
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	5	0.47
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	10	0.47
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	17	0.47
(1,188)	1:13:A:LYS:HG2	1:24:A:TYR:HE1	8	0.47
(1,188)	1:13:A:LYS:HG2	1:24:A:TYR:HE2	8	0.47
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	6	0.47
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	6	0.47
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	6	0.47
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	6	0.47
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	6	0.47
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	6	0.47
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	6	0.47
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	6	0.47
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	6	0.47
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	1	0.47
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	3	0.47
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	6	0.47
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	3	0.47
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	6	0.47
(1,129)	1:16:A:SER:HB2	1:21:A:ARG:H	2	0.47
(1,123)	1:15:A:MET:HE1	1:20:A:GLY:H	18	0.47
(1,123)	1:15:A:MET:HE2	1:20:A:GLY:H	18	0.47
(1,123)	1:15:A:MET:HE3	1:20:A:GLY:H	18	0.47
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	7	0.47
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	11	0.47
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	7	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	3	0.47
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	3	0.47
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	3	0.47
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	3	0.47
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	3	0.47
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	3	0.47
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	11	0.47
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	11	0.47
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	11	0.47
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	10	0.46
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	19	0.46
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	19	0.46
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	3	0.46
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	12	0.46
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	4	0.46
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	4	0.46
(2,68)	2:649:B:ARG:HD2	2:650:B:ASN:H	20	0.46
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	4	0.46
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	4	0.46
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	4	0.46
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	1	0.46
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	13	0.46
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	18	0.46
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	18	0.46
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	18	0.46
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	18	0.46
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	18	0.46
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	18	0.46
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	1	0.46
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	1	0.46
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	11	0.46
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	11	0.46
(1,2577)	1:23:A:TYR:HD1	2:641:B:TPO:HG21	18	0.46
(1,2577)	1:23:A:TYR:HD1	2:641:B:TPO:HG22	18	0.46
(1,2577)	1:23:A:TYR:HD1	2:641:B:TPO:HG23	18	0.46
(1,2577)	1:23:A:TYR:HD2	2:641:B:TPO:HG21	18	0.46
(1,2577)	1:23:A:TYR:HD2	2:641:B:TPO:HG22	18	0.46
(1,2577)	1:23:A:TYR:HD2	2:641:B:TPO:HG23	18	0.46
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	15	0.46
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	15	0.46
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	15	0.46
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	6	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	6	0.46
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	6	0.46
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	6	0.46
(1,2510)	2:645:B:GLN:H	2:647:B:VAL:H	9	0.46
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	15	0.46
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	14	0.46
(1,2135)	1:117:A:LYS:H	1:117:A:LYS:HD2	19	0.46
(1,1977)	1:89:A:ILE:H	1:89:A:ILE:HG12	3	0.46
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	1	0.46
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	3	0.46
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	4	0.46
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	3	0.46
(1,1400)	1:143:A:THR:HG21	1:161:A:ARG:HE	2	0.46
(1,1400)	1:143:A:THR:HG22	1:161:A:ARG:HE	2	0.46
(1,1400)	1:143:A:THR:HG23	1:161:A:ARG:HE	2	0.46
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	6	0.46
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	6	0.46
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	6	0.46
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	9	0.46
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	9	0.46
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	9	0.46
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	1	0.46
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	1	0.46
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	1	0.46
(1,1078)	1:122:A:LEU:HG	1:123:A:GLY:H	19	0.46
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	6	0.46
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	6	0.46
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	6	0.46
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	5	0.46
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	9	0.46
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	17	0.46
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	17	0.46
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	17	0.46
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	17	0.46
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	16	0.46
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	20	0.46
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	5	0.46
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	9	0.46
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	7	0.46
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	5	0.46
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	5	0.46
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	6	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	6	0.46
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	10	0.46
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	10	0.46
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	5	0.46
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	17	0.46
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	5	0.46
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	5	0.46
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	5	0.46
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	15	0.46
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	15	0.46
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	15	0.46
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	3	0.46
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	3	0.46
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	3	0.46
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD21	10	0.46
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD22	10	0.46
(1,712)	1:87:A:GLU:H	1:88:A:LEU:HD23	10	0.46
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	2	0.46
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	12	0.46
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	12	0.46
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	12	0.46
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	11	0.46
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	18	0.46
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	5	0.46
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	11	0.46
(1,549)	1:70:A:PRO:HG2	1:71:A:SER:H	7	0.46
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	12	0.46
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	15	0.46
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	15	0.46
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	15	0.46
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	15	0.46
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	1	0.46
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	1	0.46
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	1	0.46
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	2	0.46
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	10	0.46
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	5	0.46
(1,352)	1:23:A:TYR:HE1	1:32:A:SER:HA	13	0.46
(1,352)	1:23:A:TYR:HE2	1:32:A:SER:HA	13	0.46
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	2	0.46
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	2	0.46
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	2	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	3	0.46
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	3	0.46
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	19	0.46
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	19	0.46
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	8	0.46
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	11	0.46
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	12	0.46
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	13	0.46
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	19	0.46
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	7	0.46
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	7	0.46
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	16	0.46
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	16	0.46
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	20	0.46
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	20	0.46
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	12	0.46
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	10	0.46
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	17	0.46
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	10	0.46
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	20	0.46
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	20	0.46
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	12	0.46
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	12	0.46
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	12	0.46
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	12	0.46
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	12	0.46
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	12	0.46
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	12	0.46
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	12	0.46
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	12	0.46
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	11	0.46
(1,123)	1:15:A:MET:HE1	1:20:A:GLY:H	19	0.46
(1,123)	1:15:A:MET:HE2	1:20:A:GLY:H	19	0.46
(1,123)	1:15:A:MET:HE3	1:20:A:GLY:H	19	0.46
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	6	0.46
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	10	0.46
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	12	0.46
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	13	0.46
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	19	0.46
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	1	0.46
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	1	0.46
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	4	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	4	0.46
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	5	0.46
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	5	0.46
(1,44)	1:8:A:PRO:HB2	1:11:A:TRP:HE1	20	0.46
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	19	0.46
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	2	0.46
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	5	0.46
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	2	0.45
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	14	0.45
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	14	0.45
(2,88)	1:34:A:TRP:HE1	2:641:B:TPO:H	20	0.45
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	4	0.45
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	4	0.45
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	4	0.45
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	12	0.45
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	13	0.45
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	13	0.45
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	1	0.45
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	1	0.45
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	12	0.45
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	12	0.45
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	2	0.45
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	2	0.45
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	5	0.45
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	5	0.45
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	5	0.45
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD1	17	0.45
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD2	17	0.45
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	8	0.45
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	8	0.45
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	8	0.45
(1,2209)	1:131:A:GLN:HA	1:131:A:GLN:HE22	2	0.45
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	10	0.45
(1,1645)	1:29:A:THR:H	1:29:A:THR:HG21	20	0.45
(1,1645)	1:29:A:THR:H	1:29:A:THR:HG22	20	0.45
(1,1645)	1:29:A:THR:H	1:29:A:THR:HG23	20	0.45
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	5	0.45
(1,1560)	1:18:A:SER:H	1:18:A:SER:HB3	16	0.45
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	16	0.45
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	18	0.45
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	20	0.45
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	6	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD21	3	0.45
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD22	3	0.45
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD23	3	0.45
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	12	0.45
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	12	0.45
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	12	0.45
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	12	0.45
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	12	0.45
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	12	0.45
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	17	0.45
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	17	0.45
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	17	0.45
(1,1280)	1:64:A:HIS:HD2	1:156:A:ILE:HG12	3	0.45
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	16	0.45
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	3	0.45
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	18	0.45
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	18	0.45
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	18	0.45
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	11	0.45
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	11	0.45
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	11	0.45
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	16	0.45
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	16	0.45
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	16	0.45
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	5	0.45
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	4	0.45
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	19	0.45
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	3	0.45
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	3	0.45
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	3	0.45
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	3	0.45
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	3	0.45
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	3	0.45
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	10	0.45
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	14	0.45
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	16	0.45
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	15	0.45
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	13	0.45
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	10	0.45
(1,785)	1:89:A:ILE:HG21	1:93:A:ILE:H	3	0.45
(1,785)	1:89:A:ILE:HG22	1:93:A:ILE:H	3	0.45
(1,785)	1:89:A:ILE:HG23	1:93:A:ILE:H	3	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	19	0.45
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	19	0.45
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	19	0.45
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	19	0.45
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	19	0.45
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	19	0.45
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	18	0.45
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	20	0.45
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	20	0.45
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	20	0.45
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	1	0.45
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	8	0.45
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	8	0.45
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	8	0.45
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	11	0.45
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	15	0.45
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	5	0.45
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	16	0.45
(1,549)	1:70:A:PRO:HG2	1:71:A:SER:H	17	0.45
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	12	0.45
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	12	0.45
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	12	0.45
(1,471)	1:61:A:LEU:HD21	1:63:A:LYS:HA	15	0.45
(1,471)	1:61:A:LEU:HD22	1:63:A:LYS:HA	15	0.45
(1,471)	1:61:A:LEU:HD23	1:63:A:LYS:HA	15	0.45
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	8	0.45
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	11	0.45
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	19	0.45
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	5	0.45
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	5	0.45
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	14	0.45
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	14	0.45
(1,334)	1:27:A:HIS:HA	1:31:A:ALA:H	13	0.45
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	1	0.45
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	14	0.45
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	14	0.45
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	15	0.45
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	15	0.45
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	15	0.45
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	18	0.45
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	18	0.45
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	8	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	8	0.45
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	2	0.45
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	12	0.45
(1,181)	1:23:A:TYR:HB2	1:34:A:TRP:HE3	15	0.45
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	10	0.45
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	10	0.45
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	16	0.45
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	16	0.45
(1,148)	1:15:A:MET:HE1	1:22:A:VAL:HA	3	0.45
(1,148)	1:15:A:MET:HE2	1:22:A:VAL:HA	3	0.45
(1,148)	1:15:A:MET:HE3	1:22:A:VAL:HA	3	0.45
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	9	0.45
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	1	0.45
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	4	0.45
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	10	0.45
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	14	0.45
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	10	0.45
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	7	0.45
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	7	0.45
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	7	0.45
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	7	0.45
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	7	0.45
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	7	0.45
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	20	0.45
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	20	0.45
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	3	0.45
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	3	0.45
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	3	0.45
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	3	0.45
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	3	0.45
(1,16)	1:6:A:LYS:HE2	1:7:A:LEU:H	15	0.45
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	3	0.45
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	6	0.45
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	17	0.44
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	16	0.44
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	16	0.44
(2,94)	1:93:A:ILE:HG21	2:643:B:PRO:HB3	10	0.44
(2,94)	1:93:A:ILE:HG22	2:643:B:PRO:HB3	10	0.44
(2,94)	1:93:A:ILE:HG23	2:643:B:PRO:HB3	10	0.44
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	6	0.44
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	6	0.44
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	9	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	9	0.44
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	9	0.44
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	6	0.44
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	6	0.44
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE1	11	0.44
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE2	11	0.44
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	11	0.44
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	11	0.44
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	4	0.44
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	4	0.44
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	4	0.44
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	8	0.44
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	8	0.44
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	10	0.44
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	10	0.44
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	10	0.44
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	12	0.44
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	12	0.44
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	12	0.44
(1,1910)	1:82:A:LYS:H	1:82:A:LYS:HE2	20	0.44
(1,1565)	1:21:A:ARG:H	1:21:A:ARG:HG2	2	0.44
(1,1560)	1:18:A:SER:H	1:18:A:SER:HB3	4	0.44
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	9	0.44
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	11	0.44
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	12	0.44
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	13	0.44
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	10	0.44
(1,1440)	1:162:A:THR:HG21	1:163:A:GLU:HB3	11	0.44
(1,1440)	1:162:A:THR:HG22	1:163:A:GLU:HB3	11	0.44
(1,1440)	1:162:A:THR:HG23	1:163:A:GLU:HB3	11	0.44
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	14	0.44
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	14	0.44
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	14	0.44
(1,1309)	1:150:A:VAL:HB	1:157:A:HIS:H	16	0.44
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG21	4	0.44
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG22	4	0.44
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG23	4	0.44
(1,1208)	1:103:A:PHE:HD1	1:146:A:MET:HB2	19	0.44
(1,1208)	1:103:A:PHE:HD2	1:146:A:MET:HB2	19	0.44
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	5	0.44
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	5	0.44
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	5	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	17	0.44
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	5	0.44
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	5	0.44
(1,1085)	1:56:A:ARG:HE	1:124:A:ALA:H	10	0.44
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	12	0.44
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	12	0.44
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	12	0.44
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	1	0.44
(1,1031)	1:118:A:ALA:HB1	1:121:A:ASP:HB2	10	0.44
(1,1031)	1:118:A:ALA:HB2	1:121:A:ASP:HB2	10	0.44
(1,1031)	1:118:A:ALA:HB3	1:121:A:ASP:HB2	10	0.44
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	8	0.44
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	8	0.44
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	8	0.44
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	9	0.44
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	2	0.44
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	2	0.44
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	11	0.44
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	17	0.44
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	17	0.44
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	17	0.44
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	6	0.44
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	1	0.44
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	3	0.44
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	10	0.44
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	13	0.44
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	2	0.44
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	2	0.44
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	2	0.44
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	2	0.44
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	2	0.44
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	2	0.44
(1,693)	1:86:A:LEU:HD21	1:149:A:PRO:HD2	14	0.44
(1,693)	1:86:A:LEU:HD22	1:149:A:PRO:HD2	14	0.44
(1,693)	1:86:A:LEU:HD23	1:149:A:PRO:HD2	14	0.44
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	9	0.44
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	4	0.44
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	14	0.44
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	3	0.44
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	3	0.44
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	3	0.44
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	9	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	9	0.44
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	9	0.44
(1,480)	1:61:A:LEU:HD21	1:156:A:ILE:H	3	0.44
(1,480)	1:61:A:LEU:HD22	1:156:A:ILE:H	3	0.44
(1,480)	1:61:A:LEU:HD23	1:156:A:ILE:H	3	0.44
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	16	0.44
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB1	20	0.44
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB2	20	0.44
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB3	20	0.44
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	19	0.44
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	9	0.44
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	9	0.44
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	2	0.44
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	2	0.44
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	15	0.44
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	4	0.44
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	4	0.44
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	13	0.44
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	13	0.44
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	16	0.44
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	7	0.44
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	8	0.44
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	13	0.44
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	6	0.44
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	16	0.44
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	7	0.44
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	7	0.44
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	14	0.44
(1,123)	1:15:A:MET:HE1	1:20:A:GLY:H	13	0.44
(1,123)	1:15:A:MET:HE2	1:20:A:GLY:H	13	0.44
(1,123)	1:15:A:MET:HE3	1:20:A:GLY:H	13	0.44
(1,121)	1:17:A:ARG:HB2	1:18:A:SER:H	2	0.44
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	5	0.44
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	4	0.44
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	16	0.44
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	1	0.44
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	1	0.44
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	1	0.44
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	1	0.44
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	1	0.44
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	1	0.44
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	4	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	4	0.44
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	4	0.44
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	4	0.44
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	4	0.44
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	4	0.44
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	9	0.44
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	9	0.44
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	9	0.44
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	9	0.44
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	9	0.44
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	9	0.44
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	16	0.44
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	16	0.44
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	16	0.44
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	16	0.44
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	16	0.44
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	16	0.44
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	2	0.44
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	2	0.44
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	10	0.44
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	10	0.44
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	4	0.44
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	4	0.44
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	4	0.44
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	4	0.44
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	11	0.43
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	19	0.43
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	18	0.43
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	10	0.43
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	10	0.43
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	7	0.43
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	7	0.43
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	7	0.43
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	3	0.43
(1,2590)	1:122:A:LEU:HD21	2:656:B:PHE:HD1	19	0.43
(1,2590)	1:122:A:LEU:HD21	2:656:B:PHE:HD2	19	0.43
(1,2590)	1:122:A:LEU:HD22	2:656:B:PHE:HD1	19	0.43
(1,2590)	1:122:A:LEU:HD22	2:656:B:PHE:HD2	19	0.43
(1,2590)	1:122:A:LEU:HD23	2:656:B:PHE:HD1	19	0.43
(1,2590)	1:122:A:LEU:HD23	2:656:B:PHE:HD2	19	0.43
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	4	0.43
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	4	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	5	0.43
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	5	0.43
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	3	0.43
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	3	0.43
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	19	0.43
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	3	0.43
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	2	0.43
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	2	0.43
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	2	0.43
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	13	0.43
(1,1560)	1:18:A:SER:H	1:18:A:SER:HB3	6	0.43
(1,1560)	1:18:A:SER:H	1:18:A:SER:HB3	7	0.43
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	1	0.43
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	6	0.43
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	19	0.43
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	9	0.43
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	9	0.43
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	9	0.43
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	9	0.43
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	9	0.43
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	9	0.43
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	9	0.43
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	9	0.43
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	9	0.43
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	6	0.43
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	6	0.43
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	6	0.43
(1,1280)	1:64:A:HIS:HD2	1:156:A:ILE:HG12	12	0.43
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	4	0.43
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	4	0.43
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	4	0.43
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	8	0.43
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	8	0.43
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	8	0.43
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	12	0.43
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	12	0.43
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	12	0.43
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	17	0.43
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	17	0.43
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	17	0.43
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	6	0.43
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	14	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	2	0.43
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	6	0.43
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	6	0.43
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	6	0.43
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	2	0.43
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	2	0.43
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	2	0.43
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	2	0.43
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	2	0.43
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	2	0.43
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	19	0.43
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	19	0.43
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	19	0.43
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	19	0.43
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	19	0.43
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	19	0.43
(1,1085)	1:56:A:ARG:HE	1:124:A:ALA:H	13	0.43
(1,1057)	1:59:A:HIS:H	1:122:A:LEU:HG	18	0.43
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	14	0.43
(1,923)	1:106:A:LEU:HA	1:110:A:PHE:H	2	0.43
(1,834)	1:94:A:GLN:HE21	1:97:A:LYS:HD2	10	0.43
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	7	0.43
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	18	0.43
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD1	12	0.43
(1,763)	1:88:A:LEU:HG	1:92:A:TYR:HD2	12	0.43
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	17	0.43
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	17	0.43
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	17	0.43
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE1	20	0.43
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE2	20	0.43
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE1	20	0.43
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE2	20	0.43
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE1	20	0.43
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE2	20	0.43
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	16	0.43
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	16	0.43
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	16	0.43
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	2	0.43
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	10	0.43
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	1	0.43
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	14	0.43
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	17	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:71:A:SER:H	1:78:A:ILE:HD11	6	0.43
(1,557)	1:71:A:SER:H	1:78:A:ILE:HD12	6	0.43
(1,557)	1:71:A:SER:H	1:78:A:ILE:HD13	6	0.43
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	15	0.43
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	6	0.43
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	6	0.43
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	6	0.43
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	20	0.43
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	4	0.43
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	4	0.43
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	6	0.43
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	6	0.43
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	9	0.43
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	9	0.43
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	13	0.43
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	13	0.43
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	5	0.43
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	18	0.43
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	17	0.43
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	17	0.43
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	17	0.43
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	9	0.43
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	9	0.43
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	19	0.43
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	19	0.43
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	17	0.43
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	5	0.43
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	4	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	8	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	8	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	8	0.43
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	8	0.43
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	8	0.43
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	8	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	8	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	8	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	8	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	16	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	16	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	16	0.43
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	16	0.43
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	16	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	16	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	16	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	16	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	16	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	19	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	19	0.43
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	19	0.43
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	19	0.43
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	19	0.43
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	19	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	19	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	19	0.43
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	19	0.43
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	18	0.43
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	11	0.43
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	11	0.43
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	11	0.43
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	13	0.43
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	19	0.43
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	19	0.43
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	9	0.43
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	9	0.43
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	2	0.43
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	2	0.43
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	2	0.43
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	5	0.43
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	16	0.43
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	2	0.42
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	18	0.42
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	8	0.42
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	8	0.42
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	8	0.42
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	8	0.42
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	8	0.42
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	8	0.42
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	5	0.42
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	5	0.42
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	5	0.42
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	1	0.42
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	1	0.42
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	1	0.42
(2,34)	1:59:A:HIS:H	1:122:A:LEU:HB2	8	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	1	0.42
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	1	0.42
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	7	0.42
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	7	0.42
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	19	0.42
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	19	0.42
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	8	0.42
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	8	0.42
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	5	0.42
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	5	0.42
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	5	0.42
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	7	0.42
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	7	0.42
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	7	0.42
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	3	0.42
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	15	0.42
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	1	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	1	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	1	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	1	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	5	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	5	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	5	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	18	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	18	0.42
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	18	0.42
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	13	0.42
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	15	0.42
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	13	0.42
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	14	0.42
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	19	0.42
(1,1560)	1:18:A:SER:H	1:18:A:SER:HB3	8	0.42
(1,1410)	1:161:A:ARG:HE	1:163:A:GLU:HG2	13	0.42
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	1	0.42
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	1	0.42
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	1	0.42
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	5	0.42
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	5	0.42
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	5	0.42
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	13	0.42
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	13	0.42
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	13	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	6	0.42
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	6	0.42
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	6	0.42
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	15	0.42
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	15	0.42
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	15	0.42
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG21	1	0.42
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG22	1	0.42
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG23	1	0.42
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB2	18	0.42
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB3	18	0.42
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB2	18	0.42
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB3	18	0.42
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB2	18	0.42
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB3	18	0.42
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	4	0.42
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	17	0.42
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	18	0.42
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	10	0.42
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	10	0.42
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	10	0.42
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	10	0.42
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	10	0.42
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	10	0.42
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	10	0.42
(1,1024)	1:118:A:ALA:HA	1:119:A:ARG:HE	13	0.42
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	14	0.42
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	14	0.42
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	14	0.42
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	19	0.42
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	16	0.42
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	5	0.42
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	15	0.42
(1,917)	1:105:A:SER:HB2	1:106:A:LEU:H	19	0.42
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	5	0.42
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	5	0.42
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	5	0.42
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	5	0.42
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	5	0.42
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	5	0.42
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	8	0.42
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	8	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	8	0.42
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	8	0.42
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	8	0.42
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	8	0.42
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	9	0.42
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	10	0.42
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	18	0.42
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD11	4	0.42
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD12	4	0.42
(1,810)	1:94:A:GLN:H	1:96:A:ILE:HD13	4	0.42
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	19	0.42
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	19	0.42
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	19	0.42
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	20	0.42
(1,571)	1:73:A:TRP:HE1	1:74:A:ARG:HB3	18	0.42
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	1	0.42
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	3	0.42
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	8	0.42
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	8	0.42
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	8	0.42
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	8	0.42
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	1	0.42
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	7	0.42
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	11	0.42
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	12	0.42
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	20	0.42
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	3	0.42
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	11	0.42
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	2	0.42
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	7	0.42
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	1	0.42
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	1	0.42
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	3	0.42
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	3	0.42
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	8	0.42
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	8	0.42
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	3	0.42
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	3	0.42
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	20	0.42
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	20	0.42
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	20	0.42
(1,334)	1:27:A:HIS:HA	1:31:A:ALA:H	1	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	13	0.42
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	11	0.42
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	16	0.42
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	20	0.42
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	19	0.42
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	10	0.42
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	10	0.42
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	15	0.42
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	18	0.42
(1,129)	1:16:A:SER:HB2	1:21:A:ARG:H	15	0.42
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	2	0.42
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	2	0.42
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	18	0.42
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	18	0.42
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	18	0.42
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	12	0.42
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	6	0.42
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	6	0.42
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	6	0.42
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	6	0.42
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	6	0.42
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	6	0.42
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	12	0.42
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	12	0.42
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	1	0.42
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	1	0.42
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	10	0.42
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	10	0.42
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	9	0.42
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	9	0.42
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	14	0.42
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	7	0.42
(3,9)	1:16:A:SER:O	1:19:A:SER:N	19	0.41
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	8	0.41
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	8	0.41
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	8	0.41
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	8	0.41
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	8	0.41
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	8	0.41
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	6	0.41
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	6	0.41
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	6	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	6	0.41
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	6	0.41
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	6	0.41
(2,68)	2:649:B:ARG:HD2	2:650:B:ASN:H	18	0.41
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	1	0.41
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	1	0.41
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	1	0.41
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	12	0.41
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	12	0.41
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	12	0.41
(2,44)	1:131:A:GLN:HE21	1:153:A:ASP:H	20	0.41
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	8	0.41
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	8	0.41
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	6	0.41
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	14	0.41
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	14	0.41
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	18	0.41
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	18	0.41
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	18	0.41
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	18	0.41
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	18	0.41
(1,2527)	2:646:B:GLU:H	2:648:B:ILE:H	20	0.41
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	9	0.41
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	19	0.41
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	6	0.41
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	9	0.41
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	10	0.41
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	10	0.41
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	7	0.41
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	8	0.41
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	6	0.41
(1,1560)	1:18:A:SER:H	1:18:A:SER:HB3	14	0.41
(1,1406)	1:147:A:SER:H	1:161:A:ARG:H	1	0.41
(1,1399)	1:143:A:THR:H	1:161:A:ARG:HD2	18	0.41
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	20	0.41
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	12	0.41
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	12	0.41
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	12	0.41
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	7	0.41
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	7	0.41
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	7	0.41
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	3	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	3	0.41
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	3	0.41
(1,1303)	1:156:A:ILE:HG21	1:157:A:HIS:HD2	3	0.41
(1,1303)	1:156:A:ILE:HG22	1:157:A:HIS:HD2	3	0.41
(1,1303)	1:156:A:ILE:HG23	1:157:A:HIS:HD2	3	0.41
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	12	0.41
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	12	0.41
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	12	0.41
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	15	0.41
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	15	0.41
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	15	0.41
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	13	0.41
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	2	0.41
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	2	0.41
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	2	0.41
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	15	0.41
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	8	0.41
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	8	0.41
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	8	0.41
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	12	0.41
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	12	0.41
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	12	0.41
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	12	0.41
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	12	0.41
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	12	0.41
(1,1027)	1:118:A:ALA:HA	1:119:A:ARG:HG2	17	0.41
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	10	0.41
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	1	0.41
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	15	0.41
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	4	0.41
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	19	0.41
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	6	0.41
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	19	0.41
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	3	0.41
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	3	0.41
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	3	0.41
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	13	0.41
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	19	0.41
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	1	0.41
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	9	0.41
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	14	0.41
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	14	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	14	0.41
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	3	0.41
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	3	0.41
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	3	0.41
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	2	0.41
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	3	0.41
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	4	0.41
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	13	0.41
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	19	0.41
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	20	0.41
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	20	0.41
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	20	0.41
(1,385)	1:24:A:TYR:HD1	1:36:A:ARG:H	2	0.41
(1,385)	1:24:A:TYR:HD2	1:36:A:ARG:H	2	0.41
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	6	0.41
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	9	0.41
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	20	0.41
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	12	0.41
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	12	0.41
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	14	0.41
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	14	0.41
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	15	0.41
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	15	0.41
(1,362)	1:11:A:TRP:HH2	1:33:A:GLN:HE21	5	0.41
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	14	0.41
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	4	0.41
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	6	0.41
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	6	0.41
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	10	0.41
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	10	0.41
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	15	0.41
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	15	0.41
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	8	0.41
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	6	0.41
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	6	0.41
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	20	0.41
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	20	0.41
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	20	0.41
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	20	0.41
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	20	0.41
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	20	0.41
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	20	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	20	0.41
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	20	0.41
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	11	0.41
(1,129)	1:16:A:SER:HB2	1:21:A:ARG:H	17	0.41
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	5	0.41
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	5	0.41
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	14	0.41
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	14	0.41
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	14	0.41
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	14	0.41
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	15	0.41
(1,44)	1:8:A:PRO:HB2	1:11:A:TRP:HE1	12	0.41
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	18	0.41
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	19	0.41
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	13	0.4
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	19	0.4
(3,28)	1:56:A:ARG:H	1:163:A:GLU:O	17	0.4
(3,9)	1:16:A:SER:O	1:19:A:SER:N	10	0.4
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	17	0.4
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	17	0.4
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	17	0.4
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	17	0.4
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	17	0.4
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	17	0.4
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	17	0.4
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	17	0.4
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	11	0.4
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	14	0.4
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	9	0.4
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	9	0.4
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	3	0.4
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	8	0.4
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	7	0.4
(1,2514)	2:646:B:GLU:HA	2:649:B:ARG:H	10	0.4
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	6	0.4
(1,2022)	1:94:A:GLN:H	1:94:A:GLN:HG2	11	0.4
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	5	0.4
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	8	0.4
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	12	0.4
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	7	0.4
(1,1313)	1:156:A:ILE:HA	1:157:A:HIS:HD2	13	0.4
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	5	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	5	0.4
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	5	0.4
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	18	0.4
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	18	0.4
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	18	0.4
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	5	0.4
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	5	0.4
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	5	0.4
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	17	0.4
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	17	0.4
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	17	0.4
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	10	0.4
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	7	0.4
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	18	0.4
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	8	0.4
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	8	0.4
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	1	0.4
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	1	0.4
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	4	0.4
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	12	0.4
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	7	0.4
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	7	0.4
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	7	0.4
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	5	0.4
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB1	5	0.4
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB2	5	0.4
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB3	5	0.4
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB1	7	0.4
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB2	7	0.4
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB3	7	0.4
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	10	0.4
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	18	0.4
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	18	0.4
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	18	0.4
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	9	0.4
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	9	0.4
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	2	0.4
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	20	0.4
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	1	0.4
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	6	0.4
(1,748)	1:87:A:GLU:HA	1:91:A:GLY:H	18	0.4
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	13	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	13	0.4
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	13	0.4
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	19	0.4
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	19	0.4
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	19	0.4
(1,695)	1:86:A:LEU:HD21	1:149:A:PRO:HD3	11	0.4
(1,695)	1:86:A:LEU:HD22	1:149:A:PRO:HD3	11	0.4
(1,695)	1:86:A:LEU:HD23	1:149:A:PRO:HD3	11	0.4
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	4	0.4
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	4	0.4
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	4	0.4
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	10	0.4
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	10	0.4
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	10	0.4
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	10	0.4
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	17	0.4
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	5	0.4
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	12	0.4
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	19	0.4
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	5	0.4
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	9	0.4
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	14	0.4
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	1	0.4
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	7	0.4
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	10	0.4
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	7	0.4
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	7	0.4
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	5	0.4
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	5	0.4
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	5	0.4
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	8	0.4
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	8	0.4
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	8	0.4
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	6	0.4
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	6	0.4
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	6	0.4
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	11	0.4
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	11	0.4
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	11	0.4
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	11	0.4
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	12	0.4
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	16	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	16	0.4
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	9	0.4
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	9	0.4
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	9	0.4
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	9	0.4
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	9	0.4
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	9	0.4
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	9	0.4
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	9	0.4
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	9	0.4
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	9	0.4
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	9	0.4
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	15	0.4
(1,133)	1:20:A:GLY:H	1:21:A:ARG:HB2	16	0.4
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	1	0.4
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	1	0.4
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	1	0.4
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	16	0.4
(1,81)	1:12:A:GLU:H	1:14:A:ARG:H	15	0.4
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	5	0.4
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	18	0.4
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	18	0.4
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	18	0.4
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	18	0.4
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	18	0.4
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	18	0.4
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	13	0.4
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	4	0.4
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	11	0.4
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	14	0.4
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	15	0.39
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	19	0.39
(3,33)	1:60:A:LEU:N	1:158:A:ILE:O	19	0.39
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	1	0.39
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	1	0.39
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	9	0.39
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	9	0.39
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	4	0.39
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	4	0.39
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	1	0.39
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	1	0.39
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	1	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	15	0.39
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	3	0.39
(1,2589)	1:122:A:LEU:HD21	2:656:B:PHE:HE1	13	0.39
(1,2589)	1:122:A:LEU:HD21	2:656:B:PHE:HE2	13	0.39
(1,2589)	1:122:A:LEU:HD22	2:656:B:PHE:HE1	13	0.39
(1,2589)	1:122:A:LEU:HD22	2:656:B:PHE:HE2	13	0.39
(1,2589)	1:122:A:LEU:HD23	2:656:B:PHE:HE1	13	0.39
(1,2589)	1:122:A:LEU:HD23	2:656:B:PHE:HE2	13	0.39
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	7	0.39
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	7	0.39
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	7	0.39
(1,2507)	2:643:B:PRO:HA	2:645:B:GLN:H	13	0.39
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	7	0.39
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	13	0.39
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	13	0.39
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	13	0.39
(1,2209)	1:131:A:GLN:HA	1:131:A:GLN:HE22	15	0.39
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	3	0.39
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	4	0.39
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	2	0.39
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	6	0.39
(1,1525)	1:14:A:ARG:H	1:14:A:ARG:HE	1	0.39
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	10	0.39
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	4	0.39
(1,1403)	1:144:A:GLY:H	1:161:A:ARG:HG2	2	0.39
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	4	0.39
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	4	0.39
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	4	0.39
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	4	0.39
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	4	0.39
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	4	0.39
(1,1344)	1:147:A:SER:HA	1:159:A:ILE:H	3	0.39
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	11	0.39
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	11	0.39
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	11	0.39
(1,1296)	1:89:A:ILE:HG13	1:156:A:ILE:HG21	6	0.39
(1,1296)	1:89:A:ILE:HG13	1:156:A:ILE:HG22	6	0.39
(1,1296)	1:89:A:ILE:HG13	1:156:A:ILE:HG23	6	0.39
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	3	0.39
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	3	0.39
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	3	0.39
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	6	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	6	0.39
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	6	0.39
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	12	0.39
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	12	0.39
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	12	0.39
(1,1141)	1:130:A:MET:HB2	1:134:A:PHE:H	18	0.39
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	3	0.39
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	4	0.39
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	8	0.39
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	8	0.39
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	8	0.39
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	2	0.39
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	2	0.39
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	2	0.39
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	7	0.39
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	8	0.39
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	6	0.39
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	19	0.39
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	19	0.39
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	19	0.39
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	14	0.39
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	3	0.39
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	14	0.39
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	16	0.39
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	7	0.39
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	2	0.39
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	13	0.39
(1,475)	1:61:A:LEU:HD11	1:113:A:CYS:H	10	0.39
(1,475)	1:61:A:LEU:HD12	1:113:A:CYS:H	10	0.39
(1,475)	1:61:A:LEU:HD13	1:113:A:CYS:H	10	0.39
(1,475)	1:61:A:LEU:HD21	1:113:A:CYS:H	10	0.39
(1,475)	1:61:A:LEU:HD22	1:113:A:CYS:H	10	0.39
(1,475)	1:61:A:LEU:HD23	1:113:A:CYS:H	10	0.39
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	9	0.39
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	3	0.39
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	16	0.39
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	16	0.39
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	16	0.39
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	16	0.39
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	16	0.39
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	1	0.39
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	1	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	1	0.39
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	20	0.39
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	7	0.39
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	7	0.39
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	7	0.39
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	1	0.39
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	1	0.39
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	12	0.39
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	12	0.39
(1,261)	1:25:A:PHE:HE1	1:26:A:ASN:H	17	0.39
(1,261)	1:25:A:PHE:HE2	1:26:A:ASN:H	17	0.39
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	3	0.39
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	3	0.39
(1,224)	1:14:A:ARG:HE	1:25:A:PHE:HB3	5	0.39
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	19	0.39
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	20	0.39
(1,211)	1:24:A:TYR:HE1	1:36:A:ARG:HD2	14	0.39
(1,211)	1:24:A:TYR:HE2	1:36:A:ARG:HD2	14	0.39
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	14	0.39
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	14	0.39
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	5	0.39
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	5	0.39
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	14	0.39
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	11	0.39
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	18	0.38
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	1	0.38
(3,33)	1:60:A:LEU:N	1:158:A:ILE:O	18	0.38
(2,102)	1:135:A:GLU:H	2:656:B:PHE:HB2	17	0.38
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	10	0.38
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	10	0.38
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	10	0.38
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	16	0.38
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	16	0.38
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE1	16	0.38
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE2	16	0.38
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE1	16	0.38
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE2	16	0.38
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	5	0.38
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD1	9	0.38
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD2	9	0.38
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	3	0.38
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	3	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	3	0.38
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	8	0.38
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	8	0.38
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	8	0.38
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	8	0.38
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	8	0.38
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	8	0.38
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	17	0.38
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	17	0.38
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	17	0.38
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	17	0.38
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	17	0.38
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	17	0.38
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	15	0.38
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	15	0.38
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	2	0.38
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	2	0.38
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	2	0.38
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	15	0.38
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	15	0.38
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	15	0.38
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	5	0.38
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	12	0.38
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	6	0.38
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	6	0.38
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	6	0.38
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	7	0.38
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	7	0.38
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	7	0.38
(1,2022)	1:94:A:GLN:H	1:94:A:GLN:HG2	2	0.38
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	4	0.38
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	4	0.38
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	4	0.38
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	6	0.38
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	8	0.38
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	17	0.38
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	7	0.38
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	1	0.38
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	8	0.38
(1,1429)	1:143:A:THR:HG21	1:163:A:GLU:HB2	2	0.38
(1,1429)	1:143:A:THR:HG22	1:163:A:GLU:HB2	2	0.38
(1,1429)	1:143:A:THR:HG23	1:163:A:GLU:HB2	2	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	12	0.38
(1,1404)	1:144:A:GLY:HA2	1:161:A:ARG:H	7	0.38
(1,1391)	1:160:A:LEU:HD11	1:162:A:THR:HA	11	0.38
(1,1391)	1:160:A:LEU:HD12	1:162:A:THR:HA	11	0.38
(1,1391)	1:160:A:LEU:HD13	1:162:A:THR:HA	11	0.38
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	1	0.38
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	1	0.38
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	1	0.38
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	1	0.38
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	1	0.38
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	1	0.38
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	1	0.38
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	1	0.38
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	1	0.38
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	8	0.38
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	8	0.38
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	8	0.38
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	12	0.38
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	12	0.38
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	12	0.38
(1,1346)	1:148:A:GLY:H	1:159:A:ILE:H	13	0.38
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	14	0.38
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	14	0.38
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	14	0.38
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	6	0.38
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	8	0.38
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	9	0.38
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	9	0.38
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	9	0.38
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	13	0.38
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	1	0.38
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	7	0.38
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	13	0.38
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	13	0.38
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	13	0.38
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	11	0.38
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	3	0.38
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	20	0.38
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	20	0.38
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	20	0.38
(1,729)	1:89:A:ILE:HG12	1:93:A:ILE:HD11	5	0.38
(1,729)	1:89:A:ILE:HG12	1:93:A:ILE:HD12	5	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,729)	1:89:A:ILE:HG12	1:93:A:ILE:HD13	5	0.38
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	2	0.38
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	2	0.38
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	2	0.38
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	4	0.38
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	4	0.38
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	4	0.38
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	9	0.38
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	9	0.38
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	9	0.38
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	8	0.38
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	8	0.38
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	8	0.38
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	14	0.38
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	14	0.38
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	14	0.38
(1,654)	1:82:A:LYS:HG2	1:84:A:GLU:H	17	0.38
(1,654)	1:82:A:LYS:HG3	1:84:A:GLU:H	17	0.38
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	6	0.38
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	6	0.38
(1,576)	1:73:A:TRP:HE1	1:115:A:SER:H	20	0.38
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	1	0.38
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	1	0.38
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	1	0.38
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	4	0.38
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	4	0.38
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	4	0.38
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	10	0.38
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	15	0.38
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	15	0.38
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	15	0.38
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	1	0.38
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	3	0.38
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	5	0.38
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	2	0.38
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	2	0.38
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	4	0.38
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	4	0.38
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	20	0.38
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	20	0.38
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	17	0.38
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	17	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	19	0.38
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	19	0.38
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	19	0.38
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	14	0.38
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	18	0.38
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	18	0.38
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG21	12	0.38
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG22	12	0.38
(1,270)	1:26:A:ASN:HD21	1:28:A:ILE:HG23	12	0.38
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	20	0.38
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	20	0.38
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	3	0.38
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	7	0.38
(1,242)	1:10:A:GLY:H	1:26:A:ASN:HD21	20	0.38
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	12	0.38
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	14	0.38
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	4	0.38
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	15	0.38
(1,139)	1:21:A:ARG:HD2	1:34:A:TRP:HZ3	18	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	6	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	6	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	6	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	12	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	12	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	12	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	20	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	20	0.38
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	20	0.38
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB1	12	0.38
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB2	12	0.38
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB3	12	0.38
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	4	0.38
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	4	0.38
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	20	0.38
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	3	0.38
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	6	0.38
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	12	0.38
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	15	0.38
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	20	0.38
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	17	0.37
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	6	0.37
(3,9)	1:16:A:SER:O	1:19:A:SER:N	13	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,9)	1:16:A:SER:O	1:19:A:SER:N	15	0.37
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	13	0.37
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	13	0.37
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	13	0.37
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	7	0.37
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	7	0.37
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	12	0.37
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	12	0.37
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	18	0.37
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	18	0.37
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	10	0.37
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	10	0.37
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	10	0.37
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	10	0.37
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	5	0.37
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	5	0.37
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	5	0.37
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	7	0.37
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	7	0.37
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	7	0.37
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD1	12	0.37
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD2	12	0.37
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	5	0.37
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	4	0.37
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	12	0.37
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	2	0.37
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	2	0.37
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	2	0.37
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	2	0.37
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	2	0.37
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	2	0.37
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	6	0.37
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	6	0.37
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	6	0.37
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	6	0.37
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	6	0.37
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	6	0.37
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	11	0.37
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	11	0.37
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	11	0.37
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	8	0.37
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	9	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	4	0.37
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	8	0.37
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	9	0.37
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	9	0.37
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	9	0.37
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	1	0.37
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	10	0.37
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	16	0.37
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	5	0.37
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	5	0.37
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	5	0.37
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	9	0.37
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	9	0.37
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	9	0.37
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	9	0.37
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	1	0.37
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	14	0.37
(1,1399)	1:143:A:THR:H	1:161:A:ARG:HD2	5	0.37
(1,1346)	1:148:A:GLY:H	1:159:A:ILE:H	12	0.37
(1,1326)	1:89:A:ILE:HG21	1:158:A:ILE:HB	9	0.37
(1,1326)	1:89:A:ILE:HG22	1:158:A:ILE:HB	9	0.37
(1,1326)	1:89:A:ILE:HG23	1:158:A:ILE:HB	9	0.37
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	6	0.37
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	18	0.37
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	18	0.37
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	18	0.37
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	12	0.37
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	12	0.37
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	12	0.37
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	4	0.37
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	4	0.37
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	4	0.37
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	3	0.37
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	14	0.37
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	11	0.37
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	1	0.37
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	1	0.37
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	1	0.37
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	6	0.37
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	16	0.37
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	15	0.37
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	15	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	15	0.37
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	17	0.37
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	7	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	1	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	1	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	1	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	2	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	2	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	2	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	6	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	6	0.37
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	6	0.37
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	10	0.37
(1,578)	1:73:A:TRP:HE1	1:116:A:ALA:HB1	16	0.37
(1,578)	1:73:A:TRP:HE1	1:116:A:ALA:HB2	16	0.37
(1,578)	1:73:A:TRP:HE1	1:116:A:ALA:HB3	16	0.37
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	9	0.37
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	14	0.37
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	4	0.37
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	12	0.37
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	20	0.37
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	7	0.37
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	7	0.37
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	7	0.37
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	13	0.37
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	13	0.37
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	13	0.37
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	4	0.37
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	4	0.37
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	4	0.37
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	19	0.37
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	5	0.37
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	17	0.37
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	3	0.37
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	3	0.37
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	3	0.37
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	14	0.37
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	14	0.37
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	14	0.37
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	1	0.37
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	6	0.37
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	7	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	2	0.37
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	8	0.37
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	4	0.37
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB1	3	0.37
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB2	3	0.37
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB3	3	0.37
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	7	0.37
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	10	0.37
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	11	0.37
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	1	0.37
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	12	0.36
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	15	0.36
(3,35)	1:62:A:VAL:N	1:156:A:ILE:O	6	0.36
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	15	0.36
(2,105)	1:138:A:SER:H	2:656:B:PHE:HD1	5	0.36
(2,105)	1:138:A:SER:H	2:656:B:PHE:HD2	5	0.36
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	11	0.36
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	11	0.36
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	11	0.36
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG21	12	0.36
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG22	12	0.36
(2,85)	1:24:A:TYR:H	2:641:B:TPO:HG23	12	0.36
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	19	0.36
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	19	0.36
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	19	0.36
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	19	0.36
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	19	0.36
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	19	0.36
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	8	0.36
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	8	0.36
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE1	5	0.36
(2,76)	2:656:B:PHE:HE1	2:659:B:PHE:HE2	5	0.36
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE1	5	0.36
(2,76)	2:656:B:PHE:HE2	2:659:B:PHE:HE2	5	0.36
(2,66)	2:645:B:GLN:H	2:648:B:ILE:H	2	0.36
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	9	0.36
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	14	0.36
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	14	0.36
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	1	0.36
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	9	0.36
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	9	0.36
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	3	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	5	0.36
(1,2209)	1:131:A:GLN:HA	1:131:A:GLN:HE22	11	0.36
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	9	0.36
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	11	0.36
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	20	0.36
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	20	0.36
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	20	0.36
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	20	0.36
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	2	0.36
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	15	0.36
(1,1571)	1:21:A:ARG:H	1:21:A:ARG:HD2	14	0.36
(1,1456)	1:6:A:LYS:H	1:6:A:LYS:HE2	15	0.36
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	12	0.36
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	10	0.36
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	20	0.36
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	20	0.36
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	20	0.36
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	20	0.36
(1,1345)	1:147:A:SER:H	1:159:A:ILE:HB	3	0.36
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG21	9	0.36
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG22	9	0.36
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG23	9	0.36
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG21	16	0.36
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG22	16	0.36
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG23	16	0.36
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	19	0.36
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	11	0.36
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	11	0.36
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	11	0.36
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	16	0.36
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	16	0.36
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	16	0.36
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	5	0.36
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	5	0.36
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	5	0.36
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	7	0.36
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	7	0.36
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	7	0.36
(1,1152)	1:135:A:GLU:HG2	1:136:A:ASP:H	19	0.36
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	9	0.36
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	9	0.36
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	19	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	19	0.36
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	19	0.36
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	18	0.36
(1,1000)	1:113:A:CYS:H	1:116:A:ALA:H	7	0.36
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	3	0.36
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	10	0.36
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	9	0.36
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	17	0.36
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	17	0.36
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	17	0.36
(1,910)	1:102:A:ASP:H	1:106:A:LEU:HB3	17	0.36
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	3	0.36
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	3	0.36
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	17	0.36
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	20	0.36
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	18	0.36
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	18	0.36
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	18	0.36
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE1	16	0.36
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE2	16	0.36
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE1	16	0.36
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE2	16	0.36
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE1	16	0.36
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE2	16	0.36
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	17	0.36
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	17	0.36
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	17	0.36
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	12	0.36
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	7	0.36
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	8	0.36
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	17	0.36
(1,520)	1:64:A:HIS:HE1	1:66:A:GLN:HG2	7	0.36
(1,508)	1:62:A:VAL:H	1:156:A:ILE:HB	13	0.36
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	14	0.36
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	14	0.36
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	14	0.36
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	17	0.36
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	17	0.36
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	17	0.36
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	17	0.36
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB1	9	0.36
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB2	9	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:56:A:ARG:H	1:124:A:ALA:HB3	9	0.36
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	20	0.36
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	6	0.36
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	6	0.36
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	17	0.36
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	17	0.36
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	19	0.36
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	19	0.36
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	10	0.36
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	10	0.36
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	7	0.36
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	7	0.36
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	7	0.36
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	15	0.36
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	15	0.36
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	15	0.36
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	15	0.36
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	17	0.36
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	2	0.36
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	2	0.36
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	4	0.36
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	16	0.36
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	15	0.36
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	15	0.36
(1,138)	1:21:A:ARG:HE	1:34:A:TRP:HH2	10	0.36
(1,129)	1:16:A:SER:HB2	1:21:A:ARG:H	16	0.36
(1,123)	1:15:A:MET:HE1	1:20:A:GLY:H	11	0.36
(1,123)	1:15:A:MET:HE2	1:20:A:GLY:H	11	0.36
(1,123)	1:15:A:MET:HE3	1:20:A:GLY:H	11	0.36
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	19	0.36
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	19	0.36
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	19	0.36
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	3	0.36
(1,86)	1:13:A:LYS:HE2	1:14:A:ARG:H	3	0.36
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	11	0.36
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	13	0.36
(3,45)	1:70:A:PRO:O	1:78:A:ILE:N	11	0.35
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	20	0.35
(3,35)	1:62:A:VAL:N	1:156:A:ILE:O	12	0.35
(3,35)	1:62:A:VAL:N	1:156:A:ILE:O	13	0.35
(3,25)	1:55:A:VAL:N	1:125:A:PHE:O	13	0.35
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	7	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG12	16	0.35
(2,89)	1:55:A:VAL:H	2:651:B:ILE:HG13	16	0.35
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	20	0.35
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	20	0.35
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	20	0.35
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	20	0.35
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	6	0.35
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	4	0.35
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	4	0.35
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	13	0.35
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	13	0.35
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	7	0.35
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	8	0.35
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	1	0.35
(1,2022)	1:94:A:GLN:H	1:94:A:GLN:HG2	17	0.35
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	7	0.35
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	7	0.35
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	7	0.35
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	17	0.35
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	17	0.35
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	17	0.35
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	9	0.35
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	18	0.35
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	20	0.35
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	14	0.35
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	7	0.35
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	14	0.35
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	10	0.35
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	11	0.35
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	9	0.35
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	2	0.35
(1,1346)	1:148:A:GLY:H	1:159:A:ILE:H	5	0.35
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	8	0.35
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	8	0.35
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	8	0.35
(1,1276)	1:63:A:LYS:HA	1:155:A:GLY:HA2	4	0.35
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	9	0.35
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	14	0.35
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	8	0.35
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	12	0.35
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	12	0.35
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	3	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	3	0.35
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	3	0.35
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	1	0.35
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	1	0.35
(1,1112)	1:126:A:SER:H	1:129:A:GLN:HE21	12	0.35
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	4	0.35
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	4	0.35
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	4	0.35
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	1	0.35
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	1	0.35
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	1	0.35
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	3	0.35
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	3	0.35
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	3	0.35
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	17	0.35
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	17	0.35
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	17	0.35
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	9	0.35
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	5	0.35
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	5	0.35
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	5	0.35
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	9	0.35
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	9	0.35
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	9	0.35
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	18	0.35
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE1	14	0.35
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE2	14	0.35
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE3	14	0.35
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	9	0.35
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	3	0.35
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	3	0.35
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	3	0.35
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	15	0.35
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	15	0.35
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	15	0.35
(1,672)	1:64:A:HIS:HD2	1:85:A:ALA:H	15	0.35
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	17	0.35
(1,599)	1:70:A:PRO:HB2	1:78:A:ILE:H	18	0.35
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	7	0.35
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	13	0.35
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	11	0.35
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	11	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	11	0.35
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	6	0.35
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	9	0.35
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	3	0.35
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	9	0.35
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	9	0.35
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	9	0.35
(1,373)	1:34:A:TRP:HD1	1:35:A:GLU:H	12	0.35
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	15	0.35
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	8	0.35
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	8	0.35
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	1	0.35
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	1	0.35
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	9	0.35
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	9	0.35
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	9	0.35
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	9	0.35
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	9	0.35
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	10	0.35
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	10	0.35
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	10	0.35
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	18	0.35
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	20	0.35
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	19	0.35
(1,223)	1:14:A:ARG:HB2	1:25:A:PHE:H	13	0.35
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	16	0.35
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	19	0.35
(1,198)	1:23:A:TYR:HE1	1:24:A:TYR:H	20	0.35
(1,198)	1:23:A:TYR:HE2	1:24:A:TYR:H	20	0.35
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	4	0.35
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	5	0.35
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	5	0.35
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	5	0.35
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	5	0.35
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	5	0.35
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	5	0.35
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	5	0.35
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	5	0.35
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	5	0.35
(1,138)	1:21:A:ARG:HE	1:34:A:TRP:HH2	6	0.35
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	8	0.35
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	8	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	3	0.35
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	14	0.35
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	14	0.35
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	14	0.35
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	14	0.35
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	14	0.35
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	14	0.35
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	10	0.35
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	3	0.35
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	9	0.35
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	1	0.35
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	2	0.34
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	7	0.34
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	11	0.34
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	14	0.34
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	16	0.34
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	4	0.34
(3,10)	1:16:A:SER:O	1:19:A:SER:H	19	0.34
(3,9)	1:16:A:SER:O	1:19:A:SER:N	5	0.34
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	1	0.34
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	1	0.34
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	13	0.34
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	7	0.34
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	9	0.34
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	5	0.34
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	5	0.34
(2,45)	1:131:A:GLN:HE21	1:152:A:THR:HB	20	0.34
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	7	0.34
(1,2597)	1:138:A:SER:H	2:656:B:PHE:HB2	2	0.34
(1,2590)	1:122:A:LEU:HD21	2:656:B:PHE:HD1	13	0.34
(1,2590)	1:122:A:LEU:HD21	2:656:B:PHE:HD2	13	0.34
(1,2590)	1:122:A:LEU:HD22	2:656:B:PHE:HD1	13	0.34
(1,2590)	1:122:A:LEU:HD22	2:656:B:PHE:HD2	13	0.34
(1,2590)	1:122:A:LEU:HD23	2:656:B:PHE:HD1	13	0.34
(1,2590)	1:122:A:LEU:HD23	2:656:B:PHE:HD2	13	0.34
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	1	0.34
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	1	0.34
(1,2575)	1:21:A:ARG:H	2:641:B:TPO:HG21	2	0.34
(1,2575)	1:21:A:ARG:H	2:641:B:TPO:HG22	2	0.34
(1,2575)	1:21:A:ARG:H	2:641:B:TPO:HG23	2	0.34
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD1	5	0.34
(1,2568)	2:658:B:GLY:H	2:659:B:PHE:HD2	5	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	11	0.34
(1,2510)	2:645:B:GLN:H	2:647:B:VAL:H	1	0.34
(1,2384)	1:163:A:GLU:H	1:163:A:GLU:HG3	5	0.34
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	3	0.34
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	3	0.34
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	3	0.34
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	17	0.34
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	2	0.34
(1,2157)	1:119:A:ARG:H	1:119:A:ARG:HG2	13	0.34
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	5	0.34
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	14	0.34
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	19	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	6	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	6	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	6	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	7	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	7	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	7	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	17	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	17	0.34
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	17	0.34
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	11	0.34
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	11	0.34
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	11	0.34
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	12	0.34
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	16	0.34
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	17	0.34
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	11	0.34
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG21	3	0.34
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG22	3	0.34
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG23	3	0.34
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	13	0.34
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	13	0.34
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	13	0.34
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	13	0.34
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	13	0.34
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	13	0.34
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	13	0.34
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	13	0.34
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	13	0.34
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	2	0.34
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	19	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	7	0.34
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	3	0.34
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	4	0.34
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	4	0.34
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	4	0.34
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	4	0.34
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	4	0.34
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	4	0.34
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	9	0.34
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	9	0.34
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	9	0.34
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	17	0.34
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	17	0.34
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	17	0.34
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	8	0.34
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	1	0.34
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	1	0.34
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	1	0.34
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	3	0.34
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	13	0.34
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	14	0.34
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	18	0.34
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	18	0.34
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	18	0.34
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	18	0.34
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	18	0.34
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	18	0.34
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE1	1	0.34
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE2	1	0.34
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE3	1	0.34
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	11	0.34
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	11	0.34
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	11	0.34
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	11	0.34
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	11	0.34
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	11	0.34
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	14	0.34
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	12	0.34
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	10	0.34
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	7	0.34
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	7	0.34
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	7	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	12	0.34
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	12	0.34
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	12	0.34
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	6	0.34
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	12	0.34
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	17	0.34
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	17	0.34
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	15	0.34
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	17	0.34
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	1	0.34
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	1	0.34
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	1	0.34
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	7	0.34
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	7	0.34
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	7	0.34
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	14	0.34
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	14	0.34
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	14	0.34
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	14	0.34
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	14	0.34
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	14	0.34
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	14	0.34
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	14	0.34
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	14	0.34
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	18	0.34
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	18	0.34
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	18	0.34
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	4	0.34
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	4	0.34
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	12	0.34
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	12	0.34
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	19	0.34
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	19	0.34
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	5	0.34
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	7	0.34
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	7	0.34
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	11	0.34
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	11	0.34
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	17	0.34
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	6	0.34
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	20	0.34
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	6	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	19	0.34
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	6	0.34
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	12	0.34
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	2	0.34
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	1	0.33
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	6	0.33
(3,65)	1:91:A:GLY:O	1:95:A:LYS:N	4	0.33
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	14	0.33
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	5	0.33
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	12	0.33
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	14	0.33
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	20	0.33
(3,9)	1:16:A:SER:O	1:19:A:SER:N	14	0.33
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	13	0.33
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	13	0.33
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	5	0.33
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	5	0.33
(2,79)	2:659:B:PHE:HE1	2:661:B:PHE:H	12	0.33
(2,79)	2:659:B:PHE:HE2	2:661:B:PHE:H	12	0.33
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD1	4	0.33
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD2	4	0.33
(1,2615)	1:49:A:GLN:H	1:49:A:GLN:HG2	18	0.33
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	15	0.33
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	15	0.33
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	15	0.33
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	15	0.33
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	15	0.33
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	15	0.33
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	14	0.33
(1,2515)	2:645:B:GLN:HA	2:647:B:VAL:H	10	0.33
(1,2506)	2:644:B:ASP:H	2:645:B:GLN:HA	18	0.33
(1,2251)	1:141:A:LEU:H	1:141:A:LEU:HG	15	0.33
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	11	0.33
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	7	0.33
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	8	0.33
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	1	0.33
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	1	0.33
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	1	0.33
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	12	0.33
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	12	0.33
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	12	0.33
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	15	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	9	0.33
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	2	0.33
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	3	0.33
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	4	0.33
(1,1429)	1:143:A:THR:HG21	1:163:A:GLU:HB2	18	0.33
(1,1429)	1:143:A:THR:HG22	1:163:A:GLU:HB2	18	0.33
(1,1429)	1:143:A:THR:HG23	1:163:A:GLU:HB2	18	0.33
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	8	0.33
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	6	0.33
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	6	0.33
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	6	0.33
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	14	0.33
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	14	0.33
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	14	0.33
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG21	2	0.33
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG22	2	0.33
(1,1337)	1:59:A:HIS:H	1:159:A:ILE:HG23	2	0.33
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	18	0.33
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	18	0.33
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	18	0.33
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	7	0.33
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	7	0.33
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	7	0.33
(1,1208)	1:103:A:PHE:HD1	1:146:A:MET:HB2	18	0.33
(1,1208)	1:103:A:PHE:HD2	1:146:A:MET:HB2	18	0.33
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	11	0.33
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	18	0.33
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	18	0.33
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	18	0.33
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	7	0.33
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	3	0.33
(1,1141)	1:130:A:MET:HB2	1:134:A:PHE:H	11	0.33
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	1	0.33
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	15	0.33
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	5	0.33
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	5	0.33
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	5	0.33
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	9	0.33
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	9	0.33
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	9	0.33
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	2	0.33
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	11	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	3	0.33
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	6	0.33
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	15	0.33
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	17	0.33
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	17	0.33
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	1	0.33
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	2	0.33
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	4	0.33
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	4	0.33
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	17	0.33
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	17	0.33
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	20	0.33
(1,748)	1:87:A:GLU:HA	1:91:A:GLY:H	15	0.33
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD11	10	0.33
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD12	10	0.33
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD13	10	0.33
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	17	0.33
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	17	0.33
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	17	0.33
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	5	0.33
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	6	0.33
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	9	0.33
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	10	0.33
(1,646)	1:81:A:THR:HG21	1:84:A:GLU:HB2	16	0.33
(1,646)	1:81:A:THR:HG22	1:84:A:GLU:HB2	16	0.33
(1,646)	1:81:A:THR:HG23	1:84:A:GLU:HB2	16	0.33
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	16	0.33
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	19	0.33
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD11	13	0.33
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD12	13	0.33
(1,608)	1:75:A:GLN:HE22	1:78:A:ILE:HD13	13	0.33
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	15	0.33
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	14	0.33
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	16	0.33
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	5	0.33
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	3	0.33
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	3	0.33
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	3	0.33
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	1	0.33
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	10	0.33
(1,401)	1:54:A:ARG:HD2	1:55:A:VAL:HA	10	0.33
(1,393)	1:53:A:ALA:HB1	1:54:A:ARG:H	16	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:53:A:ALA:HB2	1:54:A:ARG:H	16	0.33
(1,393)	1:53:A:ALA:HB3	1:54:A:ARG:H	16	0.33
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	13	0.33
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	5	0.33
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	4	0.33
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	6	0.33
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	1	0.33
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	1	0.33
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	9	0.33
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	16	0.33
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	19	0.33
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	10	0.33
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	13	0.33
(1,278)	1:26:A:ASN:HB2	1:30:A:ASN:H	12	0.33
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	14	0.33
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	14	0.33
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	2	0.33
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	17	0.33
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	2	0.33
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	18	0.33
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	8	0.33
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	6	0.33
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	6	0.33
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	5	0.33
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	9	0.33
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	19	0.33
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	19	0.33
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	19	0.33
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	6	0.33
(3,65)	1:91:A:GLY:O	1:95:A:LYS:N	18	0.32
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	13	0.32
(3,35)	1:62:A:VAL:N	1:156:A:ILE:O	8	0.32
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	11	0.32
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	11	0.32
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	11	0.32
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	11	0.32
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	11	0.32
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	11	0.32
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	14	0.32
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	14	0.32
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	14	0.32
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	14	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	14	0.32
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	14	0.32
(2,102)	1:135:A:GLU:H	2:656:B:PHE:HB2	2	0.32
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	8	0.32
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	8	0.32
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	8	0.32
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	5	0.32
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	5	0.32
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	19	0.32
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	19	0.32
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	19	0.32
(1,2550)	2:652:B:ASP:H	2:653:B:GLN:H	16	0.32
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	8	0.32
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	4	0.32
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	4	0.32
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	4	0.32
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	17	0.32
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	17	0.32
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	17	0.32
(1,2251)	1:141:A:LEU:H	1:141:A:LEU:HG	11	0.32
(1,2209)	1:131:A:GLN:HA	1:131:A:GLN:HE22	16	0.32
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	7	0.32
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	15	0.32
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	18	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	13	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	13	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	13	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	14	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	14	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	14	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	15	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	15	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	15	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	16	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	16	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	16	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	19	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	19	0.32
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	19	0.32
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	6	0.32
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	3	0.32
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	7	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	9	0.32
(1,1441)	1:162:A:THR:HG21	1:163:A:GLU:HG3	14	0.32
(1,1441)	1:162:A:THR:HG22	1:163:A:GLU:HG3	14	0.32
(1,1441)	1:162:A:THR:HG23	1:163:A:GLU:HG3	14	0.32
(1,1428)	1:143:A:THR:HG21	1:163:A:GLU:H	20	0.32
(1,1428)	1:143:A:THR:HG22	1:163:A:GLU:H	20	0.32
(1,1428)	1:143:A:THR:HG23	1:163:A:GLU:H	20	0.32
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	3	0.32
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	11	0.32
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	11	0.32
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	9	0.32
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	9	0.32
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	9	0.32
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	7	0.32
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	7	0.32
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	7	0.32
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	16	0.32
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	16	0.32
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	16	0.32
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	7	0.32
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	7	0.32
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	7	0.32
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	11	0.32
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	8	0.32
(1,1066)	1:122:A:LEU:HD21	1:125:A:PHE:HD1	13	0.32
(1,1066)	1:122:A:LEU:HD21	1:125:A:PHE:HD2	13	0.32
(1,1066)	1:122:A:LEU:HD22	1:125:A:PHE:HD1	13	0.32
(1,1066)	1:122:A:LEU:HD22	1:125:A:PHE:HD2	13	0.32
(1,1066)	1:122:A:LEU:HD23	1:125:A:PHE:HD1	13	0.32
(1,1066)	1:122:A:LEU:HD23	1:125:A:PHE:HD2	13	0.32
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	3	0.32
(1,1027)	1:118:A:ALA:HA	1:119:A:ARG:HG2	10	0.32
(1,1027)	1:118:A:ALA:HA	1:119:A:ARG:HG2	13	0.32
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	3	0.32
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	12	0.32
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	12	0.32
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	12	0.32
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	12	0.32
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	12	0.32
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	12	0.32
(1,978)	1:107:A:ALA:HB1	1:111:A:SER:HA	17	0.32
(1,978)	1:107:A:ALA:HB2	1:111:A:SER:HA	17	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,978)	1:107:A:ALA:HB3	1:111:A:SER:HA	17	0.32
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	11	0.32
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	11	0.32
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	11	0.32
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	14	0.32
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	14	0.32
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	14	0.32
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	20	0.32
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	20	0.32
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	20	0.32
(1,917)	1:105:A:SER:HB2	1:106:A:LEU:H	15	0.32
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	13	0.32
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	19	0.32
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	19	0.32
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	19	0.32
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	19	0.32
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	19	0.32
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	19	0.32
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	20	0.32
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	20	0.32
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	20	0.32
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	20	0.32
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	20	0.32
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	20	0.32
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	12	0.32
(1,854)	1:98:A:SER:H	1:101:A:GLU:H	8	0.32
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	14	0.32
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	14	0.32
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	14	0.32
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	14	0.32
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	14	0.32
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	14	0.32
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	2	0.32
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	3	0.32
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD11	14	0.32
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD12	14	0.32
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD13	14	0.32
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	13	0.32
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	13	0.32
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	13	0.32
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	2	0.32
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	13	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	14	0.32
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	19	0.32
(1,649)	1:66:A:GLN:HE21	1:82:A:LYS:HB2	7	0.32
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	16	0.32
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	20	0.32
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	17	0.32
(1,640)	1:65:A:SER:HB3	1:81:A:THR:HA	1	0.32
(1,634)	1:80:A:ARG:HB2	1:81:A:THR:H	15	0.32
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	1	0.32
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	7	0.32
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	12	0.32
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	9	0.32
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	19	0.32
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	20	0.32
(1,444)	1:59:A:HIS:HA	1:158:A:ILE:H	6	0.32
(1,401)	1:54:A:ARG:HD2	1:55:A:VAL:HA	12	0.32
(1,393)	1:53:A:ALA:HB1	1:54:A:ARG:H	2	0.32
(1,393)	1:53:A:ALA:HB2	1:54:A:ARG:H	2	0.32
(1,393)	1:53:A:ALA:HB3	1:54:A:ARG:H	2	0.32
(1,385)	1:24:A:TYR:HD1	1:36:A:ARG:H	15	0.32
(1,385)	1:24:A:TYR:HD2	1:36:A:ARG:H	15	0.32
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE22	10	0.32
(1,366)	1:32:A:SER:H	1:33:A:GLN:HE21	10	0.32
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	9	0.32
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	9	0.32
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	11	0.32
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	11	0.32
(1,354)	1:24:A:TYR:H	1:32:A:SER:HB3	13	0.32
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	4	0.32
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	4	0.32
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	4	0.32
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	16	0.32
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	16	0.32
(1,224)	1:14:A:ARG:HE	1:25:A:PHE:HB3	12	0.32
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	2	0.32
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	15	0.32
(1,211)	1:24:A:TYR:HE1	1:36:A:ARG:HD2	12	0.32
(1,211)	1:24:A:TYR:HE2	1:36:A:ARG:HD2	12	0.32
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	12	0.32
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	4	0.32
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	14	0.32
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	7	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	2	0.32
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	2	0.32
(1,28)	1:7:A:LEU:HD21	1:13:A:LYS:HG3	19	0.32
(1,28)	1:7:A:LEU:HD22	1:13:A:LYS:HG3	19	0.32
(1,28)	1:7:A:LEU:HD23	1:13:A:LYS:HG3	19	0.32
(3,63)	1:90:A:ASN:O	1:94:A:GLN:N	2	0.31
(3,25)	1:55:A:VAL:N	1:125:A:PHE:O	10	0.31
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	10	0.31
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	11	0.31
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	12	0.31
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	16	0.31
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	16	0.31
(2,55)	1:150:A:VAL:HG21	1:158:A:ILE:HA	16	0.31
(2,55)	1:150:A:VAL:HG22	1:158:A:ILE:HA	16	0.31
(2,55)	1:150:A:VAL:HG23	1:158:A:ILE:HA	16	0.31
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	13	0.31
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	13	0.31
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	13	0.31
(2,21)	1:73:A:TRP:HE1	1:74:A:ARG:HG3	8	0.31
(2,5)	1:23:A:TYR:H	1:34:A:TRP:HZ3	8	0.31
(1,2597)	1:138:A:SER:H	2:656:B:PHE:HB2	15	0.31
(1,2578)	1:29:A:THR:HG21	2:646:B:GLU:HA	12	0.31
(1,2578)	1:29:A:THR:HG22	2:646:B:GLU:HA	12	0.31
(1,2578)	1:29:A:THR:HG23	2:646:B:GLU:HA	12	0.31
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	15	0.31
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	15	0.31
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	15	0.31
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	16	0.31
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	16	0.31
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	16	0.31
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	1	0.31
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	4	0.31
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	5	0.31
(1,2514)	2:646:B:GLU:HA	2:649:B:ARG:H	1	0.31
(1,2434)	2:648:B:ILE:H	2:648:B:ILE:HG12	13	0.31
(1,2403)	2:645:B:GLN:H	2:645:B:GLN:HG2	19	0.31
(1,2209)	1:131:A:GLN:HA	1:131:A:GLN:HE22	18	0.31
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	2	0.31
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	2	0.31
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	2	0.31
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	16	0.31
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	3	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	4	0.31
(1,1700)	1:36:A:ARG:H	1:36:A:ARG:HG2	13	0.31
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	4	0.31
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	5	0.31
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	12	0.31
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	19	0.31
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	20	0.31
(1,1439)	1:162:A:THR:HG21	1:163:A:GLU:H	11	0.31
(1,1439)	1:162:A:THR:HG22	1:163:A:GLU:H	11	0.31
(1,1439)	1:162:A:THR:HG23	1:163:A:GLU:H	11	0.31
(1,1424)	1:55:A:VAL:HG21	1:163:A:GLU:H	18	0.31
(1,1424)	1:55:A:VAL:HG22	1:163:A:GLU:H	18	0.31
(1,1424)	1:55:A:VAL:HG23	1:163:A:GLU:H	18	0.31
(1,1424)	1:55:A:VAL:HG11	1:163:A:GLU:H	18	0.31
(1,1424)	1:55:A:VAL:HG12	1:163:A:GLU:H	18	0.31
(1,1424)	1:55:A:VAL:HG13	1:163:A:GLU:H	18	0.31
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	10	0.31
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD21	15	0.31
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD22	15	0.31
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD23	15	0.31
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	3	0.31
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	3	0.31
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	3	0.31
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	8	0.31
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	8	0.31
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	8	0.31
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	2	0.31
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	2	0.31
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	2	0.31
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	7	0.31
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	10	0.31
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	10	0.31
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	10	0.31
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD21	11	0.31
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD22	11	0.31
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD23	11	0.31
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD21	11	0.31
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD22	11	0.31
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD23	11	0.31
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD21	11	0.31
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD22	11	0.31
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD23	11	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	18	0.31
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	18	0.31
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	18	0.31
(1,1143)	1:130:A:MET:HB2	1:135:A:GLU:H	11	0.31
(1,1054)	1:59:A:HIS:HD2	1:122:A:LEU:H	2	0.31
(1,1033)	1:108:A:SER:H	1:119:A:ARG:HB2	2	0.31
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	12	0.31
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	9	0.31
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	9	0.31
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	9	0.31
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB1	3	0.31
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB2	3	0.31
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB3	3	0.31
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	9	0.31
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	8	0.31
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	13	0.31
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	12	0.31
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	1	0.31
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	17	0.31
(1,909)	1:102:A:ASP:HB2	1:106:A:LEU:H	2	0.31
(1,901)	1:103:A:PHE:H	1:105:A:SER:H	19	0.31
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	20	0.31
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	10	0.31
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	2	0.31
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	10	0.31
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	17	0.31
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	17	0.31
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	17	0.31
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	8	0.31
(1,689)	1:86:A:LEU:HG	1:90:A:ASN:HD21	14	0.31
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	9	0.31
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	9	0.31
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	9	0.31
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	7	0.31
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	13	0.31
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	4	0.31
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	17	0.31
(1,612)	1:75:A:GLN:HE21	1:78:A:ILE:HA	11	0.31
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	10	0.31
(1,465)	1:60:A:LEU:HB2	1:158:A:ILE:H	18	0.31
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	11	0.31
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	11	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	11	0.31
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	18	0.31
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	18	0.31
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	18	0.31
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	13	0.31
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	12	0.31
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	12	0.31
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	15	0.31
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	15	0.31
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	8	0.31
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	8	0.31
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	8	0.31
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	18	0.31
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	18	0.31
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	18	0.31
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	16	0.31
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	18	0.31
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	8	0.31
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	16	0.31
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	3	0.31
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	3	0.31
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	3	0.31
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	3	0.31
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	3	0.31
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	3	0.31
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	3	0.31
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	3	0.31
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	3	0.31
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	9	0.31
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	11	0.31
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	5	0.31
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	5	0.31
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	5	0.31
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	5	0.31
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	5	0.31
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	5	0.31
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	3	0.31
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	3	0.31
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB1	9	0.31
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB2	9	0.31
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB3	9	0.31
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	7	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	4	0.31
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	20	0.31
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	18	0.31
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	12	0.3
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	6	0.3
(3,35)	1:62:A:VAL:N	1:156:A:ILE:O	3	0.3
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	14	0.3
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	14	0.3
(2,108)	1:140:A:ALA:HB1	2:649:B:ARG:HA	18	0.3
(2,108)	1:140:A:ALA:HB2	2:649:B:ARG:HA	18	0.3
(2,108)	1:140:A:ALA:HB3	2:649:B:ARG:HA	18	0.3
(2,106)	1:139:A:PHE:H	2:656:B:PHE:HB2	17	0.3
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	4	0.3
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	4	0.3
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	8	0.3
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	8	0.3
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	8	0.3
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	1	0.3
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	3	0.3
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	3	0.3
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	10	0.3
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	10	0.3
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG21	20	0.3
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG22	20	0.3
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG23	20	0.3
(1,2533)	2:647:B:VAL:H	2:649:B:ARG:H	19	0.3
(1,2506)	2:644:B:ASP:H	2:645:B:GLN:HA	3	0.3
(1,2506)	2:644:B:ASP:H	2:645:B:GLN:HA	20	0.3
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE1	1	0.3
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE2	1	0.3
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	15	0.3
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	1	0.3
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	3	0.3
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	6	0.3
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	5	0.3
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	15	0.3
(1,1434)	1:161:A:ARG:HD2	1:163:A:GLU:H	17	0.3
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	16	0.3
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	5	0.3
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	14	0.3
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	8	0.3
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	8	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	8	0.3
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	8	0.3
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	8	0.3
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	8	0.3
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG21	20	0.3
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG22	20	0.3
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG23	20	0.3
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG21	20	0.3
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG22	20	0.3
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG23	20	0.3
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	5	0.3
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	5	0.3
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	5	0.3
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	8	0.3
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	8	0.3
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	8	0.3
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	1	0.3
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	1	0.3
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	1	0.3
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	14	0.3
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	1	0.3
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	1	0.3
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	1	0.3
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	1	0.3
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	1	0.3
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	1	0.3
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	1	0.3
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	1	0.3
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	1	0.3
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	15	0.3
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	15	0.3
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	15	0.3
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	20	0.3
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	16	0.3
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	16	0.3
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	16	0.3
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	16	0.3
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	16	0.3
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	16	0.3
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	3	0.3
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	3	0.3
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	3	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	14	0.3
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	11	0.3
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	18	0.3
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	19	0.3
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	11	0.3
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	7	0.3
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	12	0.3
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	20	0.3
(1,901)	1:103:A:PHE:H	1:105:A:SER:H	18	0.3
(1,849)	1:98:A:SER:HB2	1:99:A:GLY:H	15	0.3
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE1	8	0.3
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE2	8	0.3
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE3	8	0.3
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	1	0.3
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	1	0.3
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	1	0.3
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	11	0.3
(1,748)	1:87:A:GLU:HA	1:91:A:GLY:H	2	0.3
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	7	0.3
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	14	0.3
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	5	0.3
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG21	10	0.3
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG22	10	0.3
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG23	10	0.3
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	4	0.3
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	4	0.3
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	4	0.3
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	18	0.3
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	18	0.3
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	18	0.3
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	14	0.3
(1,479)	1:61:A:LEU:HD21	1:155:A:GLY:H	13	0.3
(1,479)	1:61:A:LEU:HD22	1:155:A:GLY:H	13	0.3
(1,479)	1:61:A:LEU:HD23	1:155:A:GLY:H	13	0.3
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	7	0.3
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	7	0.3
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	7	0.3
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	7	0.3
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	7	0.3
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	7	0.3
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	7	0.3
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	7	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	7	0.3
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	11	0.3
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	16	0.3
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	16	0.3
(1,373)	1:34:A:TRP:HD1	1:35:A:GLU:H	17	0.3
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	14	0.3
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	9	0.3
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	9	0.3
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	9	0.3
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	20	0.3
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	8	0.3
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	10	0.3
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	3	0.3
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	7	0.3
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	6	0.3
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	13	0.3
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	13	0.3
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	8	0.3
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	7	0.3
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	7	0.3
(1,17)	1:6:A:LYS:HB3	1:7:A:LEU:H	14	0.3
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	1	0.29
(3,35)	1:62:A:VAL:N	1:156:A:ILE:O	5	0.29
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	3	0.29
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	3	0.29
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	3	0.29
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD1	1	0.29
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD2	1	0.29
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	13	0.29
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	4	0.29
(1,2589)	1:122:A:LEU:HD21	2:656:B:PHE:HE1	19	0.29
(1,2589)	1:122:A:LEU:HD21	2:656:B:PHE:HE2	19	0.29
(1,2589)	1:122:A:LEU:HD22	2:656:B:PHE:HE1	19	0.29
(1,2589)	1:122:A:LEU:HD22	2:656:B:PHE:HE2	19	0.29
(1,2589)	1:122:A:LEU:HD23	2:656:B:PHE:HE1	19	0.29
(1,2589)	1:122:A:LEU:HD23	2:656:B:PHE:HE2	19	0.29
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	3	0.29
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	3	0.29
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD1	15	0.29
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD2	15	0.29
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	6	0.29
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	14	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	3	0.29
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	12	0.29
(1,2517)	2:646:B:GLU:HG2	2:647:B:VAL:H	17	0.29
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE1	7	0.29
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE2	7	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD21	15	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD22	15	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD23	15	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD11	15	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD12	15	0.29
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD13	15	0.29
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	12	0.29
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	10	0.29
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	10	0.29
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	10	0.29
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	18	0.29
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	18	0.29
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	18	0.29
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	10	0.29
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	10	0.29
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	10	0.29
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	19	0.29
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	19	0.29
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	19	0.29
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	12	0.29
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	17	0.29
(1,1429)	1:143:A:THR:HG21	1:163:A:GLU:HB2	10	0.29
(1,1429)	1:143:A:THR:HG22	1:163:A:GLU:HB2	10	0.29
(1,1429)	1:143:A:THR:HG23	1:163:A:GLU:HB2	10	0.29
(1,1399)	1:143:A:THR:H	1:161:A:ARG:HD2	14	0.29
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	11	0.29
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD11	7	0.29
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD12	7	0.29
(1,1349)	1:158:A:ILE:H	1:159:A:ILE:HD13	7	0.29
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	19	0.29
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	19	0.29
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	19	0.29
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	19	0.29
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	19	0.29
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	19	0.29
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG21	16	0.29
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG22	16	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG23	16	0.29
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG21	16	0.29
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG22	16	0.29
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG23	16	0.29
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	6	0.29
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	6	0.29
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	6	0.29
(1,1242)	1:150:A:VAL:HG11	1:157:A:HIS:H	20	0.29
(1,1242)	1:150:A:VAL:HG12	1:157:A:HIS:H	20	0.29
(1,1242)	1:150:A:VAL:HG13	1:157:A:HIS:H	20	0.29
(1,1217)	1:145:A:GLU:HB3	1:147:A:SER:H	19	0.29
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	2	0.29
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	12	0.29
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	12	0.29
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	12	0.29
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	8	0.29
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	1	0.29
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	1	0.29
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	1	0.29
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	17	0.29
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	17	0.29
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	17	0.29
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB1	8	0.29
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB2	8	0.29
(1,1080)	1:54:A:ARG:HE	1:124:A:ALA:HB3	8	0.29
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	7	0.29
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	7	0.29
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	7	0.29
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	16	0.29
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	16	0.29
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	16	0.29
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	10	0.29
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	10	0.29
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	10	0.29
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	1	0.29
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	1	0.29
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	1	0.29
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	14	0.29
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	14	0.29
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	14	0.29
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	18	0.29
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	9	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	4	0.29
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	20	0.29
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	15	0.29
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	15	0.29
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	15	0.29
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	14	0.29
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	15	0.29
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	15	0.29
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	16	0.29
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	16	0.29
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	16	0.29
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	14	0.29
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	14	0.29
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	14	0.29
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	15	0.29
(1,737)	1:86:A:LEU:HB3	1:90:A:ASN:H	1	0.29
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	19	0.29
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	19	0.29
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	19	0.29
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD11	17	0.29
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD12	17	0.29
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD13	17	0.29
(1,640)	1:65:A:SER:HB3	1:81:A:THR:HA	20	0.29
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	8	0.29
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	7	0.29
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	13	0.29
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	13	0.29
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	13	0.29
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	19	0.29
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	19	0.29
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	19	0.29
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	16	0.29
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	16	0.29
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	16	0.29
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	10	0.29
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	10	0.29
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	10	0.29
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	16	0.29
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	16	0.29
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	16	0.29
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	4	0.29
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	4	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	4	0.29
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	4	0.29
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	4	0.29
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	4	0.29
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	4	0.29
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	4	0.29
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	4	0.29
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	1	0.29
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	10	0.29
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	10	0.29
(1,354)	1:24:A:TYR:H	1:32:A:SER:HB3	16	0.29
(1,349)	1:23:A:TYR:HD1	1:32:A:SER:HB2	13	0.29
(1,349)	1:23:A:TYR:HD2	1:32:A:SER:HB2	13	0.29
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	7	0.29
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	7	0.29
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	7	0.29
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	17	0.29
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	17	0.29
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	17	0.29
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	13	0.29
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	12	0.29
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	2	0.29
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	2	0.29
(1,103)	1:14:A:ARG:HG2	1:15:A:MET:H	10	0.29
(1,103)	1:14:A:ARG:HG2	1:15:A:MET:H	16	0.29
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	13	0.29
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	13	0.29
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	13	0.29
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	5	0.29
(3,39)	1:64:A:HIS:O	1:67:A:SER:N	1	0.28
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	3	0.28
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	3	0.28
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	8	0.28
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	8	0.28
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	9	0.28
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	9	0.28
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	14	0.28
(2,86)	1:29:A:THR:HG21	2:647:B:VAL:HA	13	0.28
(2,86)	1:29:A:THR:HG22	2:647:B:VAL:HA	13	0.28
(2,86)	1:29:A:THR:HG23	2:647:B:VAL:HA	13	0.28
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	3	0.28
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	8	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	17	0.28
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	17	0.28
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD1	7	0.28
(1,2587)	1:115:A:SER:H	2:659:B:PHE:HD2	7	0.28
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	16	0.28
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	16	0.28
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	16	0.28
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	4	0.28
(1,2553)	2:651:B:ILE:HG21	2:653:B:GLN:HE21	13	0.28
(1,2553)	2:651:B:ILE:HG21	2:653:B:GLN:HE22	13	0.28
(1,2553)	2:651:B:ILE:HG22	2:653:B:GLN:HE21	13	0.28
(1,2553)	2:651:B:ILE:HG22	2:653:B:GLN:HE22	13	0.28
(1,2553)	2:651:B:ILE:HG23	2:653:B:GLN:HE21	13	0.28
(1,2553)	2:651:B:ILE:HG23	2:653:B:GLN:HE22	13	0.28
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	17	0.28
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	17	0.28
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	17	0.28
(1,2517)	2:646:B:GLU:HG2	2:647:B:VAL:H	19	0.28
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD21	11	0.28
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD22	11	0.28
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD23	11	0.28
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD11	11	0.28
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD12	11	0.28
(1,2250)	1:141:A:LEU:H	1:141:A:LEU:HD13	11	0.28
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	3	0.28
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	5	0.28
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	3	0.28
(1,1703)	1:36:A:ARG:H	1:36:A:ARG:HD2	8	0.28
(1,1571)	1:21:A:ARG:H	1:21:A:ARG:HD2	3	0.28
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	3	0.28
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	2	0.28
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	14	0.28
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	14	0.28
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	14	0.28
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	14	0.28
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	14	0.28
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	14	0.28
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	14	0.28
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	14	0.28
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	14	0.28
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	14	0.28
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	14	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	14	0.28
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	18	0.28
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	18	0.28
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	18	0.28
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	18	0.28
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	12	0.28
(1,1178)	1:137:A:ALA:HA	1:141:A:LEU:H	1	0.28
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	1	0.28
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	11	0.28
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	16	0.28
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	16	0.28
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	16	0.28
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	15	0.28
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	15	0.28
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	15	0.28
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	19	0.28
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	18	0.28
(1,917)	1:105:A:SER:HB2	1:106:A:LEU:H	17	0.28
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	4	0.28
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	9	0.28
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	8	0.28
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	8	0.28
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	11	0.28
(1,772)	1:92:A:TYR:H	1:93:A:ILE:HB	3	0.28
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	7	0.28
(1,753)	1:90:A:ASN:HD22	1:91:A:GLY:H	5	0.28
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	6	0.28
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	14	0.28
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	14	0.28
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	14	0.28
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	20	0.28
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	20	0.28
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	20	0.28
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	3	0.28
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	3	0.28
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	3	0.28
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	20	0.28
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	20	0.28
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	20	0.28
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	2	0.28
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	8	0.28
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	13	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	2	0.28
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	2	0.28
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	2	0.28
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	5	0.28
(1,576)	1:73:A:TRP:HE1	1:115:A:SER:H	17	0.28
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	12	0.28
(1,540)	1:67:A:SER:HA	1:69:A:ARG:H	17	0.28
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	4	0.28
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	4	0.28
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	4	0.28
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	9	0.28
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	10	0.28
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	10	0.28
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	10	0.28
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	11	0.28
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	11	0.28
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	11	0.28
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	17	0.28
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	17	0.28
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	17	0.28
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	17	0.28
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	17	0.28
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	17	0.28
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	17	0.28
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	17	0.28
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	17	0.28
(1,415)	1:56:A:ARG:HA	1:124:A:ALA:H	3	0.28
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	16	0.28
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	10	0.28
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	15	0.28
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	4	0.28
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	4	0.28
(1,295)	1:27:A:HIS:H	1:29:A:THR:H	20	0.28
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	5	0.28
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	5	0.28
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	8	0.28
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	12	0.28
(1,190)	1:13:A:LYS:HB3	1:24:A:TYR:HA	3	0.28
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	18	0.28
(1,84)	1:13:A:LYS:HG2	1:14:A:ARG:H	1	0.28
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	13	0.28
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	20	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	20	0.28
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	20	0.28
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	20	0.28
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	20	0.28
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	20	0.28
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	17	0.28
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	17	0.28
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	12	0.28
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	12	0.28
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	17	0.28
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	17	0.28
(1,14)	1:6:A:LYS:HG2	1:7:A:LEU:H	1	0.28
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	10	0.27
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	16	0.27
(3,28)	1:56:A:ARG:H	1:163:A:GLU:O	16	0.27
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE1	2	0.27
(2,98)	1:124:A:ALA:H	2:656:B:PHE:HE2	2	0.27
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG12	18	0.27
(2,90)	1:56:A:ARG:H	2:651:B:ILE:HG13	18	0.27
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	2	0.27
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	19	0.27
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	4	0.27
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	4	0.27
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	4	0.27
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	4	0.27
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	20	0.27
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	20	0.27
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	20	0.27
(1,2209)	1:131:A:GLN:HA	1:131:A:GLN:HE22	20	0.27
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	1	0.27
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	5	0.27
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	6	0.27
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	7	0.27
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	8	0.27
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	14	0.27
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	9	0.27
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	9	0.27
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	9	0.27
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG21	20	0.27
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG22	20	0.27
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG23	20	0.27
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	7	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	18	0.27
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	11	0.27
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	12	0.27
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	19	0.27
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	1	0.27
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	19	0.27
(1,1413)	1:56:A:ARG:HD2	1:162:A:THR:HG21	20	0.27
(1,1413)	1:56:A:ARG:HD2	1:162:A:THR:HG22	20	0.27
(1,1413)	1:56:A:ARG:HD2	1:162:A:THR:HG23	20	0.27
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	16	0.27
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	11	0.27
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	11	0.27
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	11	0.27
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	10	0.27
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	15	0.27
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	5	0.27
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	8	0.27
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	8	0.27
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	8	0.27
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	18	0.27
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	18	0.27
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	18	0.27
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	4	0.27
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	14	0.27
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	14	0.27
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	14	0.27
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	16	0.27
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	16	0.27
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	16	0.27
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	13	0.27
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	8	0.27
(1,886)	1:103:A:PHE:HE1	1:107:A:ALA:H	15	0.27
(1,886)	1:103:A:PHE:HE2	1:107:A:ALA:H	15	0.27
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	17	0.27
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	18	0.27
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	9	0.27
(1,740)	1:89:A:ILE:HG12	1:90:A:ASN:H	5	0.27
(1,721)	1:61:A:LEU:HA	1:89:A:ILE:HD11	13	0.27
(1,721)	1:61:A:LEU:HA	1:89:A:ILE:HD12	13	0.27
(1,721)	1:61:A:LEU:HA	1:89:A:ILE:HD13	13	0.27
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	3	0.27
(1,654)	1:82:A:LYS:HG2	1:84:A:GLU:H	6	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:82:A:LYS:HG3	1:84:A:GLU:H	6	0.27
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	13	0.27
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	7	0.27
(1,593)	1:71:A:SER:HB3	1:77:A:LYS:HA	18	0.27
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	11	0.27
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	15	0.27
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	4	0.27
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	3	0.27
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	3	0.27
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	7	0.27
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	9	0.27
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	9	0.27
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	9	0.27
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	18	0.27
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	18	0.27
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	18	0.27
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	3	0.27
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	6	0.27
(1,514)	1:63:A:LYS:HB2	1:70:A:PRO:HA	1	0.27
(1,514)	1:63:A:LYS:HB2	1:70:A:PRO:HA	2	0.27
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	7	0.27
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	7	0.27
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	7	0.27
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	19	0.27
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	19	0.27
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	19	0.27
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	19	0.27
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	19	0.27
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	19	0.27
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	19	0.27
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	19	0.27
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	19	0.27
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	8	0.27
(1,393)	1:53:A:ALA:HB1	1:54:A:ARG:H	10	0.27
(1,393)	1:53:A:ALA:HB2	1:54:A:ARG:H	10	0.27
(1,393)	1:53:A:ALA:HB3	1:54:A:ARG:H	10	0.27
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	9	0.27
(1,333)	1:25:A:PHE:HA	1:31:A:ALA:H	13	0.27
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	4	0.27
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	18	0.27
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	4	0.27
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	4	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	9	0.27
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	11	0.27
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	6	0.27
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	6	0.27
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	11	0.27
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	11	0.27
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	20	0.27
(1,116)	1:16:A:SER:H	1:20:A:GLY:HA2	14	0.27
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	15	0.27
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	15	0.27
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	15	0.27
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD1	8	0.27
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD2	8	0.27
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	9	0.27
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	2	0.27
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	7	0.27
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	7	0.27
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	8	0.27
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	16	0.26
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	9	0.26
(3,47)	1:81:A:THR:O	1:85:A:ALA:N	6	0.26
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	4	0.26
(2,103)	1:137:A:ALA:H	2:656:B:PHE:HB2	8	0.26
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE1	18	0.26
(2,75)	2:656:B:PHE:HB2	2:659:B:PHE:HE2	18	0.26
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE1	18	0.26
(2,75)	2:656:B:PHE:HB3	2:659:B:PHE:HE2	18	0.26
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	17	0.26
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	17	0.26
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	17	0.26
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	17	0.26
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE1	16	0.26
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE2	16	0.26
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	14	0.26
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	14	0.26
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	14	0.26
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	13	0.26
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	13	0.26
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	13	0.26
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	5	0.26
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	20	0.26
(1,2596)	1:137:A:ALA:HB1	2:651:B:ILE:HG12	11	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2596)	1:137:A:ALA:HB1	2:651:B:ILE:HG13	11	0.26
(1,2596)	1:137:A:ALA:HB2	2:651:B:ILE:HG12	11	0.26
(1,2596)	1:137:A:ALA:HB2	2:651:B:ILE:HG13	11	0.26
(1,2596)	1:137:A:ALA:HB3	2:651:B:ILE:HG12	11	0.26
(1,2596)	1:137:A:ALA:HB3	2:651:B:ILE:HG13	11	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	1	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	1	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	1	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	10	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	10	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	10	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	15	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	15	0.26
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	15	0.26
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	9	0.26
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	9	0.26
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	9	0.26
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	12	0.26
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	8	0.26
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	9	0.26
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	3	0.26
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	4	0.26
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	9	0.26
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	6	0.26
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	4	0.26
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	4	0.26
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	4	0.26
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	19	0.26
(1,1703)	1:36:A:ARG:H	1:36:A:ARG:HD2	1	0.26
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	8	0.26
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	11	0.26
(1,1402)	1:143:A:THR:HG21	1:161:A:ARG:HD2	8	0.26
(1,1402)	1:143:A:THR:HG22	1:161:A:ARG:HD2	8	0.26
(1,1402)	1:143:A:THR:HG23	1:161:A:ARG:HD2	8	0.26
(1,1402)	1:143:A:THR:HG21	1:161:A:ARG:HD2	9	0.26
(1,1402)	1:143:A:THR:HG22	1:161:A:ARG:HD2	9	0.26
(1,1402)	1:143:A:THR:HG23	1:161:A:ARG:HD2	9	0.26
(1,1342)	1:147:A:SER:H	1:159:A:ILE:HD11	17	0.26
(1,1342)	1:147:A:SER:H	1:159:A:ILE:HD12	17	0.26
(1,1342)	1:147:A:SER:H	1:159:A:ILE:HD13	17	0.26
(1,1276)	1:63:A:LYS:HA	1:155:A:GLY:HA2	9	0.26
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	7	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	7	0.26
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	7	0.26
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	7	0.26
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	7	0.26
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	7	0.26
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	7	0.26
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	7	0.26
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	7	0.26
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	4	0.26
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	5	0.26
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	5	0.26
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	5	0.26
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	11	0.26
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	11	0.26
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	11	0.26
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	5	0.26
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	12	0.26
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	12	0.26
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	12	0.26
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	18	0.26
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD11	3	0.26
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD12	3	0.26
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD13	3	0.26
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	2	0.26
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	9	0.26
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	9	0.26
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	9	0.26
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	9	0.26
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	9	0.26
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	9	0.26
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	18	0.26
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	5	0.26
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	5	0.26
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	5	0.26
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	11	0.26
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	11	0.26
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	11	0.26
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	1	0.26
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	11	0.26
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	5	0.26
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG21	3	0.26
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG22	3	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG23	3	0.26
(1,619)	1:78:A:ILE:HB	1:80:A:ARG:H	1	0.26
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	2	0.26
(1,606)	1:75:A:GLN:HE22	1:78:A:ILE:HA	17	0.26
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	1	0.26
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	8	0.26
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	6	0.26
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	20	0.26
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	16	0.26
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	2	0.26
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	2	0.26
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	2	0.26
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	10	0.26
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	10	0.26
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	10	0.26
(1,471)	1:61:A:LEU:HD21	1:63:A:LYS:HA	13	0.26
(1,471)	1:61:A:LEU:HD22	1:63:A:LYS:HA	13	0.26
(1,471)	1:61:A:LEU:HD23	1:63:A:LYS:HA	13	0.26
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	19	0.26
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	19	0.26
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	19	0.26
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	4	0.26
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	15	0.26
(1,401)	1:54:A:ARG:HD2	1:55:A:VAL:HA	17	0.26
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	5	0.26
(1,385)	1:24:A:TYR:HD1	1:36:A:ARG:H	20	0.26
(1,385)	1:24:A:TYR:HD2	1:36:A:ARG:H	20	0.26
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	16	0.26
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	6	0.26
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	6	0.26
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	6	0.26
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	13	0.26
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	13	0.26
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	13	0.26
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	3	0.26
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	3	0.26
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	3	0.26
(1,323)	1:25:A:PHE:HZ	1:30:A:ASN:HB2	13	0.26
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	9	0.26
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	20	0.26
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	20	0.26
(1,264)	1:26:A:ASN:HD21	1:27:A:HIS:H	20	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:10:A:GLY:H	1:26:A:ASN:HD21	9	0.26
(1,214)	1:11:A:TRP:HB2	1:25:A:PHE:H	18	0.26
(1,130)	1:16:A:SER:H	1:21:A:ARG:HA	2	0.26
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	9	0.26
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	9	0.26
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	9	0.26
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	11	0.26
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	1	0.26
(1,19)	1:7:A:LEU:HD11	1:11:A:TRP:HE3	13	0.26
(1,19)	1:7:A:LEU:HD12	1:11:A:TRP:HE3	13	0.26
(1,19)	1:7:A:LEU:HD13	1:11:A:TRP:HE3	13	0.26
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	18	0.25
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	6	0.25
(3,63)	1:90:A:ASN:O	1:94:A:GLN:N	11	0.25
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	13	0.25
(2,68)	2:649:B:ARG:HD2	2:650:B:ASN:H	13	0.25
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	12	0.25
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	12	0.25
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	12	0.25
(2,34)	1:59:A:HIS:H	1:122:A:LEU:HB2	5	0.25
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	10	0.25
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	17	0.25
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	3	0.25
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	3	0.25
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	3	0.25
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	3	0.25
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	3	0.25
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	3	0.25
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	13	0.25
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	13	0.25
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	11	0.25
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	11	0.25
(1,2513)	2:646:B:GLU:HA	2:649:B:ARG:HD2	17	0.25
(1,2506)	2:644:B:ASP:H	2:645:B:GLN:HA	15	0.25
(1,2407)	2:645:B:GLN:H	2:645:B:GLN:HE21	20	0.25
(1,2385)	1:163:A:GLU:H	1:163:A:GLU:HB3	11	0.25
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	12	0.25
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	6	0.25
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	10	0.25
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	12	0.25
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	14	0.25
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	15	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	16	0.25
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	18	0.25
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	19	0.25
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	3	0.25
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	1	0.25
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	4	0.25
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	17	0.25
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	15	0.25
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	18	0.25
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	1	0.25
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	5	0.25
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	10	0.25
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	16	0.25
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	5	0.25
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	5	0.25
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	5	0.25
(1,1346)	1:148:A:GLY:H	1:159:A:ILE:H	1	0.25
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	10	0.25
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	10	0.25
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	10	0.25
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG21	9	0.25
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG22	9	0.25
(1,1263)	1:151:A:PHE:H	1:156:A:ILE:HG23	9	0.25
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	10	0.25
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	5	0.25
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	18	0.25
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	8	0.25
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	2	0.25
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	10	0.25
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	6	0.25
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	6	0.25
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	6	0.25
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	8	0.25
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	8	0.25
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	8	0.25
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	7	0.25
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	7	0.25
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	7	0.25
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	9	0.25
(1,921)	1:106:A:LEU:H	1:109:A:GLN:H	13	0.25
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	15	0.25
(1,907)	1:102:A:ASP:HB3	1:106:A:LEU:H	5	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	17	0.25
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE1	13	0.25
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE2	13	0.25
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE3	13	0.25
(1,825)	1:96:A:ILE:HD11	1:106:A:LEU:HG	18	0.25
(1,825)	1:96:A:ILE:HD12	1:106:A:LEU:HG	18	0.25
(1,825)	1:96:A:ILE:HD13	1:106:A:LEU:HG	18	0.25
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	7	0.25
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	7	0.25
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	7	0.25
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	7	0.25
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	7	0.25
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	7	0.25
(1,772)	1:92:A:TYR:H	1:93:A:ILE:HB	2	0.25
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	11	0.25
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	5	0.25
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	5	0.25
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	5	0.25
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	8	0.25
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	8	0.25
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	8	0.25
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	11	0.25
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	11	0.25
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	11	0.25
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	1	0.25
(1,649)	1:66:A:GLN:HE21	1:82:A:LYS:HB2	9	0.25
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	4	0.25
(1,571)	1:73:A:TRP:HE1	1:74:A:ARG:HB3	16	0.25
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	5	0.25
(1,510)	1:62:A:VAL:HG11	1:156:A:ILE:H	12	0.25
(1,510)	1:62:A:VAL:HG12	1:156:A:ILE:H	12	0.25
(1,510)	1:62:A:VAL:HG13	1:156:A:ILE:H	12	0.25
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	18	0.25
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	18	0.25
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	18	0.25
(1,479)	1:61:A:LEU:HD21	1:155:A:GLY:H	15	0.25
(1,479)	1:61:A:LEU:HD22	1:155:A:GLY:H	15	0.25
(1,479)	1:61:A:LEU:HD23	1:155:A:GLY:H	15	0.25
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	1	0.25
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	1	0.25
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	1	0.25
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	5	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	5	0.25
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	5	0.25
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	7	0.25
(1,379)	1:33:A:GLN:HE21	1:35:A:GLU:HB3	11	0.25
(1,379)	1:33:A:GLN:HE22	1:35:A:GLU:HB3	11	0.25
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	3	0.25
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	3	0.25
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	13	0.25
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	13	0.25
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	13	0.25
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	16	0.25
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	1	0.25
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	2	0.25
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	3	0.25
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	8	0.25
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	7	0.25
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	6	0.25
(1,204)	1:24:A:TYR:HB2	1:33:A:GLN:HE21	14	0.25
(1,181)	1:23:A:TYR:HB2	1:34:A:TRP:HE3	20	0.25
(1,129)	1:16:A:SER:HB2	1:21:A:ARG:H	13	0.25
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	8	0.25
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	8	0.25
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	8	0.25
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	11	0.25
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	20	0.25
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD1	3	0.25
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD2	3	0.25
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD1	8	0.25
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD2	8	0.25
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	11	0.24
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	3	0.24
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	3	0.24
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	3	0.24
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	3	0.24
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	3	0.24
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	3	0.24
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	10	0.24
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	13	0.24
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE1	18	0.24
(1,2586)	1:115:A:SER:H	2:659:B:PHE:HE2	18	0.24
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	17	0.24
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	17	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG21	18	0.24
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG22	18	0.24
(1,2580)	1:34:A:TRP:HE1	2:641:B:TPO:HG23	18	0.24
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG21	3	0.24
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG22	3	0.24
(1,2574)	1:20:A:GLY:H	2:641:B:TPO:HG23	3	0.24
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	8	0.24
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	5	0.24
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	5	0.24
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	5	0.24
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	4	0.24
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	7	0.24
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	11	0.24
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	13	0.24
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	17	0.24
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	20	0.24
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	17	0.24
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	11	0.24
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	11	0.24
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	11	0.24
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	16	0.24
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	16	0.24
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	16	0.24
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG21	10	0.24
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG22	10	0.24
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG23	10	0.24
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	10	0.24
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	12	0.24
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	17	0.24
(1,1625)	1:27:A:HIS:H	1:27:A:HIS:HD1	4	0.24
(1,1507)	1:13:A:LYS:H	1:13:A:LYS:HG3	2	0.24
(1,1500)	1:12:A:GLU:H	1:12:A:GLU:HB2	10	0.24
(1,1424)	1:55:A:VAL:HG21	1:163:A:GLU:H	6	0.24
(1,1424)	1:55:A:VAL:HG22	1:163:A:GLU:H	6	0.24
(1,1424)	1:55:A:VAL:HG23	1:163:A:GLU:H	6	0.24
(1,1424)	1:55:A:VAL:HG11	1:163:A:GLU:H	6	0.24
(1,1424)	1:55:A:VAL:HG12	1:163:A:GLU:H	6	0.24
(1,1424)	1:55:A:VAL:HG13	1:163:A:GLU:H	6	0.24
(1,1303)	1:156:A:ILE:HG21	1:157:A:HIS:HD2	10	0.24
(1,1303)	1:156:A:ILE:HG22	1:157:A:HIS:HD2	10	0.24
(1,1303)	1:156:A:ILE:HG23	1:157:A:HIS:HD2	10	0.24
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	20	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	20	0.24
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	20	0.24
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	11	0.24
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	11	0.24
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	11	0.24
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	7	0.24
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	11	0.24
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	13	0.24
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	13	0.24
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	13	0.24
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	13	0.24
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	2	0.24
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	2	0.24
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	2	0.24
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD1	4	0.24
(1,1109)	1:126:A:SER:HA	1:139:A:PHE:HD2	4	0.24
(1,1108)	1:54:A:ARG:HG2	1:126:A:SER:HA	15	0.24
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	14	0.24
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	20	0.24
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	9	0.24
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	4	0.24
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	4	0.24
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	4	0.24
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	16	0.24
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	16	0.24
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	16	0.24
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	13	0.24
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	1	0.24
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	11	0.24
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	5	0.24
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	17	0.24
(1,772)	1:92:A:TYR:H	1:93:A:ILE:HB	8	0.24
(1,740)	1:89:A:ILE:HG12	1:90:A:ASN:H	8	0.24
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB1	18	0.24
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB2	18	0.24
(1,676)	1:84:A:GLU:H	1:85:A:ALA:HB3	18	0.24
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	7	0.24
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	9	0.24
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	14	0.24
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	16	0.24
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	6	0.24
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB1	10	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB2	10	0.24
(1,579)	1:73:A:TRP:HD1	1:116:A:ALA:HB3	10	0.24
(1,571)	1:73:A:TRP:HE1	1:74:A:ARG:HB3	2	0.24
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	4	0.24
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	18	0.24
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	1	0.24
(1,523)	1:64:A:HIS:HE1	1:66:A:GLN:H	7	0.24
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	13	0.24
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	13	0.24
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	13	0.24
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	13	0.24
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	6	0.24
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	6	0.24
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	6	0.24
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	3	0.24
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD11	3	0.24
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD12	3	0.24
(1,305)	1:27:A:HIS:HD2	1:28:A:ILE:HD13	3	0.24
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	9	0.24
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	12	0.24
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	7	0.24
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	7	0.24
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	14	0.24
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	14	0.24
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	14	0.24
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	14	0.24
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	14	0.24
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	14	0.24
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	14	0.24
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	14	0.24
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	14	0.24
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	17	0.24
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	17	0.24
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	17	0.24
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	17	0.24
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	17	0.24
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	17	0.24
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	17	0.24
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	17	0.24
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	17	0.24
(1,103)	1:14:A:ARG:HG2	1:15:A:MET:H	14	0.24
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	17	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	8	0.24
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	8	0.24
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	18	0.23
(3,25)	1:55:A:VAL:N	1:125:A:PHE:O	4	0.23
(3,10)	1:16:A:SER:O	1:19:A:SER:H	15	0.23
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB2	15	0.23
(2,110)	1:152:A:THR:HG21	2:661:B:PHE:HB3	15	0.23
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB2	15	0.23
(2,110)	1:152:A:THR:HG22	2:661:B:PHE:HB3	15	0.23
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB2	15	0.23
(2,110)	1:152:A:THR:HG23	2:661:B:PHE:HB3	15	0.23
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	17	0.23
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	17	0.23
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	17	0.23
(2,69)	2:651:B:ILE:HG21	2:656:B:PHE:HD1	13	0.23
(2,69)	2:651:B:ILE:HG21	2:656:B:PHE:HD2	13	0.23
(2,69)	2:651:B:ILE:HG22	2:656:B:PHE:HD1	13	0.23
(2,69)	2:651:B:ILE:HG22	2:656:B:PHE:HD2	13	0.23
(2,69)	2:651:B:ILE:HG23	2:656:B:PHE:HD1	13	0.23
(2,69)	2:651:B:ILE:HG23	2:656:B:PHE:HD2	13	0.23
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	12	0.23
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	11	0.23
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	11	0.23
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	11	0.23
(1,2514)	2:646:B:GLU:HA	2:649:B:ARG:H	19	0.23
(1,2386)	1:163:A:GLU:H	1:163:A:GLU:HG2	19	0.23
(1,2302)	1:151:A:PHE:H	1:151:A:PHE:HE1	10	0.23
(1,2302)	1:151:A:PHE:H	1:151:A:PHE:HE2	10	0.23
(1,2103)	1:109:A:GLN:HG2	1:109:A:GLN:HE22	2	0.23
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	14	0.23
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	19	0.23
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	10	0.23
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG21	16	0.23
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG22	16	0.23
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG23	16	0.23
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	1	0.23
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	5	0.23
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	9	0.23
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	20	0.23
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	7	0.23
(1,1441)	1:162:A:THR:HG21	1:163:A:GLU:HG3	8	0.23
(1,1441)	1:162:A:THR:HG22	1:163:A:GLU:HG3	8	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1441)	1:162:A:THR:HG23	1:163:A:GLU:HG3	8	0.23
(1,1431)	1:161:A:ARG:HA	1:163:A:GLU:H	20	0.23
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	7	0.23
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	13	0.23
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	3	0.23
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	3	0.23
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	3	0.23
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	3	0.23
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	3	0.23
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	3	0.23
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG21	7	0.23
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG22	7	0.23
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG23	7	0.23
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	2	0.23
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	2	0.23
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	2	0.23
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	12	0.23
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	12	0.23
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	12	0.23
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	13	0.23
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	13	0.23
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	13	0.23
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG21	7	0.23
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG22	7	0.23
(1,1299)	1:152:A:THR:H	1:156:A:ILE:HG23	7	0.23
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD11	11	0.23
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD12	11	0.23
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD13	11	0.23
(1,1242)	1:150:A:VAL:HG11	1:157:A:HIS:H	9	0.23
(1,1242)	1:150:A:VAL:HG12	1:157:A:HIS:H	9	0.23
(1,1242)	1:150:A:VAL:HG13	1:157:A:HIS:H	9	0.23
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	5	0.23
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	5	0.23
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	5	0.23
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	5	0.23
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	5	0.23
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	5	0.23
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	5	0.23
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	5	0.23
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	5	0.23
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	6	0.23
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	15	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	18	0.23
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	13	0.23
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	4	0.23
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB1	4	0.23
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB2	4	0.23
(1,1154)	1:136:A:ASP:HB2	1:137:A:ALA:HB3	4	0.23
(1,1152)	1:135:A:GLU:HG2	1:136:A:ASP:H	13	0.23
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	2	0.23
(1,1107)	1:54:A:ARG:HD2	1:126:A:SER:HA	17	0.23
(1,1054)	1:59:A:HIS:HD2	1:122:A:LEU:H	11	0.23
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	12	0.23
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	15	0.23
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	7	0.23
(1,1029)	1:118:A:ALA:H	1:121:A:ASP:H	1	0.23
(1,958)	1:108:A:SER:HA	1:110:A:PHE:H	18	0.23
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	6	0.23
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	6	0.23
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	6	0.23
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	19	0.23
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	12	0.23
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	19	0.23
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	7	0.23
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	7	0.23
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	7	0.23
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	7	0.23
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	18	0.23
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	18	0.23
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	18	0.23
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	9	0.23
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	19	0.23
(1,751)	1:89:A:ILE:HG21	1:91:A:GLY:H	5	0.23
(1,751)	1:89:A:ILE:HG22	1:91:A:GLY:H	5	0.23
(1,751)	1:89:A:ILE:HG23	1:91:A:GLY:H	5	0.23
(1,748)	1:87:A:GLU:HA	1:91:A:GLY:H	13	0.23
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	1	0.23
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	4	0.23
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	16	0.23
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	20	0.23
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	10	0.23
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	10	0.23
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	10	0.23
(1,692)	1:86:A:LEU:HG	1:90:A:ASN:HD22	2	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	4	0.23
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	1	0.23
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	8	0.23
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	19	0.23
(1,654)	1:82:A:LYS:HG2	1:84:A:GLU:H	4	0.23
(1,654)	1:82:A:LYS:HG3	1:84:A:GLU:H	4	0.23
(1,618)	1:78:A:ILE:HA	1:80:A:ARG:H	19	0.23
(1,611)	1:75:A:GLN:HE21	1:78:A:ILE:HD11	13	0.23
(1,611)	1:75:A:GLN:HE21	1:78:A:ILE:HD12	13	0.23
(1,611)	1:75:A:GLN:HE21	1:78:A:ILE:HD13	13	0.23
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	3	0.23
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	11	0.23
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	1	0.23
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	14	0.23
(1,513)	1:62:A:VAL:H	1:158:A:ILE:H	6	0.23
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	20	0.23
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	20	0.23
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	20	0.23
(1,480)	1:61:A:LEU:HD21	1:156:A:ILE:H	18	0.23
(1,480)	1:61:A:LEU:HD22	1:156:A:ILE:H	18	0.23
(1,480)	1:61:A:LEU:HD23	1:156:A:ILE:H	18	0.23
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	15	0.23
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	15	0.23
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	15	0.23
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	19	0.23
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	19	0.23
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	19	0.23
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	2	0.23
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	3	0.23
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	10	0.23
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	6	0.23
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	6	0.23
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	7	0.23
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	7	0.23
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	13	0.23
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	6	0.23
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	6	0.23
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	6	0.23
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	5	0.23
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	5	0.23
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	5	0.23
(1,335)	1:29:A:THR:H	1:31:A:ALA:H	20	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:10:A:GLY:H	1:26:A:ASN:HD21	2	0.23
(1,213)	1:11:A:TRP:HA	1:25:A:PHE:H	18	0.23
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	18	0.23
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	9	0.23
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	20	0.23
(1,130)	1:16:A:SER:H	1:21:A:ARG:HA	10	0.23
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	19	0.23
(1,100)	1:14:A:ARG:HE	1:15:A:MET:H	16	0.23
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	5	0.23
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD1	11	0.23
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD2	11	0.23
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	1	0.23
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	11	0.23
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	11	0.23
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	15	0.23
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	15	0.23
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	8	0.23
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	17	0.23
(3,65)	1:91:A:GLY:O	1:95:A:LYS:N	20	0.22
(3,49)	1:82:A:LYS:O	1:86:A:LEU:N	4	0.22
(3,49)	1:82:A:LYS:O	1:86:A:LEU:N	19	0.22
(3,45)	1:70:A:PRO:O	1:78:A:ILE:N	16	0.22
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	15	0.22
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD1	9	0.22
(2,82)	2:660:B:SEP:HA	2:661:B:PHE:HD2	9	0.22
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB2	13	0.22
(2,20)	1:68:A:ARG:H	1:153:A:ASP:HB3	13	0.22
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	16	0.22
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	16	0.22
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	9	0.22
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	9	0.22
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	9	0.22
(1,2538)	2:649:B:ARG:H	2:650:B:ASN:HD21	15	0.22
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	17	0.22
(1,2510)	2:645:B:GLN:H	2:647:B:VAL:H	14	0.22
(1,2357)	1:160:A:LEU:H	1:160:A:LEU:HD11	8	0.22
(1,2357)	1:160:A:LEU:H	1:160:A:LEU:HD12	8	0.22
(1,2357)	1:160:A:LEU:H	1:160:A:LEU:HD13	8	0.22
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	18	0.22
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	5	0.22
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	5	0.22
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	5	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	4	0.22
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	4	0.22
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	4	0.22
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	5	0.22
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	5	0.22
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	5	0.22
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	17	0.22
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	14	0.22
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	14	0.22
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	14	0.22
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	5	0.22
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	17	0.22
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	19	0.22
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	8	0.22
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	4	0.22
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	11	0.22
(1,1750)	1:56:A:ARG:HA	1:56:A:ARG:HE	17	0.22
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	2	0.22
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	8	0.22
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	16	0.22
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	13	0.22
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	11	0.22
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	20	0.22
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	18	0.22
(1,1424)	1:55:A:VAL:HG21	1:163:A:GLU:H	9	0.22
(1,1424)	1:55:A:VAL:HG22	1:163:A:GLU:H	9	0.22
(1,1424)	1:55:A:VAL:HG23	1:163:A:GLU:H	9	0.22
(1,1424)	1:55:A:VAL:HG11	1:163:A:GLU:H	9	0.22
(1,1424)	1:55:A:VAL:HG12	1:163:A:GLU:H	9	0.22
(1,1424)	1:55:A:VAL:HG13	1:163:A:GLU:H	9	0.22
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	13	0.22
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	13	0.22
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	13	0.22
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	13	0.22
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	13	0.22
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	13	0.22
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	13	0.22
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	13	0.22
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	13	0.22
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	6	0.22
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	14	0.22
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	14	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	14	0.22
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	19	0.22
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	19	0.22
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	19	0.22
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	14	0.22
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	8	0.22
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	19	0.22
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	19	0.22
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	13	0.22
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	13	0.22
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	13	0.22
(1,1178)	1:137:A:ALA:HA	1:141:A:LEU:H	15	0.22
(1,1152)	1:135:A:GLU:HG2	1:136:A:ASP:H	20	0.22
(1,1141)	1:130:A:MET:HB2	1:134:A:PHE:H	7	0.22
(1,1141)	1:130:A:MET:HB2	1:134:A:PHE:H	10	0.22
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	11	0.22
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	11	0.22
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	11	0.22
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	11	0.22
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	11	0.22
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	11	0.22
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	5	0.22
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	18	0.22
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	14	0.22
(1,1000)	1:113:A:CYS:H	1:116:A:ALA:H	5	0.22
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	2	0.22
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	17	0.22
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	20	0.22
(1,934)	1:104:A:GLU:HA	1:107:A:ALA:H	19	0.22
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	13	0.22
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	20	0.22
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	20	0.22
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	9	0.22
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	9	0.22
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	9	0.22
(1,772)	1:92:A:TYR:H	1:93:A:ILE:HB	5	0.22
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	19	0.22
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	8	0.22
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	8	0.22
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	8	0.22
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	18	0.22
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	18	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	18	0.22
(1,695)	1:86:A:LEU:HD21	1:149:A:PRO:HD3	7	0.22
(1,695)	1:86:A:LEU:HD22	1:149:A:PRO:HD3	7	0.22
(1,695)	1:86:A:LEU:HD23	1:149:A:PRO:HD3	7	0.22
(1,619)	1:78:A:ILE:HB	1:80:A:ARG:H	18	0.22
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	6	0.22
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	11	0.22
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	12	0.22
(1,529)	1:64:A:HIS:HE1	1:67:A:SER:H	19	0.22
(1,521)	1:64:A:HIS:H	1:66:A:GLN:H	15	0.22
(1,514)	1:63:A:LYS:HB2	1:70:A:PRO:HA	11	0.22
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	17	0.22
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	12	0.22
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	12	0.22
(1,362)	1:11:A:TRP:HH2	1:33:A:GLN:HE21	12	0.22
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	11	0.22
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	11	0.22
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	14	0.22
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	14	0.22
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	14	0.22
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	17	0.22
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	17	0.22
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	17	0.22
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	20	0.22
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	20	0.22
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	20	0.22
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	5	0.22
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	5	0.22
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	5	0.22
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	15	0.22
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	15	0.22
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	15	0.22
(1,336)	1:29:A:THR:HG21	1:31:A:ALA:H	20	0.22
(1,336)	1:29:A:THR:HG22	1:31:A:ALA:H	20	0.22
(1,336)	1:29:A:THR:HG23	1:31:A:ALA:H	20	0.22
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	2	0.22
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	17	0.22
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	6	0.22
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	6	0.22
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	19	0.22
(1,205)	1:24:A:TYR:H	1:33:A:GLN:HG2	1	0.22
(1,205)	1:24:A:TYR:H	1:33:A:GLN:HG2	8	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,196)	1:23:A:TYR:HB3	1:24:A:TYR:H	11	0.22
(1,178)	1:23:A:TYR:HE1	1:33:A:GLN:H	10	0.22
(1,178)	1:23:A:TYR:HE2	1:33:A:GLN:H	10	0.22
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG11	15	0.22
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG12	15	0.22
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG13	15	0.22
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	2	0.22
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	2	0.22
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	2	0.22
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	2	0.22
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	2	0.22
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	2	0.22
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	2	0.22
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	2	0.22
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	2	0.22
(1,117)	1:16:A:SER:H	1:23:A:TYR:HE1	11	0.22
(1,117)	1:16:A:SER:H	1:23:A:TYR:HE2	11	0.22
(1,116)	1:16:A:SER:H	1:20:A:GLY:HA2	5	0.22
(1,69)	1:7:A:LEU:HD21	1:13:A:LYS:HE2	12	0.22
(1,69)	1:7:A:LEU:HD22	1:13:A:LYS:HE2	12	0.22
(1,69)	1:7:A:LEU:HD23	1:13:A:LYS:HE2	12	0.22
(1,69)	1:7:A:LEU:HD11	1:13:A:LYS:HE2	12	0.22
(1,69)	1:7:A:LEU:HD12	1:13:A:LYS:HE2	12	0.22
(1,69)	1:7:A:LEU:HD13	1:13:A:LYS:HE2	12	0.22
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	11	0.22
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	11	0.22
(1,16)	1:6:A:LYS:HE2	1:7:A:LEU:H	19	0.22
(3,63)	1:90:A:ASN:O	1:94:A:GLN:N	18	0.21
(3,51)	1:83:A:GLU:O	1:87:A:GLU:N	11	0.21
(3,47)	1:81:A:THR:O	1:85:A:ALA:N	19	0.21
(3,10)	1:16:A:SER:O	1:19:A:SER:H	10	0.21
(2,55)	1:150:A:VAL:HG21	1:158:A:ILE:HA	17	0.21
(2,55)	1:150:A:VAL:HG22	1:158:A:ILE:HA	17	0.21
(2,55)	1:150:A:VAL:HG23	1:158:A:ILE:HA	17	0.21
(2,25)	1:88:A:LEU:HG	1:92:A:TYR:H	16	0.21
(2,21)	1:73:A:TRP:HE1	1:74:A:ARG:HG3	4	0.21
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG21	1	0.21
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG22	1	0.21
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG23	1	0.21
(1,2527)	2:646:B:GLU:H	2:648:B:ILE:H	16	0.21
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	5	0.21
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	14	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE1	4	0.21
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE2	4	0.21
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE1	17	0.21
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE2	17	0.21
(1,2074)	1:104:A:GLU:H	1:104:A:GLU:HG2	10	0.21
(1,2046)	1:97:A:LYS:H	1:97:A:LYS:HB2	17	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	1	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	1	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	1	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	3	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	3	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	3	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	4	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	4	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	4	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	9	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	9	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	9	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	12	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	12	0.21
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	12	0.21
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	3	0.21
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	3	0.21
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	3	0.21
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	3	0.21
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	3	0.21
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	3	0.21
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	7	0.21
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	20	0.21
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	3	0.21
(1,1535)	1:14:A:ARG:HB2	1:14:A:ARG:HE	1	0.21
(1,1489)	1:11:A:TRP:H	1:11:A:TRP:HE1	8	0.21
(1,1355)	1:57:A:CYS:HB2	1:160:A:LEU:H	2	0.21
(1,1347)	1:148:A:GLY:H	1:159:A:ILE:HD11	17	0.21
(1,1347)	1:148:A:GLY:H	1:159:A:ILE:HD12	17	0.21
(1,1347)	1:148:A:GLY:H	1:159:A:ILE:HD13	17	0.21
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	10	0.21
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	10	0.21
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	10	0.21
(1,1280)	1:64:A:HIS:HD2	1:156:A:ILE:HG12	4	0.21
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	5	0.21
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB2	17	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1244)	1:150:A:VAL:HG21	1:157:A:HIS:HB3	17	0.21
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB2	17	0.21
(1,1244)	1:150:A:VAL:HG22	1:157:A:HIS:HB3	17	0.21
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB2	17	0.21
(1,1244)	1:150:A:VAL:HG23	1:157:A:HIS:HB3	17	0.21
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	4	0.21
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	4	0.21
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	4	0.21
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	4	0.21
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	4	0.21
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	4	0.21
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	4	0.21
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	4	0.21
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	4	0.21
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	3	0.21
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	9	0.21
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	6	0.21
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	2	0.21
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	2	0.21
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	2	0.21
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	2	0.21
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	2	0.21
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	2	0.21
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	16	0.21
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB1	19	0.21
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB2	19	0.21
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB3	19	0.21
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	9	0.21
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	9	0.21
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	9	0.21
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	10	0.21
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	10	0.21
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	10	0.21
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	5	0.21
(1,985)	1:61:A:LEU:HD21	1:113:A:CYS:HA	7	0.21
(1,985)	1:61:A:LEU:HD22	1:113:A:CYS:HA	7	0.21
(1,985)	1:61:A:LEU:HD23	1:113:A:CYS:HA	7	0.21
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	1	0.21
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	4	0.21
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	19	0.21
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	19	0.21
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	19	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	7	0.21
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	11	0.21
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD11	8	0.21
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD12	8	0.21
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD13	8	0.21
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	6	0.21
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	6	0.21
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	6	0.21
(1,756)	1:90:A:ASN:HD21	1:91:A:GLY:H	17	0.21
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD11	16	0.21
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD12	16	0.21
(1,747)	1:90:A:ASN:HA	1:158:A:ILE:HD13	16	0.21
(1,743)	1:89:A:ILE:HG13	1:90:A:ASN:H	17	0.21
(1,740)	1:89:A:ILE:HG12	1:90:A:ASN:H	12	0.21
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	13	0.21
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	13	0.21
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	13	0.21
(1,695)	1:86:A:LEU:HD21	1:149:A:PRO:HD3	8	0.21
(1,695)	1:86:A:LEU:HD22	1:149:A:PRO:HD3	8	0.21
(1,695)	1:86:A:LEU:HD23	1:149:A:PRO:HD3	8	0.21
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	19	0.21
(1,654)	1:82:A:LYS:HG2	1:84:A:GLU:H	16	0.21
(1,654)	1:82:A:LYS:HG3	1:84:A:GLU:H	16	0.21
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	11	0.21
(1,634)	1:80:A:ARG:HB2	1:81:A:THR:H	16	0.21
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	4	0.21
(1,531)	1:64:A:HIS:HE1	1:67:A:SER:HB2	1	0.21
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	12	0.21
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	12	0.21
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	12	0.21
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	10	0.21
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	5	0.21
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	6	0.21
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	1	0.21
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	9	0.21
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	18	0.21
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	18	0.21
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	1	0.21
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	1	0.21
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	1	0.21
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	2	0.21
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	2	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	2	0.21
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	8	0.21
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	8	0.21
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	8	0.21
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	19	0.21
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	19	0.21
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	19	0.21
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	4	0.21
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	4	0.21
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	4	0.21
(1,334)	1:27:A:HIS:HA	1:31:A:ALA:H	7	0.21
(1,333)	1:25:A:PHE:HA	1:31:A:ALA:H	1	0.21
(1,333)	1:25:A:PHE:HA	1:31:A:ALA:H	19	0.21
(1,287)	1:26:A:ASN:H	1:32:A:SER:HB2	16	0.21
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	8	0.21
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	8	0.21
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	5	0.21
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	13	0.21
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	2	0.21
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	2	0.21
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	5	0.21
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	5	0.21
(1,103)	1:14:A:ARG:HG2	1:15:A:MET:H	2	0.21
(1,87)	1:13:A:LYS:HG3	1:14:A:ARG:H	17	0.21
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	20	0.21
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE1	9	0.21
(1,66)	1:12:A:GLU:H	1:25:A:PHE:HE2	9	0.21
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB1	5	0.21
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB2	5	0.21
(1,56)	1:11:A:TRP:HE1	1:31:A:ALA:HB3	5	0.21
(1,28)	1:7:A:LEU:HD21	1:13:A:LYS:HG3	10	0.21
(1,28)	1:7:A:LEU:HD22	1:13:A:LYS:HG3	10	0.21
(1,28)	1:7:A:LEU:HD23	1:13:A:LYS:HG3	10	0.21
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	7	0.21
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	19	0.21
(3,47)	1:81:A:THR:O	1:85:A:ALA:N	4	0.2
(3,27)	1:56:A:ARG:N	1:163:A:GLU:O	11	0.2
(2,107)	1:140:A:ALA:HB1	2:651:B:ILE:HA	19	0.2
(2,107)	1:140:A:ALA:HB2	2:651:B:ILE:HA	19	0.2
(2,107)	1:140:A:ALA:HB3	2:651:B:ILE:HA	19	0.2
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	7	0.2
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	7	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	7	0.2
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	5	0.2
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	5	0.2
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	5	0.2
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	5	0.2
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	5	0.2
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	5	0.2
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	15	0.2
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	15	0.2
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	15	0.2
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	16	0.2
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	16	0.2
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	16	0.2
(2,26)	1:94:A:GLN:HE21	1:97:A:LYS:HB3	8	0.2
(2,4)	1:21:A:ARG:HE	1:22:A:VAL:H	20	0.2
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	19	0.2
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	4	0.2
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	4	0.2
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	4	0.2
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	7	0.2
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	7	0.2
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	7	0.2
(1,2510)	2:645:B:GLN:H	2:647:B:VAL:H	3	0.2
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE1	3	0.2
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE2	3	0.2
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	8	0.2
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	8	0.2
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	8	0.2
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	14	0.2
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	14	0.2
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	14	0.2
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	13	0.2
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	1	0.2
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	1	0.2
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	1	0.2
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	15	0.2
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	15	0.2
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	15	0.2
(1,1910)	1:82:A:LYS:H	1:82:A:LYS:HE2	1	0.2
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	3	0.2
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	12	0.2
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	14	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	15	0.2
(1,1703)	1:36:A:ARG:H	1:36:A:ARG:HD2	5	0.2
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	1	0.2
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	6	0.2
(1,1525)	1:14:A:ARG:H	1:14:A:ARG:HE	10	0.2
(1,1508)	1:13:A:LYS:H	1:13:A:LYS:HB3	15	0.2
(1,1457)	1:6:A:LYS:H	1:6:A:LYS:HG2	4	0.2
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	18	0.2
(1,1424)	1:55:A:VAL:HG21	1:163:A:GLU:H	19	0.2
(1,1424)	1:55:A:VAL:HG22	1:163:A:GLU:H	19	0.2
(1,1424)	1:55:A:VAL:HG23	1:163:A:GLU:H	19	0.2
(1,1424)	1:55:A:VAL:HG11	1:163:A:GLU:H	19	0.2
(1,1424)	1:55:A:VAL:HG12	1:163:A:GLU:H	19	0.2
(1,1424)	1:55:A:VAL:HG13	1:163:A:GLU:H	19	0.2
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	1	0.2
(1,1411)	1:56:A:ARG:H	1:162:A:THR:H	19	0.2
(1,1403)	1:144:A:GLY:H	1:161:A:ARG:HG2	20	0.2
(1,1399)	1:143:A:THR:H	1:161:A:ARG:HD2	15	0.2
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	4	0.2
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG21	9	0.2
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG22	9	0.2
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG23	9	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	3	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	3	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	3	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	10	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	10	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	10	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	13	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	13	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	13	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	15	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	15	0.2
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	15	0.2
(1,1320)	1:60:A:LEU:HD11	1:158:A:ILE:HB	2	0.2
(1,1320)	1:60:A:LEU:HD12	1:158:A:ILE:HB	2	0.2
(1,1320)	1:60:A:LEU:HD13	1:158:A:ILE:HB	2	0.2
(1,1320)	1:60:A:LEU:HD21	1:158:A:ILE:HB	2	0.2
(1,1320)	1:60:A:LEU:HD22	1:158:A:ILE:HB	2	0.2
(1,1320)	1:60:A:LEU:HD23	1:158:A:ILE:HB	2	0.2
(1,1276)	1:63:A:LYS:HA	1:155:A:GLY:HA2	1	0.2
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	8	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	8	0.2
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	8	0.2
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	8	0.2
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	8	0.2
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	8	0.2
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	8	0.2
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	8	0.2
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	8	0.2
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	1	0.2
(1,1212)	1:146:A:MET:HG2	1:160:A:LEU:HG	16	0.2
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	2	0.2
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	12	0.2
(1,1190)	1:141:A:LEU:HD21	1:142:A:ARG:HB2	6	0.2
(1,1190)	1:141:A:LEU:HD22	1:142:A:ARG:HB2	6	0.2
(1,1190)	1:141:A:LEU:HD23	1:142:A:ARG:HB2	6	0.2
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	15	0.2
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	15	0.2
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	15	0.2
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	15	0.2
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	15	0.2
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	15	0.2
(1,1078)	1:122:A:LEU:HG	1:123:A:GLY:H	16	0.2
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	4	0.2
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	4	0.2
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	4	0.2
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	19	0.2
(1,1032)	1:107:A:ALA:HB1	1:119:A:ARG:H	15	0.2
(1,1032)	1:107:A:ALA:HB2	1:119:A:ARG:H	15	0.2
(1,1032)	1:107:A:ALA:HB3	1:119:A:ARG:H	15	0.2
(1,1031)	1:118:A:ALA:HB1	1:121:A:ASP:HB2	5	0.2
(1,1031)	1:118:A:ALA:HB2	1:121:A:ASP:HB2	5	0.2
(1,1031)	1:118:A:ALA:HB3	1:121:A:ASP:HB2	5	0.2
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	6	0.2
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	5	0.2
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	5	0.2
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	5	0.2
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	15	0.2
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	3	0.2
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	3	0.2
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	3	0.2
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	4	0.2
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	4	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	4	0.2
(1,923)	1:106:A:LEU:HA	1:110:A:PHE:H	18	0.2
(1,921)	1:106:A:LEU:H	1:109:A:GLN:H	2	0.2
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	3	0.2
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE1	9	0.2
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE2	9	0.2
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE3	9	0.2
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE1	9	0.2
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE2	9	0.2
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE3	9	0.2
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	3	0.2
(1,854)	1:98:A:SER:H	1:101:A:GLU:H	5	0.2
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	15	0.2
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	15	0.2
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	15	0.2
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	10	0.2
(1,748)	1:87:A:GLU:HA	1:91:A:GLY:H	11	0.2
(1,740)	1:89:A:ILE:HG12	1:90:A:ASN:H	13	0.2
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	12	0.2
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	12	0.2
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	12	0.2
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	5	0.2
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	17	0.2
(1,671)	1:64:A:HIS:HB2	1:85:A:ALA:H	4	0.2
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	11	0.2
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	18	0.2
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	11	0.2
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	1	0.2
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	1	0.2
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	1	0.2
(1,592)	1:75:A:GLN:HB2	1:77:A:LYS:H	4	0.2
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	6	0.2
(1,576)	1:73:A:TRP:HE1	1:115:A:SER:H	3	0.2
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	6	0.2
(1,541)	1:67:A:SER:HB3	1:70:A:PRO:HA	17	0.2
(1,476)	1:61:A:LEU:H	1:113:A:CYS:HB2	6	0.2
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	9	0.2
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	9	0.2
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	9	0.2
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	9	0.2
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	9	0.2
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	9	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	9	0.2
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	9	0.2
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	9	0.2
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	18	0.2
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	1	0.2
(1,401)	1:54:A:ARG:HD2	1:55:A:VAL:HA	7	0.2
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	4	0.2
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	18	0.2
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	18	0.2
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	3	0.2
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	3	0.2
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	3	0.2
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	11	0.2
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	11	0.2
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	11	0.2
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	11	0.2
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	11	0.2
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	11	0.2
(1,334)	1:27:A:HIS:HA	1:31:A:ALA:H	19	0.2
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	4	0.2
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	7	0.2
(1,278)	1:26:A:ASN:HB2	1:30:A:ASN:H	11	0.2
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	3	0.2
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	3	0.2
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	9	0.2
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	9	0.2
(1,256)	1:23:A:TYR:HE1	1:26:A:ASN:H	12	0.2
(1,256)	1:23:A:TYR:HE2	1:26:A:ASN:H	12	0.2
(1,244)	1:11:A:TRP:H	1:26:A:ASN:HB2	10	0.2
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	8	0.2
(1,178)	1:23:A:TYR:HE1	1:33:A:GLN:H	15	0.2
(1,178)	1:23:A:TYR:HE2	1:33:A:GLN:H	15	0.2
(1,178)	1:23:A:TYR:HE1	1:33:A:GLN:H	16	0.2
(1,178)	1:23:A:TYR:HE2	1:33:A:GLN:H	16	0.2
(1,170)	1:16:A:SER:H	1:23:A:TYR:H	15	0.2
(1,130)	1:16:A:SER:H	1:21:A:ARG:HA	5	0.2
(1,123)	1:15:A:MET:HE1	1:20:A:GLY:H	15	0.2
(1,123)	1:15:A:MET:HE2	1:20:A:GLY:H	15	0.2
(1,123)	1:15:A:MET:HE3	1:20:A:GLY:H	15	0.2
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	3	0.2
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	10	0.2
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD1	14	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD2	14	0.2
(1,93)	1:14:A:ARG:H	1:22:A:VAL:HA	17	0.2
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	11	0.2
(1,44)	1:8:A:PRO:HB2	1:11:A:TRP:HE1	16	0.2
(1,28)	1:7:A:LEU:HD21	1:13:A:LYS:HG3	20	0.2
(1,28)	1:7:A:LEU:HD22	1:13:A:LYS:HG3	20	0.2
(1,28)	1:7:A:LEU:HD23	1:13:A:LYS:HG3	20	0.2
(1,17)	1:6:A:LYS:HB3	1:7:A:LEU:H	15	0.2
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	10	0.2
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	12	0.2
(3,79)	1:105:A:SER:O	1:109:A:GLN:N	8	0.19
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	5	0.19
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	7	0.19
(3,34)	1:60:A:LEU:H	1:158:A:ILE:O	19	0.19
(2,105)	1:138:A:SER:H	2:656:B:PHE:HD1	9	0.19
(2,105)	1:138:A:SER:H	2:656:B:PHE:HD2	9	0.19
(2,102)	1:135:A:GLU:H	2:656:B:PHE:HB2	19	0.19
(2,94)	1:93:A:ILE:HG21	2:643:B:PRO:HB3	17	0.19
(2,94)	1:93:A:ILE:HG22	2:643:B:PRO:HB3	17	0.19
(2,94)	1:93:A:ILE:HG23	2:643:B:PRO:HB3	17	0.19
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	20	0.19
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	20	0.19
(2,62)	1:160:A:LEU:HD11	1:162:A:THR:H	11	0.19
(2,62)	1:160:A:LEU:HD12	1:162:A:THR:H	11	0.19
(2,62)	1:160:A:LEU:HD13	1:162:A:THR:H	11	0.19
(2,41)	1:126:A:SER:H	1:129:A:GLN:H	17	0.19
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	4	0.19
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	16	0.19
(1,2597)	1:138:A:SER:H	2:656:B:PHE:HB2	17	0.19
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	20	0.19
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	20	0.19
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	20	0.19
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD1	2	0.19
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD2	2	0.19
(1,2532)	2:648:B:ILE:HG21	2:650:B:ASN:H	13	0.19
(1,2532)	2:648:B:ILE:HG22	2:650:B:ASN:H	13	0.19
(1,2532)	2:648:B:ILE:HG23	2:650:B:ASN:H	13	0.19
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	16	0.19
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	20	0.19
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	20	0.19
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	20	0.19
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE1	15	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE2	15	0.19
(1,2158)	1:119:A:ARG:H	1:119:A:ARG:HD2	20	0.19
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	8	0.19
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	6	0.19
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	6	0.19
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	6	0.19
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD11	8	0.19
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD12	8	0.19
(1,2013)	1:93:A:ILE:H	1:93:A:ILE:HD13	8	0.19
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	20	0.19
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	20	0.19
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	20	0.19
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	6	0.19
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	16	0.19
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	9	0.19
(1,1500)	1:12:A:GLU:H	1:12:A:GLU:HB2	20	0.19
(1,1456)	1:6:A:LYS:H	1:6:A:LYS:HE2	13	0.19
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	1	0.19
(1,1428)	1:143:A:THR:HG21	1:163:A:GLU:H	2	0.19
(1,1428)	1:143:A:THR:HG22	1:163:A:GLU:H	2	0.19
(1,1428)	1:143:A:THR:HG23	1:163:A:GLU:H	2	0.19
(1,1410)	1:161:A:ARG:HE	1:163:A:GLU:HG2	16	0.19
(1,1378)	1:147:A:SER:H	1:160:A:LEU:H	5	0.19
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	3	0.19
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	3	0.19
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	3	0.19
(1,1346)	1:148:A:GLY:H	1:159:A:ILE:H	4	0.19
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	14	0.19
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	14	0.19
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	14	0.19
(1,1276)	1:63:A:LYS:HA	1:155:A:GLY:HA2	13	0.19
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	11	0.19
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	20	0.19
(1,1242)	1:150:A:VAL:HG11	1:157:A:HIS:H	10	0.19
(1,1242)	1:150:A:VAL:HG12	1:157:A:HIS:H	10	0.19
(1,1242)	1:150:A:VAL:HG13	1:157:A:HIS:H	10	0.19
(1,1184)	1:140:A:ALA:H	1:141:A:LEU:HG	1	0.19
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	20	0.19
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	20	0.19
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	20	0.19
(1,1156)	1:136:A:ASP:HB2	1:137:A:ALA:H	1	0.19
(1,1143)	1:130:A:MET:HB2	1:135:A:GLU:H	10	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	13	0.19
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	13	0.19
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	13	0.19
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	13	0.19
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	13	0.19
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	13	0.19
(1,1066)	1:122:A:LEU:HD21	1:125:A:PHE:HD1	4	0.19
(1,1066)	1:122:A:LEU:HD21	1:125:A:PHE:HD2	4	0.19
(1,1066)	1:122:A:LEU:HD22	1:125:A:PHE:HD1	4	0.19
(1,1066)	1:122:A:LEU:HD22	1:125:A:PHE:HD2	4	0.19
(1,1066)	1:122:A:LEU:HD23	1:125:A:PHE:HD1	4	0.19
(1,1066)	1:122:A:LEU:HD23	1:125:A:PHE:HD2	4	0.19
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	2	0.19
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	8	0.19
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	11	0.19
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	13	0.19
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	11	0.19
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	19	0.19
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	2	0.19
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	2	0.19
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	2	0.19
(1,995)	1:108:A:SER:HA	1:116:A:ALA:H	6	0.19
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	13	0.19
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	1	0.19
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	1	0.19
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	19	0.19
(1,854)	1:98:A:SER:H	1:101:A:GLU:H	19	0.19
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE1	6	0.19
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE2	6	0.19
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE3	6	0.19
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	15	0.19
(1,764)	1:88:A:LEU:HA	1:92:A:TYR:H	17	0.19
(1,750)	1:88:A:LEU:H	1:91:A:GLY:H	18	0.19
(1,748)	1:87:A:GLU:HA	1:91:A:GLY:H	10	0.19
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	12	0.19
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	12	0.19
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	12	0.19
(1,742)	1:89:A:ILE:HD11	1:90:A:ASN:H	13	0.19
(1,742)	1:89:A:ILE:HD12	1:90:A:ASN:H	13	0.19
(1,742)	1:89:A:ILE:HD13	1:90:A:ASN:H	13	0.19
(1,737)	1:86:A:LEU:HB3	1:90:A:ASN:H	4	0.19
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	5	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	5	0.19
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	5	0.19
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	5	0.19
(1,654)	1:82:A:LYS:HG2	1:84:A:GLU:H	12	0.19
(1,654)	1:82:A:LYS:HG3	1:84:A:GLU:H	12	0.19
(1,649)	1:66:A:GLN:HE21	1:82:A:LYS:HB2	4	0.19
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	5	0.19
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	8	0.19
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	13	0.19
(1,549)	1:70:A:PRO:HG2	1:71:A:SER:H	12	0.19
(1,549)	1:70:A:PRO:HG2	1:71:A:SER:H	15	0.19
(1,520)	1:64:A:HIS:HE1	1:66:A:GLN:HG2	11	0.19
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	1	0.19
(1,496)	1:62:A:VAL:HG11	1:88:A:LEU:H	11	0.19
(1,496)	1:62:A:VAL:HG12	1:88:A:LEU:H	11	0.19
(1,496)	1:62:A:VAL:HG13	1:88:A:LEU:H	11	0.19
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	20	0.19
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	20	0.19
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	20	0.19
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	20	0.19
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	20	0.19
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	20	0.19
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	20	0.19
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	20	0.19
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	20	0.19
(1,402)	1:55:A:VAL:HA	1:125:A:PHE:H	4	0.19
(1,397)	1:54:A:ARG:HG2	1:126:A:SER:H	16	0.19
(1,393)	1:53:A:ALA:HB1	1:54:A:ARG:H	20	0.19
(1,393)	1:53:A:ALA:HB2	1:54:A:ARG:H	20	0.19
(1,393)	1:53:A:ALA:HB3	1:54:A:ARG:H	20	0.19
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	4	0.19
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	2	0.19
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	3	0.19
(1,344)	1:31:A:ALA:HB1	1:32:A:SER:H	13	0.19
(1,344)	1:31:A:ALA:HB2	1:32:A:SER:H	13	0.19
(1,344)	1:31:A:ALA:HB3	1:32:A:SER:H	13	0.19
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	7	0.19
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	7	0.19
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	7	0.19
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	11	0.19
(1,218)	1:12:A:GLU:HB2	1:25:A:PHE:H	4	0.19
(1,217)	1:12:A:GLU:H	1:25:A:PHE:HB3	20	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	17	0.19
(1,143)	1:15:A:MET:HA	1:22:A:VAL:H	10	0.19
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	15	0.19
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	15	0.19
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	4	0.19
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD1	19	0.19
(1,64)	1:12:A:GLU:H	1:24:A:TYR:HD2	19	0.19
(1,28)	1:7:A:LEU:HD21	1:13:A:LYS:HG3	3	0.19
(1,28)	1:7:A:LEU:HD22	1:13:A:LYS:HG3	3	0.19
(1,28)	1:7:A:LEU:HD23	1:13:A:LYS:HG3	3	0.19
(1,11)	1:4:A:GLU:H	1:6:A:LYS:H	15	0.19
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	8	0.18
(3,65)	1:91:A:GLY:O	1:95:A:LYS:N	12	0.18
(3,53)	1:84:A:GLU:O	1:88:A:LEU:N	10	0.18
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	4	0.18
(3,39)	1:64:A:HIS:O	1:67:A:SER:N	10	0.18
(3,34)	1:60:A:LEU:H	1:158:A:ILE:O	18	0.18
(2,112)	1:161:A:ARG:HE	2:651:B:ILE:HG12	18	0.18
(2,112)	1:161:A:ARG:HE	2:651:B:ILE:HG13	18	0.18
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	7	0.18
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	7	0.18
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	7	0.18
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	14	0.18
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	14	0.18
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	14	0.18
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	19	0.18
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	19	0.18
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	19	0.18
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	20	0.18
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	20	0.18
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	20	0.18
(1,2623)	1:51:A:GLU:H	1:51:A:GLU:HG2	18	0.18
(1,2597)	1:138:A:SER:H	2:656:B:PHE:HB2	18	0.18
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	4	0.18
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	4	0.18
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG21	9	0.18
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG22	9	0.18
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG23	9	0.18
(1,2557)	2:654:B:SER:H	2:655:B:GLU:H	6	0.18
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	12	0.18
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE1	14	0.18
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE2	14	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE1	2	0.18
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE2	2	0.18
(1,2383)	1:163:A:GLU:H	1:163:A:GLU:HB2	16	0.18
(1,2302)	1:151:A:PHE:H	1:151:A:PHE:HE1	11	0.18
(1,2302)	1:151:A:PHE:H	1:151:A:PHE:HE2	11	0.18
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	2	0.18
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	2	0.18
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	2	0.18
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	7	0.18
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	7	0.18
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	7	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	1	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	1	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	1	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	3	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	3	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	3	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	9	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	9	0.18
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	9	0.18
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	5	0.18
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	5	0.18
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	5	0.18
(1,1729)	1:54:A:ARG:H	1:54:A:ARG:HD2	7	0.18
(1,1703)	1:36:A:ARG:H	1:36:A:ARG:HD2	18	0.18
(1,1700)	1:36:A:ARG:H	1:36:A:ARG:HG2	15	0.18
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	13	0.18
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	20	0.18
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	3	0.18
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	14	0.18
(1,1456)	1:6:A:LYS:H	1:6:A:LYS:HE2	11	0.18
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	6	0.18
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	13	0.18
(1,1406)	1:147:A:SER:H	1:161:A:ARG:H	4	0.18
(1,1384)	1:159:A:ILE:HD11	1:160:A:LEU:H	19	0.18
(1,1384)	1:159:A:ILE:HD12	1:160:A:LEU:H	19	0.18
(1,1384)	1:159:A:ILE:HD13	1:160:A:LEU:H	19	0.18
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	1	0.18
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	12	0.18
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	4	0.18
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	4	0.18
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	4	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	11	0.18
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	11	0.18
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	11	0.18
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	5	0.18
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	5	0.18
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	5	0.18
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	14	0.18
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	14	0.18
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	14	0.18
(1,1230)	1:149:A:PRO:HD3	1:150:A:VAL:H	11	0.18
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	3	0.18
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	7	0.18
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD21	15	0.18
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD22	15	0.18
(1,1187)	1:140:A:ALA:HB1	1:141:A:LEU:HD23	15	0.18
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD21	15	0.18
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD22	15	0.18
(1,1187)	1:140:A:ALA:HB2	1:141:A:LEU:HD23	15	0.18
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD21	15	0.18
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD22	15	0.18
(1,1187)	1:140:A:ALA:HB3	1:141:A:LEU:HD23	15	0.18
(1,1178)	1:137:A:ALA:HA	1:141:A:LEU:H	11	0.18
(1,1132)	1:131:A:GLN:HG2	1:132:A:LYS:H	3	0.18
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	17	0.18
(1,1021)	1:117:A:LYS:HG3	1:118:A:ALA:H	15	0.18
(1,1021)	1:117:A:LYS:HG2	1:118:A:ALA:H	15	0.18
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	1	0.18
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	7	0.18
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	7	0.18
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	7	0.18
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	18	0.18
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	8	0.18
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	8	0.18
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	8	0.18
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	6	0.18
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	19	0.18
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	1	0.18
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	1	0.18
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	11	0.18
(1,913)	1:103:A:PHE:H	1:106:A:LEU:HB3	10	0.18
(1,846)	1:98:A:SER:HB2	1:100:A:GLU:HB2	15	0.18
(1,825)	1:96:A:ILE:HD11	1:106:A:LEU:HG	20	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,825)	1:96:A:ILE:HD12	1:106:A:LEU:HG	20	0.18
(1,825)	1:96:A:ILE:HD13	1:106:A:LEU:HG	20	0.18
(1,766)	1:89:A:ILE:HD11	1:92:A:TYR:HD1	13	0.18
(1,766)	1:89:A:ILE:HD11	1:92:A:TYR:HD2	13	0.18
(1,766)	1:89:A:ILE:HD12	1:92:A:TYR:HD1	13	0.18
(1,766)	1:89:A:ILE:HD12	1:92:A:TYR:HD2	13	0.18
(1,766)	1:89:A:ILE:HD13	1:92:A:TYR:HD1	13	0.18
(1,766)	1:89:A:ILE:HD13	1:92:A:TYR:HD2	13	0.18
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD11	3	0.18
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD12	3	0.18
(1,735)	1:89:A:ILE:HB	1:158:A:ILE:HD13	3	0.18
(1,695)	1:86:A:LEU:HD21	1:149:A:PRO:HD3	12	0.18
(1,695)	1:86:A:LEU:HD22	1:149:A:PRO:HD3	12	0.18
(1,695)	1:86:A:LEU:HD23	1:149:A:PRO:HD3	12	0.18
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	4	0.18
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	2	0.18
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	15	0.18
(1,649)	1:66:A:GLN:HE21	1:82:A:LYS:HB2	17	0.18
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	1	0.18
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	1	0.18
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	5	0.18
(1,510)	1:62:A:VAL:HG11	1:156:A:ILE:H	8	0.18
(1,510)	1:62:A:VAL:HG12	1:156:A:ILE:H	8	0.18
(1,510)	1:62:A:VAL:HG13	1:156:A:ILE:H	8	0.18
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	7	0.18
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	7	0.18
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	7	0.18
(1,475)	1:61:A:LEU:HD11	1:113:A:CYS:H	5	0.18
(1,475)	1:61:A:LEU:HD12	1:113:A:CYS:H	5	0.18
(1,475)	1:61:A:LEU:HD13	1:113:A:CYS:H	5	0.18
(1,475)	1:61:A:LEU:HD21	1:113:A:CYS:H	5	0.18
(1,475)	1:61:A:LEU:HD22	1:113:A:CYS:H	5	0.18
(1,475)	1:61:A:LEU:HD23	1:113:A:CYS:H	5	0.18
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	4	0.18
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	4	0.18
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	4	0.18
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	5	0.18
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	5	0.18
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	5	0.18
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG21	1	0.18
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG22	1	0.18
(1,452)	1:60:A:LEU:HD11	1:89:A:ILE:HG23	1	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG21	1	0.18
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG22	1	0.18
(1,452)	1:60:A:LEU:HD12	1:89:A:ILE:HG23	1	0.18
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG21	1	0.18
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG22	1	0.18
(1,452)	1:60:A:LEU:HD13	1:89:A:ILE:HG23	1	0.18
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	2	0.18
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	18	0.18
(1,383)	1:34:A:TRP:H	1:35:A:GLU:HB3	9	0.18
(1,378)	1:33:A:GLN:H	1:35:A:GLU:H	14	0.18
(1,367)	1:24:A:TYR:HD1	1:34:A:TRP:H	18	0.18
(1,367)	1:24:A:TYR:HD2	1:34:A:TRP:H	18	0.18
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	14	0.18
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	14	0.18
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	16	0.18
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	16	0.18
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	7	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	9	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	9	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	9	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	12	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	12	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	12	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	14	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	14	0.18
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	14	0.18
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	6	0.18
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	9	0.18
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	19	0.18
(1,278)	1:26:A:ASN:HB2	1:30:A:ASN:H	13	0.18
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	16	0.18
(1,242)	1:10:A:GLY:H	1:26:A:ASN:HD21	3	0.18
(1,242)	1:10:A:GLY:H	1:26:A:ASN:HD21	11	0.18
(1,194)	1:13:A:LYS:HG2	1:24:A:TYR:HA	17	0.18
(1,188)	1:13:A:LYS:HG2	1:24:A:TYR:HE1	13	0.18
(1,188)	1:13:A:LYS:HG2	1:24:A:TYR:HE2	13	0.18
(1,143)	1:15:A:MET:HA	1:22:A:VAL:H	18	0.18
(1,130)	1:16:A:SER:H	1:21:A:ARG:HA	20	0.18
(1,116)	1:16:A:SER:H	1:20:A:GLY:HA2	7	0.18
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE1	16	0.18
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE2	16	0.18
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	13	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	12	0.18
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD1	9	0.18
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD2	9	0.18
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	19	0.18
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	18	0.18
(1,27)	1:7:A:LEU:HD21	1:13:A:LYS:H	18	0.18
(1,27)	1:7:A:LEU:HD22	1:13:A:LYS:H	18	0.18
(1,27)	1:7:A:LEU:HD23	1:13:A:LYS:H	18	0.18
(1,17)	1:6:A:LYS:HB3	1:7:A:LEU:H	8	0.18
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	17	0.18
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	15	0.18
(3,81)	1:106:A:LEU:O	1:110:A:PHE:N	2	0.17
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	7	0.17
(3,63)	1:90:A:ASN:O	1:94:A:GLN:N	13	0.17
(3,45)	1:70:A:PRO:O	1:78:A:ILE:N	6	0.17
(3,44)	1:72:A:SER:O	1:75:A:GLN:H	12	0.17
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	2	0.17
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	7	0.17
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	7	0.17
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	4	0.17
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	4	0.17
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	4	0.17
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD11	6	0.17
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD12	6	0.17
(2,87)	1:31:A:ALA:H	2:640:B:LEU:HD13	6	0.17
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	8	0.17
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	8	0.17
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	8	0.17
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	8	0.17
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	8	0.17
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	8	0.17
(2,9)	1:53:A:ALA:H	1:54:A:ARG:HD2	17	0.17
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	5	0.17
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD1	15	0.17
(1,2584)	1:114:A:SER:H	2:659:B:PHE:HD2	15	0.17
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	6	0.17
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	6	0.17
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	6	0.17
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	8	0.17
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	8	0.17
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	8	0.17
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	9	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	9	0.17
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	9	0.17
(1,2520)	2:646:B:GLU:HG3	2:647:B:VAL:H	14	0.17
(1,2517)	2:646:B:GLU:HG2	2:647:B:VAL:H	7	0.17
(1,2513)	2:646:B:GLU:HA	2:649:B:ARG:HD2	19	0.17
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE1	6	0.17
(1,2496)	2:659:B:PHE:H	2:659:B:PHE:HE2	6	0.17
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD11	19	0.17
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD12	19	0.17
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD13	19	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	10	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	10	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	10	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	11	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	11	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	11	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	13	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	13	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	13	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	16	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	16	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	16	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	17	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	17	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	17	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	18	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	18	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	18	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	20	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	20	0.17
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	20	0.17
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	6	0.17
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	6	0.17
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	6	0.17
(1,1910)	1:82:A:LYS:H	1:82:A:LYS:HE2	2	0.17
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG21	1	0.17
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG22	1	0.17
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG23	1	0.17
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG21	2	0.17
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG22	2	0.17
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG23	2	0.17
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG21	17	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG22	17	0.17
(1,1906)	1:81:A:THR:H	1:81:A:THR:HG23	17	0.17
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	4	0.17
(1,1700)	1:36:A:ARG:H	1:36:A:ARG:HG2	2	0.17
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	14	0.17
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	18	0.17
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	5	0.17
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	15	0.17
(1,1425)	1:56:A:ARG:H	1:163:A:GLU:H	11	0.17
(1,1410)	1:161:A:ARG:HE	1:163:A:GLU:HG2	20	0.17
(1,1384)	1:159:A:ILE:HD11	1:160:A:LEU:H	5	0.17
(1,1384)	1:159:A:ILE:HD12	1:160:A:LEU:H	5	0.17
(1,1384)	1:159:A:ILE:HD13	1:160:A:LEU:H	5	0.17
(1,1384)	1:159:A:ILE:HD11	1:160:A:LEU:H	18	0.17
(1,1384)	1:159:A:ILE:HD12	1:160:A:LEU:H	18	0.17
(1,1384)	1:159:A:ILE:HD13	1:160:A:LEU:H	18	0.17
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	3	0.17
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	6	0.17
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	8	0.17
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	12	0.17
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	14	0.17
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	15	0.17
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	15	0.17
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	15	0.17
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	19	0.17
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	19	0.17
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	19	0.17
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD21	17	0.17
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD22	17	0.17
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD23	17	0.17
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	15	0.17
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	15	0.17
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	15	0.17
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	19	0.17
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	19	0.17
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	19	0.17
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	19	0.17
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	19	0.17
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	19	0.17
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	19	0.17
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	19	0.17
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	19	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1346)	1:148:A:GLY:H	1:159:A:ILE:H	14	0.17
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	17	0.17
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	17	0.17
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	17	0.17
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD11	1	0.17
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD12	1	0.17
(1,1282)	1:82:A:LYS:HE2	1:156:A:ILE:HD13	1	0.17
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	15	0.17
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	1	0.17
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	12	0.17
(1,1242)	1:150:A:VAL:HG11	1:157:A:HIS:H	1	0.17
(1,1242)	1:150:A:VAL:HG12	1:157:A:HIS:H	1	0.17
(1,1242)	1:150:A:VAL:HG13	1:157:A:HIS:H	1	0.17
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	4	0.17
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	5	0.17
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	6	0.17
(1,1178)	1:137:A:ALA:HA	1:141:A:LEU:H	17	0.17
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	5	0.17
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	5	0.17
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	5	0.17
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	5	0.17
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	5	0.17
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	5	0.17
(1,1078)	1:122:A:LEU:HG	1:123:A:GLY:H	2	0.17
(1,1078)	1:122:A:LEU:HG	1:123:A:GLY:H	20	0.17
(1,1031)	1:118:A:ALA:HB1	1:121:A:ASP:HB2	15	0.17
(1,1031)	1:118:A:ALA:HB2	1:121:A:ASP:HB2	15	0.17
(1,1031)	1:118:A:ALA:HB3	1:121:A:ASP:HB2	15	0.17
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	7	0.17
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	11	0.17
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	11	0.17
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	11	0.17
(1,1011)	1:116:A:ALA:HB1	1:119:A:ARG:H	19	0.17
(1,1011)	1:116:A:ALA:HB2	1:119:A:ARG:H	19	0.17
(1,1011)	1:116:A:ALA:HB3	1:119:A:ARG:H	19	0.17
(1,978)	1:107:A:ALA:HB1	1:111:A:SER:HA	13	0.17
(1,978)	1:107:A:ALA:HB2	1:111:A:SER:HA	13	0.17
(1,978)	1:107:A:ALA:HB3	1:111:A:SER:HA	13	0.17
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	8	0.17
(1,960)	1:108:A:SER:H	1:111:A:SER:H	20	0.17
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	6	0.17
(1,959)	1:108:A:SER:HA	1:111:A:SER:H	12	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	10	0.17
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	10	0.17
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	10	0.17
(1,940)	1:106:A:LEU:HG	1:107:A:ALA:H	12	0.17
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	10	0.17
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	20	0.17
(1,843)	1:97:A:LYS:HB2	1:98:A:SER:H	17	0.17
(1,824)	1:96:A:ILE:HG21	1:98:A:SER:H	19	0.17
(1,824)	1:96:A:ILE:HG22	1:98:A:SER:H	19	0.17
(1,824)	1:96:A:ILE:HG23	1:98:A:SER:H	19	0.17
(1,805)	1:93:A:ILE:HG21	1:94:A:GLN:H	19	0.17
(1,805)	1:93:A:ILE:HG22	1:94:A:GLN:H	19	0.17
(1,805)	1:93:A:ILE:HG23	1:94:A:GLN:H	19	0.17
(1,751)	1:89:A:ILE:HG21	1:91:A:GLY:H	8	0.17
(1,751)	1:89:A:ILE:HG22	1:91:A:GLY:H	8	0.17
(1,751)	1:89:A:ILE:HG23	1:91:A:GLY:H	8	0.17
(1,750)	1:88:A:LEU:H	1:91:A:GLY:H	6	0.17
(1,750)	1:88:A:LEU:H	1:91:A:GLY:H	15	0.17
(1,695)	1:86:A:LEU:HD21	1:149:A:PRO:HD3	9	0.17
(1,695)	1:86:A:LEU:HD22	1:149:A:PRO:HD3	9	0.17
(1,695)	1:86:A:LEU:HD23	1:149:A:PRO:HD3	9	0.17
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD11	20	0.17
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD12	20	0.17
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD13	20	0.17
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	3	0.17
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	12	0.17
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	6	0.17
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	11	0.17
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG21	12	0.17
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG22	12	0.17
(1,641)	1:65:A:SER:HB2	1:81:A:THR:HG23	12	0.17
(1,637)	1:80:A:ARG:HE	1:85:A:ALA:H	15	0.17
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG21	16	0.17
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG22	16	0.17
(1,624)	1:66:A:GLN:H	1:79:A:THR:HG23	16	0.17
(1,619)	1:78:A:ILE:HB	1:80:A:ARG:H	6	0.17
(1,571)	1:73:A:TRP:HE1	1:74:A:ARG:HB3	20	0.17
(1,569)	1:73:A:TRP:HE1	1:74:A:ARG:HB2	5	0.17
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	3	0.17
(1,564)	1:72:A:SER:H	1:78:A:ILE:HG12	9	0.17
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	12	0.17
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	14	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	14	0.17
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	14	0.17
(1,440)	1:59:A:HIS:H	1:115:A:SER:HB3	11	0.17
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	3	0.17
(1,435)	1:58:A:SER:HA	1:122:A:LEU:HG	20	0.17
(1,393)	1:53:A:ALA:HB1	1:54:A:ARG:H	11	0.17
(1,393)	1:53:A:ALA:HB2	1:54:A:ARG:H	11	0.17
(1,393)	1:53:A:ALA:HB3	1:54:A:ARG:H	11	0.17
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	13	0.17
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	14	0.17
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	19	0.17
(1,362)	1:11:A:TRP:HH2	1:33:A:GLN:HE21	7	0.17
(1,355)	1:25:A:PHE:HE1	1:32:A:SER:HB2	8	0.17
(1,355)	1:25:A:PHE:HE2	1:32:A:SER:HB2	8	0.17
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	12	0.17
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	12	0.17
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	12	0.17
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	17	0.17
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	17	0.17
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	17	0.17
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	18	0.17
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	18	0.17
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	18	0.17
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	7	0.17
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	18	0.17
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	19	0.17
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	14	0.17
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	5	0.17
(1,311)	1:27:A:HIS:HB2	1:29:A:THR:H	12	0.17
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	6	0.17
(1,211)	1:24:A:TYR:HE1	1:36:A:ARG:HD2	8	0.17
(1,211)	1:24:A:TYR:HE2	1:36:A:ARG:HD2	8	0.17
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	7	0.17
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	16	0.17
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	18	0.17
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	18	0.17
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	18	0.17
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	18	0.17
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	18	0.17
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	18	0.17
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	18	0.17
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	18	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	18	0.17
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD1	1	0.17
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD2	1	0.17
(1,28)	1:7:A:LEU:HD21	1:13:A:LYS:HG3	18	0.17
(1,28)	1:7:A:LEU:HD22	1:13:A:LYS:HG3	18	0.17
(1,28)	1:7:A:LEU:HD23	1:13:A:LYS:HG3	18	0.17
(1,20)	1:7:A:LEU:HD11	1:11:A:TRP:H	2	0.17
(1,20)	1:7:A:LEU:HD12	1:11:A:TRP:H	2	0.17
(1,20)	1:7:A:LEU:HD13	1:11:A:TRP:H	2	0.17
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	9	0.17
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	13	0.17
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	14	0.17
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	20	0.17
(4,2774)	1:26:A:ASN:H	1:31:A:ALA:O	16	0.16
(3,46)	1:70:A:PRO:O	1:78:A:ILE:H	11	0.16
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	8	0.16
(2,101)	1:129:A:GLN:HE21	2:657:B:GLU:HB2	15	0.16
(2,101)	1:129:A:GLN:HE21	2:657:B:GLU:HB3	15	0.16
(2,97)	1:94:A:GLN:HE21	2:640:B:LEU:HG	8	0.16
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	1	0.16
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	1	0.16
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	1	0.16
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	5	0.16
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	5	0.16
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	5	0.16
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	5	0.16
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE1	6	0.16
(2,72)	2:653:B:GLN:HA	2:656:B:PHE:HE2	6	0.16
(2,58)	1:152:A:THR:HG21	1:157:A:HIS:HB3	19	0.16
(2,58)	1:152:A:THR:HG22	1:157:A:HIS:HB3	19	0.16
(2,58)	1:152:A:THR:HG23	1:157:A:HIS:HB3	19	0.16
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD1	14	0.16
(2,42)	1:130:A:MET:HB2	1:134:A:PHE:HD2	14	0.16
(2,38)	1:126:A:SER:H	1:129:A:GLN:HB2	15	0.16
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	18	0.16
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB2	11	0.16
(1,2598)	1:146:A:MET:HE1	2:642:B:PRO:HB3	11	0.16
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB2	11	0.16
(1,2598)	1:146:A:MET:HE2	2:642:B:PRO:HB3	11	0.16
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB2	11	0.16
(1,2598)	1:146:A:MET:HE3	2:642:B:PRO:HB3	11	0.16
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	6	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	6	0.16
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD1	16	0.16
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD2	16	0.16
(1,2517)	2:646:B:GLU:HG2	2:647:B:VAL:H	8	0.16
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	13	0.16
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	13	0.16
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE1	16	0.16
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE2	16	0.16
(1,2276)	1:146:A:MET:H	1:146:A:MET:HE3	16	0.16
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	1	0.16
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	5	0.16
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	9	0.16
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	15	0.16
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	15	0.16
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	15	0.16
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG21	19	0.16
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG22	19	0.16
(1,2043)	1:96:A:ILE:H	1:96:A:ILE:HG23	19	0.16
(1,2033)	1:95:A:LYS:H	1:95:A:LYS:HD2	12	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	2	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	2	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	2	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	8	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	8	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	8	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	12	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	12	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	12	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	18	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	18	0.16
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	18	0.16
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	4	0.16
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	11	0.16
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	20	0.16
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	2	0.16
(1,1703)	1:36:A:ARG:H	1:36:A:ARG:HD2	19	0.16
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	4	0.16
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	14	0.16
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	15	0.16
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	11	0.16
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	17	0.16
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	14	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	9	0.16
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG21	7	0.16
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG22	7	0.16
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG23	7	0.16
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	15	0.16
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	15	0.16
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	15	0.16
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	6	0.16
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	17	0.16
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	8	0.16
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	14	0.16
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	19	0.16
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	3	0.16
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	3	0.16
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	3	0.16
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	3	0.16
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	3	0.16
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	3	0.16
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	3	0.16
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	3	0.16
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	3	0.16
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	13	0.16
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	20	0.16
(1,1085)	1:56:A:ARG:HE	1:124:A:ALA:H	18	0.16
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	7	0.16
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	16	0.16
(1,1031)	1:118:A:ALA:HB1	1:121:A:ASP:HB2	16	0.16
(1,1031)	1:118:A:ALA:HB2	1:121:A:ASP:HB2	16	0.16
(1,1031)	1:118:A:ALA:HB3	1:121:A:ASP:HB2	16	0.16
(1,1029)	1:118:A:ALA:H	1:121:A:ASP:H	9	0.16
(1,1015)	1:116:A:ALA:HB1	1:120:A:GLY:H	4	0.16
(1,1015)	1:116:A:ALA:HB2	1:120:A:GLY:H	4	0.16
(1,1015)	1:116:A:ALA:HB3	1:120:A:GLY:H	4	0.16
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB1	1	0.16
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB2	1	0.16
(1,996)	1:108:A:SER:H	1:116:A:ALA:HB3	1	0.16
(1,978)	1:107:A:ALA:HB1	1:111:A:SER:HA	10	0.16
(1,978)	1:107:A:ALA:HB2	1:111:A:SER:HA	10	0.16
(1,978)	1:107:A:ALA:HB3	1:111:A:SER:HA	10	0.16
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	12	0.16
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	5	0.16
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	5	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	5	0.16
(1,926)	1:60:A:LEU:HD11	1:107:A:ALA:H	6	0.16
(1,926)	1:60:A:LEU:HD12	1:107:A:ALA:H	6	0.16
(1,926)	1:60:A:LEU:HD13	1:107:A:ALA:H	6	0.16
(1,921)	1:106:A:LEU:H	1:109:A:GLN:H	12	0.16
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	9	0.16
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	8	0.16
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE1	12	0.16
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE2	12	0.16
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE3	12	0.16
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	14	0.16
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	19	0.16
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE1	3	0.16
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE2	3	0.16
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE3	3	0.16
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE1	18	0.16
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE2	18	0.16
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE3	18	0.16
(1,772)	1:92:A:TYR:H	1:93:A:ILE:HB	12	0.16
(1,751)	1:89:A:ILE:HG21	1:91:A:GLY:H	12	0.16
(1,751)	1:89:A:ILE:HG22	1:91:A:GLY:H	12	0.16
(1,751)	1:89:A:ILE:HG23	1:91:A:GLY:H	12	0.16
(1,698)	1:86:A:LEU:HD11	1:87:A:GLU:H	11	0.16
(1,698)	1:86:A:LEU:HD12	1:87:A:GLU:H	11	0.16
(1,698)	1:86:A:LEU:HD13	1:87:A:GLU:H	11	0.16
(1,692)	1:86:A:LEU:HG	1:90:A:ASN:HD22	13	0.16
(1,668)	1:83:A:GLU:HB2	1:84:A:GLU:H	10	0.16
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	8	0.16
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	15	0.16
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	4	0.16
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG21	13	0.16
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG22	13	0.16
(1,639)	1:65:A:SER:HB3	1:81:A:THR:HG23	13	0.16
(1,634)	1:80:A:ARG:HB2	1:81:A:THR:H	11	0.16
(1,540)	1:67:A:SER:HA	1:69:A:ARG:H	11	0.16
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	12	0.16
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	12	0.16
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	12	0.16
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	12	0.16
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	12	0.16
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	12	0.16
(1,469)	1:60:A:LEU:HB2	1:61:A:LEU:H	5	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,402)	1:55:A:VAL:HA	1:125:A:PHE:H	11	0.16
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	9	0.16
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	20	0.16
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	1	0.16
(1,383)	1:34:A:TRP:H	1:35:A:GLU:HB3	3	0.16
(1,373)	1:34:A:TRP:HD1	1:35:A:GLU:H	10	0.16
(1,369)	1:33:A:GLN:HG2	1:34:A:TRP:H	13	0.16
(1,367)	1:24:A:TYR:HD1	1:34:A:TRP:H	10	0.16
(1,367)	1:24:A:TYR:HD2	1:34:A:TRP:H	10	0.16
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	19	0.16
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	19	0.16
(1,347)	1:31:A:ALA:HB1	1:33:A:GLN:H	11	0.16
(1,347)	1:31:A:ALA:HB2	1:33:A:GLN:H	11	0.16
(1,347)	1:31:A:ALA:HB3	1:33:A:GLN:H	11	0.16
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	15	0.16
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	15	0.16
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	15	0.16
(1,333)	1:25:A:PHE:HA	1:31:A:ALA:H	2	0.16
(1,296)	1:27:A:HIS:HA	1:30:A:ASN:HD21	13	0.16
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	17	0.16
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	17	0.16
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	5	0.16
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	7	0.16
(1,112)	1:15:A:MET:H	1:23:A:TYR:H	13	0.16
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD1	12	0.16
(1,111)	1:15:A:MET:H	1:23:A:TYR:HD2	12	0.16
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	20	0.16
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	18	0.16
(1,2)	1:2:A:ALA:HA	1:3:A:ASP:H	19	0.16
(3,46)	1:70:A:PRO:O	1:78:A:ILE:H	16	0.15
(3,45)	1:70:A:PRO:O	1:78:A:ILE:N	17	0.15
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	3	0.15
(2,108)	1:140:A:ALA:HB1	2:649:B:ARG:HA	2	0.15
(2,108)	1:140:A:ALA:HB2	2:649:B:ARG:HA	2	0.15
(2,108)	1:140:A:ALA:HB3	2:649:B:ARG:HA	2	0.15
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG11	9	0.15
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG12	9	0.15
(2,95)	1:90:A:ASN:HD21	2:639:B:VAL:HG13	9	0.15
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG11	11	0.15
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG12	11	0.15
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG13	11	0.15
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG21	11	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG22	11	0.15
(2,83)	1:14:A:ARG:H	2:639:B:VAL:HG23	11	0.15
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD1	15	0.15
(2,74)	2:656:B:PHE:HB2	2:659:B:PHE:HD2	15	0.15
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD1	15	0.15
(2,74)	2:656:B:PHE:HB3	2:659:B:PHE:HD2	15	0.15
(2,39)	1:55:A:VAL:HG11	1:127:A:ARG:H	17	0.15
(2,39)	1:55:A:VAL:HG12	1:127:A:ARG:H	17	0.15
(2,39)	1:55:A:VAL:HG13	1:127:A:ARG:H	17	0.15
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG21	3	0.15
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG22	3	0.15
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG23	3	0.15
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG21	6	0.15
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG22	6	0.15
(1,2572)	1:16:A:SER:HB2	2:641:B:TPO:HG23	6	0.15
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	2	0.15
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	2	0.15
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	2	0.15
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	3	0.15
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	3	0.15
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	3	0.15
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD1	20	0.15
(1,2561)	2:655:B:GLU:H	2:656:B:PHE:HD2	20	0.15
(1,2523)	2:647:B:VAL:HA	2:649:B:ARG:H	3	0.15
(1,2517)	2:646:B:GLU:HG2	2:647:B:VAL:H	3	0.15
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE1	20	0.15
(1,2481)	2:656:B:PHE:H	2:656:B:PHE:HE2	20	0.15
(1,2386)	1:163:A:GLU:H	1:163:A:GLU:HG2	11	0.15
(1,2383)	1:163:A:GLU:H	1:163:A:GLU:HB2	2	0.15
(1,2161)	1:119:A:ARG:H	1:119:A:ARG:HD3	13	0.15
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	12	0.15
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	12	0.15
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	12	0.15
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD11	13	0.15
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD12	13	0.15
(1,1950)	1:86:A:LEU:H	1:86:A:LEU:HD13	13	0.15
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	6	0.15
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	12	0.15
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	14	0.15
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	16	0.15
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	13	0.15
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	5	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	4	0.15
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	9	0.15
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	10	0.15
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	19	0.15
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	16	0.15
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	16	0.15
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	12	0.15
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	20	0.15
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	9	0.15
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	10	0.15
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	15	0.15
(1,1406)	1:147:A:SER:H	1:161:A:ARG:H	5	0.15
(1,1402)	1:143:A:THR:HG21	1:161:A:ARG:HD2	10	0.15
(1,1402)	1:143:A:THR:HG22	1:161:A:ARG:HD2	10	0.15
(1,1402)	1:143:A:THR:HG23	1:161:A:ARG:HD2	10	0.15
(1,1402)	1:143:A:THR:HG21	1:161:A:ARG:HD2	14	0.15
(1,1402)	1:143:A:THR:HG22	1:161:A:ARG:HD2	14	0.15
(1,1402)	1:143:A:THR:HG23	1:161:A:ARG:HD2	14	0.15
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	18	0.15
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	18	0.15
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	18	0.15
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	18	0.15
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	18	0.15
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	18	0.15
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG21	4	0.15
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG22	4	0.15
(1,1330)	1:92:A:TYR:HD1	1:158:A:ILE:HG23	4	0.15
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG21	4	0.15
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG22	4	0.15
(1,1330)	1:92:A:TYR:HD2	1:158:A:ILE:HG23	4	0.15
(1,1309)	1:150:A:VAL:HB	1:157:A:HIS:H	17	0.15
(1,1306)	1:89:A:ILE:HD11	1:157:A:HIS:HD2	19	0.15
(1,1306)	1:89:A:ILE:HD12	1:157:A:HIS:HD2	19	0.15
(1,1306)	1:89:A:ILE:HD13	1:157:A:HIS:HD2	19	0.15
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD11	4	0.15
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD12	4	0.15
(1,1292)	1:87:A:GLU:H	1:156:A:ILE:HD13	4	0.15
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	3	0.15
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	7	0.15
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	10	0.15
(1,1190)	1:141:A:LEU:HD21	1:142:A:ARG:HB2	8	0.15
(1,1190)	1:141:A:LEU:HD22	1:142:A:ARG:HB2	8	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1190)	1:141:A:LEU:HD23	1:142:A:ARG:HB2	8	0.15
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	2	0.15
(1,1114)	1:126:A:SER:HB2	1:127:A:ARG:H	13	0.15
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE1	7	0.15
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE2	7	0.15
(1,1103)	1:125:A:PHE:HD1	1:130:A:MET:HE3	7	0.15
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE1	7	0.15
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE2	7	0.15
(1,1103)	1:125:A:PHE:HD2	1:130:A:MET:HE3	7	0.15
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	3	0.15
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	14	0.15
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	11	0.15
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	19	0.15
(1,1012)	1:116:A:ALA:H	1:119:A:ARG:H	7	0.15
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB1	12	0.15
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB2	12	0.15
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB3	12	0.15
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	6	0.15
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	19	0.15
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	20	0.15
(1,934)	1:104:A:GLU:HA	1:107:A:ALA:H	10	0.15
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	13	0.15
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	3	0.15
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	6	0.15
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	11	0.15
(1,871)	1:96:A:ILE:HB	1:103:A:PHE:H	16	0.15
(1,862)	1:101:A:GLU:HG2	1:102:A:ASP:H	4	0.15
(1,845)	1:97:A:LYS:HD2	1:98:A:SER:H	19	0.15
(1,844)	1:97:A:LYS:HG2	1:98:A:SER:H	19	0.15
(1,843)	1:97:A:LYS:HB2	1:98:A:SER:H	14	0.15
(1,822)	1:96:A:ILE:HD11	1:97:A:LYS:H	12	0.15
(1,822)	1:96:A:ILE:HD12	1:97:A:LYS:H	12	0.15
(1,822)	1:96:A:ILE:HD13	1:97:A:LYS:H	12	0.15
(1,811)	1:94:A:GLN:H	1:96:A:ILE:H	16	0.15
(1,805)	1:93:A:ILE:HG21	1:94:A:GLN:H	12	0.15
(1,805)	1:93:A:ILE:HG22	1:94:A:GLN:H	12	0.15
(1,805)	1:93:A:ILE:HG23	1:94:A:GLN:H	12	0.15
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	11	0.15
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	11	0.15
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	11	0.15
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD11	13	0.15
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD12	13	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:92:A:TYR:HE1	1:158:A:ILE:HD13	13	0.15
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD11	13	0.15
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD12	13	0.15
(1,783)	1:92:A:TYR:HE2	1:158:A:ILE:HD13	13	0.15
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD11	12	0.15
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD12	12	0.15
(1,778)	1:92:A:TYR:H	1:106:A:LEU:HD13	12	0.15
(1,750)	1:88:A:LEU:H	1:91:A:GLY:H	13	0.15
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	7	0.15
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	7	0.15
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	7	0.15
(1,723)	1:86:A:LEU:HD21	1:89:A:ILE:HB	18	0.15
(1,723)	1:86:A:LEU:HD22	1:89:A:ILE:HB	18	0.15
(1,723)	1:86:A:LEU:HD23	1:89:A:ILE:HB	18	0.15
(1,692)	1:86:A:LEU:HG	1:90:A:ASN:HD22	1	0.15
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	3	0.15
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	5	0.15
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	7	0.15
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	3	0.15
(1,619)	1:78:A:ILE:HB	1:80:A:ARG:H	13	0.15
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	4	0.15
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	5	0.15
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG21	6	0.15
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG22	6	0.15
(1,527)	1:66:A:GLN:HG2	1:81:A:THR:HG23	6	0.15
(1,514)	1:63:A:LYS:HB2	1:70:A:PRO:HA	15	0.15
(1,510)	1:62:A:VAL:HG11	1:156:A:ILE:H	4	0.15
(1,510)	1:62:A:VAL:HG12	1:156:A:ILE:H	4	0.15
(1,510)	1:62:A:VAL:HG13	1:156:A:ILE:H	4	0.15
(1,469)	1:60:A:LEU:HB2	1:61:A:LEU:H	12	0.15
(1,457)	1:60:A:LEU:HD11	1:108:A:SER:H	3	0.15
(1,457)	1:60:A:LEU:HD12	1:108:A:SER:H	3	0.15
(1,457)	1:60:A:LEU:HD13	1:108:A:SER:H	3	0.15
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	3	0.15
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	3	0.15
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	5	0.15
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	17	0.15
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	18	0.15
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	4	0.15
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	4	0.15
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	4	0.15
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	2	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	8	0.15
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	17	0.15
(1,205)	1:24:A:TYR:H	1:33:A:GLN:HG2	11	0.15
(1,170)	1:16:A:SER:H	1:23:A:TYR:H	13	0.15
(1,129)	1:16:A:SER:HB2	1:21:A:ARG:H	10	0.15
(1,129)	1:16:A:SER:HB2	1:21:A:ARG:H	11	0.15
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	13	0.15
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	13	0.15
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	13	0.15
(1,75)	1:13:A:LYS:HA	1:23:A:TYR:H	17	0.15
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	11	0.15
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	11	0.15
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	12	0.15
(1,23)	1:7:A:LEU:HA	1:11:A:TRP:HB3	2	0.15
(3,80)	1:105:A:SER:O	1:109:A:GLN:H	1	0.14
(3,80)	1:105:A:SER:O	1:109:A:GLN:H	20	0.14
(3,47)	1:81:A:THR:O	1:85:A:ALA:N	17	0.14
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	17	0.14
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	5	0.14
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	5	0.14
(2,93)	1:93:A:ILE:HD11	2:643:B:PRO:HA	12	0.14
(2,93)	1:93:A:ILE:HD12	2:643:B:PRO:HA	12	0.14
(2,93)	1:93:A:ILE:HD13	2:643:B:PRO:HA	12	0.14
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	10	0.14
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	13	0.14
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	10	0.14
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	10	0.14
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB2	12	0.14
(1,2582)	1:34:A:TRP:HE1	2:642:B:PRO:HB3	12	0.14
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	1	0.14
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	1	0.14
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	1	0.14
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	17	0.14
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	17	0.14
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	17	0.14
(1,2532)	2:648:B:ILE:HG21	2:650:B:ASN:H	19	0.14
(1,2532)	2:648:B:ILE:HG22	2:650:B:ASN:H	19	0.14
(1,2532)	2:648:B:ILE:HG23	2:650:B:ASN:H	19	0.14
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	8	0.14
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	8	0.14
(1,2383)	1:163:A:GLU:H	1:163:A:GLU:HB2	13	0.14
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	4	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	12	0.14
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	12	0.14
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	13	0.14
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	19	0.14
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	20	0.14
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	18	0.14
(1,1703)	1:36:A:ARG:H	1:36:A:ARG:HD2	11	0.14
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	2	0.14
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	3	0.14
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	7	0.14
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	8	0.14
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	17	0.14
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	5	0.14
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	5	0.14
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	10	0.14
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	10	0.14
(1,1547)	1:15:A:MET:H	1:15:A:MET:HB2	3	0.14
(1,1456)	1:6:A:LYS:H	1:6:A:LYS:HE2	4	0.14
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	17	0.14
(1,1441)	1:162:A:THR:HG21	1:163:A:GLU:HG3	9	0.14
(1,1441)	1:162:A:THR:HG22	1:163:A:GLU:HG3	9	0.14
(1,1441)	1:162:A:THR:HG23	1:163:A:GLU:HG3	9	0.14
(1,1423)	1:55:A:VAL:HB	1:163:A:GLU:H	15	0.14
(1,1402)	1:143:A:THR:HG21	1:161:A:ARG:HD2	3	0.14
(1,1402)	1:143:A:THR:HG22	1:161:A:ARG:HD2	3	0.14
(1,1402)	1:143:A:THR:HG23	1:161:A:ARG:HD2	3	0.14
(1,1382)	1:159:A:ILE:HG12	1:160:A:LEU:H	7	0.14
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD21	1	0.14
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD22	1	0.14
(1,1368)	1:103:A:PHE:HB3	1:160:A:LEU:HD23	1	0.14
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD11	4	0.14
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD12	4	0.14
(1,1366)	1:103:A:PHE:H	1:160:A:LEU:HD13	4	0.14
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD11	1	0.14
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD12	1	0.14
(1,1348)	1:157:A:HIS:HB2	1:159:A:ILE:HD13	1	0.14
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD11	1	0.14
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD12	1	0.14
(1,1348)	1:157:A:HIS:HB3	1:159:A:ILE:HD13	1	0.14
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG21	19	0.14
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG22	19	0.14
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG23	19	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	1	0.14
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	1	0.14
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	1	0.14
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	15	0.14
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	15	0.14
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	15	0.14
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	7	0.14
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	7	0.14
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	7	0.14
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	7	0.14
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	7	0.14
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	7	0.14
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	3	0.14
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	4	0.14
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	6	0.14
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	9	0.14
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	2	0.14
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	2	0.14
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	2	0.14
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	2	0.14
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	2	0.14
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	2	0.14
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	2	0.14
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	2	0.14
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	2	0.14
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	9	0.14
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	9	0.14
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	9	0.14
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	9	0.14
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	9	0.14
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	9	0.14
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	9	0.14
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	9	0.14
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	9	0.14
(1,1232)	1:149:A:PRO:HB3	1:150:A:VAL:H	13	0.14
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	16	0.14
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	15	0.14
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	15	0.14
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	11	0.14
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	11	0.14
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	11	0.14
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	2	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1020)	1:116:A:ALA:HA	1:118:A:ALA:H	8	0.14
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB1	10	0.14
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB2	10	0.14
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB3	10	0.14
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	7	0.14
(1,920)	1:106:A:LEU:HB3	1:108:A:SER:H	15	0.14
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE1	8	0.14
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE2	8	0.14
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE3	8	0.14
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE1	8	0.14
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE2	8	0.14
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE3	8	0.14
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE1	16	0.14
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE2	16	0.14
(1,889)	1:103:A:PHE:HE1	1:146:A:MET:HE3	16	0.14
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE1	16	0.14
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE2	16	0.14
(1,889)	1:103:A:PHE:HE2	1:146:A:MET:HE3	16	0.14
(1,854)	1:98:A:SER:H	1:101:A:GLU:H	6	0.14
(1,854)	1:98:A:SER:H	1:101:A:GLU:H	18	0.14
(1,843)	1:97:A:LYS:HB2	1:98:A:SER:H	13	0.14
(1,831)	1:93:A:ILE:HG21	1:97:A:LYS:HB3	2	0.14
(1,831)	1:93:A:ILE:HG22	1:97:A:LYS:HB3	2	0.14
(1,831)	1:93:A:ILE:HG23	1:97:A:LYS:HB3	2	0.14
(1,807)	1:93:A:ILE:HD11	1:94:A:GLN:H	4	0.14
(1,807)	1:93:A:ILE:HD12	1:94:A:GLN:H	4	0.14
(1,807)	1:93:A:ILE:HD13	1:94:A:GLN:H	4	0.14
(1,800)	1:93:A:ILE:HB	1:158:A:ILE:HD11	8	0.14
(1,800)	1:93:A:ILE:HB	1:158:A:ILE:HD12	8	0.14
(1,800)	1:93:A:ILE:HB	1:158:A:ILE:HD13	8	0.14
(1,737)	1:86:A:LEU:HB3	1:90:A:ASN:H	3	0.14
(1,654)	1:82:A:LYS:HG2	1:84:A:GLU:H	8	0.14
(1,654)	1:82:A:LYS:HG3	1:84:A:GLU:H	8	0.14
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	1	0.14
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	14	0.14
(1,619)	1:78:A:ILE:HB	1:80:A:ARG:H	2	0.14
(1,605)	1:72:A:SER:HA	1:78:A:ILE:HD11	17	0.14
(1,605)	1:72:A:SER:HA	1:78:A:ILE:HD12	17	0.14
(1,605)	1:72:A:SER:HA	1:78:A:ILE:HD13	17	0.14
(1,589)	1:74:A:ARG:H	1:112:A:ASP:HA	8	0.14
(1,520)	1:64:A:HIS:HE1	1:66:A:GLN:HG2	5	0.14
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	20	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	20	0.14
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	20	0.14
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	2	0.14
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	2	0.14
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	2	0.14
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	1	0.14
(1,422)	1:56:A:ARG:HG2	1:162:A:THR:HB	18	0.14
(1,393)	1:53:A:ALA:HB1	1:54:A:ARG:H	17	0.14
(1,393)	1:53:A:ALA:HB2	1:54:A:ARG:H	17	0.14
(1,393)	1:53:A:ALA:HB3	1:54:A:ARG:H	17	0.14
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	7	0.14
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	6	0.14
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	13	0.14
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	10	0.14
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	10	0.14
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	10	0.14
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	20	0.14
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	20	0.14
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	20	0.14
(1,334)	1:27:A:HIS:HA	1:31:A:ALA:H	2	0.14
(1,333)	1:25:A:PHE:HA	1:31:A:ALA:H	10	0.14
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	18	0.14
(1,265)	1:26:A:ASN:H	1:27:A:HIS:H	14	0.14
(1,265)	1:26:A:ASN:H	1:27:A:HIS:H	20	0.14
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	13	0.14
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	13	0.14
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	10	0.14
(1,178)	1:23:A:TYR:HE1	1:33:A:GLN:H	6	0.14
(1,178)	1:23:A:TYR:HE2	1:33:A:GLN:H	6	0.14
(1,165)	1:22:A:VAL:H	1:23:A:TYR:H	17	0.14
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG11	13	0.14
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG12	13	0.14
(1,157)	1:16:A:SER:H	1:22:A:VAL:HG13	13	0.14
(1,130)	1:16:A:SER:H	1:21:A:ARG:HA	7	0.14
(1,116)	1:16:A:SER:H	1:20:A:GLY:HA2	17	0.14
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	12	0.14
(1,102)	1:14:A:ARG:HD2	1:15:A:MET:H	13	0.14
(1,102)	1:14:A:ARG:HD3	1:15:A:MET:H	13	0.14
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	5	0.14
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	6	0.14
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	12	0.14
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	14	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD1	20	0.14
(1,79)	1:13:A:LYS:H	1:24:A:TYR:HD2	20	0.14
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	6	0.14
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	10	0.14
(1,28)	1:7:A:LEU:HD21	1:13:A:LYS:HG3	14	0.14
(1,28)	1:7:A:LEU:HD22	1:13:A:LYS:HG3	14	0.14
(1,28)	1:7:A:LEU:HD23	1:13:A:LYS:HG3	14	0.14
(1,20)	1:7:A:LEU:HD11	1:11:A:TRP:H	13	0.14
(1,20)	1:7:A:LEU:HD12	1:11:A:TRP:H	13	0.14
(1,20)	1:7:A:LEU:HD13	1:11:A:TRP:H	13	0.14
(4,2593)	2:640:B:LEU:H	2:641:B:TPO:H	10	0.13
(4,2532)	2:649:B:ARG:H	2:649:B:ARG:HD2	10	0.13
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	17	0.13
(3,63)	1:90:A:ASN:O	1:94:A:GLN:N	4	0.13
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG12	4	0.13
(2,111)	1:160:A:LEU:H	2:651:B:ILE:HG13	4	0.13
(2,102)	1:135:A:GLU:H	2:656:B:PHE:HB2	6	0.13
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE1	5	0.13
(2,70)	2:651:B:ILE:HG21	2:656:B:PHE:HE2	5	0.13
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE1	5	0.13
(2,70)	2:651:B:ILE:HG22	2:656:B:PHE:HE2	5	0.13
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE1	5	0.13
(2,70)	2:651:B:ILE:HG23	2:656:B:PHE:HE2	5	0.13
(2,34)	1:59:A:HIS:H	1:122:A:LEU:HB2	15	0.13
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE1	5	0.13
(1,2591)	1:123:A:GLY:H	2:656:B:PHE:HE2	5	0.13
(1,2589)	1:122:A:LEU:HD21	2:656:B:PHE:HE1	20	0.13
(1,2589)	1:122:A:LEU:HD21	2:656:B:PHE:HE2	20	0.13
(1,2589)	1:122:A:LEU:HD22	2:656:B:PHE:HE1	20	0.13
(1,2589)	1:122:A:LEU:HD22	2:656:B:PHE:HE2	20	0.13
(1,2589)	1:122:A:LEU:HD23	2:656:B:PHE:HE1	20	0.13
(1,2589)	1:122:A:LEU:HD23	2:656:B:PHE:HE2	20	0.13
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE1	10	0.13
(1,2588)	1:122:A:LEU:H	2:656:B:PHE:HE2	10	0.13
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG21	13	0.13
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG22	13	0.13
(1,2576)	1:23:A:TYR:HB3	2:641:B:TPO:HG23	13	0.13
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG21	12	0.13
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG22	12	0.13
(1,2571)	1:16:A:SER:H	2:641:B:TPO:HG23	12	0.13
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	12	0.13
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	12	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	12	0.13
(1,2524)	2:647:B:VAL:HG11	2:650:B:ASN:HD22	9	0.13
(1,2524)	2:647:B:VAL:HG12	2:650:B:ASN:HD22	9	0.13
(1,2524)	2:647:B:VAL:HG13	2:650:B:ASN:HD22	9	0.13
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	9	0.13
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	9	0.13
(1,2383)	1:163:A:GLU:H	1:163:A:GLU:HB2	17	0.13
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	17	0.13
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	7	0.13
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	1	0.13
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	6	0.13
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	1	0.13
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	1	0.13
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	13	0.13
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	13	0.13
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	8	0.13
(1,1456)	1:6:A:LYS:H	1:6:A:LYS:HE2	20	0.13
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	14	0.13
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	16	0.13
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	7	0.13
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	14	0.13
(1,1428)	1:143:A:THR:HG21	1:163:A:GLU:H	19	0.13
(1,1428)	1:143:A:THR:HG22	1:163:A:GLU:H	19	0.13
(1,1428)	1:143:A:THR:HG23	1:163:A:GLU:H	19	0.13
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG21	8	0.13
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG22	8	0.13
(1,1335)	1:57:A:CYS:HA	1:159:A:ILE:HG23	8	0.13
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	6	0.13
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	6	0.13
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	6	0.13
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG21	6	0.13
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG22	6	0.13
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG23	6	0.13
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	16	0.13
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	16	0.13
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	16	0.13
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG21	3	0.13
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG22	3	0.13
(1,1293)	1:89:A:ILE:H	1:156:A:ILE:HG23	3	0.13
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	2	0.13
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG21	13	0.13
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG22	13	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG23	13	0.13
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	11	0.13
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	11	0.13
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	11	0.13
(1,1208)	1:103:A:PHE:HD1	1:146:A:MET:HB2	8	0.13
(1,1208)	1:103:A:PHE:HD2	1:146:A:MET:HB2	8	0.13
(1,1193)	1:141:A:LEU:HD11	1:148:A:GLY:H	16	0.13
(1,1193)	1:141:A:LEU:HD12	1:148:A:GLY:H	16	0.13
(1,1193)	1:141:A:LEU:HD13	1:148:A:GLY:H	16	0.13
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	7	0.13
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	7	0.13
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	7	0.13
(1,1192)	1:141:A:LEU:HD21	1:146:A:MET:H	18	0.13
(1,1192)	1:141:A:LEU:HD22	1:146:A:MET:H	18	0.13
(1,1192)	1:141:A:LEU:HD23	1:146:A:MET:H	18	0.13
(1,1184)	1:140:A:ALA:H	1:141:A:LEU:HG	20	0.13
(1,1177)	1:137:A:ALA:HB1	1:141:A:LEU:H	4	0.13
(1,1177)	1:137:A:ALA:HB2	1:141:A:LEU:H	4	0.13
(1,1177)	1:137:A:ALA:HB3	1:141:A:LEU:H	4	0.13
(1,1072)	1:121:A:ASP:HB2	1:123:A:GLY:H	14	0.13
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	6	0.13
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	20	0.13
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	5	0.13
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	5	0.13
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	5	0.13
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	8	0.13
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	8	0.13
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	8	0.13
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	10	0.13
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	10	0.13
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	10	0.13
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	13	0.13
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	13	0.13
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	13	0.13
(1,978)	1:107:A:ALA:HB1	1:111:A:SER:HA	20	0.13
(1,978)	1:107:A:ALA:HB2	1:111:A:SER:HA	20	0.13
(1,978)	1:107:A:ALA:HB3	1:111:A:SER:HA	20	0.13
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	6	0.13
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	12	0.13
(1,952)	1:107:A:ALA:HB1	1:111:A:SER:H	3	0.13
(1,952)	1:107:A:ALA:HB2	1:111:A:SER:H	3	0.13
(1,952)	1:107:A:ALA:HB3	1:111:A:SER:H	3	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,923)	1:106:A:LEU:HA	1:110:A:PHE:H	17	0.13
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	9	0.13
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	7	0.13
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	7	0.13
(1,878)	1:102:A:ASP:H	1:103:A:PHE:H	1	0.13
(1,878)	1:102:A:ASP:H	1:103:A:PHE:H	9	0.13
(1,854)	1:98:A:SER:H	1:101:A:GLU:H	15	0.13
(1,832)	1:93:A:ILE:HG21	1:97:A:LYS:HG2	13	0.13
(1,832)	1:93:A:ILE:HG22	1:97:A:LYS:HG2	13	0.13
(1,832)	1:93:A:ILE:HG23	1:97:A:LYS:HG2	13	0.13
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE1	14	0.13
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE2	14	0.13
(1,799)	1:93:A:ILE:HB	1:146:A:MET:HE3	14	0.13
(1,737)	1:86:A:LEU:HB3	1:90:A:ASN:H	9	0.13
(1,698)	1:86:A:LEU:HD11	1:87:A:GLU:H	16	0.13
(1,698)	1:86:A:LEU:HD12	1:87:A:GLU:H	16	0.13
(1,698)	1:86:A:LEU:HD13	1:87:A:GLU:H	16	0.13
(1,674)	1:81:A:THR:H	1:85:A:ALA:H	16	0.13
(1,654)	1:82:A:LYS:HG2	1:84:A:GLU:H	3	0.13
(1,654)	1:82:A:LYS:HG3	1:84:A:GLU:H	3	0.13
(1,649)	1:66:A:GLN:HE21	1:82:A:LYS:HB2	5	0.13
(1,649)	1:66:A:GLN:HE21	1:82:A:LYS:HB2	6	0.13
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	18	0.13
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	2	0.13
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	7	0.13
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	11	0.13
(1,591)	1:74:A:ARG:HE	1:75:A:GLN:H	6	0.13
(1,586)	1:73:A:TRP:HB3	1:74:A:ARG:H	17	0.13
(1,551)	1:70:A:PRO:HB3	1:71:A:SER:H	10	0.13
(1,523)	1:64:A:HIS:HE1	1:66:A:GLN:H	5	0.13
(1,510)	1:62:A:VAL:HG11	1:156:A:ILE:H	1	0.13
(1,510)	1:62:A:VAL:HG12	1:156:A:ILE:H	1	0.13
(1,510)	1:62:A:VAL:HG13	1:156:A:ILE:H	1	0.13
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	8	0.13
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	8	0.13
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	8	0.13
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	13	0.13
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	13	0.13
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	13	0.13
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	4	0.13
(1,424)	1:56:A:ARG:HE	1:57:A:CYS:H	13	0.13
(1,388)	1:35:A:GLU:HG2	1:36:A:ARG:H	11	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:34:A:TRP:H	1:35:A:GLU:HB3	11	0.13
(1,378)	1:33:A:GLN:H	1:35:A:GLU:H	3	0.13
(1,378)	1:33:A:GLN:H	1:35:A:GLU:H	18	0.13
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	17	0.13
(1,317)	1:28:A:ILE:HG12	1:29:A:THR:H	8	0.13
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	5	0.13
(1,302)	1:27:A:HIS:HD2	1:28:A:ILE:H	14	0.13
(1,284)	1:26:A:ASN:HA	1:31:A:ALA:HB1	11	0.13
(1,284)	1:26:A:ASN:HA	1:31:A:ALA:HB2	11	0.13
(1,284)	1:26:A:ASN:HA	1:31:A:ALA:HB3	11	0.13
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	4	0.13
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	5	0.13
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	15	0.13
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	15	0.13
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	10	0.13
(1,205)	1:24:A:TYR:H	1:33:A:GLN:HG2	13	0.13
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	12	0.13
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	3	0.13
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	17	0.13
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	17	0.13
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD1	19	0.13
(1,176)	1:23:A:TYR:HB3	1:24:A:TYR:HD2	19	0.13
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG11	7	0.13
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG12	7	0.13
(1,149)	1:15:A:MET:HE1	1:22:A:VAL:HG13	7	0.13
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG11	7	0.13
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG12	7	0.13
(1,149)	1:15:A:MET:HE2	1:22:A:VAL:HG13	7	0.13
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG11	7	0.13
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG12	7	0.13
(1,149)	1:15:A:MET:HE3	1:22:A:VAL:HG13	7	0.13
(1,134)	1:20:A:GLY:H	1:21:A:ARG:HA	13	0.13
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	6	0.13
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD1	7	0.13
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD2	7	0.13
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	2	0.13
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	20	0.13
(1,87)	1:13:A:LYS:HG3	1:14:A:ARG:H	11	0.13
(1,81)	1:12:A:GLU:H	1:14:A:ARG:H	4	0.13
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	4	0.13
(1,12)	1:5:A:GLU:HB2	1:6:A:LYS:H	13	0.13
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	2	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:3:A:ASP:HA	1:4:A:GLU:H	3	0.13
(4,2784)	1:56:A:ARG:H	1:163:A:GLU:O	2	0.12
(4,2760)	1:12:A:GLU:H	1:25:A:PHE:O	7	0.12
(4,2672)	2:657:B:GLU:HG2	2:658:B:GLY:H	7	0.12
(4,1761)	1:33:A:GLN:HB3	1:33:A:GLN:HE21	11	0.12
(4,1761)	1:33:A:GLN:HB2	1:33:A:GLN:HE21	11	0.12
(4,1761)	1:33:A:GLN:HB3	1:33:A:GLN:HE22	11	0.12
(3,59)	1:88:A:LEU:O	1:92:A:TYR:N	6	0.12
(3,43)	1:72:A:SER:O	1:75:A:GLN:N	9	0.12
(3,10)	1:16:A:SER:O	1:19:A:SER:H	13	0.12
(2,34)	1:59:A:HIS:H	1:122:A:LEU:HB2	6	0.12
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	2	0.12
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	12	0.12
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	1	0.12
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	2	0.12
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	2	0.12
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	2	0.12
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	5	0.12
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	5	0.12
(1,2477)	2:653:B:GLN:HA	2:653:B:GLN:HE22	2	0.12
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD11	6	0.12
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD12	6	0.12
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD13	6	0.12
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	6	0.12
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	6	0.12
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	6	0.12
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	11	0.12
(1,1751)	1:56:A:ARG:H	1:56:A:ARG:HG3	18	0.12
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	11	0.12
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	19	0.12
(1,1703)	1:36:A:ARG:H	1:36:A:ARG:HD2	7	0.12
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	20	0.12
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	4	0.12
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	4	0.12
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	15	0.12
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	15	0.12
(1,1568)	1:21:A:ARG:HB2	1:21:A:ARG:HE	9	0.12
(1,1547)	1:15:A:MET:H	1:15:A:MET:HB2	4	0.12
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	12	0.12
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	2	0.12
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	4	0.12
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	19	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	4	0.12
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	12	0.12
(1,1441)	1:162:A:THR:HG21	1:163:A:GLU:HG3	5	0.12
(1,1441)	1:162:A:THR:HG22	1:163:A:GLU:HG3	5	0.12
(1,1441)	1:162:A:THR:HG23	1:163:A:GLU:HG3	5	0.12
(1,1431)	1:161:A:ARG:HA	1:163:A:GLU:H	10	0.12
(1,1361)	1:59:A:HIS:HB2	1:160:A:LEU:H	16	0.12
(1,1361)	1:59:A:HIS:HB3	1:160:A:LEU:H	16	0.12
(1,1353)	1:57:A:CYS:HB3	1:160:A:LEU:H	4	0.12
(1,1346)	1:148:A:GLY:H	1:159:A:ILE:H	17	0.12
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG21	20	0.12
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG22	20	0.12
(1,1329)	1:90:A:ASN:H	1:158:A:ILE:HG23	20	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	6	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	6	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	6	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	6	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	6	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	6	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	6	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	6	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	6	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	14	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	14	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	14	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	14	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	14	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	14	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	14	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	14	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	14	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	15	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	15	0.12
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	15	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	15	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	15	0.12
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	15	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	15	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	15	0.12
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	15	0.12
(1,1233)	1:149:A:PRO:HD2	1:150:A:VAL:H	2	0.12
(1,1231)	1:149:A:PRO:HG2	1:150:A:VAL:H	11	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1199)	1:142:A:ARG:HG2	1:143:A:THR:H	16	0.12
(1,1178)	1:137:A:ALA:HA	1:141:A:LEU:H	12	0.12
(1,1161)	1:136:A:ASP:HB2	1:138:A:SER:H	18	0.12
(1,1096)	1:56:A:ARG:HA	1:125:A:PHE:HD1	2	0.12
(1,1096)	1:56:A:ARG:HA	1:125:A:PHE:HD2	2	0.12
(1,1072)	1:121:A:ASP:HB2	1:123:A:GLY:H	13	0.12
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD21	1	0.12
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD22	1	0.12
(1,1051)	1:57:A:CYS:H	1:122:A:LEU:HD23	1	0.12
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	4	0.12
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	17	0.12
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	17	0.12
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	17	0.12
(1,1026)	1:118:A:ALA:H	1:119:A:ARG:HA	1	0.12
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB1	9	0.12
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB2	9	0.12
(1,1001)	1:113:A:CYS:H	1:116:A:ALA:HB3	9	0.12
(1,961)	1:108:A:SER:H	1:119:A:ARG:HG2	19	0.12
(1,921)	1:106:A:LEU:H	1:109:A:GLN:H	20	0.12
(1,914)	1:104:A:GLU:H	1:106:A:LEU:HB3	16	0.12
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	12	0.12
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	12	0.12
(1,888)	1:103:A:PHE:HE1	1:120:A:GLY:H	16	0.12
(1,888)	1:103:A:PHE:HE2	1:120:A:GLY:H	16	0.12
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD11	2	0.12
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD12	2	0.12
(1,885)	1:103:A:PHE:HA	1:106:A:LEU:HD13	2	0.12
(1,878)	1:102:A:ASP:H	1:103:A:PHE:H	3	0.12
(1,878)	1:102:A:ASP:H	1:103:A:PHE:H	19	0.12
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	10	0.12
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	10	0.12
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	10	0.12
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	10	0.12
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	10	0.12
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	10	0.12
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD11	12	0.12
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD12	12	0.12
(1,857)	1:101:A:GLU:HG2	1:106:A:LEU:HD13	12	0.12
(1,807)	1:93:A:ILE:HD11	1:94:A:GLN:H	5	0.12
(1,807)	1:93:A:ILE:HD12	1:94:A:GLN:H	5	0.12
(1,807)	1:93:A:ILE:HD13	1:94:A:GLN:H	5	0.12
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE1	14	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,728)	1:89:A:ILE:HD11	1:92:A:TYR:HE2	14	0.12
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE1	14	0.12
(1,728)	1:89:A:ILE:HD12	1:92:A:TYR:HE2	14	0.12
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE1	14	0.12
(1,728)	1:89:A:ILE:HD13	1:92:A:TYR:HE2	14	0.12
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD11	7	0.12
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD12	7	0.12
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD13	7	0.12
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	6	0.12
(1,648)	1:66:A:GLN:HE22	1:82:A:LYS:HG3	6	0.12
(1,647)	1:65:A:SER:H	1:82:A:LYS:H	14	0.12
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	3	0.12
(1,599)	1:70:A:PRO:HB2	1:78:A:ILE:H	11	0.12
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	18	0.12
(1,537)	1:66:A:GLN:HB3	1:67:A:SER:H	17	0.12
(1,532)	1:64:A:HIS:H	1:67:A:SER:H	1	0.12
(1,531)	1:64:A:HIS:HE1	1:67:A:SER:HB2	6	0.12
(1,523)	1:64:A:HIS:HE1	1:66:A:GLN:H	2	0.12
(1,515)	1:63:A:LYS:H	1:156:A:ILE:H	4	0.12
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD11	9	0.12
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD12	9	0.12
(1,492)	1:62:A:VAL:HA	1:78:A:ILE:HD13	9	0.12
(1,469)	1:60:A:LEU:HB2	1:61:A:LEU:H	13	0.12
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	13	0.12
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	13	0.12
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	13	0.12
(1,450)	1:60:A:LEU:HD11	1:89:A:ILE:HD11	8	0.12
(1,450)	1:60:A:LEU:HD11	1:89:A:ILE:HD12	8	0.12
(1,450)	1:60:A:LEU:HD11	1:89:A:ILE:HD13	8	0.12
(1,450)	1:60:A:LEU:HD12	1:89:A:ILE:HD11	8	0.12
(1,450)	1:60:A:LEU:HD12	1:89:A:ILE:HD12	8	0.12
(1,450)	1:60:A:LEU:HD12	1:89:A:ILE:HD13	8	0.12
(1,450)	1:60:A:LEU:HD13	1:89:A:ILE:HD11	8	0.12
(1,450)	1:60:A:LEU:HD13	1:89:A:ILE:HD12	8	0.12
(1,450)	1:60:A:LEU:HD13	1:89:A:ILE:HD13	8	0.12
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	2	0.12
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	14	0.12
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	19	0.12
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	5	0.12
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	12	0.12
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	17	0.12
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	8	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	15	0.12
(1,365)	1:32:A:SER:H	1:33:A:GLN:H	5	0.12
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	5	0.12
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	5	0.12
(1,363)	1:11:A:TRP:HE3	1:33:A:GLN:H	11	0.12
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	16	0.12
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	16	0.12
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	16	0.12
(1,321)	1:25:A:PHE:HZ	1:30:A:ASN:H	8	0.12
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	11	0.12
(1,317)	1:28:A:ILE:HG12	1:29:A:THR:H	12	0.12
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	2	0.12
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	19	0.12
(1,223)	1:14:A:ARG:HB2	1:25:A:PHE:H	17	0.12
(1,208)	1:24:A:TYR:H	1:34:A:TRP:HB3	12	0.12
(1,205)	1:24:A:TYR:H	1:33:A:GLN:HG2	9	0.12
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	7	0.12
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	1	0.12
(1,189)	1:13:A:LYS:H	1:24:A:TYR:HA	14	0.12
(1,143)	1:15:A:MET:HA	1:22:A:VAL:H	11	0.12
(1,125)	1:15:A:MET:HA	1:21:A:ARG:H	18	0.12
(1,121)	1:17:A:ARG:HB2	1:18:A:SER:H	5	0.12
(1,121)	1:17:A:ARG:HB2	1:18:A:SER:H	10	0.12
(1,121)	1:17:A:ARG:HB2	1:18:A:SER:H	20	0.12
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG21	10	0.12
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG22	10	0.12
(1,109)	1:15:A:MET:H	1:22:A:VAL:HG23	10	0.12
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	7	0.12
(1,89)	1:14:A:ARG:H	1:15:A:MET:HA	8	0.12
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	17	0.12
(1,20)	1:7:A:LEU:HD11	1:11:A:TRP:H	19	0.12
(1,20)	1:7:A:LEU:HD12	1:11:A:TRP:H	19	0.12
(1,20)	1:7:A:LEU:HD13	1:11:A:TRP:H	19	0.12
(4,2798)	1:72:A:SER:H	1:75:A:GLN:O	7	0.11
(4,2798)	1:72:A:SER:H	1:75:A:GLN:O	8	0.11
(4,2774)	1:26:A:ASN:H	1:31:A:ALA:O	11	0.11
(4,1958)	1:75:A:GLN:HB2	1:75:A:GLN:HE21	2	0.11
(4,1958)	1:75:A:GLN:HB2	1:75:A:GLN:HE22	2	0.11
(4,1958)	1:75:A:GLN:HB2	1:75:A:GLN:HE21	15	0.11
(4,1958)	1:75:A:GLN:HB2	1:75:A:GLN:HE22	15	0.11
(4,1958)	1:75:A:GLN:HB2	1:75:A:GLN:HE21	18	0.11
(4,1958)	1:75:A:GLN:HB2	1:75:A:GLN:HE22	18	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,71)	1:94:A:GLN:O	1:98:A:SER:N	10	0.11
(3,63)	1:90:A:ASN:O	1:94:A:GLN:N	16	0.11
(3,10)	1:16:A:SER:O	1:19:A:SER:H	5	0.11
(3,9)	1:16:A:SER:O	1:19:A:SER:N	18	0.11
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG12	20	0.11
(2,113)	1:162:A:THR:H	2:651:B:ILE:HG13	20	0.11
(2,107)	1:140:A:ALA:HB1	2:651:B:ILE:HA	15	0.11
(2,107)	1:140:A:ALA:HB2	2:651:B:ILE:HA	15	0.11
(2,107)	1:140:A:ALA:HB3	2:651:B:ILE:HA	15	0.11
(2,91)	1:57:A:CYS:H	2:651:B:ILE:HG12	13	0.11
(2,91)	1:57:A:CYS:H	2:651:B:ILE:HG13	13	0.11
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG11	1	0.11
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG12	1	0.11
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG13	1	0.11
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG11	9	0.11
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG12	9	0.11
(2,67)	2:646:B:GLU:HA	2:647:B:VAL:HG13	9	0.11
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	3	0.11
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	3	0.11
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	3	0.11
(2,52)	1:141:A:LEU:HD21	1:148:A:GLY:H	18	0.11
(2,52)	1:141:A:LEU:HD22	1:148:A:GLY:H	18	0.11
(2,52)	1:141:A:LEU:HD23	1:148:A:GLY:H	18	0.11
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	1	0.11
(2,1)	1:10:A:GLY:H	1:11:A:TRP:HB3	9	0.11
(1,2597)	1:138:A:SER:H	2:656:B:PHE:HB2	5	0.11
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE1	20	0.11
(1,2593)	1:129:A:GLN:HE21	2:656:B:PHE:HE2	20	0.11
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	5	0.11
(1,2551)	2:652:B:ASP:H	2:654:B:SER:H	17	0.11
(1,2527)	2:646:B:GLU:H	2:648:B:ILE:H	19	0.11
(1,2526)	2:646:B:GLU:HB2	2:648:B:ILE:H	2	0.11
(1,2506)	2:644:B:ASP:H	2:645:B:GLN:HA	16	0.11
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	3	0.11
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	3	0.11
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	4	0.11
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	4	0.11
(1,2386)	1:163:A:GLU:H	1:163:A:GLU:HG2	14	0.11
(1,2074)	1:104:A:GLU:H	1:104:A:GLU:HG2	19	0.11
(1,2056)	1:101:A:GLU:H	1:101:A:GLU:HG2	6	0.11
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD11	8	0.11
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD12	8	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2036)	1:96:A:ILE:H	1:96:A:ILE:HD13	8	0.11
(1,1913)	1:82:A:LYS:H	1:82:A:LYS:HD2	16	0.11
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	14	0.11
(1,1747)	1:56:A:ARG:H	1:56:A:ARG:HD2	2	0.11
(1,1660)	1:32:A:SER:H	1:32:A:SER:HB3	12	0.11
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	18	0.11
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	18	0.11
(1,1571)	1:21:A:ARG:H	1:21:A:ARG:HD2	5	0.11
(1,1571)	1:21:A:ARG:H	1:21:A:ARG:HD2	8	0.11
(1,1571)	1:21:A:ARG:H	1:21:A:ARG:HD2	15	0.11
(1,1571)	1:21:A:ARG:H	1:21:A:ARG:HD2	16	0.11
(1,1521)	1:14:A:ARG:H	1:14:A:ARG:HG3	15	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	1	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	2	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	3	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	4	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	5	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	6	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	7	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	8	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	9	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	10	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	11	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	14	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	15	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	16	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	17	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	18	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	19	0.11
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	20	0.11
(1,1455)	1:6:A:LYS:H	1:6:A:LYS:HB3	15	0.11
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	1	0.11
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	10	0.11
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	15	0.11
(1,1452)	1:5:A:GLU:H	1:5:A:GLU:HB3	16	0.11
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	5	0.11
(1,1450)	1:4:A:GLU:HA	1:4:A:GLU:HG2	6	0.11
(1,1435)	1:161:A:ARG:HG3	1:163:A:GLU:H	19	0.11
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD11	16	0.11
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD12	16	0.11
(1,1369)	1:104:A:GLU:H	1:160:A:LEU:HD13	16	0.11
(1,1340)	1:147:A:SER:HB2	1:159:A:ILE:HD11	17	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:147:A:SER:HB2	1:159:A:ILE:HD12	17	0.11
(1,1340)	1:147:A:SER:HB2	1:159:A:ILE:HD13	17	0.11
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG21	1	0.11
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG22	1	0.11
(1,1324)	1:89:A:ILE:HA	1:158:A:ILE:HG23	1	0.11
(1,1322)	1:61:A:LEU:HA	1:158:A:ILE:H	6	0.11
(1,1311)	1:152:A:THR:HG21	1:157:A:HIS:H	10	0.11
(1,1311)	1:152:A:THR:HG22	1:157:A:HIS:H	10	0.11
(1,1311)	1:152:A:THR:HG23	1:157:A:HIS:H	10	0.11
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG21	19	0.11
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG22	19	0.11
(1,1298)	1:90:A:ASN:H	1:156:A:ILE:HG23	19	0.11
(1,1262)	1:151:A:PHE:H	1:156:A:ILE:HA	18	0.11
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	13	0.11
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	15	0.11
(1,1259)	1:151:A:PHE:HB2	1:152:A:THR:H	16	0.11
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG11	18	0.11
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG12	18	0.11
(1,1228)	1:148:A:GLY:H	1:150:A:VAL:HG13	18	0.11
(1,1141)	1:130:A:MET:HB2	1:134:A:PHE:H	13	0.11
(1,1088)	1:56:A:ARG:HD2	1:124:A:ALA:HA	13	0.11
(1,1079)	1:123:A:GLY:H	1:125:A:PHE:HD1	15	0.11
(1,1079)	1:123:A:GLY:H	1:125:A:PHE:HD2	15	0.11
(1,1052)	1:58:A:SER:HB2	1:122:A:LEU:H	17	0.11
(1,1038)	1:119:A:ARG:HA	1:121:A:ASP:H	12	0.11
(1,1026)	1:118:A:ALA:H	1:119:A:ARG:HA	9	0.11
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB1	2	0.11
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB2	2	0.11
(1,998)	1:111:A:SER:H	1:116:A:ALA:HB3	2	0.11
(1,970)	1:108:A:SER:H	1:110:A:PHE:H	14	0.11
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	16	0.11
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	16	0.11
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	16	0.11
(1,926)	1:60:A:LEU:HD11	1:107:A:ALA:H	1	0.11
(1,926)	1:60:A:LEU:HD12	1:107:A:ALA:H	1	0.11
(1,926)	1:60:A:LEU:HD13	1:107:A:ALA:H	1	0.11
(1,926)	1:60:A:LEU:HD11	1:107:A:ALA:H	18	0.11
(1,926)	1:60:A:LEU:HD12	1:107:A:ALA:H	18	0.11
(1,926)	1:60:A:LEU:HD13	1:107:A:ALA:H	18	0.11
(1,925)	1:60:A:LEU:HG	1:107:A:ALA:H	17	0.11
(1,921)	1:106:A:LEU:H	1:109:A:GLN:H	7	0.11
(1,878)	1:102:A:ASP:H	1:103:A:PHE:H	7	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE1	16	0.11
(1,868)	1:60:A:LEU:HD21	1:103:A:PHE:HE2	16	0.11
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE1	16	0.11
(1,868)	1:60:A:LEU:HD22	1:103:A:PHE:HE2	16	0.11
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE1	16	0.11
(1,868)	1:60:A:LEU:HD23	1:103:A:PHE:HE2	16	0.11
(1,843)	1:97:A:LYS:HB2	1:98:A:SER:H	7	0.11
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE1	19	0.11
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE2	19	0.11
(1,828)	1:96:A:ILE:H	1:146:A:MET:HE3	19	0.11
(1,816)	1:95:A:LYS:HD2	1:96:A:ILE:H	4	0.11
(1,772)	1:92:A:TYR:H	1:93:A:ILE:HB	17	0.11
(1,750)	1:88:A:LEU:H	1:91:A:GLY:H	2	0.11
(1,669)	1:84:A:GLU:H	1:87:A:GLU:H	20	0.11
(1,663)	1:82:A:LYS:HB3	1:83:A:GLU:H	20	0.11
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	1	0.11
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	7	0.11
(1,659)	1:81:A:THR:HA	1:83:A:GLU:H	16	0.11
(1,619)	1:78:A:ILE:HB	1:80:A:ARG:H	11	0.11
(1,619)	1:78:A:ILE:HB	1:80:A:ARG:H	17	0.11
(1,586)	1:73:A:TRP:HB3	1:74:A:ARG:H	2	0.11
(1,586)	1:73:A:TRP:HB3	1:74:A:ARG:H	18	0.11
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	11	0.11
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	3	0.11
(1,469)	1:60:A:LEU:HB2	1:61:A:LEU:H	8	0.11
(1,469)	1:60:A:LEU:HB2	1:61:A:LEU:H	10	0.11
(1,469)	1:60:A:LEU:HB2	1:61:A:LEU:H	14	0.11
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	6	0.11
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	7	0.11
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	9	0.11
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	11	0.11
(1,387)	1:35:A:GLU:HB2	1:36:A:ARG:H	18	0.11
(1,384)	1:7:A:LEU:HD21	1:36:A:ARG:HA	18	0.11
(1,384)	1:7:A:LEU:HD22	1:36:A:ARG:HA	18	0.11
(1,384)	1:7:A:LEU:HD23	1:36:A:ARG:HA	18	0.11
(1,378)	1:33:A:GLN:H	1:35:A:GLU:H	1	0.11
(1,378)	1:33:A:GLN:H	1:35:A:GLU:H	6	0.11
(1,377)	1:33:A:GLN:HG2	1:35:A:GLU:H	17	0.11
(1,373)	1:34:A:TRP:HD1	1:35:A:GLU:H	11	0.11
(1,373)	1:34:A:TRP:HD1	1:35:A:GLU:H	15	0.11
(1,367)	1:24:A:TYR:HD1	1:34:A:TRP:H	16	0.11
(1,367)	1:24:A:TYR:HD2	1:34:A:TRP:H	16	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	1:24:A:TYR:HD1	1:33:A:GLN:H	17	0.11
(1,364)	1:24:A:TYR:HD2	1:33:A:GLN:H	17	0.11
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB1	16	0.11
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB2	16	0.11
(1,340)	1:30:A:ASN:H	1:31:A:ALA:HB3	16	0.11
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	12	0.11
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	12	0.11
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	12	0.11
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB1	19	0.11
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB2	19	0.11
(1,338)	1:29:A:THR:H	1:31:A:ALA:HB3	19	0.11
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	10	0.11
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	13	0.11
(1,278)	1:26:A:ASN:HB2	1:30:A:ASN:H	5	0.11
(1,278)	1:26:A:ASN:HB2	1:30:A:ASN:H	17	0.11
(1,265)	1:26:A:ASN:H	1:27:A:HIS:H	5	0.11
(1,265)	1:26:A:ASN:H	1:27:A:HIS:H	7	0.11
(1,262)	1:25:A:PHE:HE1	1:26:A:ASN:HA	20	0.11
(1,262)	1:25:A:PHE:HE2	1:26:A:ASN:HA	20	0.11
(1,242)	1:10:A:GLY:H	1:26:A:ASN:HD21	7	0.11
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB1	13	0.11
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB2	13	0.11
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB3	13	0.11
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	6	0.11
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	8	0.11
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	9	0.11
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	11	0.11
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	15	0.11
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	16	0.11
(1,181)	1:23:A:TYR:HB2	1:34:A:TRP:HE3	19	0.11
(1,180)	1:23:A:TYR:HD1	1:33:A:GLN:HA	12	0.11
(1,180)	1:23:A:TYR:HD2	1:33:A:GLN:HA	12	0.11
(1,165)	1:22:A:VAL:H	1:23:A:TYR:H	2	0.11
(1,165)	1:22:A:VAL:H	1:23:A:TYR:H	3	0.11
(1,130)	1:16:A:SER:H	1:21:A:ARG:HA	14	0.11
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE1	10	0.11
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE2	10	0.11
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE1	19	0.11
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE2	19	0.11
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	9	0.11
(1,104)	1:15:A:MET:H	1:16:A:SER:H	13	0.11
(1,98)	1:14:A:ARG:H	1:24:A:TYR:H	9	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:13:A:LYS:HG2	1:14:A:ARG:H	9	0.11
(1,67)	1:12:A:GLU:HB3	1:27:A:HIS:HD2	13	0.11
(1,61)	1:11:A:TRP:HA	1:12:A:GLU:HB3	17	0.11
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB2	6	0.11
(1,52)	1:11:A:TRP:HE1	1:26:A:ASN:HB3	6	0.11
(1,42)	1:10:A:GLY:H	1:28:A:ILE:HD11	20	0.11
(1,42)	1:10:A:GLY:H	1:28:A:ILE:HD12	20	0.11
(1,42)	1:10:A:GLY:H	1:28:A:ILE:HD13	20	0.11
(1,41)	1:10:A:GLY:H	1:27:A:HIS:HD2	18	0.11
(1,20)	1:7:A:LEU:HD11	1:11:A:TRP:H	14	0.11
(1,20)	1:7:A:LEU:HD12	1:11:A:TRP:H	14	0.11
(1,20)	1:7:A:LEU:HD13	1:11:A:TRP:H	14	0.11
(1,2)	1:2:A:ALA:HA	1:3:A:ASP:H	10	0.11
(4,2764)	1:16:A:SER:H	1:21:A:ARG:O	3	0.1
(4,2764)	1:16:A:SER:H	1:21:A:ARG:O	12	0.1
(4,2656)	2:654:B:SER:H	2:655:B:GLU:H	19	0.1
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG12	1	0.1
(2,92)	1:58:A:SER:H	2:651:B:ILE:HG13	1	0.1
(1,2530)	2:648:B:ILE:HD11	2:649:B:ARG:H	14	0.1
(1,2530)	2:648:B:ILE:HD12	2:649:B:ARG:H	14	0.1
(1,2530)	2:648:B:ILE:HD13	2:649:B:ARG:H	14	0.1
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	1	0.1
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	1	0.1
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE1	6	0.1
(1,2488)	2:656:B:PHE:HA	2:656:B:PHE:HE2	6	0.1
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD11	14	0.1
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD12	14	0.1
(1,2466)	2:651:B:ILE:H	2:651:B:ILE:HD13	14	0.1
(1,2083)	1:106:A:LEU:H	1:106:A:LEU:HG	7	0.1
(1,2083)	1:106:A:LEU:H	1:106:A:LEU:HG	19	0.1
(1,2074)	1:104:A:GLU:H	1:104:A:GLU:HG2	5	0.1
(1,1869)	1:75:A:GLN:H	1:75:A:GLN:HE22	5	0.1
(1,1694)	1:35:A:GLU:H	1:35:A:GLU:HG3	19	0.1
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	6	0.1
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	6	0.1
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD1	8	0.1
(1,1611)	1:25:A:PHE:H	1:25:A:PHE:HD2	8	0.1
(1,1547)	1:15:A:MET:H	1:15:A:MET:HB2	1	0.1
(1,1485)	1:11:A:TRP:HD1	1:11:A:TRP:HE3	13	0.1
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	5	0.1
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	9	0.1
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	13	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1453)	1:5:A:GLU:H	1:5:A:GLU:HA	18	0.1
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG21	13	0.1
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG22	13	0.1
(1,1412)	1:56:A:ARG:HB2	1:162:A:THR:HG23	13	0.1
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD11	7	0.1
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD12	7	0.1
(1,1363)	1:96:A:ILE:HG21	1:160:A:LEU:HD13	7	0.1
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD11	7	0.1
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD12	7	0.1
(1,1363)	1:96:A:ILE:HG22	1:160:A:LEU:HD13	7	0.1
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD11	7	0.1
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD12	7	0.1
(1,1363)	1:96:A:ILE:HG23	1:160:A:LEU:HD13	7	0.1
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG21	14	0.1
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG22	14	0.1
(1,1331)	1:146:A:MET:HG2	1:158:A:ILE:HG23	14	0.1
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG21	12	0.1
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG22	12	0.1
(1,1236)	1:150:A:VAL:HG21	1:152:A:THR:HG23	12	0.1
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG21	12	0.1
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG22	12	0.1
(1,1236)	1:150:A:VAL:HG22	1:152:A:THR:HG23	12	0.1
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG21	12	0.1
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG22	12	0.1
(1,1236)	1:150:A:VAL:HG23	1:152:A:THR:HG23	12	0.1
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG21	17	0.1
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG22	17	0.1
(1,1235)	1:150:A:VAL:H	1:152:A:THR:HG23	17	0.1
(1,1206)	1:145:A:GLU:HB3	1:146:A:MET:HB2	15	0.1
(1,1200)	1:143:A:THR:H	1:144:A:GLY:H	20	0.1
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	4	0.1
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	4	0.1
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB2	9	0.1
(1,1130)	1:131:A:GLN:HE21	1:153:A:ASP:HB3	9	0.1
(1,1089)	1:57:A:CYS:H	1:124:A:ALA:HA	9	0.1
(1,1085)	1:56:A:ARG:HE	1:124:A:ALA:H	15	0.1
(1,1085)	1:56:A:ARG:HE	1:124:A:ALA:H	16	0.1
(1,1047)	1:119:A:ARG:HD2	1:121:A:ASP:H	16	0.1
(1,1036)	1:118:A:ALA:HB1	1:119:A:ARG:H	3	0.1
(1,1036)	1:118:A:ALA:HB2	1:119:A:ARG:H	3	0.1
(1,1036)	1:118:A:ALA:HB3	1:119:A:ARG:H	3	0.1
(1,941)	1:106:A:LEU:HD11	1:107:A:ALA:H	2	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,941)	1:106:A:LEU:HD12	1:107:A:ALA:H	2	0.1
(1,941)	1:106:A:LEU:HD13	1:107:A:ALA:H	2	0.1
(1,843)	1:97:A:LYS:HB2	1:98:A:SER:H	8	0.1
(1,843)	1:97:A:LYS:HB2	1:98:A:SER:H	10	0.1
(1,841)	1:97:A:LYS:HB3	1:98:A:SER:H	11	0.1
(1,805)	1:93:A:ILE:HG21	1:94:A:GLN:H	8	0.1
(1,805)	1:93:A:ILE:HG22	1:94:A:GLN:H	8	0.1
(1,805)	1:93:A:ILE:HG23	1:94:A:GLN:H	8	0.1
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE1	5	0.1
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE2	5	0.1
(1,797)	1:93:A:ILE:H	1:146:A:MET:HE3	5	0.1
(1,702)	1:87:A:GLU:HA	1:90:A:ASN:H	20	0.1
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD11	11	0.1
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD12	11	0.1
(1,681)	1:85:A:ALA:H	1:88:A:LEU:HD13	11	0.1
(1,644)	1:81:A:THR:HA	1:84:A:GLU:H	12	0.1
(1,554)	1:70:A:PRO:HG3	1:71:A:SER:H	18	0.1
(1,538)	1:66:A:GLN:HG2	1:67:A:SER:H	8	0.1
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB1	17	0.1
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB2	17	0.1
(1,455)	1:60:A:LEU:HB2	1:107:A:ALA:HB3	17	0.1
(1,436)	1:58:A:SER:H	1:160:A:LEU:HG	9	0.1
(1,391)	1:35:A:GLU:HB3	1:36:A:ARG:H	4	0.1
(1,354)	1:24:A:TYR:H	1:32:A:SER:HB3	8	0.1
(1,320)	1:25:A:PHE:HE1	1:30:A:ASN:H	1	0.1
(1,320)	1:25:A:PHE:HE2	1:30:A:ASN:H	1	0.1
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	4	0.1
(1,318)	1:29:A:THR:H	1:30:A:ASN:HB3	5	0.1
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	11	0.1
(1,277)	1:26:A:ASN:H	1:30:A:ASN:H	15	0.1
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB1	2	0.1
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB2	2	0.1
(1,236)	1:25:A:PHE:HA	1:31:A:ALA:HB3	2	0.1
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	1	0.1
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	4	0.1
(1,199)	1:23:A:TYR:H	1:24:A:TYR:H	18	0.1
(1,165)	1:22:A:VAL:H	1:23:A:TYR:H	8	0.1
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE1	14	0.1
(1,110)	1:15:A:MET:H	1:23:A:TYR:HE2	14	0.1
(1,108)	1:15:A:MET:H	1:22:A:VAL:HA	8	0.1
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD1	5	0.1
(1,96)	1:14:A:ARG:H	1:23:A:TYR:HD2	5	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:14:A:ARG:H	1:15:A:MET:H	19	0.1
(1,35)	1:9:A:PRO:HG2	1:10:A:GLY:H	3	0.1

10 Dihedral-angle violation analysis

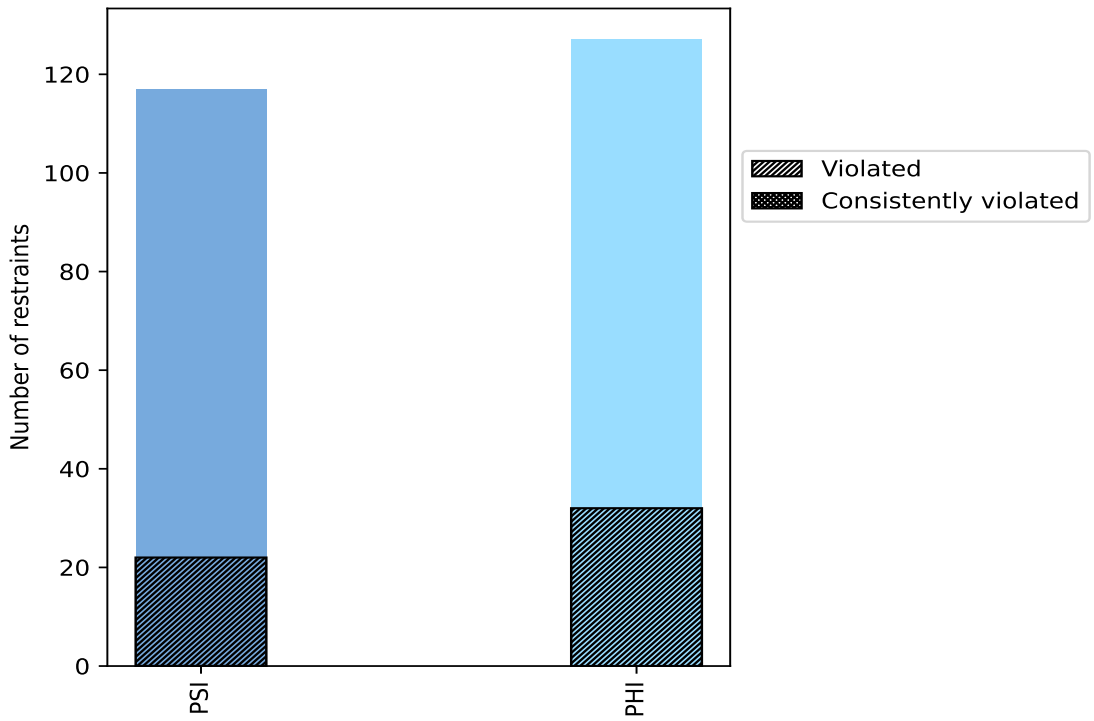
10.1 Summary of dihedral-angle violations

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	117	48.0	22	18.8	9.0	0	0.0	0.0
PHI	127	52.0	32	25.2	13.1	0	0.0	0.0
Total	244	100.0	54	22.1	22.1	0	0.0	0.0

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations



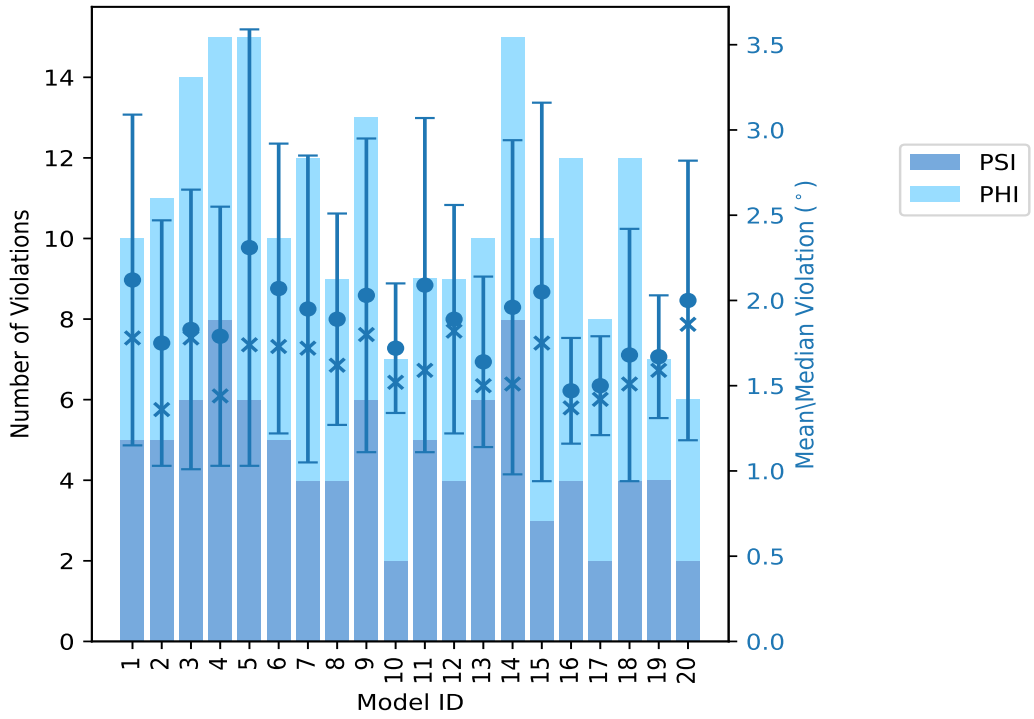
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	5	5	10	2.12	4.52	0.97	1.78
2	5	6	11	1.75	3.45	0.72	1.36
3	6	8	14	1.83	4.56	0.82	1.78
4	8	7	15	1.79	3.34	0.76	1.44
5	6	9	15	2.31	5.69	1.28	1.74
6	5	5	10	2.07	4.2	0.85	1.73
7	4	8	12	1.95	4.06	0.9	1.72
8	4	5	9	1.89	3.18	0.62	1.62
9	6	7	13	2.03	4.38	0.92	1.8
10	2	5	7	1.72	2.3	0.38	1.52
11	5	4	9	2.09	3.26	0.98	1.59
12	4	5	9	1.89	3.44	0.67	1.82
13	6	4	10	1.64	2.44	0.5	1.5
14	8	7	15	1.96	4.09	0.98	1.51
15	3	7	10	2.05	4.89	1.11	1.75
16	4	8	12	1.47	2.1	0.31	1.37
17	2	6	8	1.5	2.2	0.29	1.42
18	4	8	12	1.68	3.69	0.74	1.51
19	4	3	7	1.67	2.3	0.36	1.59
20	2	4	6	2.0	3.59	0.82	1.86

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
12	11	23	1	5.0
1	7	8	2	10.0
0	5	5	3	15.0
3	2	5	4	20.0
1	1	2	5	25.0
0	1	1	6	30.0
1	0	1	7	35.0
0	2	2	8	40.0
0	0	0	9	45.0
1	0	1	10	50.0
0	0	0	11	55.0

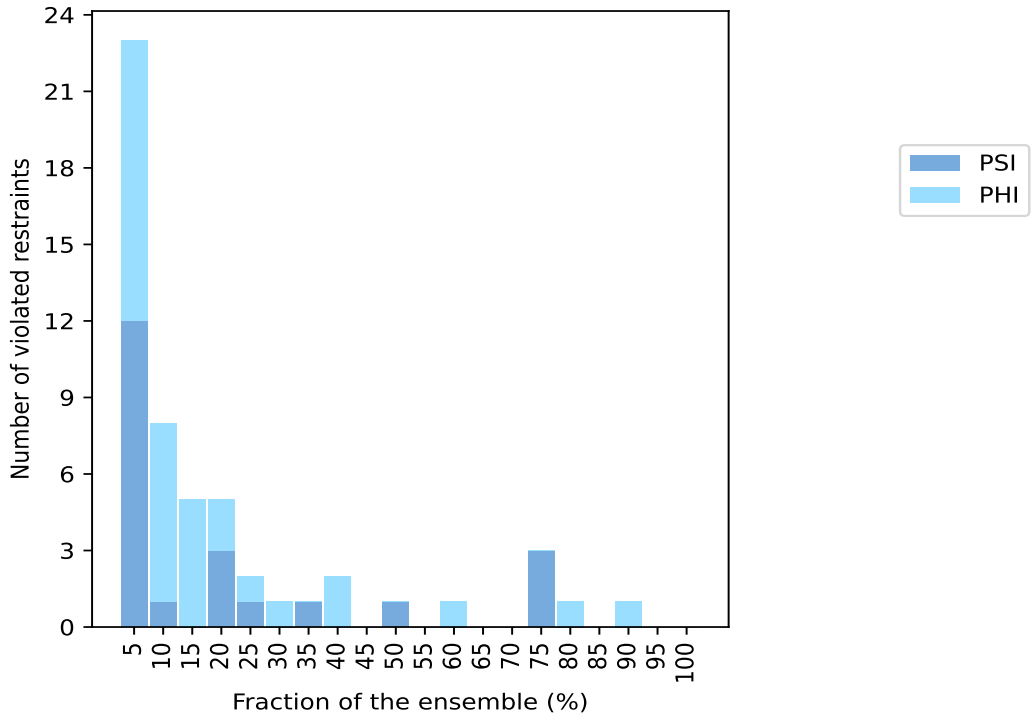
Continued on next page...

Continued from previous page...

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	1	1	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
3	0	3	15	75.0
0	1	1	16	80.0
0	0	0	17	85.0
0	1	1	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

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

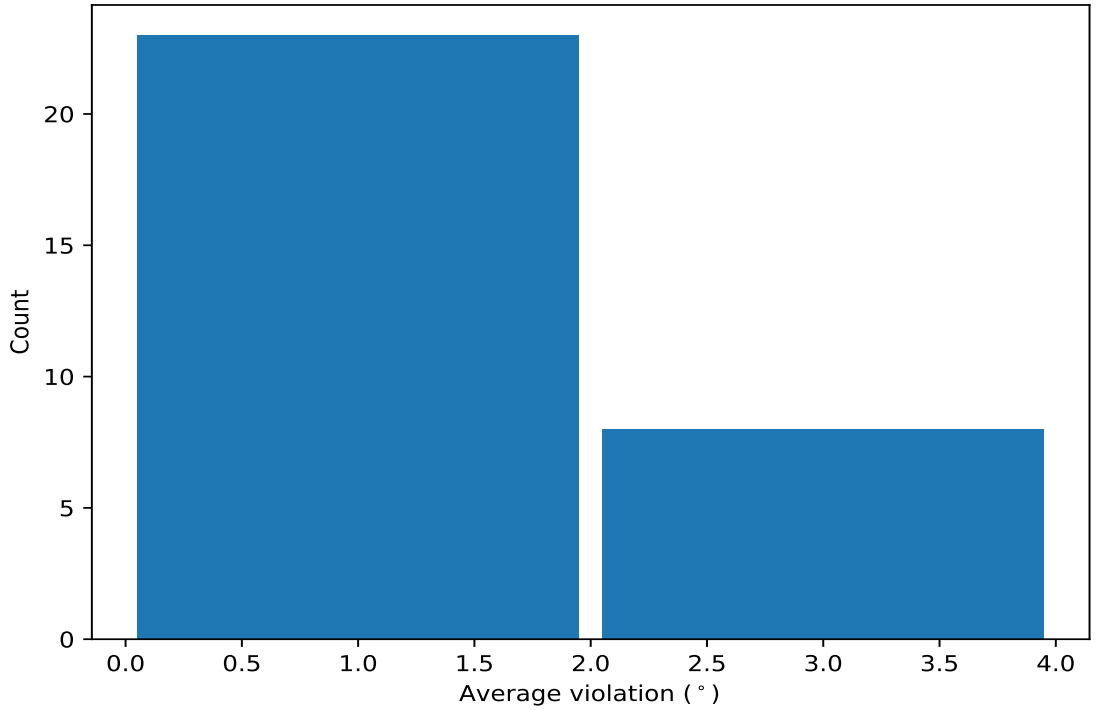


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	18	2.09	0.6	1.92
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	16	1.71	0.39	1.72
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	15	2.55	1.32	1.99
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	15	2.49	1.04	2.13
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	15	1.82	0.5	1.87
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	12	3.36	1.11	3.39
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	10	1.77	0.59	1.82
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	8	1.68	0.44	1.86
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	8	1.64	0.43	1.54
(1,213)	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1:141:A:LEU:N	7	1.44	0.23	1.44
(1,235)	1:156:A:ILE:C	1:157:A:HIS:N	1:157:A:HIS:CA	1:157:A:HIS:C	6	1.85	0.4	1.8
(1,61)	1:42:A:SER:N	1:42:A:SER:CA	1:42:A:SER:C	1:43:A:SER:N	5	2.13	0.7	1.88
(1,110)	1:79:A:THR:C	1:80:A:ARG:N	1:80:A:ARG:CA	1:80:A:ARG:C	5	1.37	0.15	1.29
(1,201)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLU:N	4	2.42	1.03	2.46
(1,205)	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	1:137:A:ALA:N	4	2.03	0.74	1.73
(1,62)	1:42:A:SER:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	4	1.66	0.62	1.46
(1,204)	1:135:A:GLU:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	4	1.35	0.24	1.33
(1,96)	1:65:A:SER:N	1:65:A:SER:CA	1:65:A:SER:C	1:66:A:GLN:N	4	1.28	0.21	1.23
(1,51)	1:34:A:TRP:C	1:35:A:GLU:N	1:35:A:GLU:CA	1:35:A:GLU:C	3	1.53	0.53	1.35
(1,66)	1:46:A:LYS:C	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	3	1.53	0.38	1.47

Continued on next page...

Continued from previous page...

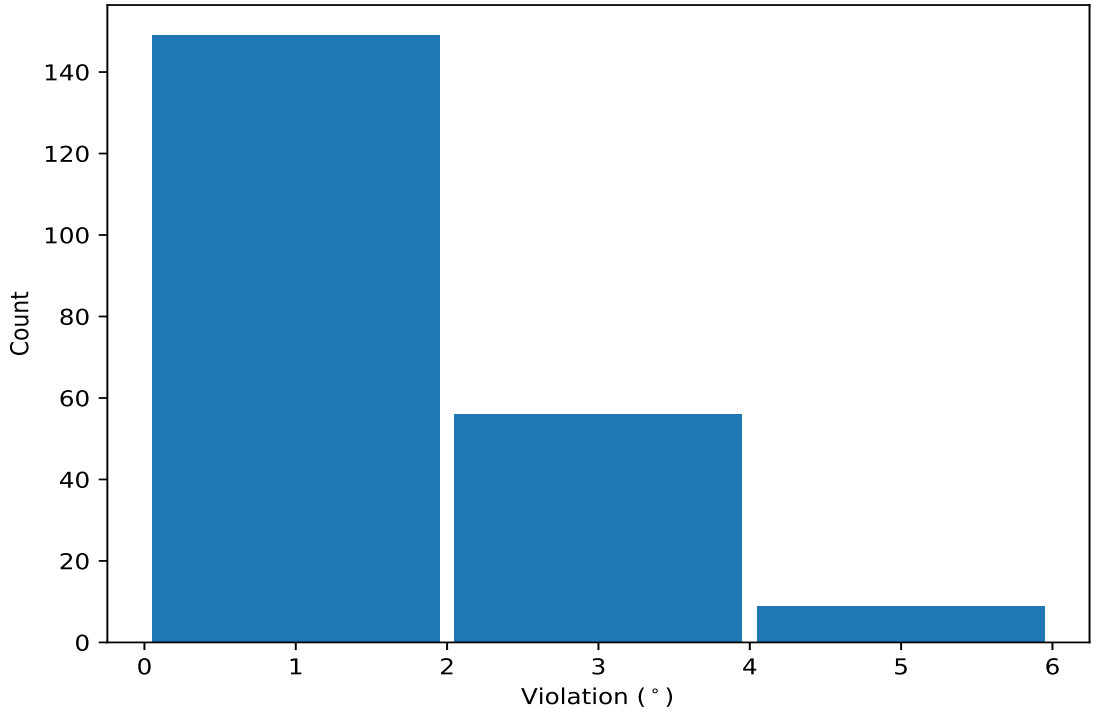
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,168)	1:112:A:ASP:C	1:113:A:CYS:N	1:113:A:CYS:CA	1:113:A:CYS:C	3	1.31	0.14	1.39
(1,210)	1:138:A:SER:C	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	3	1.3	0.19	1.34
(1,10)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	3	1.26	0.12	1.35
(1,108)	1:77:A:LYS:C	1:78:A:ILE:N	1:78:A:ILE:CA	1:78:A:ILE:C	2	2.04	0.78	2.04
(1,1)	1:2:A:ALA:C	1:3:A:ASP:N	1:3:A:ASP:CA	1:3:A:ASP:C	2	1.93	0.13	1.93
(1,69)	1:49:A:GLN:C	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	2	1.56	0.3	1.56
(1,45)	1:31:A:ALA:C	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	2	1.54	0.17	1.54
(1,35)	1:26:A:ASN:C	1:27:A:HIS:N	1:27:A:HIS:CA	1:27:A:HIS:C	2	1.42	0.08	1.42
(1,5)	1:4:A:GLU:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	2	1.42	0.12	1.42
(1,64)	1:44:A:GLY:C	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	2	1.22	0.11	1.22
(1,167)	1:110:A:PHE:N	1:110:A:PHE:CA	1:110:A:PHE:C	1:111:A:SER:N	2	1.19	0.0	1.19

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

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

restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	5	5.69
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	15	4.89
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	3	4.56
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	1	4.52
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	5	4.5
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	9	4.38
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	6	4.2
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	14	4.09
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	7	4.06
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	14	3.97
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	18	3.69
(1,201)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLU:N	20	3.59
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	2	3.45
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	12	3.44
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	4	3.34
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	4	3.26
(1,201)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLU:N	11	3.26
(1,205)	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	1:137:A:ALA:N	11	3.24
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	5	3.23
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	7	3.23
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	8	3.18
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	11	3.16
(1,61)	1:42:A:SER:N	1:42:A:SER:CA	1:42:A:SER:C	1:43:A:SER:N	9	3.14
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	1	3.07
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	11	3.01
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	5	3.0
(1,108)	1:77:A:LYS:C	1:78:A:ILE:N	1:78:A:ILE:CA	1:78:A:ILE:C	15	2.82
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	8	2.8
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	2	2.79
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	9	2.75
(1,61)	1:42:A:SER:N	1:42:A:SER:CA	1:42:A:SER:C	1:43:A:SER:N	14	2.7
(1,62)	1:42:A:SER:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	14	2.69
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	4	2.68
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	15	2.68
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	4	2.64
(1,87)	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	1:61:A:LEU:N	6	2.57
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	14	2.55
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	1	2.54
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	5	2.52
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	9	2.5
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	7	2.47
(1,235)	1:156:A:ILE:C	1:157:A:HIS:N	1:157:A:HIS:CA	1:157:A:HIS:C	6	2.44
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	13	2.44
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	7	2.42
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	5	2.41
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	6	2.41
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	12	2.34
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	19	2.3
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	10	2.3
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	20	2.25
(1,51)	1:34:A:TRP:C	1:35:A:GLU:N	1:35:A:GLU:CA	1:35:A:GLU:C	18	2.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,235)	1:156:A:ILE:C	1:157:A:HIS:N	1:157:A:HIS:CA	1:157:A:HIS:C	13	2.22
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	17	2.2
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	13	2.13
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	9	2.13
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	3	2.12
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	16	2.1
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	2	2.09
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	5	2.09
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	13	2.06
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	18	2.06
(1,1)	1:2:A:ALA:C	1:3:A:ASP:N	1:3:A:ASP:CA	1:3:A:ASP:C	10	2.06
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	10	2.03
(1,66)	1:46:A:LYS:C	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	18	2.02
(1,205)	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	1:137:A:ALA:N	20	2.01
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	19	1.99
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	12	1.98
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	16	1.96
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	3	1.95
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	3	1.95
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1	1.94
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	7	1.91
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	8	1.88
(1,61)	1:42:A:SER:N	1:42:A:SER:CA	1:42:A:SER:C	1:43:A:SER:N	3	1.88
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	4	1.87
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	3	1.86
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	12	1.86
(1,69)	1:49:A:GLN:C	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	9	1.85
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	15	1.84
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	6	1.84
(1,235)	1:156:A:ILE:C	1:157:A:HIS:N	1:157:A:HIS:CA	1:157:A:HIS:C	12	1.82
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	7	1.82
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	15	1.82
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1	1.81
(1,216)	1:141:A:LEU:C	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	18	1.8
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	9	1.8
(1,1)	1:2:A:ALA:C	1:3:A:ASP:N	1:3:A:ASP:CA	1:3:A:ASP:C	19	1.8
(1,213)	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1:141:A:LEU:N	3	1.79
(1,235)	1:156:A:ILE:C	1:157:A:HIS:N	1:157:A:HIS:CA	1:157:A:HIS:C	8	1.78
(1,192)	1:128:A:GLY:C	1:129:A:GLN:N	1:129:A:GLN:CA	1:129:A:GLN:C	3	1.76
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	1	1.75
(1,148)	1:100:A:GLU:C	1:101:A:GLU:N	1:101:A:GLU:CA	1:101:A:GLU:C	2	1.75
(1,61)	1:42:A:SER:N	1:42:A:SER:CA	1:42:A:SER:C	1:43:A:SER:N	5	1.74
(1,45)	1:31:A:ALA:C	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	2	1.71
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	12	1.7
(1,204)	1:135:A:GLU:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	20	1.7
(1,200)	1:133:A:PRO:C	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	12	1.7
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	15	1.68
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	17	1.67
(1,235)	1:156:A:ILE:C	1:157:A:HIS:N	1:157:A:HIS:CA	1:157:A:HIS:C	9	1.65
(1,201)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLU:N	16	1.65
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	16	1.65

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	1	1.64
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	14	1.64
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	6	1.62
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	14	1.62
(1,213)	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1:141:A:LEU:N	8	1.62
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	7	1.61
(1,96)	1:65:A:SER:N	1:65:A:SER:CA	1:65:A:SER:C	1:66:A:GLN:N	6	1.61
(1,213)	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1:141:A:LEU:N	1	1.6
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	11	1.59
(1,110)	1:79:A:THR:C	1:80:A:ARG:N	1:80:A:ARG:CA	1:80:A:ARG:C	13	1.59
(1,58)	1:40:A:ASN:N	1:40:A:ASN:CA	1:40:A:ASN:C	1:41:A:SER:N	19	1.59
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	18	1.56
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	8	1.55
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	8	1.54
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	4	1.54
(1,5)	1:4:A:GLU:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	16	1.54
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	10	1.52
(1,210)	1:138:A:SER:C	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	10	1.51
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	14	1.51
(1,35)	1:26:A:ASN:C	1:27:A:HIS:N	1:27:A:HIS:CA	1:27:A:HIS:C	10	1.51
(1,110)	1:79:A:THR:C	1:80:A:ARG:N	1:80:A:ARG:CA	1:80:A:ARG:C	5	1.5
(1,62)	1:42:A:SER:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	9	1.5
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	4	1.49
(1,66)	1:46:A:LYS:C	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	17	1.47
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	18	1.46
(1,205)	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	1:137:A:ALA:N	19	1.45
(1,213)	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1:141:A:LEU:N	4	1.44
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	9	1.44
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	17	1.44
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	5	1.43
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	20	1.43
(1,168)	1:112:A:ASP:C	1:113:A:CYS:N	1:113:A:CYS:CA	1:113:A:CYS:C	3	1.42
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	8	1.42
(1,205)	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	1:137:A:ALA:N	13	1.41
(1,62)	1:42:A:SER:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	5	1.41
(1,204)	1:135:A:GLU:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	17	1.39
(1,168)	1:112:A:ASP:C	1:113:A:CYS:N	1:113:A:CYS:CA	1:113:A:CYS:C	6	1.39
(1,208)	1:137:A:ALA:C	1:138:A:SER:N	1:138:A:SER:CA	1:138:A:SER:C	5	1.38
(1,45)	1:31:A:ALA:C	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	16	1.38
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	2	1.36
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	16	1.36
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	16	1.36
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	3	1.36
(1,68)	1:49:A:GLN:N	1:49:A:GLN:CA	1:49:A:GLN:C	1:50:A:GLY:N	14	1.36
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1	1.35
(1,51)	1:34:A:TRP:C	1:35:A:GLU:N	1:35:A:GLU:CA	1:35:A:GLU:C	15	1.35
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	7	1.35
(1,10)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	3	1.35
(1,10)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	14	1.35
(1,210)	1:138:A:SER:C	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	14	1.34
(1,35)	1:26:A:ASN:C	1:27:A:HIS:N	1:27:A:HIS:CA	1:27:A:HIS:C	15	1.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,176)	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	1:118:A:ALA:N	4	1.33
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	4	1.33
(1,86)	1:59:A:HIS:C	1:60:A:LEU:N	1:60:A:LEU:CA	1:60:A:LEU:C	11	1.33
(1,64)	1:44:A:GLY:C	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	16	1.33
(1,213)	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1:141:A:LEU:N	5	1.32
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	4	1.31
(1,170)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:SER:N	4	1.31
(1,213)	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1:141:A:LEU:N	6	1.3
(1,5)	1:4:A:GLU:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	2	1.3
(1,110)	1:79:A:THR:C	1:80:A:ARG:N	1:80:A:ARG:CA	1:80:A:ARG:C	6	1.29
(1,228)	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	1:153:A:ASP:N	17	1.28
(1,242)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:ARG:N	19	1.27
(1,204)	1:135:A:GLU:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	2	1.27
(1,126)	1:87:A:GLU:C	1:88:A:LEU:N	1:88:A:LEU:CA	1:88:A:LEU:C	17	1.27
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	19	1.27
(1,96)	1:65:A:SER:N	1:65:A:SER:CA	1:65:A:SER:C	1:66:A:GLN:N	8	1.27
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	16	1.26
(1,108)	1:77:A:LYS:C	1:78:A:ILE:N	1:78:A:ILE:CA	1:78:A:ILE:C	5	1.26
(1,69)	1:49:A:GLN:C	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	17	1.26
(1,110)	1:79:A:THR:C	1:80:A:ARG:N	1:80:A:ARG:CA	1:80:A:ARG:C	2	1.24
(1,227)	1:151:A:PHE:C	1:152:A:THR:N	1:152:A:THR:CA	1:152:A:THR:C	3	1.22
(1,110)	1:79:A:THR:C	1:80:A:ARG:N	1:80:A:ARG:CA	1:80:A:ARG:C	7	1.22
(1,235)	1:156:A:ILE:C	1:157:A:HIS:N	1:157:A:HIS:CA	1:157:A:HIS:C	3	1.21
(1,6)	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	1:6:A:LYS:N	2	1.21
(1,96)	1:65:A:SER:N	1:65:A:SER:CA	1:65:A:SER:C	1:66:A:GLN:N	4	1.2
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	13	1.2
(1,57)	1:39:A:GLY:C	1:40:A:ASN:N	1:40:A:ASN:CA	1:40:A:ASN:C	7	1.2
(1,167)	1:110:A:PHE:N	1:110:A:PHE:CA	1:110:A:PHE:C	1:111:A:SER:N	3	1.19
(1,167)	1:110:A:PHE:N	1:110:A:PHE:CA	1:110:A:PHE:C	1:111:A:SER:N	14	1.19
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	9	1.18
(1,201)	1:134:A:PHE:N	1:134:A:PHE:CA	1:134:A:PHE:C	1:135:A:GLU:N	14	1.18
(1,106)	1:76:A:GLU:C	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	5	1.17
(1,61)	1:42:A:SER:N	1:42:A:SER:CA	1:42:A:SER:C	1:43:A:SER:N	13	1.17
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	18	1.14
(1,91)	1:62:A:VAL:C	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	10	1.14
(1,105)	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:C	1:77:A:LYS:N	13	1.13
(1,168)	1:112:A:ASP:C	1:113:A:CYS:N	1:113:A:CYS:CA	1:113:A:CYS:C	18	1.11
(1,64)	1:44:A:GLY:C	1:45:A:GLY:N	1:45:A:GLY:CA	1:45:A:GLY:C	4	1.11
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	14	1.11
(1,97)	1:66:A:GLN:C	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	12	1.1
(1,66)	1:46:A:LYS:C	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	15	1.1
(1,21)	1:18:A:SER:C	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	11	1.09
(1,10)	1:9:A:PRO:C	1:10:A:GLY:N	1:10:A:GLY:CA	1:10:A:GLY:C	11	1.09
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	9	1.08
(1,210)	1:138:A:SER:C	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	16	1.06
(1,109)	1:78:A:ILE:N	1:78:A:ILE:CA	1:78:A:ILE:C	1:79:A:THR:N	18	1.05
(1,107)	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1:78:A:ILE:N	13	1.05
(1,62)	1:42:A:SER:C	1:43:A:SER:N	1:43:A:SER:CA	1:43:A:SER:C	7	1.05
(1,217)	1:142:A:ARG:N	1:142:A:ARG:CA	1:142:A:ARG:C	1:143:A:THR:N	2	1.04
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	14	1.04
(1,99)	1:68:A:ARG:C	1:69:A:ARG:N	1:69:A:ARG:CA	1:69:A:ARG:C	16	1.04

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,96)	1:65:A:SER:N	1:65:A:SER:CA	1:65:A:SER:C	1:66:A:GLN:N	12	1.04
(1,213)	1:140:A:ALA:N	1:140:A:ALA:CA	1:140:A:ALA:C	1:141:A:LEU:N	9	1.03
(1,204)	1:135:A:GLU:C	1:136:A:ASP:N	1:136:A:ASP:CA	1:136:A:ASP:C	7	1.03
(1,42)	1:30:A:ASN:N	1:30:A:ASN:CA	1:30:A:ASN:C	1:31:A:ALA:N	18	1.03
(1,223)	1:149:A:PRO:C	1:150:A:VAL:N	1:150:A:VAL:CA	1:150:A:VAL:C	15	1.02
(1,211)	1:139:A:PHE:N	1:139:A:PHE:CA	1:139:A:PHE:C	1:140:A:ALA:N	11	1.02
(1,19)	1:16:A:SER:N	1:16:A:SER:CA	1:16:A:SER:C	1:17:A:ARG:N	18	1.01
(1,220)	1:144:A:GLY:C	1:145:A:GLU:N	1:145:A:GLU:CA	1:145:A:GLU:C	20	1.0
(1,51)	1:34:A:TRP:C	1:35:A:GLU:N	1:35:A:GLU:CA	1:35:A:GLU:C	4	1.0
(1,8)	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	1:7:A:LEU:N	1	1.0