



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 09:37 AM UTC

PDB ID : 2JQG / pdb_00002jqg
BMRB ID : 15278
Title : Leader Protease
Authors : Cencic, R.; Mayer, C.; Juliano, M.A.; Juliano, L.; Konrat, R.; Kontaxis, G.; Skern, T.
Deposited on : 2007-06-01

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

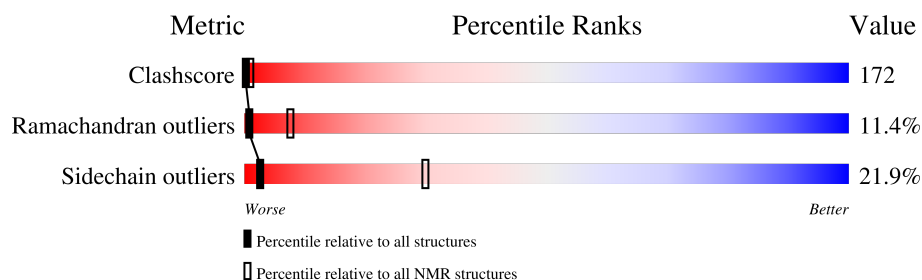
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 34%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	R	167	

2 Ensemble composition and analysis

This entry contains 5 models. Model 2 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	R:29-R:184 (156)	2.22	2

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2
2	3, 5
Single-model clusters	4

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2612 atoms, of which 1266 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms						Trace
1	R	167	Total	C	H	N	O	S	0
			2612	871	1266	214	256	5	

There are 2 discrepancies between the modelled and reference sequences:

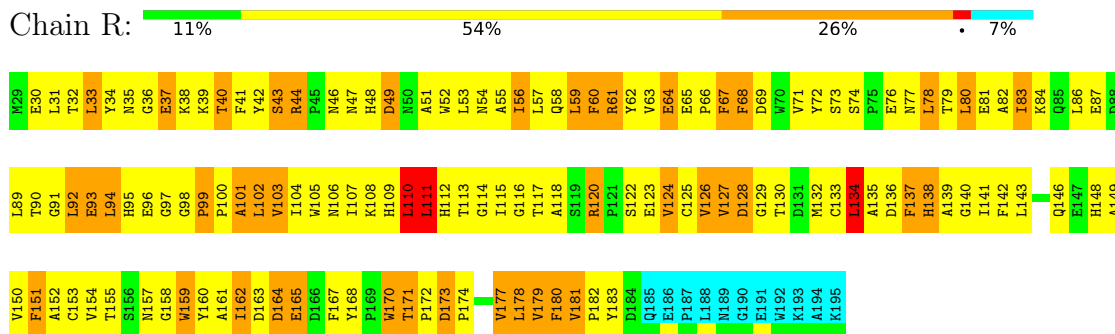
Chain	Residue	Modelled	Actual	Comment	Reference
R	51	ALA	CYS	engineered mutation	UNP P03305
R	126	VAL	MET	engineered mutation	UNP P03305

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Genome polyprotein

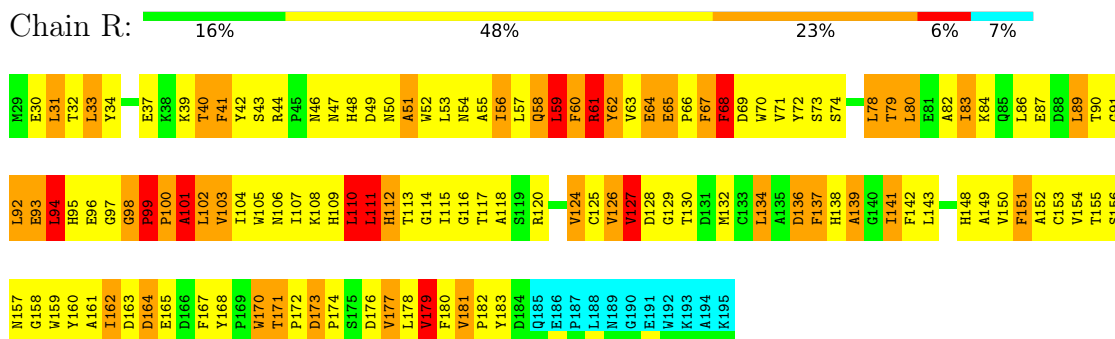


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

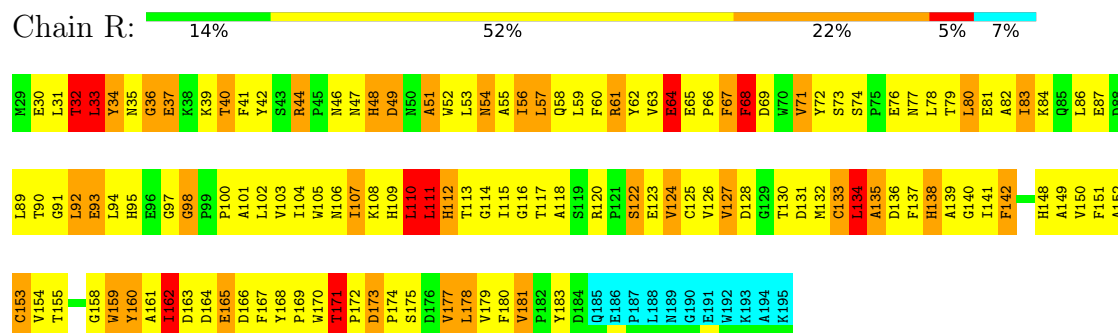
4.2.1 Score per residue for model 1

- Molecule 1: Genome polyprotein



4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Genome polyprotein



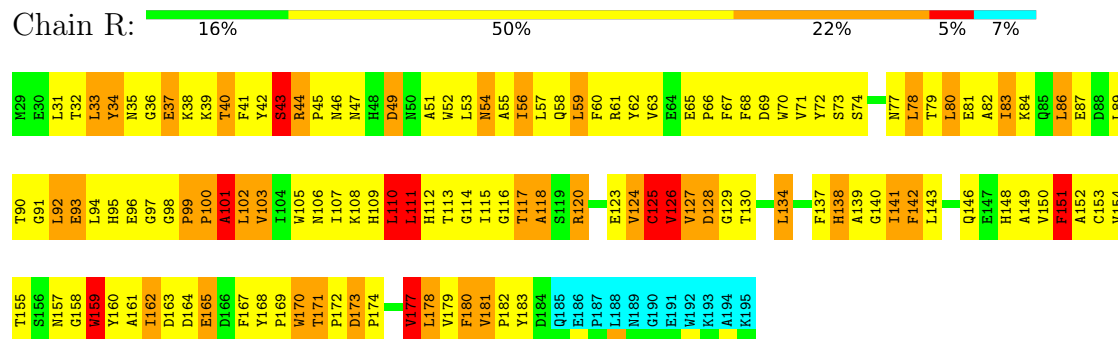
4.2.3 Score per residue for model 3

- Molecule 1: Genome polyprotein



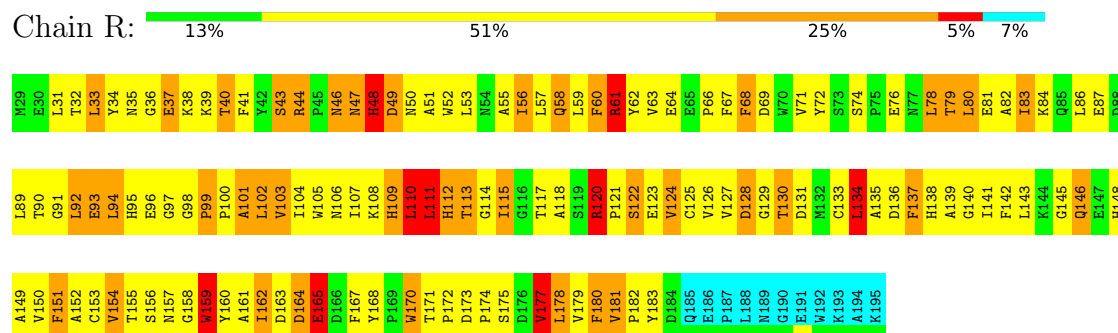
4.2.4 Score per residue for model 4

- Molecule 1: Genome polyprotein



4.2.5 Score per residue for model 5

• Molecule 1: Genome polypeptide



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 5 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	774
Number of shifts mapped to atoms	774
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	34%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	R	1.51±0.01	2±1/1296 (0.1± 0.1%)	1.64±0.02	10±2/1776 (0.5± 0.1%)
All	All	1.51	9/6480 (0.1%)	1.64	48/8880 (0.5%)

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

Mol	Chain	Chirality	Planarity
1	R	0.0±0.0	3.0±0.0
All	All	0	15

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
1	R	33	LEU	N-CA	6.08	1.54	1.46	2	1
1	R	180	PHE	C-N	-5.68	1.26	1.33	3	1
1	R	134	LEU	N-CA	5.39	1.53	1.46	2	1
1	R	101	ALA	C-N	-5.35	1.26	1.33	1	2
1	R	43	SER	N-CA	5.16	1.52	1.46	4	1
1	R	99	PRO	CA-C	5.04	1.56	1.52	1	1
1	R	64	GLU	N-CA	5.03	1.52	1.46	2	1
1	R	165	GLU	N-CA	5.01	1.52	1.46	5	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	R	115	ILE	N-CA-CB	-8.99	97.34	112.44	5	1
1	R	168	TYR	N-CA-CB	-8.69	102.34	111.29	3	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	R	180	PHE	CA-CB-CG	-7.97	105.83	113.80	4	1
1	R	127	VAL	N-CA-CB	-7.46	102.66	112.36	3	3
1	R	110	LEU	N-CA-C	-6.76	105.03	113.55	5	4
1	R	103	VAL	N-CA-C	-6.71	103.77	110.62	5	3
1	R	177	VAL	N-CA-CB	-6.31	104.88	112.07	5	2
1	R	56	ILE	N-CA-CB	-6.30	101.97	110.54	4	1
1	R	118	ALA	N-CA-CB	-6.14	101.08	110.16	4	1
1	R	111	LEU	N-CA-CB	-6.08	101.02	110.57	4	2
1	R	162	ILE	N-CA-CB	-6.00	105.64	111.89	1	3
1	R	171	THR	N-CA-CB	-5.98	99.72	110.37	3	1
1	R	100	PRO	N-CA-C	-5.95	106.11	113.84	1	2
1	R	32	THR	N-CA-C	5.82	118.96	109.24	2	1
1	R	165	GLU	N-CA-CB	-5.65	104.14	112.78	2	1
1	R	68	PHE	CA-CB-CG	-5.62	108.19	113.80	5	2
1	R	51	ALA	N-CA-CB	-5.51	102.00	110.16	1	2
1	R	151	PHE	N-CA-CB	-5.45	101.66	110.71	4	1
1	R	180	PHE	N-CA-CB	-5.37	102.74	111.22	4	1
1	R	67	PHE	N-CA-C	-5.28	106.34	112.89	2	1
1	R	137	PHE	N-CA-CB	-5.27	103.39	111.56	5	1
1	R	151	PHE	CA-CB-CG	-5.25	108.55	113.80	5	2
1	R	138	HIS	N-CA-CB	-5.24	103.62	111.64	4	1
1	R	71	VAL	N-CA-CB	-5.22	104.75	110.65	3	1
1	R	59	LEU	N-CA-C	-5.22	105.67	111.36	1	1
1	R	173	ASP	CA-CB-CG	-5.20	107.40	112.60	4	1
1	R	161	ALA	N-CA-CB	-5.20	102.54	110.85	3	1
1	R	141	ILE	N-CA-CB	-5.17	104.95	111.46	1	1
1	R	86	LEU	N-CA-CB	-5.12	102.60	110.12	4	1
1	R	57	LEU	N-CA-CB	-5.10	102.07	109.82	2	1
1	R	181	VAL	N-CA-CB	-5.05	104.14	111.21	3	1
1	R	168	TYR	N-CA-C	5.04	112.56	108.07	3	1
1	R	48	HIS	N-CA-CB	-5.03	104.78	112.28	1	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	R	44	ARG	Sidechain	5
1	R	61	ARG	Sidechain	5
1	R	120	ARG	Sidechain	5

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	R	1254	1178	1175	417±14
All	All	6270	5890	5875	2084

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 172.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:115:ILE:HG23	1:R:124:VAL:O	1.22	1.28	5	2
1:R:36:GLY:O	1:R:37:GLU:O	1.22	1.56	2	3
1:R:115:ILE:HD12	1:R:124:VAL:HG22	1.15	1.17	2	3
1:R:134:LEU:HD11	1:R:171:THR:HG22	1.11	1.12	1	4
1:R:86:LEU:HD11	1:R:103:VAL:HG13	1.08	1.23	4	4
1:R:152:ALA:HB2	1:R:161:ALA:HB2	1.06	1.26	1	4
1:R:41:PHE:CE2	1:R:162:ILE:HD11	1.06	1.85	3	1
1:R:33:LEU:N	1:R:33:LEU:HD22	1.05	1.67	2	2
1:R:92:LEU:HD13	1:R:94:LEU:HD23	1.04	1.18	2	3
1:R:115:ILE:CG2	1:R:124:VAL:O	1.04	2.04	5	2
1:R:113:THR:HG23	1:R:115:ILE:HD11	1.03	1.26	2	2
1:R:127:VAL:HG21	1:R:177:VAL:O	1.02	1.54	4	2
1:R:31:LEU:HD13	1:R:162:ILE:HG21	1.01	1.26	3	1
1:R:117:THR:HG23	1:R:126:VAL:HG21	1.01	1.28	5	2
1:R:134:LEU:HD11	1:R:171:THR:HG23	1.00	1.26	5	1
1:R:127:VAL:CG2	1:R:178:LEU:HA	0.98	1.88	4	5
1:R:162:ILE:HG22	1:R:167:PHE:HA	0.98	1.34	3	2
1:R:113:THR:CG2	1:R:115:ILE:HD11	0.98	1.87	2	4
1:R:31:LEU:CD1	1:R:162:ILE:HG21	0.98	1.89	4	2
1:R:141:ILE:HG23	1:R:151:PHE:CE1	0.98	1.94	3	2
1:R:134:LEU:CA	1:R:173:ASP:HB2	0.98	1.88	2	1
1:R:134:LEU:HD11	1:R:171:THR:CG2	0.97	1.89	3	5
1:R:83:ILE:HG21	1:R:94:LEU:HD11	0.96	1.36	2	2
1:R:111:LEU:O	1:R:113:THR:N	0.95	2.00	5	3
1:R:142:PHE:CG	1:R:177:VAL:HB	0.95	1.95	3	5
1:R:100:PRO:O	1:R:102:LEU:N	0.95	1.99	5	4
1:R:53:LEU:HD11	1:R:83:ILE:HG12	0.95	1.33	4	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:134:LEU:HA	1:R:173:ASP:HB2	0.94	1.34	2	1
1:R:141:ILE:HG23	1:R:151:PHE:CE2	0.94	1.98	1	1
1:R:33:LEU:HD13	1:R:33:LEU:H	0.94	1.17	2	2
1:R:134:LEU:HD13	1:R:172:PRO:CD	0.93	1.92	2	1
1:R:138:HIS:HB3	1:R:181:VAL:O	0.93	1.62	3	1
1:R:92:LEU:CD1	1:R:94:LEU:HD23	0.93	1.93	2	2
1:R:41:PHE:CZ	1:R:162:ILE:HD11	0.93	1.98	3	1
1:R:142:PHE:CE2	1:R:177:VAL:HG11	0.93	1.99	3	4
1:R:152:ALA:HB1	1:R:160:TYR:O	0.92	1.64	2	2
1:R:31:LEU:HD11	1:R:162:ILE:HD13	0.92	1.39	4	2
1:R:138:HIS:CB	1:R:181:VAL:O	0.92	2.16	3	1
1:R:118:ALA:HB1	1:R:130:THR:HG21	0.91	1.39	1	3
1:R:57:LEU:HG	1:R:71:VAL:HG11	0.91	1.41	5	4
1:R:57:LEU:HD12	1:R:72:TYR:CE1	0.90	2.00	4	1
1:R:118:ALA:HB1	1:R:130:THR:CG2	0.90	1.97	1	3
1:R:115:ILE:HD12	1:R:124:VAL:CG2	0.90	1.97	2	4
1:R:83:ILE:CG2	1:R:94:LEU:HD11	0.90	1.97	4	2
1:R:152:ALA:HA	1:R:161:ALA:HA	0.89	1.42	2	5
1:R:134:LEU:HD13	1:R:172:PRO:HD2	0.89	1.45	2	2
1:R:31:LEU:HD11	1:R:162:ILE:CD1	0.89	1.97	5	3
1:R:31:LEU:HD23	1:R:41:PHE:CD1	0.89	2.02	2	1
1:R:55:ALA:O	1:R:59:LEU:HD23	0.89	1.67	5	1
1:R:52:TRP:CE3	1:R:149:ALA:HB2	0.89	2.03	3	3
1:R:57:LEU:HD12	1:R:72:TYR:CD1	0.88	2.04	4	1
1:R:33:LEU:HD13	1:R:33:LEU:N	0.88	1.82	4	4
1:R:152:ALA:CB	1:R:161:ALA:HB2	0.88	1.97	3	4
1:R:113:THR:HG22	1:R:123:GLU:HA	0.88	1.41	5	1
1:R:115:ILE:HD12	1:R:124:VAL:CA	0.88	1.98	5	1
1:R:126:VAL:CG1	1:R:127:VAL:HG13	0.88	1.99	4	1
1:R:139:ALA:HB3	1:R:181:VAL:CG1	0.87	1.99	4	4
1:R:101:ALA:O	1:R:103:VAL:N	0.87	2.07	3	4
1:R:92:LEU:HD12	1:R:101:ALA:O	0.87	1.69	3	1
1:R:31:LEU:HD22	1:R:167:PHE:CZ	0.87	2.04	4	3
1:R:55:ALA:HB1	1:R:151:PHE:CE1	0.87	2.04	3	1
1:R:141:ILE:O	1:R:177:VAL:HG23	0.86	1.70	3	2
1:R:86:LEU:CD1	1:R:103:VAL:HG13	0.86	2.00	1	4
1:R:115:ILE:HD12	1:R:124:VAL:HA	0.86	1.46	5	1
1:R:113:THR:HG23	1:R:115:ILE:CD1	0.86	2.00	2	2
1:R:174:PRO:HA	1:R:177:VAL:HG13	0.85	1.48	2	2
1:R:86:LEU:HD22	1:R:90:THR:CG2	0.85	2.01	2	1
1:R:168:TYR:HH	1:R:170:TRP:CG	0.85	1.89	3	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:103:VAL:O	1:R:107:ILE:HB	0.85	1.72	3	1
1:R:86:LEU:HD13	1:R:103:VAL:HG13	0.84	1.47	2	1
1:R:92:LEU:HD11	1:R:94:LEU:HD21	0.84	1.46	3	2
1:R:127:VAL:HG23	1:R:178:LEU:HD13	0.84	1.48	3	3
1:R:103:VAL:O	1:R:107:ILE:HG12	0.84	1.73	4	1
1:R:115:ILE:HG23	1:R:124:VAL:CG2	0.84	2.02	3	3
1:R:56:ILE:HG23	1:R:60:PHE:CE2	0.84	2.07	4	1
1:R:134:LEU:CD1	1:R:171:THR:HG23	0.83	2.03	5	1
1:R:86:LEU:HD22	1:R:90:THR:HG23	0.83	1.49	2	1
1:R:53:LEU:CD1	1:R:83:ILE:HG12	0.83	2.03	3	2
1:R:31:LEU:HD13	1:R:162:ILE:CD1	0.83	2.03	1	1
1:R:31:LEU:HD11	1:R:162:ILE:HD11	0.83	1.47	5	1
1:R:86:LEU:C	1:R:86:LEU:HD13	0.83	1.98	5	2
1:R:31:LEU:HD11	1:R:167:PHE:CZ	0.83	2.09	1	1
1:R:57:LEU:HD11	1:R:71:VAL:HB	0.82	1.49	5	4
1:R:33:LEU:O	1:R:34:TYR:C	0.82	2.20	2	2
1:R:57:LEU:CD2	1:R:71:VAL:HG21	0.82	2.04	2	2
1:R:115:ILE:HG13	1:R:123:GLU:C	0.82	1.99	5	1
1:R:115:ILE:HG23	1:R:124:VAL:C	0.82	2.00	5	1
1:R:57:LEU:HD12	1:R:72:TYR:CE2	0.82	2.08	1	1
1:R:127:VAL:CG2	1:R:178:LEU:HD13	0.82	2.04	2	4
1:R:86:LEU:HD12	1:R:94:LEU:HD21	0.82	1.49	4	3
1:R:33:LEU:HA	1:R:37:GLU:CA	0.82	2.05	2	1
1:R:139:ALA:HB3	1:R:181:VAL:HG12	0.82	1.52	4	3
1:R:57:LEU:HD21	1:R:71:VAL:HG21	0.81	1.50	1	5
1:R:32:THR:C	1:R:33:LEU:HD22	0.81	2.00	2	1
1:R:126:VAL:HA	1:R:179:VAL:HA	0.81	1.53	2	2
1:R:126:VAL:HG12	1:R:178:LEU:O	0.81	1.73	4	1
1:R:60:PHE:CE1	1:R:111:LEU:HD21	0.81	2.10	2	1
1:R:113:THR:HG22	1:R:115:ILE:CD1	0.80	2.07	4	1
1:R:55:ALA:O	1:R:59:LEU:HB2	0.80	1.75	1	4
1:R:31:LEU:CD1	1:R:162:ILE:HD13	0.80	2.07	4	2
1:R:115:ILE:HG13	1:R:123:GLU:CA	0.80	2.07	5	1
1:R:113:THR:HG23	1:R:115:ILE:HG12	0.80	1.52	5	1
1:R:63:VAL:HG22	1:R:124:VAL:CG1	0.80	2.06	1	2
1:R:134:LEU:HD21	1:R:171:THR:CG2	0.79	2.07	5	2
1:R:33:LEU:CA	1:R:37:GLU:HA	0.79	2.07	2	1
1:R:33:LEU:HA	1:R:37:GLU:HA	0.79	1.54	2	1
1:R:31:LEU:HD21	1:R:41:PHE:CD1	0.79	2.13	5	3
1:R:62:TYR:CZ	1:R:63:VAL:HG23	0.79	2.13	5	2
1:R:62:TYR:HB3	1:R:181:VAL:HG21	0.79	1.52	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:113:THR:HG23	1:R:115:ILE:CG1	0.79	2.07	5	1
1:R:162:ILE:O	1:R:162:ILE:HG23	0.78	1.75	2	1
1:R:86:LEU:HD12	1:R:94:LEU:CD2	0.78	2.09	5	2
1:R:109:HIS:C	1:R:110:LEU:HD13	0.78	2.04	2	4
1:R:99:PRO:HB2	1:R:100:PRO:CD	0.78	2.09	4	2
1:R:90:THR:OG1	1:R:92:LEU:HD22	0.78	1.79	3	1
1:R:117:THR:HG23	1:R:126:VAL:CG2	0.78	2.06	5	1
1:R:63:VAL:O	1:R:64:GLU:CB	0.78	2.31	1	4
1:R:126:VAL:HG13	1:R:127:VAL:HG13	0.78	1.55	4	1
1:R:162:ILE:HG23	1:R:167:PHE:CE1	0.78	2.14	1	1
1:R:142:PHE:CE1	1:R:177:VAL:HG21	0.77	2.14	3	2
1:R:168:TYR:HH	1:R:170:TRP:CD1	0.77	1.96	3	2
1:R:57:LEU:HD13	1:R:68:PHE:CG	0.77	2.13	4	1
1:R:117:THR:HA	1:R:126:VAL:HG22	0.77	1.53	2	3
1:R:63:VAL:HG22	1:R:124:VAL:HG12	0.77	1.55	1	2
1:R:59:LEU:HD13	1:R:151:PHE:CE2	0.77	2.13	3	1
1:R:171:THR:HG22	1:R:171:THR:O	0.77	1.79	3	1
1:R:71:VAL:HG23	1:R:82:ALA:HB1	0.77	1.55	3	5
1:R:134:LEU:CD1	1:R:171:THR:HG22	0.77	2.08	2	2
1:R:92:LEU:CD1	1:R:94:LEU:HD21	0.77	2.09	3	2
1:R:99:PRO:HG2	1:R:100:PRO:HD2	0.77	1.57	1	2
1:R:53:LEU:HD13	1:R:71:VAL:HG22	0.77	1.56	5	3
1:R:114:GLY:C	1:R:115:ILE:HD13	0.77	2.05	2	3
1:R:86:LEU:HD13	1:R:103:VAL:CG1	0.77	2.08	2	1
1:R:53:LEU:O	1:R:57:LEU:HD23	0.76	1.79	3	4
1:R:142:PHE:CZ	1:R:177:VAL:HG11	0.76	2.15	1	5
1:R:127:VAL:HG22	1:R:178:LEU:C	0.76	2.05	3	2
1:R:138:HIS:HB2	1:R:154:VAL:HG23	0.76	1.54	2	2
1:R:55:ALA:HA	1:R:151:PHE:CD1	0.76	2.16	3	2
1:R:159:TRP:O	1:R:169:PRO:HA	0.76	1.80	2	1
1:R:93:GLU:C	1:R:94:LEU:HD13	0.76	2.05	3	1
1:R:118:ALA:HB1	1:R:130:THR:CB	0.76	2.11	2	1
1:R:159:TRP:CG	1:R:171:THR:O	0.76	2.39	3	1
1:R:92:LEU:HD22	1:R:101:ALA:O	0.75	1.82	5	3
1:R:33:LEU:H	1:R:33:LEU:CD1	0.75	1.91	2	1
1:R:137:PHE:CE1	1:R:180:PHE:HB2	0.75	2.16	2	2
1:R:162:ILE:HG22	1:R:162:ILE:O	0.75	1.81	5	1
1:R:55:ALA:HB2	1:R:151:PHE:CZ	0.75	2.16	1	2
1:R:31:LEU:N	1:R:31:LEU:HD23	0.75	1.96	4	3
1:R:110:LEU:HD13	1:R:110:LEU:N	0.75	1.96	4	5
1:R:53:LEU:HD11	1:R:83:ILE:HG13	0.74	1.58	2	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:118:ALA:HB2	1:R:130:THR:CG2	0.74	2.12	5	1
1:R:152:ALA:CB	1:R:160:TYR:O	0.74	2.35	2	1
1:R:116:GLY:C	1:R:125:CYS:HB3	0.74	2.05	4	1
1:R:60:PHE:CD1	1:R:60:PHE:C	0.74	2.66	1	3
1:R:113:THR:CG2	1:R:123:GLU:HA	0.74	2.12	5	1
1:R:53:LEU:HD13	1:R:71:VAL:CG2	0.74	2.12	5	4
1:R:116:GLY:O	1:R:125:CYS:HB3	0.74	1.83	4	1
1:R:62:TYR:CZ	1:R:139:ALA:HB1	0.73	2.18	3	2
1:R:99:PRO:CG	1:R:100:PRO:HD2	0.73	2.13	1	4
1:R:83:ILE:CG2	1:R:94:LEU:HD13	0.73	2.14	1	2
1:R:89:LEU:HD23	1:R:90:THR:N	0.72	1.98	1	4
1:R:142:PHE:CD1	1:R:177:VAL:HB	0.72	2.19	5	5
1:R:60:PHE:HA	1:R:66:PRO:HD3	0.72	1.60	1	2
1:R:86:LEU:HD13	1:R:90:THR:OG1	0.72	1.84	3	2
1:R:127:VAL:O	1:R:129:GLY:N	0.72	2.23	4	2
1:R:151:PHE:CD1	1:R:151:PHE:C	0.72	2.66	4	1
1:R:53:LEU:HD11	1:R:83:ILE:CG1	0.72	2.14	5	4
1:R:31:LEU:HD11	1:R:162:ILE:HG21	0.72	1.60	4	1
1:R:117:THR:CG2	1:R:126:VAL:HG21	0.72	2.13	5	1
1:R:123:GLU:O	1:R:124:VAL:HG13	0.72	1.84	5	1
1:R:53:LEU:HD12	1:R:79:THR:OG1	0.72	1.85	2	3
1:R:170:TRP:O	1:R:171:THR:HG23	0.72	1.83	2	1
1:R:31:LEU:CD1	1:R:41:PHE:CD1	0.71	2.73	1	1
1:R:55:ALA:HA	1:R:151:PHE:CE2	0.71	2.20	1	1
1:R:59:LEU:HD13	1:R:151:PHE:HE2	0.71	1.45	3	1
1:R:89:LEU:HD12	1:R:89:LEU:H	0.71	1.46	3	1
1:R:142:PHE:CD2	1:R:177:VAL:CG1	0.71	2.73	2	5
1:R:137:PHE:CG	1:R:180:PHE:CD2	0.71	2.78	4	2
1:R:41:PHE:CD2	1:R:151:PHE:CE2	0.71	2.78	4	1
1:R:150:VAL:C	1:R:151:PHE:CD1	0.71	2.68	1	1
1:R:163:ASP:O	1:R:164:ASP:C	0.71	2.34	3	5
1:R:31:LEU:CD2	1:R:41:PHE:CD1	0.71	2.74	2	2
1:R:34:TYR:N	1:R:154:VAL:O	0.71	2.24	3	2
1:R:177:VAL:O	1:R:178:LEU:HD22	0.71	1.85	1	4
1:R:139:ALA:HB2	1:R:153:CYS:SG	0.71	2.25	3	1
1:R:162:ILE:HG22	1:R:167:PHE:CA	0.71	2.15	3	2
1:R:125:CYS:O	1:R:126:VAL:HG23	0.71	1.85	4	1
1:R:57:LEU:HD13	1:R:68:PHE:HD2	0.71	1.45	1	1
1:R:42:TYR:O	1:R:165:GLU:HB3	0.71	1.86	2	1
1:R:31:LEU:HD21	1:R:41:PHE:CE1	0.71	2.19	3	1
1:R:57:LEU:HD21	1:R:71:VAL:CG2	0.71	2.15	2	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:149:ALA:HB1	1:R:151:PHE:HZ	0.71	1.44	5	1
1:R:111:LEU:O	1:R:112:HIS:C	0.71	2.33	1	3
1:R:153:CYS:HB2	1:R:160:TYR:CE2	0.71	2.21	2	1
1:R:51:ALA:C	1:R:149:ALA:HB3	0.70	2.11	2	3
1:R:142:PHE:CE1	1:R:177:VAL:HG11	0.70	2.20	1	2
1:R:152:ALA:HB2	1:R:161:ALA:CB	0.70	2.15	4	5
1:R:33:LEU:N	1:R:33:LEU:CD2	0.70	2.41	2	1
1:R:107:ILE:HG23	1:R:111:LEU:CG	0.70	2.16	3	1
1:R:134:LEU:HD13	1:R:173:ASP:CG	0.70	2.10	4	1
1:R:44:ARG:HA	1:R:164:ASP:HA	0.70	1.63	5	1
1:R:59:LEU:CD2	1:R:141:ILE:HD11	0.70	2.16	2	1
1:R:107:ILE:HG21	1:R:111:LEU:HD23	0.70	1.63	4	1
1:R:164:ASP:O	1:R:165:GLU:CB	0.70	2.40	4	2
1:R:138:HIS:CG	1:R:181:VAL:HG12	0.70	2.21	3	1
1:R:42:TYR:O	1:R:165:GLU:O	0.69	2.09	2	1
1:R:92:LEU:CG	1:R:94:LEU:HD21	0.69	2.16	3	1
1:R:126:VAL:HG13	1:R:127:VAL:H	0.69	1.47	4	1
1:R:56:ILE:HD12	1:R:103:VAL:HG11	0.69	1.64	3	1
1:R:90:THR:HG22	1:R:106:ASN:HB2	0.69	1.62	4	4
1:R:155:THR:OG1	1:R:160:TYR:HB2	0.69	1.88	3	4
1:R:162:ILE:HA	1:R:166:ASP:O	0.69	1.88	2	2
1:R:43:SER:O	1:R:44:ARG:O	0.69	2.10	3	1
1:R:162:ILE:O	1:R:162:ILE:CG2	0.69	2.39	2	2
1:R:41:PHE:CE2	1:R:162:ILE:HD13	0.69	2.22	5	2
1:R:137:PHE:CG	1:R:180:PHE:CD1	0.69	2.80	5	2
1:R:152:ALA:CA	1:R:161:ALA:HA	0.69	2.17	2	2
1:R:51:ALA:HB1	1:R:149:ALA:HB3	0.68	1.66	4	5
1:R:114:GLY:O	1:R:115:ILE:HD13	0.68	1.88	5	3
1:R:142:PHE:CD2	1:R:177:VAL:HG12	0.68	2.23	4	3
1:R:127:VAL:CB	1:R:178:LEU:HD13	0.68	2.19	1	1
1:R:33:LEU:N	1:R:33:LEU:CD1	0.68	2.56	4	3
1:R:142:PHE:CG	1:R:177:VAL:CG1	0.68	2.76	2	2
1:R:126:VAL:C	1:R:179:VAL:HA	0.68	2.13	1	1
1:R:31:LEU:HD21	1:R:162:ILE:HD13	0.68	1.65	4	1
1:R:31:LEU:HD13	1:R:167:PHE:CG	0.68	2.22	4	1
1:R:139:ALA:HA	1:R:152:ALA:O	0.68	1.88	1	5
1:R:41:PHE:CD2	1:R:162:ILE:HD11	0.68	2.24	2	1
1:R:71:VAL:HG23	1:R:82:ALA:CB	0.68	2.18	2	3
1:R:90:THR:HA	1:R:106:ASN:CB	0.68	2.18	2	1
1:R:57:LEU:O	1:R:60:PHE:CD2	0.68	2.47	1	3
1:R:71:VAL:CG2	1:R:82:ALA:HB1	0.68	2.18	1	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:142:PHE:CE2	1:R:177:VAL:CG1	0.68	2.76	3	4
1:R:118:ALA:CB	1:R:130:THR:HG23	0.68	2.19	3	2
1:R:63:VAL:O	1:R:64:GLU:HB2	0.68	1.89	1	2
1:R:31:LEU:HD13	1:R:162:ILE:HD13	0.67	1.66	1	1
1:R:31:LEU:HD22	1:R:162:ILE:HD11	0.67	1.65	1	1
1:R:31:LEU:HD11	1:R:167:PHE:CE2	0.67	2.24	1	1
1:R:41:PHE:CD2	1:R:162:ILE:CD1	0.67	2.76	2	3
1:R:142:PHE:O	1:R:150:VAL:HG22	0.67	1.90	2	5
1:R:59:LEU:HD12	1:R:151:PHE:CE1	0.67	2.25	2	1
1:R:127:VAL:CG2	1:R:177:VAL:O	0.67	2.40	4	1
1:R:127:VAL:HG23	1:R:178:LEU:HA	0.67	1.66	1	1
1:R:161:ALA:HB3	1:R:168:TYR:CE1	0.67	2.24	1	1
1:R:53:LEU:O	1:R:57:LEU:CB	0.67	2.43	2	1
1:R:150:VAL:O	1:R:151:PHE:CD1	0.67	2.48	5	2
1:R:48:HIS:CD2	1:R:79:THR:HG21	0.67	2.25	5	1
1:R:115:ILE:HB	1:R:122:SER:H	0.67	1.49	5	1
1:R:115:ILE:CD1	1:R:124:VAL:HG22	0.66	2.08	2	2
1:R:98:GLY:O	1:R:101:ALA:HB3	0.66	1.89	3	2
1:R:53:LEU:HD22	1:R:57:LEU:HD21	0.66	1.65	4	2
1:R:55:ALA:O	1:R:59:LEU:HD22	0.66	1.91	1	1
1:R:49:ASP:O	1:R:79:THR:HG21	0.66	1.89	4	2
1:R:43:SER:C	1:R:164:ASP:HA	0.66	2.16	3	1
1:R:57:LEU:HD12	1:R:72:TYR:CD2	0.66	2.26	1	1
1:R:56:ILE:HG21	1:R:100:PRO:O	0.66	1.91	2	1
1:R:31:LEU:HB3	1:R:167:PHE:CD2	0.66	2.26	3	1
1:R:115:ILE:CG1	1:R:123:GLU:C	0.66	2.69	5	1
1:R:33:LEU:HD21	1:R:37:GLU:HB3	0.66	1.68	3	2
1:R:63:VAL:HG13	1:R:124:VAL:HG11	0.66	1.67	1	1
1:R:32:THR:HG22	1:R:38:LYS:HB3	0.66	1.68	4	1
1:R:50:ASN:HA	1:R:79:THR:OG1	0.65	1.92	1	1
1:R:134:LEU:HD23	1:R:175:SER:OG	0.65	1.91	2	1
1:R:116:GLY:O	1:R:125:CYS:CB	0.65	2.44	4	1
1:R:44:ARG:N	1:R:165:GLU:CB	0.65	2.59	5	1
1:R:94:LEU:CD2	1:R:103:VAL:HG22	0.65	2.21	5	3
1:R:137:PHE:CE1	1:R:173:ASP:HA	0.65	2.26	2	2
1:R:55:ALA:C	1:R:59:LEU:HD22	0.65	2.17	1	1
1:R:92:LEU:HD12	1:R:93:GLU:N	0.65	2.06	2	3
1:R:138:HIS:CG	1:R:159:TRP:CE3	0.65	2.85	5	1
1:R:142:PHE:HA	1:R:177:VAL:HA	0.65	1.66	4	4
1:R:33:LEU:HA	1:R:37:GLU:N	0.65	2.07	2	1
1:R:31:LEU:HD13	1:R:162:ILE:HD11	0.65	1.69	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:150:VAL:C	1:R:151:PHE:CG	0.65	2.73	5	2
1:R:126:VAL:HG13	1:R:127:VAL:N	0.65	2.05	4	1
1:R:127:VAL:HG21	1:R:178:LEU:HA	0.65	1.66	4	3
1:R:107:ILE:HG23	1:R:111:LEU:CD1	0.65	2.22	3	1
1:R:162:ILE:HG23	1:R:167:PHE:CD1	0.65	2.27	1	1
1:R:93:GLU:C	1:R:94:LEU:HG	0.65	2.11	5	2
1:R:137:PHE:HB2	1:R:183:TYR:CE2	0.65	2.27	3	1
1:R:41:PHE:CD2	1:R:162:ILE:HD13	0.64	2.27	1	2
1:R:68:PHE:CD1	1:R:68:PHE:C	0.64	2.75	4	2
1:R:136:ASP:O	1:R:137:PHE:CD2	0.64	2.50	3	1
1:R:31:LEU:HD21	1:R:162:ILE:CD1	0.64	2.22	4	1
1:R:58:GLN:CD	1:R:162:ILE:HG21	0.64	2.17	2	1
1:R:127:VAL:HG21	1:R:178:LEU:HD13	0.64	1.68	1	1
1:R:124:VAL:O	1:R:125:CYS:HB2	0.64	1.91	4	1
1:R:134:LEU:HD23	1:R:173:ASP:OD2	0.64	1.91	5	1
1:R:160:TYR:CD1	1:R:161:ALA:N	0.64	2.65	2	1
1:R:55:ALA:CB	1:R:151:PHE:CE1	0.64	2.80	5	2
1:R:57:LEU:HD22	1:R:68:PHE:HB2	0.64	1.70	1	1
1:R:141:ILE:HG23	1:R:151:PHE:CZ	0.64	2.27	1	2
1:R:50:ASN:HB3	1:R:79:THR:HG21	0.64	1.68	5	1
1:R:31:LEU:HD12	1:R:41:PHE:CD1	0.64	2.28	1	1
1:R:55:ALA:O	1:R:59:LEU:CD2	0.64	2.45	5	2
1:R:59:LEU:O	1:R:62:TYR:CD1	0.64	2.50	2	2
1:R:31:LEU:HD23	1:R:31:LEU:H	0.64	1.51	4	2
1:R:31:LEU:CG	1:R:162:ILE:HD13	0.64	2.21	4	1
1:R:53:LEU:HD21	1:R:83:ILE:HG13	0.64	1.68	1	2
1:R:53:LEU:CD1	1:R:79:THR:HA	0.64	2.23	2	4
1:R:126:VAL:CG1	1:R:127:VAL:N	0.64	2.61	4	1
1:R:113:THR:HG22	1:R:115:ILE:HD13	0.64	1.70	4	2
1:R:55:ALA:HA	1:R:141:ILE:CG1	0.64	2.23	4	1
1:R:94:LEU:HD23	1:R:103:VAL:HG22	0.64	1.70	5	1
1:R:42:TYR:O	1:R:43:SER:CB	0.63	2.46	4	2
1:R:99:PRO:CB	1:R:100:PRO:CD	0.63	2.76	4	2
1:R:173:ASP:O	1:R:177:VAL:CG1	0.63	2.45	4	3
1:R:31:LEU:HG	1:R:41:PHE:CE1	0.63	2.28	2	1
1:R:134:LEU:O	1:R:173:ASP:OD2	0.63	2.16	4	1
1:R:57:LEU:HD11	1:R:71:VAL:CG1	0.63	2.24	1	2
1:R:55:ALA:HB2	1:R:151:PHE:CE1	0.63	2.29	5	1
1:R:142:PHE:HB2	1:R:150:VAL:HG23	0.63	1.69	2	3
1:R:78:LEU:O	1:R:82:ALA:HB2	0.63	1.94	2	2
1:R:137:PHE:CB	1:R:180:PHE:CE1	0.63	2.82	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:56:ILE:O	1:R:60:PHE:CG	0.63	2.52	4	1
1:R:58:GLN:OE1	1:R:140:GLY:O	0.63	2.17	4	1
1:R:117:THR:HB	1:R:120:ARG:O	0.63	1.93	5	1
1:R:57:LEU:HD11	1:R:71:VAL:CB	0.62	2.24	4	4
1:R:83:ILE:HD13	1:R:95:HIS:HA	0.62	1.71	2	2
1:R:31:LEU:CD2	1:R:162:ILE:HD13	0.62	2.24	4	1
1:R:54:ASN:OD1	1:R:54:ASN:C	0.62	2.41	4	1
1:R:33:LEU:O	1:R:35:ASN:N	0.62	2.31	2	1
1:R:127:VAL:HG22	1:R:178:LEU:HA	0.62	1.71	2	3
1:R:94:LEU:HD13	1:R:94:LEU:N	0.62	2.09	3	1
1:R:86:LEU:CD2	1:R:90:THR:HG23	0.62	2.24	2	1
1:R:107:ILE:CG2	1:R:111:LEU:HD11	0.62	2.24	3	1
1:R:160:TYR:OH	1:R:162:ILE:HD13	0.62	1.94	2	1
1:R:63:VAL:HG11	1:R:113:THR:HG23	0.62	1.71	4	1
1:R:53:LEU:HD11	1:R:79:THR:O	0.62	1.95	1	1
1:R:42:TYR:O	1:R:165:GLU:CB	0.62	2.47	2	1
1:R:137:PHE:CZ	1:R:173:ASP:HA	0.62	2.29	2	1
1:R:138:HIS:HB2	1:R:154:VAL:CG2	0.62	2.24	2	3
1:R:142:PHE:CD1	1:R:142:PHE:N	0.62	2.67	4	3
1:R:118:ALA:CA	1:R:126:VAL:HG22	0.62	2.24	4	1
1:R:107:ILE:HG22	1:R:107:ILE:O	0.62	1.95	1	2
1:R:137:PHE:CE2	1:R:174:PRO:HD3	0.62	2.30	2	2
1:R:83:ILE:HD12	1:R:95:HIS:HA	0.62	1.72	4	1
1:R:115:ILE:CD1	1:R:123:GLU:C	0.62	2.72	5	1
1:R:107:ILE:HG23	1:R:111:LEU:HG	0.62	1.70	3	1
1:R:118:ALA:HB2	1:R:130:THR:OG1	0.62	1.94	3	2
1:R:116:GLY:C	1:R:125:CYS:CB	0.62	2.72	4	1
1:R:126:VAL:CG2	1:R:180:PHE:CD1	0.62	2.82	4	1
1:R:41:PHE:CD1	1:R:41:PHE:N	0.61	2.68	1	4
1:R:90:THR:OG1	1:R:92:LEU:HD11	0.61	1.94	1	4
1:R:53:LEU:O	1:R:57:LEU:HB2	0.61	1.96	5	3
1:R:60:PHE:CG	1:R:61:ARG:N	0.61	2.68	1	2
1:R:59:LEU:HD12	1:R:62:TYR:CZ	0.61	2.30	3	1
1:R:94:LEU:HG	1:R:103:VAL:CG2	0.61	2.25	3	1
1:R:118:ALA:CB	1:R:130:THR:HG21	0.61	2.25	4	1
1:R:139:ALA:HB3	1:R:181:VAL:HB	0.61	1.71	1	3
1:R:33:LEU:HD22	1:R:33:LEU:O	0.61	1.95	5	2
1:R:43:SER:CB	1:R:163:ASP:HA	0.61	2.25	4	1
1:R:124:VAL:O	1:R:125:CYS:CB	0.61	2.48	4	1
1:R:180:PHE:CD1	1:R:180:PHE:C	0.61	2.78	5	2
1:R:31:LEU:CD1	1:R:162:ILE:HD11	0.61	2.24	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:74:SER:OG	1:R:78:LEU:HD22	0.61	1.96	1	1
1:R:57:LEU:HD22	1:R:68:PHE:HB3	0.61	1.71	3	1
1:R:127:VAL:HG22	1:R:178:LEU:O	0.61	1.95	5	2
1:R:142:PHE:O	1:R:150:VAL:CG2	0.61	2.49	3	4
1:R:79:THR:O	1:R:83:ILE:HG12	0.61	1.96	3	2
1:R:136:ASP:O	1:R:183:TYR:CZ	0.61	2.54	2	3
1:R:139:ALA:HB3	1:R:181:VAL:CB	0.61	2.26	1	4
1:R:33:LEU:N	1:R:33:LEU:HD13	0.61	2.00	2	1
1:R:57:LEU:HD12	1:R:72:TYR:CZ	0.61	2.31	1	1
1:R:118:ALA:CB	1:R:130:THR:CG2	0.61	2.78	1	3
1:R:152:ALA:HA	1:R:161:ALA:CA	0.61	2.26	5	3
1:R:31:LEU:HD11	1:R:162:ILE:CG1	0.61	2.24	4	1
1:R:107:ILE:CG2	1:R:111:LEU:HD23	0.60	2.26	4	1
1:R:126:VAL:CG1	1:R:178:LEU:O	0.60	2.48	4	1
1:R:127:VAL:CG2	1:R:178:LEU:CA	0.60	2.78	3	2
1:R:60:PHE:HB2	1:R:66:PRO:HD2	0.60	1.72	3	2
1:R:100:PRO:HA	1:R:104:ILE:HD12	0.60	1.73	5	1
1:R:180:PHE:CD1	1:R:181:VAL:N	0.60	2.70	5	1
1:R:57:LEU:CG	1:R:71:VAL:HG11	0.60	2.23	5	4
1:R:125:CYS:O	1:R:180:PHE:CD1	0.60	2.55	4	3
1:R:41:PHE:CZ	1:R:162:ILE:CD1	0.60	2.82	3	1
1:R:107:ILE:HA	1:R:110:LEU:HD23	0.60	1.74	3	1
1:R:126:VAL:C	1:R:127:VAL:HG22	0.60	2.19	4	1
1:R:51:ALA:CB	1:R:149:ALA:HB3	0.60	2.26	4	5
1:R:90:THR:HG22	1:R:106:ASN:CB	0.60	2.26	4	1
1:R:154:VAL:HG13	1:R:158:GLY:HA2	0.60	1.74	4	1
1:R:86:LEU:C	1:R:86:LEU:CD1	0.60	2.74	5	1
1:R:103:VAL:O	1:R:107:ILE:CG1	0.60	2.48	4	2
1:R:62:TYR:OH	1:R:151:PHE:CD1	0.60	2.55	4	1
1:R:168:TYR:CE2	1:R:170:TRP:CD1	0.60	2.90	5	1
1:R:54:ASN:OD1	1:R:58:GLN:NE2	0.60	2.35	4	2
1:R:63:VAL:HG13	1:R:124:VAL:CG1	0.60	2.26	1	1
1:R:58:GLN:HB2	1:R:151:PHE:CD1	0.60	2.32	4	1
1:R:55:ALA:CB	1:R:151:PHE:CZ	0.60	2.85	1	2
1:R:155:THR:CG2	1:R:160:TYR:HB2	0.60	2.27	5	3
1:R:134:LEU:O	1:R:172:PRO:HG2	0.60	1.97	2	1
1:R:167:PHE:N	1:R:167:PHE:CD1	0.60	2.69	3	2
1:R:53:LEU:HD22	1:R:57:LEU:CD2	0.60	2.26	4	2
1:R:53:LEU:O	1:R:57:LEU:N	0.59	2.35	2	1
1:R:56:ILE:HB	1:R:68:PHE:CE2	0.59	2.32	3	1
1:R:99:PRO:CD	1:R:100:PRO:HD2	0.59	2.27	3	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:113:THR:CG2	1:R:115:ILE:CG1	0.59	2.79	5	1
1:R:31:LEU:HD11	1:R:167:PHE:CB	0.59	2.28	2	1
1:R:183:TYR:N	1:R:183:TYR:CD1	0.59	2.70	3	1
1:R:115:ILE:HG23	1:R:124:VAL:HG21	0.59	1.73	3	1
1:R:151:PHE:CZ	1:R:162:ILE:HG13	0.59	2.32	4	1
1:R:118:ALA:HB2	1:R:128:ASP:HA	0.59	1.74	1	1
1:R:63:VAL:HG21	1:R:124:VAL:CG1	0.59	2.27	2	3
1:R:159:TRP:CD1	1:R:172:PRO:HB3	0.59	2.33	2	1
1:R:99:PRO:HG2	1:R:100:PRO:CD	0.59	2.28	5	2
1:R:137:PHE:CE1	1:R:159:TRP:NE1	0.59	2.70	3	1
1:R:60:PHE:HB2	1:R:68:PHE:CD2	0.59	2.32	4	1
1:R:115:ILE:CG2	1:R:124:VAL:N	0.59	2.66	5	1
1:R:138:HIS:O	1:R:139:ALA:HB2	0.59	1.98	1	2
1:R:33:LEU:CA	1:R:37:GLU:CA	0.59	2.77	2	1
1:R:134:LEU:HD21	1:R:142:PHE:CZ	0.59	2.33	3	1
1:R:99:PRO:CB	1:R:100:PRO:HD2	0.59	2.28	4	1
1:R:31:LEU:HD12	1:R:160:TYR:CZ	0.59	2.33	2	1
1:R:86:LEU:O	1:R:90:THR:N	0.59	2.35	2	1
1:R:104:ILE:HG22	1:R:111:LEU:HD11	0.59	1.74	2	1
1:R:173:ASP:CB	1:R:174:PRO:CD	0.59	2.81	2	1
1:R:33:LEU:CB	1:R:154:VAL:O	0.59	2.50	1	3
1:R:83:ILE:HG22	1:R:94:LEU:HD13	0.59	1.74	5	1
1:R:152:ALA:CB	1:R:161:ALA:CB	0.59	2.76	1	4
1:R:154:VAL:HA	1:R:158:GLY:O	0.59	1.98	2	2
1:R:118:ALA:CA	1:R:130:THR:HG23	0.59	2.26	3	1
1:R:33:LEU:CD1	1:R:37:GLU:O	0.58	2.51	1	1
1:R:60:PHE:CD2	1:R:68:PHE:CD2	0.58	2.90	1	1
1:R:118:ALA:HB3	1:R:130:THR:CB	0.58	2.27	4	1
1:R:67:PHE:O	1:R:69:ASP:N	0.58	2.36	1	1
1:R:69:ASP:O	1:R:73:SER:CB	0.58	2.51	1	3
1:R:107:ILE:HG23	1:R:110:LEU:HD23	0.58	1.75	1	2
1:R:43:SER:HB2	1:R:163:ASP:HA	0.58	1.75	4	1
1:R:104:ILE:HG23	1:R:111:LEU:CD1	0.58	2.27	5	1
1:R:53:LEU:CD1	1:R:82:ALA:HB3	0.58	2.28	3	2
1:R:92:LEU:HD23	1:R:102:LEU:HB2	0.58	1.75	1	1
1:R:142:PHE:CZ	1:R:171:THR:O	0.58	2.56	1	1
1:R:55:ALA:O	1:R:151:PHE:CD2	0.58	2.56	3	1
1:R:115:ILE:HD12	1:R:124:VAL:N	0.58	2.12	5	1
1:R:56:ILE:HG22	1:R:57:LEU:HD22	0.58	1.74	4	1
1:R:55:ALA:HB3	1:R:99:PRO:HB3	0.58	1.75	5	1
1:R:67:PHE:CG	1:R:111:LEU:CD2	0.58	2.87	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:86:LEU:HD13	1:R:86:LEU:O	0.58	1.97	5	1
1:R:142:PHE:CZ	1:R:172:PRO:HA	0.58	2.33	4	3
1:R:57:LEU:CD1	1:R:68:PHE:HB2	0.58	2.28	2	1
1:R:31:LEU:CD1	1:R:162:ILE:CG2	0.58	2.75	4	2
1:R:66:PRO:O	1:R:68:PHE:HD1	0.58	1.82	1	1
1:R:133:CYS:O	1:R:134:LEU:C	0.58	2.47	2	1
1:R:126:VAL:HG22	1:R:179:VAL:HA	0.58	1.76	5	1
1:R:162:ILE:HG13	1:R:167:PHE:CD1	0.58	2.34	5	1
1:R:56:ILE:O	1:R:60:PHE:HB3	0.58	1.98	5	2
1:R:107:ILE:O	1:R:111:LEU:N	0.58	2.37	4	2
1:R:134:LEU:HD13	1:R:172:PRO:HD3	0.58	1.72	2	1
1:R:62:TYR:CE1	1:R:181:VAL:HG21	0.58	2.34	3	1
1:R:79:THR:O	1:R:83:ILE:CG1	0.58	2.52	3	2
1:R:126:VAL:HG12	1:R:179:VAL:HB	0.58	1.75	3	1
1:R:170:TRP:CE3	1:R:170:TRP:HA	0.58	2.33	3	1
1:R:52:TRP:CD2	1:R:97:GLY:HA2	0.58	2.33	4	1
1:R:134:LEU:HD22	1:R:173:ASP:CB	0.58	2.28	4	1
1:R:94:LEU:O	1:R:95:HIS:C	0.58	2.46	5	5
1:R:141:ILE:HB	1:R:179:VAL:CG1	0.58	2.29	1	2
1:R:141:ILE:O	1:R:177:VAL:CG2	0.58	2.49	3	2
1:R:83:ILE:CB	1:R:94:LEU:HD13	0.58	2.29	1	2
1:R:31:LEU:HD13	1:R:162:ILE:CG2	0.58	2.18	3	1
1:R:59:LEU:HD12	1:R:62:TYR:OH	0.58	1.99	3	1
1:R:31:LEU:HD11	1:R:162:ILE:CG2	0.58	2.27	4	1
1:R:44:ARG:CB	1:R:164:ASP:O	0.58	2.52	4	1
1:R:94:LEU:HD12	1:R:94:LEU:O	0.58	1.99	4	1
1:R:151:PHE:CD2	1:R:162:ILE:O	0.58	2.57	4	1
1:R:149:ALA:HB1	1:R:151:PHE:CZ	0.58	2.30	5	1
1:R:89:LEU:CD2	1:R:107:ILE:HG23	0.57	2.29	2	1
1:R:134:LEU:HD13	1:R:173:ASP:OD2	0.57	1.98	4	1
1:R:124:VAL:HB	1:R:180:PHE:O	0.57	1.99	5	1
1:R:51:ALA:HB1	1:R:149:ALA:O	0.57	1.99	1	1
1:R:69:ASP:O	1:R:73:SER:HB3	0.57	1.99	2	2
1:R:92:LEU:HD13	1:R:94:LEU:CD2	0.57	2.29	1	1
1:R:83:ILE:HG21	1:R:94:LEU:CD1	0.57	2.20	2	2
1:R:52:TRP:CG	1:R:97:GLY:HA2	0.57	2.35	1	2
1:R:137:PHE:CD1	1:R:137:PHE:C	0.57	2.82	2	3
1:R:68:PHE:CE1	1:R:72:TYR:CD2	0.57	2.92	4	1
1:R:86:LEU:CG	1:R:103:VAL:HG13	0.57	2.28	1	2
1:R:68:PHE:CD1	1:R:68:PHE:N	0.57	2.71	3	2
1:R:142:PHE:CA	1:R:177:VAL:HB	0.57	2.28	2	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:51:ALA:HA	1:R:54:ASN:HB3	0.57	1.75	2	2
1:R:107:ILE:HG23	1:R:111:LEU:HD11	0.57	1.74	3	1
1:R:141:ILE:HG12	1:R:151:PHE:CZ	0.57	2.34	3	1
1:R:151:PHE:CE2	1:R:162:ILE:HG13	0.57	2.34	4	1
1:R:53:LEU:HD12	1:R:79:THR:CA	0.57	2.29	2	2
1:R:127:VAL:HG22	1:R:178:LEU:CA	0.57	2.29	3	3
1:R:64:GLU:O	1:R:66:PRO:HD3	0.57	2.00	3	2
1:R:142:PHE:CG	1:R:177:VAL:CB	0.57	2.81	3	4
1:R:152:ALA:CA	1:R:160:TYR:O	0.57	2.53	2	1
1:R:142:PHE:CD2	1:R:177:VAL:HG11	0.57	2.35	2	2
1:R:134:LEU:HD21	1:R:171:THR:HG23	0.57	1.76	3	1
1:R:53:LEU:HD22	1:R:71:VAL:HG21	0.57	1.76	3	4
1:R:33:LEU:HD23	1:R:35:ASN:OD1	0.57	1.99	3	1
1:R:31:LEU:HD21	1:R:167:PHE:CG	0.57	2.34	1	1
1:R:33:LEU:CD2	1:R:36:GLY:C	0.57	2.78	4	2
1:R:40:THR:O	1:R:72:TYR:CD1	0.57	2.58	4	1
1:R:32:THR:C	1:R:33:LEU:HD13	0.56	2.25	4	3
1:R:112:HIS:HA	1:R:122:SER:O	0.56	2.00	5	1
1:R:141:ILE:HD12	1:R:179:VAL:HG11	0.56	1.76	2	3
1:R:170:TRP:O	1:R:171:THR:CG2	0.56	2.52	2	1
1:R:57:LEU:HG	1:R:71:VAL:CG1	0.56	2.24	5	2
1:R:137:PHE:CE1	1:R:159:TRP:CD1	0.56	2.93	3	1
1:R:43:SER:N	1:R:164:ASP:HB2	0.56	2.15	4	1
1:R:57:LEU:CD2	1:R:57:LEU:N	0.56	2.68	4	1
1:R:33:LEU:CA	1:R:154:VAL:O	0.56	2.53	5	1
1:R:107:ILE:CG2	1:R:110:LEU:HB2	0.56	2.30	1	2
1:R:118:ALA:HA	1:R:130:THR:HG23	0.56	1.77	3	1
1:R:101:ALA:C	1:R:103:VAL:N	0.56	2.63	5	4
1:R:141:ILE:O	1:R:177:VAL:CB	0.56	2.53	2	2
1:R:171:THR:CG2	1:R:171:THR:O	0.56	2.52	3	1
1:R:164:ASP:O	1:R:165:GLU:HB2	0.56	2.01	4	1
1:R:53:LEU:HD21	1:R:83:ILE:CG1	0.56	2.30	1	3
1:R:92:LEU:HD23	1:R:92:LEU:C	0.56	2.23	3	1
1:R:102:LEU:HA	1:R:105:TRP:HB3	0.56	1.77	3	1
1:R:118:ALA:CB	1:R:130:THR:CB	0.56	2.84	4	2
1:R:139:ALA:HB1	1:R:153:CYS:SG	0.56	2.41	2	1
1:R:31:LEU:N	1:R:31:LEU:CD2	0.56	2.68	4	1
1:R:134:LEU:N	1:R:173:ASP:CB	0.56	2.69	2	1
1:R:57:LEU:HD13	1:R:60:PHE:CD2	0.56	2.35	3	1
1:R:42:TYR:HA	1:R:164:ASP:HB2	0.56	1.77	4	1
1:R:71:VAL:CG2	1:R:82:ALA:CB	0.56	2.84	3	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:102:LEU:O	1:R:103:VAL:C	0.55	2.46	1	3
1:R:31:LEU:N	1:R:31:LEU:HD22	0.55	2.16	2	1
1:R:83:ILE:CG2	1:R:94:LEU:HD21	0.55	2.30	2	1
1:R:126:VAL:N	1:R:179:VAL:HA	0.55	2.16	4	1
1:R:107:ILE:HG22	1:R:110:LEU:HB2	0.55	1.78	1	2
1:R:118:ALA:CB	1:R:130:THR:HB	0.55	2.31	4	1
1:R:31:LEU:HD13	1:R:41:PHE:CD1	0.55	2.35	1	1
1:R:31:LEU:HD21	1:R:167:PHE:CD2	0.55	2.36	1	1
1:R:55:ALA:O	1:R:59:LEU:CB	0.55	2.53	1	2
1:R:103:VAL:HG12	1:R:107:ILE:HD11	0.55	1.77	4	2
1:R:102:LEU:N	1:R:102:LEU:HD12	0.55	2.17	3	1
1:R:137:PHE:CG	1:R:180:PHE:HD2	0.55	2.19	4	1
1:R:86:LEU:HD11	1:R:90:THR:CG2	0.55	2.31	5	1
1:R:134:LEU:HD21	1:R:171:THR:HB	0.55	1.77	1	2
1:R:137:PHE:CZ	1:R:174:PRO:CD	0.55	2.89	4	2
1:R:155:THR:CG2	1:R:160:TYR:HB3	0.55	2.31	2	1
1:R:118:ALA:HB1	1:R:130:THR:HG23	0.55	1.76	3	1
1:R:43:SER:CA	1:R:165:GLU:HB2	0.55	2.31	5	1
1:R:32:THR:O	1:R:156:SER:N	0.55	2.39	1	2
1:R:137:PHE:CB	1:R:180:PHE:CD1	0.55	2.90	1	2
1:R:59:LEU:HD22	1:R:141:ILE:HD11	0.55	1.78	2	1
1:R:142:PHE:HA	1:R:177:VAL:HB	0.55	1.77	2	3
1:R:138:HIS:CG	1:R:154:VAL:HG21	0.55	2.37	1	1
1:R:163:ASP:O	1:R:165:GLU:N	0.55	2.39	3	2
1:R:138:HIS:CB	1:R:154:VAL:HG23	0.55	2.32	5	2
1:R:137:PHE:HA	1:R:183:TYR:CD2	0.55	2.37	4	1
1:R:57:LEU:N	1:R:57:LEU:CD2	0.55	2.69	1	1
1:R:142:PHE:HA	1:R:177:VAL:CA	0.55	2.32	4	3
1:R:58:GLN:CD	1:R:162:ILE:CG2	0.55	2.79	2	1
1:R:94:LEU:HB2	1:R:97:GLY:O	0.55	2.02	2	2
1:R:99:PRO:HG2	1:R:100:PRO:HD3	0.55	1.77	5	2
1:R:60:PHE:CD2	1:R:68:PHE:CE2	0.55	2.95	1	1
1:R:89:LEU:HD12	1:R:89:LEU:N	0.55	2.14	3	1
1:R:92:LEU:CD2	1:R:92:LEU:H	0.55	2.15	3	1
1:R:87:GLU:O	1:R:91:GLY:N	0.54	2.39	1	3
1:R:62:TYR:CD2	1:R:153:CYS:SG	0.54	3.00	2	2
1:R:137:PHE:O	1:R:172:PRO:HB2	0.54	2.03	2	1
1:R:141:ILE:O	1:R:177:VAL:HB	0.54	2.02	2	2
1:R:142:PHE:N	1:R:142:PHE:HD1	0.54	1.98	4	2
1:R:161:ALA:O	1:R:168:TYR:CD1	0.54	2.60	2	3
1:R:138:HIS:CG	1:R:181:VAL:O	0.54	2.60	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:83:ILE:HG22	1:R:94:LEU:HD11	0.54	1.77	4	1
1:R:123:GLU:O	1:R:124:VAL:CG1	0.54	2.55	5	1
1:R:126:VAL:HG12	1:R:128:ASP:H	0.54	1.63	5	1
1:R:102:LEU:HA	1:R:105:TRP:CB	0.54	2.32	1	4
1:R:125:CYS:O	1:R:180:PHE:O	0.54	2.25	2	2
1:R:138:HIS:HA	1:R:172:PRO:CG	0.54	2.32	5	1
1:R:63:VAL:HG13	1:R:113:THR:HG21	0.54	1.79	1	2
1:R:115:ILE:HD13	1:R:115:ILE:N	0.54	2.16	4	3
1:R:92:LEU:HD12	1:R:93:GLU:H	0.54	1.63	4	2
1:R:127:VAL:HG11	1:R:174:PRO:HB3	0.54	1.78	2	1
1:R:153:CYS:N	1:R:160:TYR:O	0.54	2.40	2	1
1:R:120:ARG:CB	1:R:121:PRO:CD	0.54	2.85	5	1
1:R:33:LEU:HD22	1:R:33:LEU:H	0.54	1.62	1	3
1:R:56:ILE:HD13	1:R:56:ILE:N	0.54	2.17	1	1
1:R:101:ALA:O	1:R:104:ILE:HG12	0.54	2.03	2	1
1:R:115:ILE:HG23	1:R:124:VAL:HG23	0.54	1.79	2	1
1:R:55:ALA:CA	1:R:141:ILE:HD11	0.54	2.33	4	1
1:R:31:LEU:HD21	1:R:41:PHE:CG	0.54	2.37	5	1
1:R:31:LEU:HD21	1:R:162:ILE:HD11	0.54	1.80	5	1
1:R:86:LEU:HD12	1:R:94:LEU:HD22	0.54	1.80	5	1
1:R:101:ALA:C	1:R:103:VAL:H	0.54	2.11	5	4
1:R:109:HIS:CD2	1:R:110:LEU:HD22	0.54	2.38	1	1
1:R:53:LEU:HD22	1:R:57:LEU:HD23	0.54	1.79	2	1
1:R:60:PHE:CE2	1:R:67:PHE:HB3	0.54	2.38	2	2
1:R:35:ASN:O	1:R:62:TYR:HA	0.54	2.02	4	1
1:R:126:VAL:O	1:R:128:ASP:N	0.54	2.41	4	1
1:R:123:GLU:C	1:R:124:VAL:HG13	0.54	2.27	5	1
1:R:89:LEU:HD23	1:R:89:LEU:C	0.54	2.27	4	4
1:R:138:HIS:CG	1:R:154:VAL:CG2	0.54	2.91	2	2
1:R:31:LEU:CD2	1:R:31:LEU:N	0.54	2.70	2	1
1:R:31:LEU:HD12	1:R:160:TYR:CE2	0.54	2.37	2	1
1:R:71:VAL:HG12	1:R:72:TYR:CD1	0.54	2.38	2	1
1:R:160:TYR:CD1	1:R:160:TYR:C	0.54	2.86	2	1
1:R:180:PHE:CD2	1:R:181:VAL:N	0.54	2.75	4	1
1:R:128:ASP:C	1:R:130:THR:N	0.54	2.64	1	1
1:R:40:THR:HG22	1:R:40:THR:O	0.54	2.02	2	2
1:R:54:ASN:HA	1:R:58:GLN:CD	0.54	2.28	2	1
1:R:128:ASP:HB2	1:R:178:LEU:HD12	0.54	1.80	3	1
1:R:155:THR:HG21	1:R:160:TYR:HB3	0.54	1.79	4	2
1:R:90:THR:OG1	1:R:92:LEU:CD1	0.54	2.56	1	3
1:R:160:TYR:HA	1:R:168:TYR:O	0.54	2.02	5	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:141:ILE:C	1:R:177:VAL:HG23	0.54	2.28	3	1
1:R:134:LEU:HD22	1:R:173:ASP:HB2	0.54	1.80	4	1
1:R:55:ALA:CA	1:R:151:PHE:CD1	0.54	2.91	3	1
1:R:67:PHE:CE1	1:R:89:LEU:HD21	0.54	2.38	3	1
1:R:85:GLN:O	1:R:88:ASP:HB2	0.54	2.03	3	1
1:R:116:GLY:H	1:R:125:CYS:HB2	0.54	1.62	4	1
1:R:124:VAL:O	1:R:124:VAL:CG2	0.54	2.56	4	1
1:R:137:PHE:CZ	1:R:174:PRO:N	0.54	2.76	4	1
1:R:161:ALA:CB	1:R:170:TRP:CD1	0.53	2.91	3	1
1:R:51:ALA:O	1:R:54:ASN:HB3	0.53	2.03	1	1
1:R:115:ILE:HG23	1:R:124:VAL:HG22	0.53	1.80	2	1
1:R:92:LEU:HD11	1:R:103:VAL:CG2	0.53	2.33	3	1
1:R:134:LEU:HD21	1:R:142:PHE:HZ	0.53	1.63	3	1
1:R:31:LEU:HD11	1:R:162:ILE:CB	0.53	2.33	4	1
1:R:59:LEU:HD13	1:R:62:TYR:CE1	0.53	2.38	5	1
1:R:33:LEU:HB2	1:R:154:VAL:O	0.53	2.03	1	3
1:R:58:GLN:OE1	1:R:162:ILE:CG2	0.53	2.56	2	1
1:R:40:THR:O	1:R:40:THR:CG2	0.53	2.57	3	1
1:R:107:ILE:HG12	1:R:111:LEU:HD21	0.53	1.80	3	1
1:R:125:CYS:O	1:R:180:PHE:HD1	0.53	1.85	4	1
1:R:117:THR:HA	1:R:126:VAL:HB	0.53	1.80	5	1
1:R:53:LEU:HG	1:R:83:ILE:HG12	0.53	1.81	2	3
1:R:99:PRO:CG	1:R:100:PRO:CD	0.53	2.86	3	3
1:R:128:ASP:C	1:R:130:THR:H	0.53	2.11	1	1
1:R:153:CYS:O	1:R:160:TYR:CD2	0.53	2.61	2	1
1:R:118:ALA:HB3	1:R:128:ASP:O	0.53	2.04	1	1
1:R:138:HIS:CD2	1:R:183:TYR:CD2	0.53	2.97	1	1
1:R:134:LEU:N	1:R:173:ASP:HB2	0.53	2.18	2	1
1:R:162:ILE:CG2	1:R:167:PHE:CD1	0.53	2.92	3	1
1:R:137:PHE:CD1	1:R:180:PHE:CD1	0.53	2.96	5	1
1:R:41:PHE:N	1:R:41:PHE:CD1	0.53	2.77	3	1
1:R:142:PHE:CE2	1:R:172:PRO:HA	0.53	2.39	5	2
1:R:62:TYR:CE2	1:R:181:VAL:HG21	0.53	2.38	5	1
1:R:58:GLN:O	1:R:62:TYR:CE2	0.53	2.62	3	2
1:R:89:LEU:CD2	1:R:90:THR:HG23	0.53	2.33	4	3
1:R:36:GLY:O	1:R:37:GLU:C	0.53	2.42	2	2
1:R:48:HIS:O	1:R:49:ASP:CB	0.53	2.55	2	1
1:R:53:LEU:CG	1:R:83:ILE:HG12	0.53	2.34	2	2
1:R:59:LEU:HA	1:R:62:TYR:CE1	0.53	2.38	2	2
1:R:127:VAL:HG22	1:R:178:LEU:HD13	0.53	1.80	2	1
1:R:65:GLU:HB2	1:R:68:PHE:CE1	0.53	2.39	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:67:PHE:CE2	1:R:70:TRP:CD1	0.53	2.97	1	1
1:R:83:ILE:O	1:R:86:LEU:N	0.53	2.41	2	5
1:R:154:VAL:CG2	1:R:159:TRP:CD1	0.53	2.92	1	1
1:R:86:LEU:HD13	1:R:90:THR:HG1	0.53	1.63	3	1
1:R:113:THR:CG2	1:R:115:ILE:CD1	0.53	2.83	4	2
1:R:52:TRP:O	1:R:55:ALA:HB3	0.53	2.04	5	5
1:R:109:HIS:CD2	1:R:110:LEU:CD2	0.53	2.92	1	1
1:R:168:TYR:CD1	1:R:170:TRP:CD1	0.53	2.97	1	1
1:R:151:PHE:O	1:R:162:ILE:N	0.53	2.41	2	1
1:R:77:ASN:O	1:R:78:LEU:CB	0.53	2.56	3	1
1:R:123:GLU:C	1:R:124:VAL:CG1	0.53	2.82	4	1
1:R:55:ALA:C	1:R:59:LEU:HD23	0.53	2.27	5	1
1:R:138:HIS:HB3	1:R:172:PRO:HB3	0.52	1.80	2	1
1:R:159:TRP:CD1	1:R:159:TRP:N	0.52	2.75	2	1
1:R:43:SER:O	1:R:164:ASP:CA	0.52	2.57	3	1
1:R:86:LEU:HD11	1:R:90:THR:HG21	0.52	1.79	5	1
1:R:62:TYR:N	1:R:62:TYR:CD1	0.52	2.75	1	1
1:R:31:LEU:CD1	1:R:160:TYR:CZ	0.52	2.92	2	1
1:R:62:TYR:CE1	1:R:63:VAL:HG23	0.52	2.38	5	2
1:R:155:THR:CG2	1:R:160:TYR:CD2	0.52	2.92	2	1
1:R:92:LEU:HD11	1:R:103:VAL:HG22	0.52	1.79	3	1
1:R:43:SER:HA	1:R:51:ALA:HA	0.52	1.80	4	1
1:R:53:LEU:C	1:R:57:LEU:CB	0.52	2.82	2	1
1:R:132:MET:O	1:R:173:ASP:OD2	0.52	2.27	2	1
1:R:62:TYR:CZ	1:R:139:ALA:CB	0.52	2.90	3	1
1:R:31:LEU:CD1	1:R:162:ILE:CD1	0.52	2.84	1	3
1:R:42:TYR:N	1:R:42:TYR:CD1	0.52	2.77	1	1
1:R:127:VAL:HG13	1:R:128:ASP:N	0.52	2.19	1	1
1:R:138:HIS:O	1:R:153:CYS:HA	0.52	2.04	1	2
1:R:87:GLU:O	1:R:91:GLY:HA2	0.52	2.04	2	4
1:R:138:HIS:HA	1:R:172:PRO:O	0.52	2.04	4	1
1:R:53:LEU:CG	1:R:83:ILE:CG1	0.52	2.88	2	3
1:R:134:LEU:HD12	1:R:159:TRP:CE2	0.52	2.39	1	1
1:R:139:ALA:CB	1:R:181:VAL:CG1	0.52	2.84	4	2
1:R:161:ALA:O	1:R:168:TYR:CD2	0.52	2.62	3	1
1:R:47:ASN:C	1:R:48:HIS:CG	0.52	2.85	5	1
1:R:68:PHE:CE2	1:R:103:VAL:HG11	0.52	2.39	5	1
1:R:142:PHE:HB2	1:R:150:VAL:CG2	0.52	2.33	1	2
1:R:48:HIS:O	1:R:49:ASP:HB3	0.52	2.03	2	1
1:R:138:HIS:ND1	1:R:154:VAL:CG2	0.52	2.73	2	1
1:R:92:LEU:HD21	1:R:94:LEU:HD21	0.52	1.82	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:68:PHE:CZ	1:R:103:VAL:HG11	0.52	2.39	5	1
1:R:118:ALA:HB2	1:R:130:THR:HG23	0.52	1.82	5	1
1:R:124:VAL:CG1	1:R:181:VAL:HG23	0.52	2.35	5	1
1:R:31:LEU:HD11	1:R:160:TYR:CE1	0.52	2.39	2	1
1:R:92:LEU:O	1:R:93:GLU:O	0.52	2.28	4	2
1:R:181:VAL:O	1:R:181:VAL:HG12	0.52	2.05	3	1
1:R:60:PHE:HB2	1:R:68:PHE:CE2	0.52	2.39	4	1
1:R:74:SER:OG	1:R:78:LEU:HD23	0.52	2.05	4	1
1:R:50:ASN:HB3	1:R:79:THR:CG2	0.52	2.35	5	1
1:R:54:ASN:O	1:R:58:GLN:HB2	0.52	2.04	2	2
1:R:92:LEU:CD1	1:R:94:LEU:CD2	0.52	2.88	1	2
1:R:53:LEU:HD12	1:R:79:THR:CB	0.52	2.35	2	2
1:R:32:THR:HG22	1:R:38:LYS:CB	0.52	2.35	4	1
1:R:42:TYR:O	1:R:54:ASN:HB2	0.52	2.04	4	1
1:R:80:LEU:O	1:R:84:LYS:CB	0.52	2.58	5	1
1:R:117:THR:CB	1:R:120:ARG:O	0.52	2.58	5	1
1:R:31:LEU:HD22	1:R:167:PHE:CE2	0.52	2.39	3	2
1:R:163:ASP:OD2	1:R:168:TYR:OH	0.52	2.28	3	1
1:R:42:TYR:O	1:R:43:SER:HB2	0.52	2.05	4	1
1:R:49:ASP:CB	1:R:95:HIS:O	0.52	2.58	5	1
1:R:115:ILE:HG21	1:R:124:VAL:H	0.52	1.65	5	1
1:R:53:LEU:HD22	1:R:71:VAL:CG2	0.52	2.35	1	1
1:R:104:ILE:HG22	1:R:111:LEU:CD1	0.52	2.35	2	1
1:R:92:LEU:CD1	1:R:101:ALA:O	0.52	2.52	3	1
1:R:99:PRO:CG	1:R:141:ILE:HG21	0.52	2.35	3	1
1:R:65:GLU:CG	1:R:112:HIS:CE1	0.52	2.93	4	1
1:R:160:TYR:HA	1:R:170:TRP:H	0.52	1.64	4	1
1:R:60:PHE:HA	1:R:66:PRO:CD	0.51	2.34	1	1
1:R:79:THR:O	1:R:82:ALA:HB3	0.51	2.05	1	3
1:R:178:LEU:C	1:R:179:VAL:HG12	0.51	2.28	1	2
1:R:48:HIS:CD2	1:R:80:LEU:HD23	0.51	2.39	2	1
1:R:161:ALA:N	1:R:168:TYR:O	0.51	2.43	2	1
1:R:40:THR:O	1:R:72:TYR:CE1	0.51	2.63	4	1
1:R:35:ASN:HB2	1:R:154:VAL:N	0.51	2.20	2	1
1:R:57:LEU:C	1:R:57:LEU:HD13	0.51	2.31	2	1
1:R:138:HIS:HA	1:R:172:PRO:HA	0.51	1.81	2	1
1:R:53:LEU:CD1	1:R:83:ILE:CG1	0.51	2.88	5	5
1:R:79:THR:HG23	1:R:80:LEU:N	0.51	2.19	4	3
1:R:42:TYR:O	1:R:43:SER:OG	0.51	2.29	3	1
1:R:59:LEU:CD1	1:R:62:TYR:OH	0.51	2.58	3	1
1:R:92:LEU:CD2	1:R:94:LEU:HD21	0.51	2.35	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:98:GLY:O	1:R:101:ALA:CB	0.51	2.58	5	2
1:R:58:GLN:NE2	1:R:151:PHE:HB2	0.51	2.20	4	1
1:R:48:HIS:HD2	1:R:79:THR:HG21	0.51	1.64	5	1
1:R:53:LEU:CD1	1:R:83:ILE:HG13	0.51	2.34	1	2
1:R:79:THR:O	1:R:83:ILE:CD1	0.51	2.58	5	3
1:R:137:PHE:CZ	1:R:180:PHE:CB	0.51	2.93	2	1
1:R:138:HIS:ND1	1:R:138:HIS:N	0.51	2.58	2	1
1:R:55:ALA:O	1:R:151:PHE:CE2	0.51	2.63	3	1
1:R:181:VAL:O	1:R:181:VAL:CG1	0.51	2.58	3	1
1:R:62:TYR:CE2	1:R:139:ALA:HB1	0.51	2.40	5	2
1:R:44:ARG:HA	1:R:164:ASP:CA	0.51	2.35	5	1
1:R:31:LEU:CD1	1:R:167:PHE:CE2	0.51	2.93	1	1
1:R:41:PHE:CZ	1:R:61:ARG:CB	0.51	2.93	2	1
1:R:69:ASP:HA	1:R:72:TYR:CD1	0.51	2.40	5	1
1:R:31:LEU:HD11	1:R:162:ILE:HD12	0.51	1.77	5	2
1:R:57:LEU:HA	1:R:60:PHE:CD2	0.51	2.40	2	1
1:R:90:THR:HA	1:R:106:ASN:HB3	0.51	1.81	2	1
1:R:173:ASP:HB3	1:R:174:PRO:CD	0.51	2.36	2	2
1:R:137:PHE:C	1:R:138:HIS:CD2	0.51	2.89	5	1
1:R:86:LEU:CD1	1:R:94:LEU:HD21	0.51	2.36	5	2
1:R:168:TYR:CD1	1:R:168:TYR:N	0.51	2.78	4	3
1:R:137:PHE:CD2	1:R:180:PHE:CD1	0.51	2.99	1	1
1:R:53:LEU:O	1:R:57:LEU:HB3	0.51	2.06	2	1
1:R:79:THR:HG23	1:R:80:LEU:H	0.51	1.66	2	4
1:R:137:PHE:C	1:R:138:HIS:CG	0.51	2.87	2	2
1:R:161:ALA:O	1:R:168:TYR:CE1	0.51	2.64	2	2
1:R:69:ASP:O	1:R:73:SER:HB2	0.51	2.06	4	1
1:R:168:TYR:CE1	1:R:170:TRP:CD1	0.51	2.99	1	1
1:R:54:ASN:CB	1:R:58:GLN:OE1	0.51	2.59	2	1
1:R:137:PHE:CB	1:R:183:TYR:CD1	0.51	2.94	2	1
1:R:155:THR:OG1	1:R:160:TYR:CB	0.51	2.58	4	4
1:R:107:ILE:O	1:R:111:LEU:HG	0.51	2.06	3	1
1:R:68:PHE:CZ	1:R:72:TYR:CD2	0.51	2.98	4	1
1:R:48:HIS:CD2	1:R:79:THR:CG2	0.51	2.93	5	1
1:R:55:ALA:HA	1:R:151:PHE:CE1	0.51	2.41	5	1
1:R:115:ILE:CG1	1:R:122:SER:O	0.51	2.59	5	1
1:R:180:PHE:HD1	1:R:181:VAL:N	0.51	2.02	5	1
1:R:60:PHE:CD1	1:R:61:ARG:N	0.50	2.78	1	2
1:R:67:PHE:CZ	1:R:70:TRP:CD1	0.50	2.99	1	1
1:R:101:ALA:O	1:R:102:LEU:C	0.50	2.54	5	3
1:R:142:PHE:CD1	1:R:177:VAL:CB	0.50	2.94	5	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:63:VAL:CG2	1:R:124:VAL:HG12	0.50	2.36	2	1
1:R:94:LEU:O	1:R:94:LEU:HD12	0.50	2.06	2	1
1:R:127:VAL:HG12	1:R:180:PHE:CD1	0.50	2.40	2	1
1:R:141:ILE:H	1:R:179:VAL:HG13	0.50	1.65	2	1
1:R:60:PHE:CZ	1:R:72:TYR:CD2	0.50	2.99	3	1
1:R:62:TYR:CE1	1:R:153:CYS:HB3	0.50	2.40	4	1
1:R:94:LEU:HD22	1:R:103:VAL:CG2	0.50	2.36	4	1
1:R:125:CYS:O	1:R:126:VAL:CG2	0.50	2.56	4	1
1:R:160:TYR:CE1	1:R:162:ILE:N	0.50	2.79	2	1
1:R:170:TRP:C	1:R:171:THR:OG1	0.50	2.52	2	1
1:R:52:TRP:CD2	1:R:97:GLY:O	0.50	2.65	3	2
1:R:92:LEU:HD21	1:R:94:LEU:CD2	0.50	2.36	3	1
1:R:141:ILE:C	1:R:142:PHE:HD1	0.50	2.14	4	1
1:R:104:ILE:HG23	1:R:111:LEU:HG	0.50	1.81	5	1
1:R:53:LEU:CD1	1:R:79:THR:CA	0.50	2.90	2	2
1:R:130:THR:O	1:R:131:ASP:HB2	0.50	2.06	2	1
1:R:170:TRP:O	1:R:171:THR:CB	0.50	2.58	2	1
1:R:173:ASP:HB3	1:R:174:PRO:HD2	0.50	1.84	4	2
1:R:53:LEU:C	1:R:57:LEU:HD23	0.50	2.30	3	2
1:R:94:LEU:N	1:R:94:LEU:HD22	0.50	2.22	3	1
1:R:67:PHE:CD1	1:R:111:LEU:HD22	0.50	2.41	5	1
1:R:115:ILE:CG2	1:R:124:VAL:H	0.50	2.19	5	1
1:R:141:ILE:HG23	1:R:151:PHE:HE1	0.50	1.64	5	1
1:R:43:SER:O	1:R:44:ARG:C	0.50	2.54	3	1
1:R:92:LEU:O	1:R:93:GLU:HB2	0.50	2.05	5	1
1:R:55:ALA:CA	1:R:151:PHE:CZ	0.50	2.95	1	2
1:R:60:PHE:CD1	1:R:65:GLU:HB3	0.50	2.42	3	2
1:R:104:ILE:HA	1:R:111:LEU:HG	0.50	1.83	1	1
1:R:56:ILE:CG1	1:R:60:PHE:CZ	0.50	2.94	2	1
1:R:60:PHE:HB3	1:R:65:GLU:O	0.50	2.07	2	1
1:R:53:LEU:HD21	1:R:83:ILE:HG23	0.50	1.82	4	2
1:R:137:PHE:O	1:R:183:TYR:CD2	0.50	2.64	3	1
1:R:43:SER:HA	1:R:165:GLU:HB2	0.50	1.83	5	1
1:R:58:GLN:HE21	1:R:59:LEU:HD22	0.50	1.66	5	1
1:R:107:ILE:O	1:R:110:LEU:N	0.50	2.37	2	2
1:R:107:ILE:HG22	1:R:110:LEU:HD23	0.50	1.82	2	1
1:R:155:THR:CG2	1:R:160:TYR:CB	0.50	2.89	2	4
1:R:160:TYR:CD1	1:R:167:PHE:HB2	0.50	2.42	2	1
1:R:33:LEU:O	1:R:33:LEU:CD2	0.50	2.60	5	2
1:R:52:TRP:CD1	1:R:96:GLU:C	0.50	2.90	4	1
1:R:138:HIS:CE1	1:R:159:TRP:CD1	0.50	3.00	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:44:ARG:N	1:R:165:GLU:HB3	0.50	2.22	5	1
1:R:56:ILE:HG13	1:R:68:PHE:CD1	0.50	2.42	5	1
1:R:63:VAL:CG1	1:R:124:VAL:HG11	0.50	2.35	1	1
1:R:57:LEU:O	1:R:60:PHE:HB2	0.50	2.06	2	1
1:R:123:GLU:O	1:R:181:VAL:HG23	0.50	2.05	4	1
1:R:53:LEU:O	1:R:54:ASN:C	0.50	2.52	2	3
1:R:111:LEU:CD1	1:R:111:LEU:C	0.50	2.84	1	4
1:R:71:VAL:HG12	1:R:72:TYR:N	0.50	2.20	2	1
1:R:137:PHE:CZ	1:R:174:PRO:HD3	0.50	2.41	2	2
1:R:137:PHE:HB3	1:R:183:TYR:CD1	0.50	2.42	2	1
1:R:57:LEU:CD1	1:R:68:PHE:CG	0.50	2.92	4	1
1:R:124:VAL:HA	1:R:180:PHE:O	0.50	2.07	4	1
1:R:33:LEU:HA	1:R:155:THR:HA	0.50	1.84	5	1
1:R:94:LEU:HD12	1:R:94:LEU:C	0.49	2.31	4	2
1:R:89:LEU:HD21	1:R:107:ILE:HG23	0.49	1.84	2	1
1:R:57:LEU:HA	1:R:68:PHE:CD2	0.49	2.41	4	1
1:R:141:ILE:CG2	1:R:151:PHE:CE2	0.49	2.85	1	1
1:R:167:PHE:CD1	1:R:167:PHE:N	0.49	2.77	1	2
1:R:181:VAL:HG12	1:R:181:VAL:O	0.49	2.06	1	1
1:R:125:CYS:C	1:R:179:VAL:HA	0.49	2.33	4	1
1:R:58:GLN:OE1	1:R:58:GLN:CA	0.49	2.60	1	1
1:R:79:THR:CG2	1:R:80:LEU:N	0.49	2.75	1	1
1:R:49:ASP:O	1:R:79:THR:CG2	0.49	2.61	2	2
1:R:53:LEU:HD11	1:R:83:ILE:HG23	0.49	1.84	3	1
1:R:170:TRP:HA	1:R:170:TRP:HE3	0.49	1.66	3	1
1:R:56:ILE:HA	1:R:59:LEU:HB2	0.49	1.83	2	1
1:R:155:THR:HG23	1:R:160:TYR:CD2	0.49	2.42	2	1
1:R:160:TYR:HA	1:R:169:PRO:HA	0.49	1.84	2	1
1:R:43:SER:O	1:R:164:ASP:HA	0.49	2.06	3	1
1:R:141:ILE:O	1:R:177:VAL:HA	0.49	2.07	3	1
1:R:142:PHE:CZ	1:R:171:THR:CG2	0.49	2.94	3	1
1:R:159:TRP:HB3	1:R:172:PRO:HD2	0.49	1.84	4	1
1:R:137:PHE:CG	1:R:180:PHE:CE1	0.49	3.00	5	1
1:R:117:THR:C	1:R:125:CYS:SG	0.49	2.95	1	1
1:R:60:PHE:CZ	1:R:61:ARG:HG2	0.49	2.42	3	1
1:R:56:ILE:HG12	1:R:60:PHE:CZ	0.49	2.43	2	1
1:R:127:VAL:O	1:R:130:THR:CB	0.49	2.60	2	1
1:R:34:TYR:HB2	1:R:154:VAL:CG1	0.49	2.37	1	1
1:R:57:LEU:HD11	1:R:71:VAL:HG11	0.49	1.84	2	1
1:R:55:ALA:CA	1:R:151:PHE:CE1	0.49	2.95	5	2
1:R:92:LEU:CG	1:R:94:LEU:CD2	0.49	2.89	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:142:PHE:CD1	1:R:177:VAL:CG2	0.49	2.96	3	1
1:R:86:LEU:HD21	1:R:107:ILE:HD11	0.49	1.84	1	1
1:R:107:ILE:O	1:R:108:LYS:C	0.49	2.55	2	5
1:R:111:LEU:C	1:R:111:LEU:HD13	0.49	2.33	1	4
1:R:163:ASP:HB2	1:R:168:TYR:CE2	0.49	2.43	1	1
1:R:31:LEU:CG	1:R:41:PHE:CE1	0.49	2.95	2	1
1:R:31:LEU:HD11	1:R:167:PHE:HB2	0.49	1.82	2	1
1:R:56:ILE:CG1	1:R:103:VAL:HG11	0.49	2.38	4	1
1:R:137:PHE:CD2	1:R:180:PHE:CD2	0.49	3.00	2	2
1:R:47:ASN:O	1:R:48:HIS:HB2	0.49	2.08	3	1
1:R:57:LEU:CD1	1:R:60:PHE:CD2	0.49	2.96	3	1
1:R:161:ALA:HB3	1:R:170:TRP:HB2	0.49	1.83	3	1
1:R:157:ASN:HB2	1:R:160:TYR:CE1	0.49	2.43	4	1
1:R:67:PHE:CE1	1:R:111:LEU:HD22	0.49	2.43	5	1
1:R:134:LEU:CD2	1:R:171:THR:CG2	0.49	2.89	5	1
1:R:105:TRP:O	1:R:108:LYS:HG3	0.48	2.08	1	1
1:R:66:PRO:HG2	1:R:68:PHE:CE2	0.48	2.43	3	1
1:R:62:TYR:CE1	1:R:153:CYS:CB	0.48	2.96	4	1
1:R:92:LEU:CD2	1:R:102:LEU:HB2	0.48	2.37	5	1
1:R:137:PHE:HB2	1:R:181:VAL:O	0.48	2.08	5	1
1:R:134:LEU:CD1	1:R:171:THR:CG2	0.48	2.79	1	2
1:R:142:PHE:CE2	1:R:177:VAL:HG12	0.48	2.43	1	1
1:R:153:CYS:CB	1:R:160:TYR:CE2	0.48	2.96	2	1
1:R:43:SER:C	1:R:164:ASP:CA	0.48	2.87	3	1
1:R:65:GLU:CG	1:R:65:GLU:O	0.48	2.61	3	1
1:R:177:VAL:HG23	1:R:178:LEU:N	0.48	2.23	4	1
1:R:115:ILE:HG13	1:R:122:SER:C	0.48	2.33	5	1
1:R:31:LEU:CD1	1:R:160:TYR:CE1	0.48	2.96	2	1
1:R:39:LYS:O	1:R:41:PHE:CE1	0.48	2.66	4	2
1:R:102:LEU:HD23	1:R:106:ASN:HD21	0.48	1.67	3	1
1:R:138:HIS:CD2	1:R:183:TYR:CA	0.48	2.95	3	1
1:R:79:THR:O	1:R:83:ILE:HD12	0.48	2.08	5	1
1:R:31:LEU:CD1	1:R:41:PHE:CG	0.48	2.96	1	1
1:R:116:GLY:O	1:R:126:VAL:HG13	0.48	2.08	1	1
1:R:118:ALA:CB	1:R:128:ASP:HA	0.48	2.38	1	1
1:R:138:HIS:ND1	1:R:154:VAL:HG21	0.48	2.23	2	2
1:R:142:PHE:CZ	1:R:177:VAL:CG1	0.48	2.93	1	1
1:R:99:PRO:HD2	1:R:101:ALA:HB2	0.48	1.85	4	1
1:R:31:LEU:HD22	1:R:167:PHE:CE1	0.48	2.43	5	1
1:R:56:ILE:CB	1:R:68:PHE:CE1	0.48	2.96	5	1
1:R:126:VAL:HG12	1:R:127:VAL:HG13	0.48	1.81	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:142:PHE:CG	1:R:177:VAL:HG12	0.48	2.43	4	1
1:R:104:ILE:HG23	1:R:111:LEU:CG	0.48	2.38	5	1
1:R:83:ILE:HB	1:R:94:LEU:HD13	0.48	1.85	1	1
1:R:160:TYR:OH	1:R:162:ILE:HB	0.48	2.08	2	1
1:R:31:LEU:HD11	1:R:41:PHE:CZ	0.48	2.44	3	1
1:R:54:ASN:O	1:R:58:GLN:HG3	0.48	2.08	3	1
1:R:66:PRO:HG2	1:R:68:PHE:CD2	0.48	2.43	3	1
1:R:80:LEU:HD12	1:R:81:GLU:N	0.48	2.24	4	1
1:R:142:PHE:CZ	1:R:172:PRO:CA	0.48	2.97	5	1
1:R:33:LEU:HD11	1:R:37:GLU:O	0.48	2.07	1	1
1:R:157:ASN:CB	1:R:160:TYR:CE1	0.48	2.97	4	2
1:R:127:VAL:HG23	1:R:128:ASP:N	0.48	2.23	2	1
1:R:92:LEU:CD2	1:R:92:LEU:N	0.48	2.77	3	1
1:R:41:PHE:CD1	1:R:162:ILE:CD1	0.48	2.97	4	1
1:R:134:LEU:O	1:R:138:HIS:CE1	0.48	2.67	5	1
1:R:164:ASP:O	1:R:165:GLU:HB3	0.48	2.09	5	1
1:R:53:LEU:CD2	1:R:83:ILE:HG13	0.48	2.39	1	1
1:R:38:LYS:O	1:R:38:LYS:HG3	0.48	2.09	5	3
1:R:90:THR:HB	1:R:92:LEU:HD21	0.48	1.86	5	1
1:R:137:PHE:CB	1:R:183:TYR:CE2	0.48	2.96	3	1
1:R:115:ILE:CD1	1:R:124:VAL:N	0.48	2.77	5	1
1:R:58:GLN:CG	1:R:59:LEU:HD13	0.47	2.38	4	1
1:R:62:TYR:OH	1:R:151:PHE:CE1	0.47	2.66	4	1
1:R:92:LEU:HD21	1:R:103:VAL:HA	0.47	1.86	4	1
1:R:111:LEU:HD11	1:R:113:THR:OG1	0.47	2.09	4	1
1:R:117:THR:HG23	1:R:126:VAL:CB	0.47	2.38	5	1
1:R:34:TYR:HB2	1:R:154:VAL:HG11	0.47	1.84	1	1
1:R:57:LEU:CD1	1:R:72:TYR:CD2	0.47	2.97	1	1
1:R:159:TRP:CD1	1:R:171:THR:O	0.47	2.67	3	1
1:R:107:ILE:O	1:R:111:LEU:HB2	0.47	2.09	4	1
1:R:111:LEU:HD13	1:R:112:HIS:N	0.47	2.24	4	1
1:R:112:HIS:O	1:R:112:HIS:CD2	0.47	2.67	4	1
1:R:62:TYR:CE2	1:R:181:VAL:CG2	0.47	2.97	2	1
1:R:43:SER:HB3	1:R:164:ASP:O	0.47	2.08	3	1
1:R:72:TYR:CD1	1:R:72:TYR:C	0.47	2.92	3	1
1:R:56:ILE:HG21	1:R:68:PHE:CE1	0.47	2.44	5	1
1:R:137:PHE:HB3	1:R:180:PHE:CE1	0.47	2.45	5	1
1:R:48:HIS:CD2	1:R:80:LEU:HD22	0.47	2.45	3	1
1:R:89:LEU:HD23	1:R:90:THR:CG2	0.47	2.40	5	2
1:R:63:VAL:O	1:R:64:GLU:HB3	0.47	2.07	2	2
1:R:99:PRO:HB2	1:R:141:ILE:HD13	0.47	1.86	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:52:TRP:CG	1:R:97:GLY:N	0.47	2.83	4	1
1:R:60:PHE:CB	1:R:68:PHE:CE2	0.47	2.97	4	1
1:R:56:ILE:HB	1:R:68:PHE:CD1	0.47	2.45	5	1
1:R:115:ILE:HB	1:R:122:SER:N	0.47	2.23	5	1
1:R:59:LEU:HD21	1:R:141:ILE:HD11	0.47	1.86	1	2
1:R:136:ASP:O	1:R:183:TYR:CE2	0.47	2.67	2	3
1:R:111:LEU:CD1	1:R:112:HIS:N	0.47	2.78	2	1
1:R:139:ALA:CB	1:R:153:CYS:SG	0.47	3.03	2	1
1:R:160:TYR:CE1	1:R:162:ILE:HB	0.47	2.45	2	1
1:R:55:ALA:HB2	1:R:141:ILE:CD1	0.47	2.40	4	1
1:R:49:ASP:HB2	1:R:95:HIS:O	0.47	2.10	5	1
1:R:57:LEU:HD22	1:R:57:LEU:N	0.47	2.24	4	2
1:R:127:VAL:HB	1:R:178:LEU:HD13	0.47	1.85	1	1
1:R:141:ILE:HB	1:R:179:VAL:HG13	0.47	1.87	1	1
1:R:162:ILE:HG12	1:R:167:PHE:CD1	0.47	2.45	1	1
1:R:67:PHE:CE2	1:R:86:LEU:HD11	0.47	2.45	2	1
1:R:83:ILE:HG22	1:R:94:LEU:HD21	0.47	1.85	2	1
1:R:153:CYS:O	1:R:160:TYR:HD2	0.47	1.91	2	1
1:R:163:ASP:HB2	1:R:168:TYR:CE1	0.47	2.44	5	2
1:R:33:LEU:HD22	1:R:33:LEU:N	0.47	2.23	3	1
1:R:34:TYR:HB3	1:R:154:VAL:CG1	0.47	2.40	3	1
1:R:71:VAL:HG13	1:R:77:ASN:ND2	0.47	2.24	3	1
1:R:127:VAL:C	1:R:130:THR:OG1	0.47	2.58	3	1
1:R:137:PHE:CB	1:R:180:PHE:CD2	0.47	2.97	4	1
1:R:46:ASN:HB3	1:R:48:HIS:CE1	0.47	2.45	5	2
1:R:53:LEU:O	1:R:57:LEU:CD2	0.47	2.59	3	1
1:R:87:GLU:O	1:R:91:GLY:CA	0.47	2.63	3	4
1:R:125:CYS:SG	1:R:180:PHE:CZ	0.47	3.06	1	2
1:R:57:LEU:HD13	1:R:60:PHE:HD2	0.47	1.70	3	1
1:R:59:LEU:HD12	1:R:62:TYR:CE1	0.47	2.45	3	1
1:R:157:ASN:CB	1:R:160:TYR:CZ	0.47	2.98	5	1
1:R:94:LEU:HD12	1:R:94:LEU:N	0.47	2.24	1	1
1:R:69:ASP:HA	1:R:73:SER:CB	0.47	2.40	2	1
1:R:141:ILE:C	1:R:177:VAL:HB	0.47	2.34	2	1
1:R:98:GLY:O	1:R:103:VAL:HG21	0.47	2.10	4	1
1:R:74:SER:CB	1:R:78:LEU:HB2	0.47	2.40	5	1
1:R:115:ILE:HG13	1:R:123:GLU:N	0.47	2.24	5	1
1:R:125:CYS:O	1:R:180:PHE:CD2	0.47	2.68	5	1
1:R:134:LEU:CA	1:R:173:ASP:CB	0.46	2.79	2	1
1:R:67:PHE:CZ	1:R:89:LEU:CD2	0.46	2.97	3	1
1:R:138:HIS:CD2	1:R:181:VAL:CG1	0.46	2.98	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:126:VAL:CG1	1:R:127:VAL:H	0.46	2.20	4	1
1:R:127:VAL:HG21	1:R:177:VAL:C	0.46	2.35	5	1
1:R:68:PHE:CD1	1:R:69:ASP:N	0.46	2.84	1	1
1:R:127:VAL:CB	1:R:178:LEU:HA	0.46	2.39	1	1
1:R:62:TYR:CE2	1:R:140:GLY:N	0.46	2.83	4	1
1:R:170:TRP:O	1:R:172:PRO:HD3	0.46	2.10	4	1
1:R:142:PHE:HA	1:R:177:VAL:CB	0.46	2.39	2	1
1:R:155:THR:OG1	1:R:160:TYR:HB3	0.46	2.10	2	1
1:R:31:LEU:CD2	1:R:41:PHE:CE1	0.46	2.97	3	1
1:R:60:PHE:CB	1:R:68:PHE:CD2	0.46	2.98	4	1
1:R:71:VAL:HG22	1:R:82:ALA:CB	0.46	2.41	1	2
1:R:94:LEU:C	1:R:96:GLU:N	0.46	2.70	3	4
1:R:104:ILE:CA	1:R:111:LEU:HG	0.46	2.41	1	1
1:R:57:LEU:HD22	1:R:68:PHE:CB	0.46	2.40	2	1
1:R:104:ILE:HB	1:R:111:LEU:HD12	0.46	1.86	2	1
1:R:114:GLY:O	1:R:123:GLU:N	0.46	2.48	2	3
1:R:117:THR:O	1:R:125:CYS:SG	0.46	2.73	2	1
1:R:161:ALA:HB3	1:R:170:TRP:CB	0.46	2.41	3	1
1:R:116:GLY:O	1:R:117:THR:HG23	0.46	2.11	4	1
1:R:44:ARG:HB3	1:R:164:ASP:C	0.46	2.35	5	1
1:R:102:LEU:HB3	1:R:105:TRP:HB3	0.46	1.87	5	1
1:R:136:ASP:C	1:R:183:TYR:CZ	0.46	2.93	2	1
1:R:132:MET:CB	1:R:180:PHE:CZ	0.46	2.98	3	1
1:R:52:TRP:CE3	1:R:97:GLY:HA2	0.46	2.46	4	1
1:R:126:VAL:C	1:R:127:VAL:CG2	0.46	2.89	4	1
1:R:177:VAL:CG2	1:R:178:LEU:N	0.46	2.79	5	2
1:R:65:GLU:CB	1:R:68:PHE:CE1	0.46	2.98	1	1
1:R:155:THR:OG1	1:R:160:TYR:CG	0.46	2.67	5	1
1:R:56:ILE:HG12	1:R:60:PHE:CE2	0.46	2.46	2	1
1:R:83:ILE:O	1:R:84:LYS:C	0.46	2.58	3	4
1:R:107:ILE:HG12	1:R:111:LEU:CD2	0.46	2.41	3	1
1:R:142:PHE:CE2	1:R:171:THR:HG23	0.46	2.46	3	1
1:R:58:GLN:HG2	1:R:151:PHE:HB2	0.46	1.86	5	1
1:R:41:PHE:N	1:R:41:PHE:HD1	0.46	2.06	1	1
1:R:67:PHE:C	1:R:69:ASP:H	0.46	2.18	2	3
1:R:127:VAL:HG23	1:R:177:VAL:O	0.46	2.11	1	1
1:R:141:ILE:HG12	1:R:151:PHE:CE2	0.46	2.46	3	2
1:R:159:TRP:CD2	1:R:172:PRO:HG3	0.46	2.46	2	1
1:R:53:LEU:HD13	1:R:82:ALA:HB3	0.46	1.88	3	1
1:R:58:GLN:HG2	1:R:151:PHE:CB	0.46	2.40	5	1
1:R:160:TYR:CA	1:R:168:TYR:O	0.46	2.64	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:33:LEU:CD1	1:R:61:ARG:NH1	0.46	2.79	1	1
1:R:57:LEU:CD1	1:R:71:VAL:HG11	0.46	2.41	1	2
1:R:108:LYS:HA	1:R:112:HIS:H	0.46	1.70	1	1
1:R:137:PHE:CD2	1:R:180:PHE:CE1	0.46	3.04	1	1
1:R:41:PHE:CG	1:R:162:ILE:HD11	0.46	2.45	2	1
1:R:59:LEU:O	1:R:62:TYR:CE1	0.46	2.69	2	1
1:R:117:THR:CA	1:R:126:VAL:HG22	0.46	2.33	2	1
1:R:138:HIS:CB	1:R:181:VAL:HG12	0.46	2.40	3	1
1:R:150:VAL:HG12	1:R:163:ASP:CG	0.46	2.35	3	1
1:R:41:PHE:CD2	1:R:72:TYR:OH	0.46	2.65	4	1
1:R:51:ALA:O	1:R:54:ASN:ND2	0.46	2.49	4	1
1:R:115:ILE:CB	1:R:122:SER:C	0.46	2.89	5	1
1:R:41:PHE:CE2	1:R:162:ILE:CD1	0.46	2.99	2	3
1:R:62:TYR:CZ	1:R:153:CYS:HB2	0.46	2.46	1	1
1:R:57:LEU:CD2	1:R:68:PHE:HB2	0.46	2.41	2	2
1:R:138:HIS:CB	1:R:154:VAL:CG2	0.46	2.94	2	2
1:R:168:TYR:CE2	1:R:170:TRP:CG	0.46	3.04	2	1
1:R:89:LEU:CD2	1:R:90:THR:CG2	0.46	2.94	5	1
1:R:43:SER:O	1:R:164:ASP:CB	0.45	2.63	3	1
1:R:152:ALA:HA	1:R:161:ALA:CB	0.45	2.40	5	2
1:R:170:TRP:CG	1:R:171:THR:N	0.45	2.84	3	1
1:R:31:LEU:HB3	1:R:167:PHE:CE2	0.45	2.45	4	1
1:R:43:SER:OG	1:R:54:ASN:CG	0.45	2.60	4	1
1:R:33:LEU:CA	1:R:37:GLU:N	0.45	2.79	2	1
1:R:159:TRP:CG	1:R:172:PRO:HG3	0.45	2.45	2	1
1:R:30:GLU:HG2	1:R:40:THR:OG1	0.45	2.11	3	1
1:R:138:HIS:HB3	1:R:181:VAL:HG12	0.45	1.88	3	1
1:R:126:VAL:CB	1:R:178:LEU:O	0.45	2.64	4	1
1:R:173:ASP:O	1:R:177:VAL:HG11	0.45	2.12	4	1
1:R:92:LEU:O	1:R:93:GLU:HB3	0.45	2.12	1	1
1:R:138:HIS:O	1:R:139:ALA:CB	0.45	2.63	1	1
1:R:66:PRO:HB3	1:R:68:PHE:CZ	0.45	2.46	4	1
1:R:168:TYR:CZ	1:R:170:TRP:CD1	0.45	3.05	5	1
1:R:30:GLU:HA	1:R:40:THR:HA	0.45	1.88	1	1
1:R:104:ILE:O	1:R:111:LEU:HG	0.45	2.12	1	1
1:R:109:HIS:NE2	1:R:110:LEU:CD2	0.45	2.80	1	1
1:R:168:TYR:CE1	1:R:170:TRP:CG	0.45	3.04	1	1
1:R:117:THR:HA	1:R:126:VAL:CG2	0.45	2.37	2	1
1:R:161:ALA:CB	1:R:170:TRP:CB	0.45	2.95	3	1
1:R:58:GLN:HG3	1:R:59:LEU:HD22	0.45	1.87	5	1
1:R:107:ILE:O	1:R:107:ILE:CG2	0.45	2.64	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:58:GLN:OE1	1:R:162:ILE:HG21	0.45	2.10	2	1
1:R:63:VAL:HG21	1:R:124:VAL:HG12	0.45	1.88	2	1
1:R:118:ALA:CB	1:R:130:THR:OG1	0.45	2.63	3	2
1:R:38:LYS:C	1:R:39:LYS:HG2	0.45	2.37	4	1
1:R:92:LEU:CD2	1:R:101:ALA:O	0.45	2.65	4	1
1:R:159:TRP:O	1:R:160:TYR:CD1	0.45	2.69	4	1
1:R:67:PHE:CD2	1:R:111:LEU:CD2	0.45	2.99	5	1
1:R:53:LEU:CD1	1:R:79:THR:O	0.45	2.64	1	1
1:R:98:GLY:HA2	1:R:101:ALA:HB2	0.45	1.88	1	1
1:R:53:LEU:CG	1:R:83:ILE:HG23	0.45	2.42	3	1
1:R:138:HIS:CG	1:R:181:VAL:CG1	0.45	2.96	3	1
1:R:150:VAL:CG1	1:R:163:ASP:OD2	0.45	2.65	3	1
1:R:153:CYS:O	1:R:155:THR:HG23	0.45	2.11	3	1
1:R:168:TYR:CD1	1:R:168:TYR:C	0.45	2.94	3	1
1:R:99:PRO:C	1:R:101:ALA:N	0.45	2.75	4	2
1:R:62:TYR:CZ	1:R:63:VAL:CG2	0.45	2.96	5	2
1:R:56:ILE:O	1:R:59:LEU:CB	0.45	2.64	3	1
1:R:142:PHE:CE2	1:R:171:THR:OG1	0.45	2.55	3	1
1:R:103:VAL:HG12	1:R:107:ILE:CD1	0.45	2.42	5	1
1:R:44:ARG:N	1:R:164:ASP:O	0.45	2.50	3	1
1:R:54:ASN:CA	1:R:57:LEU:HB2	0.45	2.41	3	1
1:R:31:LEU:HD12	1:R:155:THR:HG22	0.45	1.89	5	1
1:R:134:LEU:HG	1:R:173:ASP:CA	0.45	2.42	3	1
1:R:67:PHE:CZ	1:R:70:TRP:NE1	0.45	2.85	1	1
1:R:57:LEU:CG	1:R:71:VAL:HG21	0.45	2.42	2	1
1:R:62:TYR:CE2	1:R:63:VAL:HG23	0.45	2.46	2	2
1:R:159:TRP:HA	1:R:172:PRO:CD	0.45	2.42	4	1
1:R:120:ARG:CG	1:R:121:PRO:CD	0.45	2.95	5	1
1:R:162:ILE:HG13	1:R:167:PHE:CE1	0.45	2.46	5	1
1:R:173:ASP:C	1:R:175:SER:H	0.45	2.20	5	1
1:R:54:ASN:ND2	1:R:163:ASP:HA	0.44	2.26	1	1
1:R:94:LEU:N	1:R:94:LEU:CD1	0.44	2.78	1	1
1:R:90:THR:OG1	1:R:92:LEU:CG	0.44	2.65	2	2
1:R:29:MET:HB2	1:R:167:PHE:CE2	0.44	2.47	3	1
1:R:161:ALA:O	1:R:168:TYR:CE2	0.44	2.70	3	1
1:R:42:TYR:CD2	1:R:71:VAL:HG12	0.44	2.47	4	1
1:R:160:TYR:CD2	1:R:168:TYR:C	0.44	2.95	4	2
1:R:60:PHE:CE1	1:R:66:PRO:HB3	0.44	2.47	5	1
1:R:143:LEU:HD21	1:R:146:GLN:HG2	0.44	1.87	5	1
1:R:41:PHE:CG	1:R:162:ILE:HD13	0.44	2.48	1	1
1:R:90:THR:CB	1:R:92:LEU:HG	0.44	2.42	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:54:ASN:HA	1:R:57:LEU:HB2	0.44	1.88	3	1
1:R:107:ILE:HA	1:R:110:LEU:CD2	0.44	2.40	3	1
1:R:33:LEU:HB3	1:R:155:THR:HA	0.44	1.90	4	1
1:R:115:ILE:HG22	1:R:125:CYS:SG	0.44	2.52	4	1
1:R:33:LEU:CD2	1:R:37:GLU:O	0.44	2.66	1	1
1:R:162:ILE:CG2	1:R:167:PHE:CE1	0.44	2.97	1	1
1:R:57:LEU:CD2	1:R:68:PHE:CB	0.44	2.95	2	1
1:R:59:LEU:HD12	1:R:151:PHE:HE1	0.44	1.67	2	1
1:R:34:TYR:CG	1:R:35:ASN:N	0.44	2.85	3	1
1:R:58:GLN:OE1	1:R:151:PHE:CD1	0.44	2.70	4	1
1:R:112:HIS:O	1:R:112:HIS:CG	0.44	2.70	4	1
1:R:125:CYS:O	1:R:126:VAL:CB	0.44	2.63	4	1
1:R:78:LEU:HD12	1:R:81:GLU:OE1	0.44	2.13	5	1
1:R:118:ALA:CB	1:R:128:ASP:O	0.44	2.66	1	1
1:R:37:GLU:O	1:R:39:LYS:N	0.44	2.50	2	1
1:R:59:LEU:O	1:R:62:TYR:HD1	0.44	1.93	2	1
1:R:80:LEU:HD12	1:R:81:GLU:HG3	0.44	1.89	3	2
1:R:56:ILE:HD11	1:R:103:VAL:HB	0.44	1.89	4	1
1:R:130:THR:HG23	1:R:132:MET:HG3	0.44	1.89	1	1
1:R:35:ASN:ND2	1:R:181:VAL:HG11	0.44	2.27	2	1
1:R:40:THR:O	1:R:61:ARG:NH2	0.44	2.51	2	1
1:R:67:PHE:CE1	1:R:89:LEU:CD2	0.44	3.00	3	1
1:R:33:LEU:HD11	1:R:41:PHE:CE1	0.44	2.47	4	1
1:R:56:ILE:CD1	1:R:56:ILE:N	0.44	2.80	4	1
1:R:103:VAL:O	1:R:107:ILE:CD1	0.44	2.65	4	1
1:R:49:ASP:O	1:R:79:THR:HG23	0.44	2.12	1	1
1:R:63:VAL:CG2	1:R:124:VAL:CG1	0.44	2.89	1	1
1:R:132:MET:HB3	1:R:180:PHE:CZ	0.44	2.46	3	1
1:R:53:LEU:HD11	1:R:83:ILE:CD1	0.44	2.41	5	1
1:R:66:PRO:O	1:R:68:PHE:N	0.44	2.51	3	2
1:R:67:PHE:C	1:R:69:ASP:N	0.44	2.74	1	2
1:R:98:GLY:CA	1:R:101:ALA:CB	0.44	2.95	1	1
1:R:126:VAL:O	1:R:180:PHE:CD2	0.44	2.71	1	1
1:R:31:LEU:CD1	1:R:167:PHE:CB	0.44	2.96	2	1
1:R:168:TYR:CD2	1:R:170:TRP:CE3	0.44	3.06	2	1
1:R:142:PHE:CD1	1:R:177:VAL:HG21	0.44	2.47	3	1
1:R:44:ARG:HB3	1:R:165:GLU:CB	0.44	2.43	4	1
1:R:58:GLN:CG	1:R:59:LEU:N	0.44	2.81	4	1
1:R:113:THR:HG23	1:R:114:GLY:H	0.44	1.73	5	1
1:R:170:TRP:O	1:R:171:THR:OG1	0.44	2.35	2	1
1:R:86:LEU:HD11	1:R:103:VAL:CG1	0.44	2.16	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:126:VAL:HG21	1:R:180:PHE:CD1	0.44	2.46	4	1
1:R:55:ALA:CA	1:R:151:PHE:CE2	0.44	2.96	1	1
1:R:143:LEU:N	1:R:143:LEU:CD2	0.44	2.80	4	2
1:R:152:ALA:CA	1:R:161:ALA:CB	0.44	2.95	3	3
1:R:33:LEU:N	1:R:37:GLU:HA	0.44	2.27	2	1
1:R:53:LEU:C	1:R:57:LEU:HB2	0.44	2.37	2	1
1:R:66:PRO:CB	1:R:68:PHE:CE1	0.44	3.01	2	1
1:R:143:LEU:N	1:R:143:LEU:HD22	0.43	2.27	4	2
1:R:94:LEU:HB2	1:R:98:GLY:HA3	0.43	1.88	4	1
1:R:137:PHE:HA	1:R:183:TYR:CE2	0.43	2.48	4	1
1:R:146:GLN:O	1:R:148:HIS:CD2	0.43	2.71	4	2
1:R:58:GLN:CD	1:R:151:PHE:HB2	0.43	2.38	5	1
1:R:125:CYS:HB2	1:R:182:PRO:HG3	0.43	1.89	5	1
1:R:143:LEU:N	1:R:176:ASP:O	0.43	2.48	1	1
1:R:49:ASP:O	1:R:49:ASP:OD1	0.43	2.36	2	1
1:R:90:THR:OG1	1:R:92:LEU:HG	0.43	2.13	2	2
1:R:139:ALA:O	1:R:181:VAL:N	0.43	2.49	3	1
1:R:170:TRP:CG	1:R:171:THR:H	0.43	2.28	3	1
1:R:47:ASN:ND2	1:R:80:LEU:HD23	0.43	2.27	1	1
1:R:103:VAL:O	1:R:107:ILE:HG13	0.43	2.13	1	1
1:R:30:GLU:C	1:R:31:LEU:HD22	0.43	2.37	2	1
1:R:68:PHE:CE2	1:R:72:TYR:HB2	0.43	2.48	2	1
1:R:71:VAL:HG22	1:R:79:THR:HA	0.43	1.89	2	1
1:R:139:ALA:H	1:R:181:VAL:HG12	0.43	1.72	3	1
1:R:43:SER:HA	1:R:165:GLU:HA	0.43	1.90	5	1
1:R:60:PHE:CE2	1:R:61:ARG:HG2	0.43	2.48	5	1
1:R:40:THR:O	1:R:40:THR:HG22	0.43	2.13	1	2
1:R:33:LEU:N	1:R:37:GLU:CA	0.43	2.81	2	1
1:R:127:VAL:O	1:R:128:ASP:C	0.43	2.60	2	1
1:R:60:PHE:HD1	1:R:65:GLU:HB3	0.43	1.72	3	1
1:R:58:GLN:OE1	1:R:151:PHE:HD1	0.43	1.96	4	1
1:R:92:LEU:HD11	1:R:94:LEU:CD2	0.43	2.44	5	1
1:R:41:PHE:CZ	1:R:61:ARG:HB2	0.43	2.49	1	1
1:R:137:PHE:O	1:R:138:HIS:ND1	0.43	2.52	1	1
1:R:137:PHE:HA	1:R:183:TYR:CD1	0.43	2.48	2	1
1:R:58:GLN:OE1	1:R:151:PHE:O	0.43	2.37	3	1
1:R:138:HIS:CD2	1:R:181:VAL:O	0.43	2.71	3	1
1:R:65:GLU:HG3	1:R:112:HIS:CE1	0.43	2.48	4	1
1:R:43:SER:HA	1:R:164:ASP:O	0.43	2.14	1	1
1:R:68:PHE:CE1	1:R:69:ASP:OD1	0.43	2.71	1	1
1:R:126:VAL:CA	1:R:179:VAL:HA	0.43	2.43	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:42:TYR:CD2	1:R:72:TYR:O	0.43	2.72	3	1
1:R:99:PRO:HD2	1:R:100:PRO:HD2	0.43	1.89	3	2
1:R:138:HIS:ND1	1:R:183:TYR:CE2	0.43	2.86	4	1
1:R:32:THR:O	1:R:155:THR:HA	0.43	2.14	5	2
1:R:67:PHE:CG	1:R:86:LEU:HD23	0.43	2.49	1	1
1:R:180:PHE:CE2	1:R:182:PRO:HB3	0.43	2.48	3	1
1:R:51:ALA:O	1:R:54:ASN:CG	0.43	2.62	4	1
1:R:68:PHE:O	1:R:69:ASP:C	0.43	2.61	4	1
1:R:180:PHE:CE2	1:R:182:PRO:N	0.43	2.87	4	1
1:R:86:LEU:CD1	1:R:94:LEU:CD2	0.43	2.91	5	1
1:R:61:ARG:NH1	1:R:61:ARG:CG	0.43	2.78	1	1
1:R:31:LEU:CD1	1:R:167:PHE:HB2	0.43	2.44	2	1
1:R:53:LEU:C	1:R:57:LEU:HB3	0.43	2.39	2	1
1:R:140:GLY:HA3	1:R:179:VAL:O	0.43	2.14	2	1
1:R:77:ASN:O	1:R:78:LEU:HB2	0.43	2.14	3	1
1:R:128:ASP:CA	1:R:178:LEU:CD1	0.43	2.97	3	1
1:R:33:LEU:HD21	1:R:36:GLY:O	0.43	2.14	4	1
1:R:159:TRP:C	1:R:170:TRP:O	0.43	2.62	4	1
1:R:44:ARG:CA	1:R:164:ASP:C	0.43	2.92	5	1
1:R:58:GLN:NE2	1:R:162:ILE:O	0.43	2.51	1	1
1:R:107:ILE:HG23	1:R:110:LEU:CD2	0.43	2.43	1	1
1:R:155:THR:HG23	1:R:160:TYR:HB3	0.43	1.91	2	1
1:R:33:LEU:C	1:R:33:LEU:CD2	0.43	2.92	3	1
1:R:59:LEU:CD1	1:R:62:TYR:CE1	0.43	3.01	5	1
1:R:181:VAL:CG1	1:R:181:VAL:O	0.43	2.64	5	1
1:R:53:LEU:C	1:R:55:ALA:N	0.43	2.74	4	2
1:R:134:LEU:HD21	1:R:171:THR:CB	0.43	2.42	1	1
1:R:67:PHE:CZ	1:R:86:LEU:HD21	0.43	2.49	2	1
1:R:33:LEU:HD21	1:R:37:GLU:CB	0.43	2.41	3	1
1:R:62:TYR:CD1	1:R:181:VAL:HG21	0.43	2.49	3	1
1:R:69:ASP:HA	1:R:72:TYR:CD2	0.43	2.49	3	1
1:R:83:ILE:HG21	1:R:94:LEU:HB2	0.43	1.90	3	1
1:R:118:ALA:HB3	1:R:130:THR:HB	0.43	1.90	4	1
1:R:115:ILE:HG23	1:R:124:VAL:N	0.43	2.29	5	1
1:R:115:ILE:CG1	1:R:122:SER:C	0.43	2.92	5	1
1:R:128:ASP:CG	1:R:129:GLY:H	0.42	2.22	1	1
1:R:69:ASP:HA	1:R:73:SER:HB3	0.42	1.90	2	1
1:R:33:LEU:HD13	1:R:37:GLU:O	0.42	2.13	3	1
1:R:43:SER:C	1:R:44:ARG:O	0.42	2.62	3	1
1:R:89:LEU:N	1:R:89:LEU:CD1	0.42	2.79	3	1
1:R:158:GLY:O	1:R:160:TYR:N	0.42	2.51	3	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:51:ALA:HB1	1:R:149:ALA:H	0.42	1.74	2	1
1:R:41:PHE:CD2	1:R:151:PHE:CZ	0.42	3.07	4	1
1:R:151:PHE:CE2	1:R:162:ILE:O	0.42	2.71	4	1
1:R:168:TYR:OH	1:R:170:TRP:CD1	0.42	2.72	5	1
1:R:53:LEU:HD11	1:R:82:ALA:HB3	0.42	1.92	4	2
1:R:70:TRP:HB3	1:R:82:ALA:HA	0.42	1.91	1	1
1:R:80:LEU:N	1:R:80:LEU:HD12	0.42	2.29	1	1
1:R:98:GLY:HA2	1:R:101:ALA:CB	0.42	2.44	1	1
1:R:136:ASP:HB3	1:R:173:ASP:OD1	0.42	2.14	2	1
1:R:31:LEU:HD22	1:R:167:PHE:CD1	0.42	2.49	5	1
1:R:69:ASP:O	1:R:72:TYR:CD1	0.42	2.72	5	1
1:R:33:LEU:HA	1:R:155:THR:C	0.42	2.38	1	1
1:R:57:LEU:O	1:R:60:PHE:N	0.42	2.52	3	2
1:R:155:THR:N	1:R:158:GLY:O	0.42	2.47	1	2
1:R:66:PRO:HB2	1:R:68:PHE:CE1	0.42	2.49	2	1
1:R:133:CYS:O	1:R:135:ALA:N	0.42	2.52	5	2
1:R:183:TYR:N	1:R:183:TYR:HD1	0.42	2.10	3	1
1:R:53:LEU:CD2	1:R:57:LEU:CD2	0.42	2.98	4	1
1:R:55:ALA:HB1	1:R:99:PRO:HA	0.42	1.91	4	1
1:R:58:GLN:NE2	1:R:141:ILE:HG12	0.42	2.29	4	1
1:R:60:PHE:N	1:R:60:PHE:CD1	0.42	2.86	4	1
1:R:41:PHE:CD2	1:R:58:GLN:HB2	0.42	2.49	5	1
1:R:53:LEU:CD2	1:R:68:PHE:CD2	0.42	3.02	5	1
1:R:59:LEU:HG	1:R:141:ILE:CG1	0.42	2.44	5	1
1:R:62:TYR:HE2	1:R:181:VAL:CB	0.42	2.27	5	1
1:R:151:PHE:CD1	1:R:151:PHE:N	0.42	2.88	1	1
1:R:159:TRP:CD1	1:R:172:PRO:HD3	0.42	2.50	1	1
1:R:76:GLU:O	1:R:78:LEU:HD13	0.42	2.13	2	1
1:R:86:LEU:O	1:R:87:GLU:C	0.42	2.59	2	1
1:R:159:TRP:C	1:R:169:PRO:HA	0.42	2.37	2	1
1:R:127:VAL:HA	1:R:130:THR:OG1	0.42	2.14	3	1
1:R:55:ALA:CB	1:R:141:ILE:CD1	0.42	2.98	4	1
1:R:56:ILE:HG23	1:R:60:PHE:CD2	0.42	2.48	4	1
1:R:39:LYS:HB3	1:R:61:ARG:HD3	0.42	1.92	1	1
1:R:100:PRO:HA	1:R:104:ILE:HG12	0.42	1.92	3	1
1:R:141:ILE:O	1:R:177:VAL:CA	0.42	2.68	3	1
1:R:52:TRP:CD1	1:R:96:GLU:HA	0.42	2.50	4	1
1:R:32:THR:HG22	1:R:38:LYS:HA	0.42	1.91	5	1
1:R:115:ILE:HG23	1:R:124:VAL:CA	0.42	2.44	5	1
1:R:55:ALA:HB2	1:R:99:PRO:HB3	0.42	1.89	1	1
1:R:102:LEU:HD22	1:R:105:TRP:CG	0.42	2.49	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:104:ILE:HG13	1:R:105:TRP:N	0.42	2.29	2	2
1:R:142:PHE:CE1	1:R:177:VAL:CG1	0.42	2.99	1	1
1:R:104:ILE:CB	1:R:111:LEU:HD12	0.42	2.44	2	1
1:R:33:LEU:H	1:R:33:LEU:HD13	0.42	1.74	3	1
1:R:136:ASP:O	1:R:137:PHE:CG	0.42	2.73	3	1
1:R:56:ILE:HG13	1:R:68:PHE:CG	0.42	2.50	5	1
1:R:86:LEU:HG	1:R:103:VAL:CG1	0.42	2.44	5	1
1:R:94:LEU:O	1:R:97:GLY:N	0.42	2.52	5	1
1:R:56:ILE:HA	1:R:59:LEU:CB	0.42	2.44	2	1
1:R:127:VAL:CG2	1:R:128:ASP:N	0.42	2.82	2	1
1:R:58:GLN:CB	1:R:151:PHE:HB3	0.42	2.44	3	1
1:R:62:TYR:CE1	1:R:139:ALA:CB	0.42	3.02	3	1
1:R:150:VAL:HB	1:R:163:ASP:CG	0.42	2.40	3	1
1:R:183:TYR:CD1	1:R:183:TYR:C	0.42	2.97	4	2
1:R:32:THR:HG22	1:R:38:LYS:CA	0.42	2.45	4	1
1:R:58:GLN:O	1:R:62:TYR:CG	0.42	2.73	4	1
1:R:116:GLY:O	1:R:125:CYS:SG	0.42	2.78	4	1
1:R:163:ASP:CG	1:R:168:TYR:CE1	0.42	2.98	5	1
1:R:83:ILE:CG2	1:R:94:LEU:CD1	0.42	2.95	1	1
1:R:84:LYS:O	1:R:87:GLU:HG2	0.42	2.14	1	1
1:R:34:TYR:HB2	1:R:154:VAL:HG12	0.42	1.90	2	1
1:R:42:TYR:CD2	1:R:42:TYR:N	0.42	2.88	2	1
1:R:127:VAL:O	1:R:130:THR:HB	0.42	2.15	2	1
1:R:34:TYR:CB	1:R:154:VAL:CG1	0.42	2.97	3	1
1:R:69:ASP:HA	1:R:72:TYR:CE2	0.42	2.49	3	1
1:R:140:GLY:HA3	1:R:180:PHE:HA	0.42	1.91	5	1
1:R:157:ASN:HB2	1:R:160:TYR:CZ	0.42	2.50	5	1
1:R:52:TRP:CD1	1:R:97:GLY:HA2	0.42	2.49	1	1
1:R:60:PHE:HB2	1:R:68:PHE:CG	0.42	2.50	1	1
1:R:31:LEU:CG	1:R:41:PHE:CD1	0.42	3.02	2	1
1:R:32:THR:OG1	1:R:155:THR:CB	0.42	2.68	2	1
1:R:59:LEU:CD1	1:R:151:PHE:CE1	0.42	3.01	2	1
1:R:53:LEU:HD12	1:R:79:THR:HA	0.42	1.92	5	1
1:R:134:LEU:CD2	1:R:173:ASP:CB	0.42	2.98	5	1
1:R:39:LYS:HG2	1:R:60:PHE:CZ	0.41	2.50	1	1
1:R:39:LYS:O	1:R:41:PHE:CD1	0.41	2.73	4	2
1:R:86:LEU:CD1	1:R:103:VAL:CG1	0.41	2.92	2	1
1:R:134:LEU:CD1	1:R:172:PRO:CD	0.41	2.84	2	1
1:R:42:TYR:CE1	1:R:75:PRO:O	0.41	2.73	3	1
1:R:59:LEU:HD13	1:R:151:PHE:CD2	0.41	2.48	3	1
1:R:60:PHE:CD1	1:R:65:GLU:CB	0.41	3.03	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:92:LEU:HG	1:R:93:GLU:N	0.41	2.29	3	1
1:R:164:ASP:O	1:R:165:GLU:C	0.41	2.63	3	1
1:R:46:ASN:CB	1:R:164:ASP:CG	0.41	2.92	4	1
1:R:47:ASN:O	1:R:48:HIS:CB	0.41	2.67	5	1
1:R:89:LEU:HD23	1:R:90:THR:HG23	0.41	1.91	1	1
1:R:94:LEU:HD12	1:R:95:HIS:N	0.41	2.29	1	1
1:R:35:ASN:HB3	1:R:153:CYS:CB	0.41	2.45	2	1
1:R:137:PHE:CD1	1:R:180:PHE:HB2	0.41	2.50	2	1
1:R:144:LYS:O	1:R:148:HIS:CB	0.41	2.68	3	1
1:R:126:VAL:C	1:R:180:PHE:CD2	0.41	2.98	5	1
1:R:53:LEU:CD2	1:R:83:ILE:CG1	0.41	2.98	1	2
1:R:99:PRO:HB2	1:R:100:PRO:HD3	0.41	1.92	1	2
1:R:60:PHE:CZ	1:R:72:TYR:CG	0.41	3.07	3	1
1:R:118:ALA:HA	1:R:130:THR:CG2	0.41	2.45	3	1
1:R:53:LEU:HD13	1:R:79:THR:HA	0.41	1.93	1	1
1:R:55:ALA:CB	1:R:99:PRO:HB3	0.41	2.46	4	2
1:R:63:VAL:HG21	1:R:124:VAL:HG11	0.41	1.89	2	1
1:R:101:ALA:O	1:R:104:ILE:CG1	0.41	2.67	2	1
1:R:33:LEU:CD2	1:R:35:ASN:OD1	0.41	2.67	3	1
1:R:102:LEU:HD12	1:R:102:LEU:H	0.41	1.73	3	1
1:R:127:VAL:CA	1:R:130:THR:OG1	0.41	2.68	3	1
1:R:41:PHE:HA	1:R:72:TYR:CE1	0.41	2.51	4	1
1:R:41:PHE:CG	1:R:162:ILE:HD12	0.41	2.50	4	1
1:R:33:LEU:HD12	1:R:61:ARG:NH1	0.41	2.30	1	1
1:R:92:LEU:HD23	1:R:102:LEU:C	0.41	2.41	2	1
1:R:163:ASP:O	1:R:166:ASP:N	0.41	2.43	2	1
1:R:64:GLU:O	1:R:66:PRO:CD	0.41	2.69	3	1
1:R:76:GLU:O	1:R:78:LEU:N	0.41	2.54	3	1
1:R:94:LEU:O	1:R:96:GLU:N	0.41	2.53	4	1
1:R:55:ALA:CB	1:R:99:PRO:HG3	0.41	2.45	5	1
1:R:58:GLN:CG	1:R:151:PHE:HB2	0.41	2.46	5	1
1:R:60:PHE:HB2	1:R:65:GLU:HA	0.41	1.93	1	1
1:R:102:LEU:HA	1:R:105:TRP:HB2	0.41	1.91	4	3
1:R:125:CYS:HB2	1:R:182:PRO:HD3	0.41	1.93	1	1
1:R:134:LEU:HD12	1:R:159:TRP:CD2	0.41	2.51	1	1
1:R:61:ARG:HD3	1:R:68:PHE:CZ	0.41	2.50	2	1
1:R:100:PRO:C	1:R:102:LEU:N	0.41	2.76	3	1
1:R:139:ALA:CB	1:R:181:VAL:HG12	0.41	2.36	4	1
1:R:39:LYS:HG2	1:R:61:ARG:CA	0.41	2.46	5	1
1:R:54:ASN:OD1	1:R:58:GLN:CG	0.41	2.69	1	1
1:R:84:LYS:O	1:R:87:GLU:CG	0.41	2.69	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:111:LEU:HD12	1:R:112:HIS:N	0.41	2.31	2	1
1:R:142:PHE:CE2	1:R:173:ASP:O	0.41	2.74	2	2
1:R:39:LYS:HB3	1:R:61:ARG:HD2	0.41	1.93	3	1
1:R:46:ASN:ND2	1:R:76:GLU:O	0.41	2.54	3	1
1:R:92:LEU:C	1:R:92:LEU:CD2	0.41	2.89	3	1
1:R:142:PHE:CD2	1:R:171:THR:OG1	0.41	2.73	3	1
1:R:44:ARG:CB	1:R:45:PRO:HD2	0.41	2.46	4	1
1:R:57:LEU:HD13	1:R:68:PHE:CD2	0.41	2.50	4	1
1:R:70:TRP:CZ3	1:R:81:GLU:OE2	0.41	2.74	4	1
1:R:137:PHE:O	1:R:138:HIS:CD2	0.41	2.73	4	1
1:R:35:ASN:O	1:R:62:TYR:O	0.41	2.38	5	1
1:R:57:LEU:O	1:R:60:PHE:CB	0.41	2.68	1	1
1:R:138:HIS:HB3	1:R:154:VAL:CG2	0.41	2.46	1	1
1:R:97:GLY:O	1:R:98:GLY:O	0.41	2.39	2	1
1:R:44:ARG:HA	1:R:164:ASP:C	0.41	2.41	3	1
1:R:36:GLY:HA3	1:R:62:TYR:HA	0.41	1.92	5	1
1:R:44:ARG:H	1:R:165:GLU:CB	0.41	2.26	5	1
1:R:117:THR:N	1:R:120:ARG:O	0.41	2.54	5	1
1:R:56:ILE:CA	1:R:59:LEU:HB2	0.41	2.46	2	1
1:R:56:ILE:CG2	1:R:100:PRO:O	0.41	2.68	2	1
1:R:57:LEU:CD1	1:R:57:LEU:C	0.41	2.94	2	1
1:R:62:TYR:HE2	1:R:181:VAL:CG2	0.41	2.29	2	1
1:R:76:GLU:O	1:R:77:ASN:C	0.41	2.64	2	1
1:R:177:VAL:O	1:R:178:LEU:CD2	0.41	2.69	2	1
1:R:40:THR:O	1:R:40:THR:HG23	0.41	2.15	3	1
1:R:48:HIS:O	1:R:49:ASP:O	0.41	2.39	3	1
1:R:56:ILE:HD12	1:R:103:VAL:CG1	0.41	2.42	3	1
1:R:93:GLU:O	1:R:94:LEU:HD13	0.41	2.16	3	1
1:R:168:TYR:CE1	1:R:170:TRP:CB	0.41	3.04	3	1
1:R:107:ILE:HG22	1:R:111:LEU:HB2	0.41	1.93	4	1
1:R:138:HIS:CB	1:R:172:PRO:HG2	0.41	2.46	4	1
1:R:155:THR:HG1	1:R:160:TYR:CB	0.41	2.29	4	1
1:R:69:ASP:HA	1:R:72:TYR:CE1	0.41	2.51	5	1
1:R:90:THR:HB	1:R:92:LEU:CD2	0.41	2.45	5	1
1:R:127:VAL:HG13	1:R:180:PHE:HD2	0.41	1.76	5	1
1:R:54:ASN:ND2	1:R:55:ALA:N	0.41	2.69	2	1
1:R:61:ARG:CD	1:R:68:PHE:CE2	0.41	3.03	2	1
1:R:102:LEU:N	1:R:102:LEU:CD1	0.41	2.83	3	1
1:R:117:THR:HG22	1:R:118:ALA:H	0.41	1.76	3	1
1:R:42:TYR:CD2	1:R:71:VAL:CG1	0.41	3.04	4	1
1:R:173:ASP:O	1:R:177:VAL:HG13	0.41	2.13	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:115:ILE:HG21	1:R:123:GLU:N	0.41	2.31	5	1
1:R:179:VAL:HG23	1:R:179:VAL:O	0.41	2.15	5	1
1:R:55:ALA:CB	1:R:99:PRO:CB	0.40	2.99	1	1
1:R:128:ASP:CG	1:R:174:PRO:CG	0.40	2.94	1	1
1:R:51:ALA:CA	1:R:164:ASP:OD2	0.40	2.69	3	1
1:R:44:ARG:HB3	1:R:164:ASP:O	0.40	2.16	5	1
1:R:83:ILE:HD13	1:R:95:HIS:HB3	0.40	1.92	5	1
1:R:54:ASN:CG	1:R:151:PHE:CD1	0.40	3.00	1	1
1:R:60:PHE:CB	1:R:66:PRO:HD2	0.40	2.46	1	1
1:R:49:ASP:CG	1:R:95:HIS:O	0.40	2.64	2	1
1:R:38:LYS:O	1:R:38:LYS:CG	0.40	2.69	3	1
1:R:71:VAL:O	1:R:77:ASN:O	0.40	2.39	3	1
1:R:78:LEU:HD12	1:R:81:GLU:HB2	0.40	1.93	3	1
1:R:86:LEU:CD1	1:R:90:THR:OG1	0.40	2.64	3	1
1:R:92:LEU:HG	1:R:94:LEU:CD2	0.40	2.46	3	1
1:R:68:PHE:CZ	1:R:103:VAL:CG1	0.40	3.04	5	1
1:R:145:GLY:O	1:R:146:GLN:O	0.40	2.40	5	1
1:R:98:GLY:C	1:R:101:ALA:HB3	0.40	2.41	1	1
1:R:154:VAL:HG22	1:R:159:TRP:CD1	0.40	2.52	1	1
1:R:157:ASN:HB3	1:R:160:TYR:CZ	0.40	2.51	1	1
1:R:58:GLN:HB3	1:R:151:PHE:CD2	0.40	2.52	2	1
1:R:100:PRO:HA	1:R:104:ILE:CG1	0.40	2.46	3	1
1:R:137:PHE:CZ	1:R:159:TRP:NE1	0.40	2.89	3	1
1:R:62:TYR:CB	1:R:181:VAL:HG21	0.40	2.35	4	1
1:R:68:PHE:O	1:R:71:VAL:N	0.40	2.49	4	1
1:R:69:ASP:O	1:R:73:SER:OG	0.40	2.39	4	1
1:R:56:ILE:HB	1:R:68:PHE:CE1	0.40	2.52	5	1
1:R:67:PHE:HB2	1:R:68:PHE:CD1	0.40	2.51	5	1
1:R:76:GLU:CG	1:R:78:LEU:HD23	0.40	2.47	5	1
1:R:178:LEU:HA	1:R:178:LEU:HD13	0.40	1.74	5	1
1:R:60:PHE:CG	1:R:68:PHE:CD2	0.40	3.09	1	1
1:R:94:LEU:CD1	1:R:94:LEU:C	0.40	2.95	1	1
1:R:51:ALA:HB1	1:R:149:ALA:CB	0.40	2.46	2	1
1:R:116:GLY:N	1:R:122:SER:HB2	0.40	2.31	2	1
1:R:137:PHE:CE1	1:R:180:PHE:CB	0.40	2.97	2	1
1:R:142:PHE:CD1	1:R:177:VAL:CG1	0.40	3.04	2	1
1:R:86:LEU:HD11	1:R:103:VAL:HA	0.40	1.93	3	1
1:R:141:ILE:C	1:R:142:PHE:CD1	0.40	2.97	4	1
1:R:33:LEU:CA	1:R:155:THR:HA	0.40	2.45	5	1
1:R:58:GLN:CG	1:R:151:PHE:CB	0.40	2.99	5	1
1:R:59:LEU:CD2	1:R:141:ILE:HG12	0.40	2.46	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:R:92:LEU:O	1:R:93:GLU:CB	0.40	2.69	5	1
1:R:47:ASN:OD1	1:R:80:LEU:CD2	0.40	2.70	1	1
1:R:59:LEU:N	1:R:59:LEU:CD1	0.40	2.83	1	1
1:R:94:LEU:HD12	1:R:94:LEU:H	0.40	1.76	1	1
1:R:53:LEU:CD2	1:R:83:ILE:HG12	0.40	2.47	2	1
1:R:52:TRP:CG	1:R:97:GLY:CA	0.40	3.05	4	1
1:R:59:LEU:HD21	1:R:179:VAL:CG2	0.40	2.46	4	1
1:R:160:TYR:CZ	1:R:169:PRO:HB3	0.40	2.51	4	1
1:R:33:LEU:HD22	1:R:36:GLY:C	0.40	2.40	5	1
1:R:94:LEU:C	1:R:97:GLY:H	0.40	2.25	5	1
1:R:139:ALA:O	1:R:180:PHE:HA	0.40	2.17	5	1
1:R:155:THR:HG23	1:R:160:TYR:HB2	0.40	1.91	5	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	155/167 (93%)	109±3 (70±2%)	29±2 (19±2%)	18±3 (11±2%)	1	7
All	All	775/835 (93%)	543 (70%)	144 (19%)	88 (11%)	1	7

All 48 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	R	93	GLU	4
1	R	99	PRO	4
1	R	101	ALA	4
1	R	102	LEU	4
1	R	49	ASP	4
1	R	64	GLU	3
1	R	112	HIS	3
1	R	164	ASP	3
1	R	37	GLU	3
1	R	43	SER	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	R	128	ASP	3
1	R	159	TRP	3
1	R	67	PHE	2
1	R	68	PHE	2
1	R	98	GLY	2
1	R	111	LEU	2
1	R	126	VAL	2
1	R	127	VAL	2
1	R	179	VAL	2
1	R	34	TYR	2
1	R	48	HIS	2
1	R	134	LEU	2
1	R	77	ASN	2
1	R	94	LEU	1
1	R	139	ALA	1
1	R	33	LEU	1
1	R	36	GLY	1
1	R	71	VAL	1
1	R	135	ALA	1
1	R	171	THR	1
1	R	44	ARG	1
1	R	45	PRO	1
1	R	78	LEU	1
1	R	136	ASP	1
1	R	138	HIS	1
1	R	147	GLU	1
1	R	172	PRO	1
1	R	183	TYR	1
1	R	125	CYS	1
1	R	165	GLU	1
1	R	46	ASN	1
1	R	113	THR	1
1	R	120	ARG	1
1	R	122	SER	1
1	R	124	VAL	1
1	R	131	ASP	1
1	R	146	GLN	1
1	R	154	VAL	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	136/145 (94%)	106±2 (78±1%)	30±2 (22±1%)	2	30
All	All	680/725 (94%)	531 (78%)	149 (22%)	2	30

All 62 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	R	33	LEU	5
1	R	80	LEU	5
1	R	83	ILE	5
1	R	92	LEU	5
1	R	110	LEU	5
1	R	134	LEU	5
1	R	181	VAL	5
1	R	40	THR	4
1	R	56	ILE	4
1	R	78	LEU	4
1	R	111	LEU	4
1	R	170	TRP	4
1	R	171	THR	4
1	R	177	VAL	4
1	R	47	ASN	4
1	R	159	TRP	4
1	R	178	LEU	4
1	R	59	LEU	3
1	R	60	PHE	3
1	R	94	LEU	3
1	R	124	VAL	3
1	R	162	ILE	3
1	R	120	ARG	3
1	R	41	PHE	2
1	R	58	GLN	2
1	R	61	ARG	2
1	R	79	THR	2
1	R	89	LEU	2
1	R	137	PHE	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	R	148	HIS	2
1	R	173	ASP	2
1	R	179	VAL	2
1	R	54	ASN	2
1	R	74	SER	2
1	R	107	ILE	2
1	R	122	SER	2
1	R	138	HIS	2
1	R	142	PHE	2
1	R	160	TYR	2
1	R	109	HIS	2
1	R	31	LEU	1
1	R	46	ASN	1
1	R	62	TYR	1
1	R	65	GLU	1
1	R	136	ASP	1
1	R	32	THR	1
1	R	44	ARG	1
1	R	68	PHE	1
1	R	133	CYS	1
1	R	153	CYS	1
1	R	86	LEU	1
1	R	183	TYR	1
1	R	43	SER	1
1	R	117	THR	1
1	R	125	CYS	1
1	R	126	VAL	1
1	R	141	ILE	1
1	R	151	PHE	1
1	R	48	HIS	1
1	R	130	THR	1
1	R	165	GLU	1
1	R	180	PHE	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 34% for the well-defined parts and 34% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	774
Number of shifts mapped to atoms	774
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

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	162	-0.27 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	151	0.18 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	161	0.08 ± 0.11	None needed (< 0.5 ppm)
^{15}N	150	0.67 ± 0.32	Should be applied

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 34%, i.e. 722 atoms were assigned a chemical shift out of a possible 2099. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	581/770 (75%)	140/312 (45%)	301/312 (96%)	140/146 (96%)
Sidechain	141/1074 (13%)	0/702 (0%)	141/347 (41%)	0/25 (0%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Aromatic	0/255 (0%)	0/127 (0%)	0/117 (0%)	0/11 (0%)
Overall	722/2099 (34%)	140/1141 (12%)	442/776 (57%)	140/182 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 34%, i.e. 774 atoms were assigned a chemical shift out of a possible 2251. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	623/824 (76%)	150/334 (45%)	323/334 (97%)	150/156 (96%)
Sidechain	151/1160 (13%)	0/756 (0%)	151/375 (40%)	0/29 (0%)
Aromatic	0/267 (0%)	0/133 (0%)	0/122 (0%)	0/12 (0%)
Overall	774/2251 (34%)	150/1223 (12%)	474/831 (57%)	150/197 (76%)

7.1.4 Statistically unusual chemical shifts [i](#)

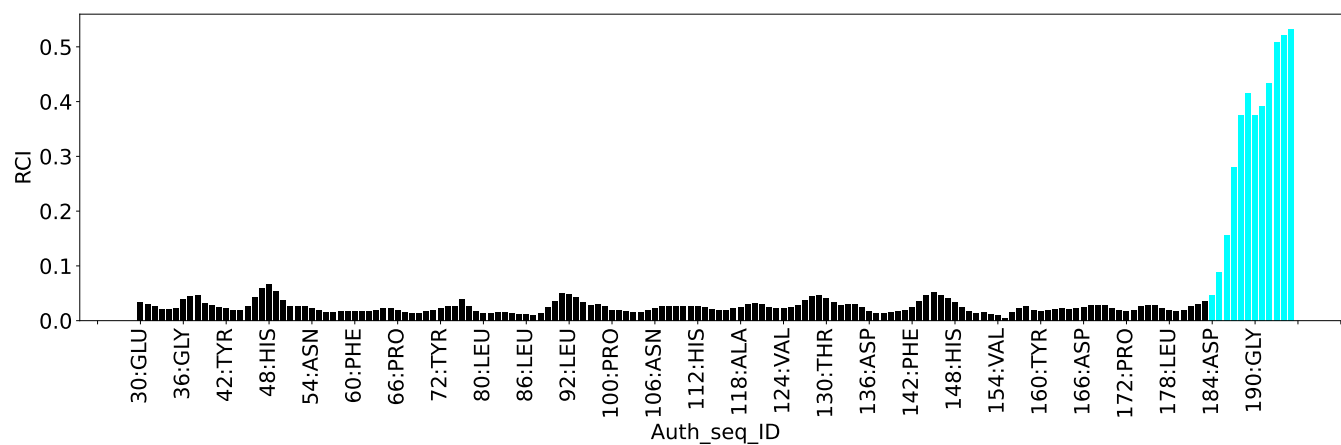
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	R	155	THR	CB	15.33	61.12 – 78.27	-31.7

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 R:



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	2439
Intra-residue ($ i-j =0$)	806
Sequential ($ i-j =1$)	686
Medium range ($ i-j >1$ and $ i-j <5$)	390
Long range ($ i-j \geq 5$)	439
Inter-chain	0
Hydrogen bond restraints	118
Disulfide bond restraints	0
Total dihedral-angle restraints	216
Number of unmapped restraints	0
Number of restraints per residue	15.9
Number of long range restraints per residue ¹	2.9

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	100.4	0.2
0.2-0.5 (Medium)	153.2	0.5
>0.5 (Large)	93.2	2.54

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)	72.6	9.67
10.0-20.0 (Medium)	25.8	20.0
>20.0 (Large)	25.4	114.55

9 Distance violation analysis ⓘ

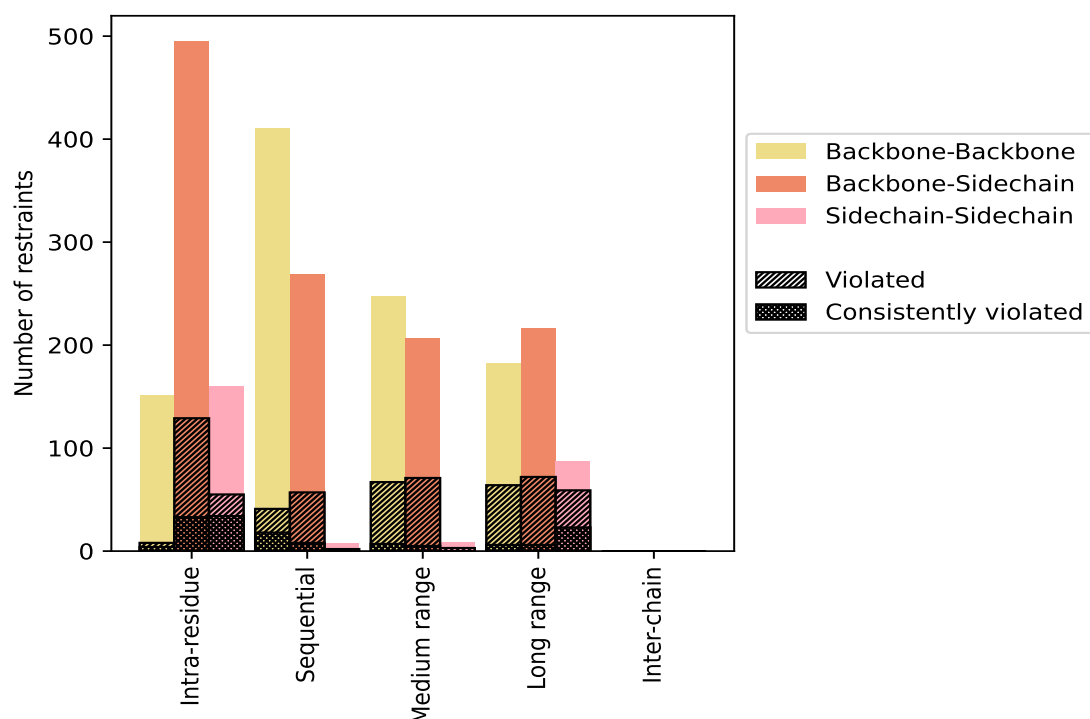
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	806	33.0	192	23.8	7.9	71	8.8	2.9
Backbone-Backbone	151	6.2	8	5.3	0.3	4	2.6	0.2
Backbone-Sidechain	495	20.3	129	26.1	5.3	33	6.7	1.4
Sidechain-Sidechain	160	6.6	55	34.4	2.3	34	21.2	1.4
Sequential ($i-j =1$)	686	28.1	100	14.6	4.1	26	3.8	1.1
Backbone-Backbone	410	16.8	41	10.0	1.7	18	4.4	0.7
Backbone-Sidechain	269	11.0	57	21.2	2.3	8	3.0	0.3
Sidechain-Sidechain	7	0.3	2	28.6	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	390	16.0	102	26.2	4.2	10	2.6	0.4
Backbone-Backbone	247	10.1	67	27.1	2.7	7	2.8	0.3
Backbone-Sidechain	135	5.5	32	23.7	1.3	3	2.2	0.1
Sidechain-Sidechain	8	0.3	3	37.5	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	439	18.0	178	40.5	7.3	34	7.7	1.4
Backbone-Backbone	182	7.5	64	35.2	2.6	6	3.3	0.2
Backbone-Sidechain	170	7.0	55	32.4	2.3	5	2.9	0.2
Sidechain-Sidechain	87	3.6	59	67.8	2.4	23	26.4	0.9
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	118	4.8	56	47.5	2.3	3	2.5	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2439	100.0	628	25.7	25.7	144	5.9	5.9
Backbone-Backbone	990	40.6	180	18.2	7.4	35	3.5	1.4
Backbone-Sidechain	1187	48.7	329	27.7	13.5	52	4.4	2.1
Sidechain-Sidechain	262	10.7	119	45.4	4.9	57	21.8	2.3

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

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



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

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

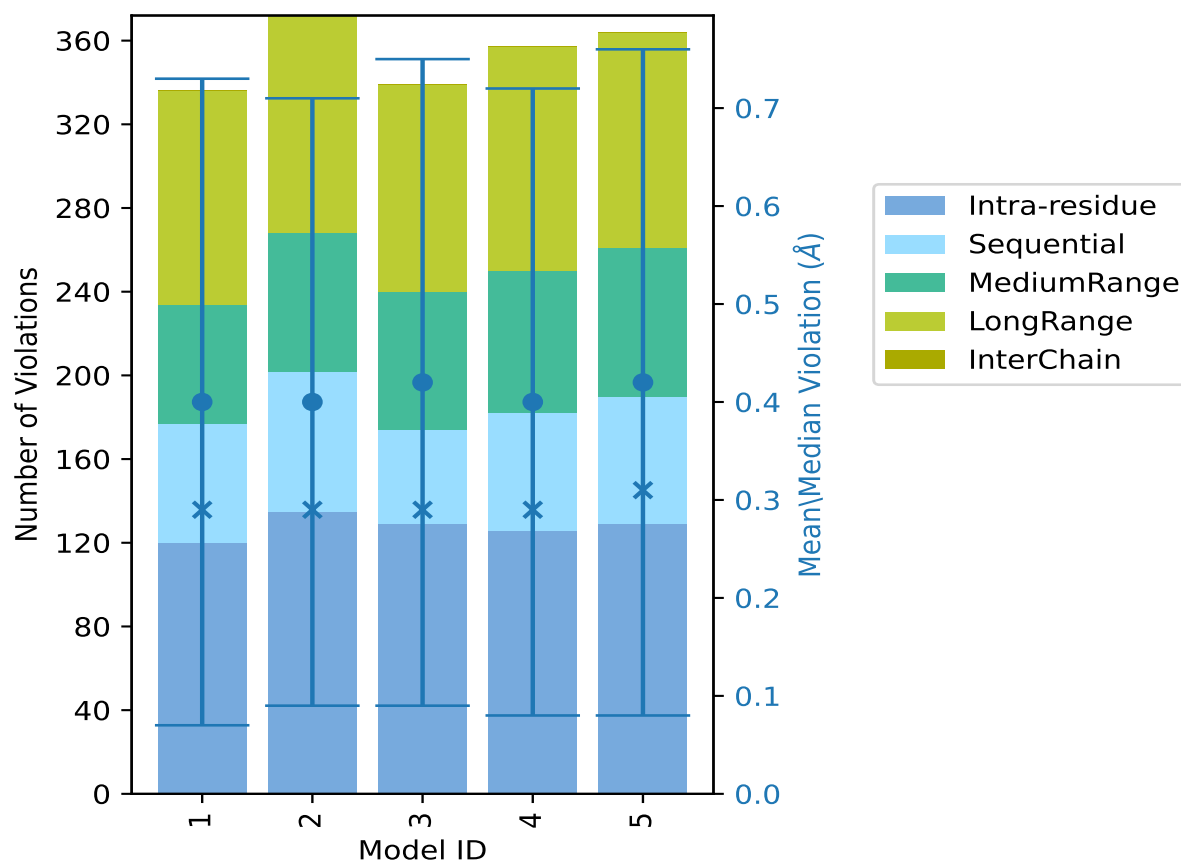
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	120	57	57	102	0	336	0.4	2.54	0.33	0.29
2	135	67	66	104	0	372	0.4	2.09	0.31	0.29
3	129	45	66	99	0	339	0.42	2.14	0.33	0.29
4	126	56	68	107	0	357	0.4	2.15	0.32	0.29
5	129	61	71	103	0	364	0.42	2.51	0.34	0.31

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

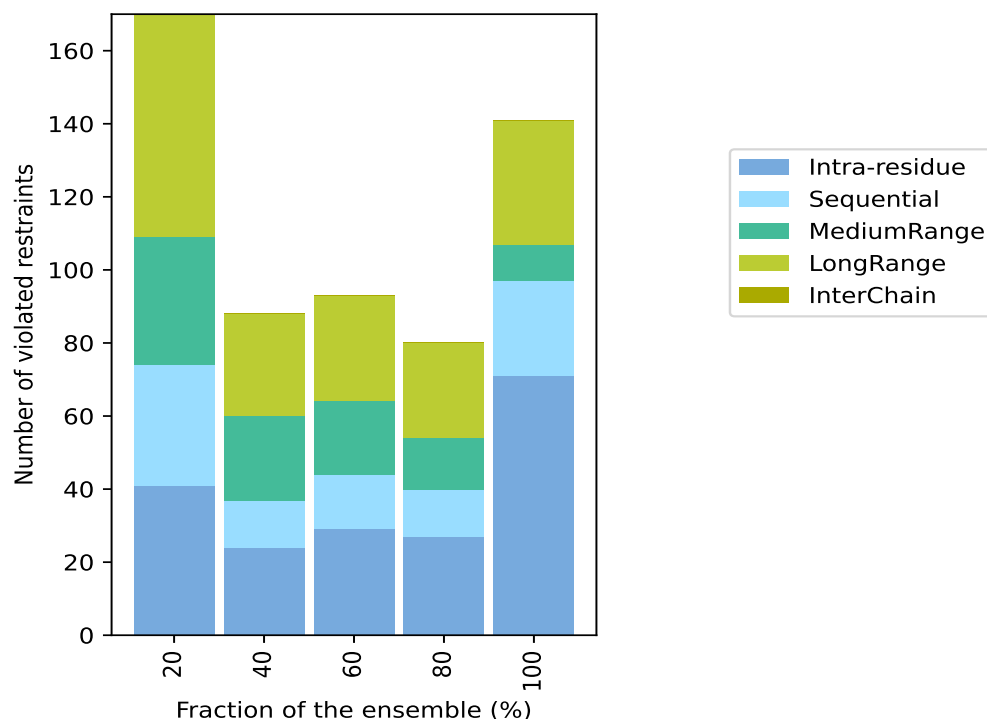
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1749(IR:614, SQ:586, MR:288, LR:261, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
41	33	35	61	0	170	1	20.0
24	13	23	28	0	88	2	40.0
29	15	20	29	0	93	3	60.0
27	13	14	26	0	80	4	80.0
71	26	10	34	0	141	5	100.0

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

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

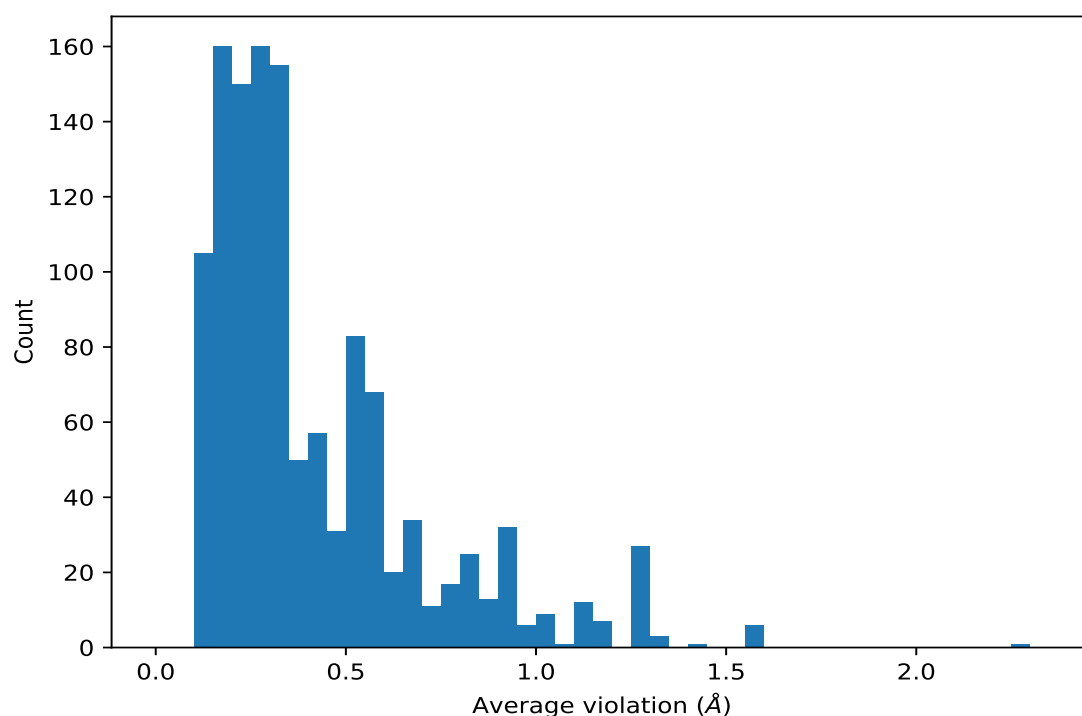
9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ



9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1222)	1:153:R:CYS:H	1:158:R:GLY:HA3	5	2.28	0.19	2.15
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD11	5	1.58	0.26	1.62
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD12	5	1.58	0.26	1.62
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD13	5	1.58	0.26	1.62
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD21	5	1.58	0.26	1.62
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD22	5	1.58	0.26	1.62
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD23	5	1.58	0.26	1.62
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG21	5	1.33	0.15	1.34
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG22	5	1.33	0.15	1.34
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG23	5	1.33	0.15	1.34
(1,29)	1:79:R:THR:H	1:80:R:LEU:HA	5	1.29	0.04	1.32
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD11	5	1.28	0.03	1.27
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD12	5	1.28	0.03	1.27
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD13	5	1.28	0.03	1.27
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD21	5	1.28	0.03	1.27
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD22	5	1.28	0.03	1.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD23	5	1.28	0.03	1.27
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD11	5	1.28	0.03	1.27
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD12	5	1.28	0.03	1.27
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD13	5	1.28	0.03	1.27
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD21	5	1.28	0.03	1.27
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD22	5	1.28	0.03	1.27
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD23	5	1.28	0.03	1.27
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD11	5	1.28	0.03	1.27
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD12	5	1.28	0.03	1.27
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD13	5	1.28	0.03	1.27
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD21	5	1.28	0.03	1.27
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD22	5	1.28	0.03	1.27
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD23	5	1.28	0.03	1.27
(1,1698)	1:42:R:TYR:HE1	1:42:R:TYR:HA	5	1.27	0.09	1.28
(1,1698)	1:42:R:TYR:HE2	1:42:R:TYR:HA	5	1.27	0.09	1.28
(1,2076)	1:49:R:ASP:HB2	1:49:R:ASP:HB3	5	1.17	0.0	1.17
(1,2081)	1:52:R:TRP:HB3	1:52:R:TRP:HB2	5	1.17	0.0	1.17
(1,2088)	1:56:R:ILE:HG13	1:56:R:ILE:HG12	5	1.17	0.0	1.17
(1,2210)	1:153:R:CYS:HB2	1:153:R:CYS:HB3	5	1.17	0.0	1.17
(1,2101)	1:70:R:TRP:HB2	1:70:R:TRP:HB3	5	1.16	0.0	1.16
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD11	5	1.13	0.22	1.13
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD12	5	1.13	0.22	1.13
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD13	5	1.13	0.22	1.13
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD21	5	1.13	0.22	1.13
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD22	5	1.13	0.22	1.13
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD23	5	1.13	0.22	1.13
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD11	5	1.13	0.22	1.13
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD12	5	1.13	0.22	1.13
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD13	5	1.13	0.22	1.13
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD21	5	1.13	0.22	1.13
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD22	5	1.13	0.22	1.13
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD23	5	1.13	0.22	1.13
(1,606)	1:139:R:ALA:H	1:180:R:PHE:HB3	5	1.07	0.42	1.05
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD21	5	0.96	0.12	0.98
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD22	5	0.96	0.12	0.98
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD23	5	0.96	0.12	0.98
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD11	5	0.92	0.35	1.06
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD12	5	0.92	0.35	1.06
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD13	5	0.92	0.35	1.06
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD21	5	0.92	0.35	1.06
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD22	5	0.92	0.35	1.06
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD23	5	0.92	0.35	1.06

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD11	5	0.92	0.35	1.06
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD12	5	0.92	0.35	1.06
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD13	5	0.92	0.35	1.06
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD21	5	0.92	0.35	1.06
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD22	5	0.92	0.35	1.06
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD23	5	0.92	0.35	1.06
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB1	5	0.9	0.13	0.86
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB2	5	0.9	0.13	0.86
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB3	5	0.9	0.13	0.86
(1,2134)	1:94:R:LEU:HD21	1:94:R:LEU:HG	5	0.9	0.02	0.89
(1,2134)	1:94:R:LEU:HD22	1:94:R:LEU:HG	5	0.9	0.02	0.89
(1,2134)	1:94:R:LEU:HD23	1:94:R:LEU:HG	5	0.9	0.02	0.89
(1,2112)	1:53:R:LEU:HD11	1:83:R:ILE:HG13	5	0.89	0.51	1.24
(1,2112)	1:53:R:LEU:HD12	1:83:R:ILE:HG13	5	0.89	0.51	1.24
(1,2112)	1:53:R:LEU:HD13	1:83:R:ILE:HG13	5	0.89	0.51	1.24
(1,2154)	1:111:R:LEU:HD21	1:111:R:LEU:HG	5	0.87	0.01	0.87
(1,2154)	1:111:R:LEU:HD22	1:111:R:LEU:HG	5	0.87	0.01	0.87
(1,2154)	1:111:R:LEU:HD23	1:111:R:LEU:HG	5	0.87	0.01	0.87
(1,2086)	1:56:R:ILE:HD11	1:56:R:ILE:HG13	5	0.85	0.01	0.86
(1,2086)	1:56:R:ILE:HD12	1:56:R:ILE:HG13	5	0.85	0.01	0.86
(1,2086)	1:56:R:ILE:HD13	1:56:R:ILE:HG13	5	0.85	0.01	0.86
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB1	5	0.85	0.0	0.85
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB2	5	0.85	0.0	0.85
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB3	5	0.85	0.0	0.85
(1,2087)	1:56:R:ILE:HD11	1:56:R:ILE:HG12	5	0.84	0.01	0.83
(1,2087)	1:56:R:ILE:HD12	1:56:R:ILE:HG12	5	0.84	0.01	0.83
(1,2087)	1:56:R:ILE:HD13	1:56:R:ILE:HG12	5	0.84	0.01	0.83
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD21	5	0.82	0.03	0.81
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD22	5	0.82	0.03	0.81
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD23	5	0.82	0.03	0.81
(1,1966)	1:70:R:TRP:HB2	1:70:R:TRP:HA	5	0.8	0.0	0.8
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG21	5	0.78	0.09	0.8
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG22	5	0.78	0.09	0.8
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG23	5	0.78	0.09	0.8
(1,1470)	1:81:R:GLU:H	1:80:R:LEU:H	5	0.78	0.02	0.78
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG21	5	0.78	0.09	0.74
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG22	5	0.78	0.09	0.74
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG23	5	0.78	0.09	0.74
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD21	5	0.77	0.32	0.95
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD22	5	0.77	0.32	0.95
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD23	5	0.77	0.32	0.95
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD11	5	0.76	0.03	0.77

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD12	5	0.76	0.03	0.77
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD13	5	0.76	0.03	0.77
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB1	5	0.68	0.03	0.68
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB2	5	0.68	0.03	0.68
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB3	5	0.68	0.03	0.68
(1,1137)	1:126:R:VAL:H	1:124:R:VAL:HA	5	0.67	0.09	0.61
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB1	5	0.67	0.08	0.69
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB2	5	0.67	0.08	0.69
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB3	5	0.67	0.08	0.69
(1,2203)	1:152:R:ALA:H	1:151:R:PHE:HA	5	0.66	0.02	0.67
(1,1361)	1:35:R:ASN:H	1:36:R:GLY:H	5	0.66	0.21	0.76
(1,2212)	1:34:R:TYR:HB2	1:154:R:VAL:HB	5	0.65	0.25	0.58
(1,2212)	1:34:R:TYR:HB3	1:154:R:VAL:HB	5	0.65	0.25	0.58
(1,2191)	1:150:R:VAL:HG11	1:150:R:VAL:HA	5	0.64	0.06	0.66
(1,2191)	1:150:R:VAL:HG12	1:150:R:VAL:HA	5	0.64	0.06	0.66
(1,2191)	1:150:R:VAL:HG13	1:150:R:VAL:HA	5	0.64	0.06	0.66
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG11	5	0.64	0.06	0.66
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG12	5	0.64	0.06	0.66
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG13	5	0.64	0.06	0.66
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD11	5	0.64	0.02	0.65
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD12	5	0.64	0.02	0.65
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD13	5	0.64	0.02	0.65
(1,2208)	1:154:R:VAL:H	1:153:R:CYS:HA	5	0.63	0.07	0.66
(1,2252)	1:178:R:LEU:H	1:177:R:VAL:HA	5	0.63	0.03	0.62
(1,2258)	1:180:R:PHE:HB2	1:180:R:PHE:HA	5	0.62	0.02	0.62
(1,180)	1:33:R:LEU:H	1:36:R:GLY:HA3	5	0.61	0.33	0.38
(1,603)	1:138:R:HIS:H	1:139:R:ALA:HA	5	0.6	0.15	0.67
(1,1356)	1:34:R:TYR:H	1:35:R:ASN:H	5	0.6	0.04	0.58
(1,1359)	1:35:R:ASN:H	1:34:R:TYR:H	5	0.6	0.04	0.58
(1,2215)	1:154:R:VAL:H	1:154:R:VAL:HB	5	0.6	0.02	0.59
(1,2096)	1:64:R:GLU:HB2	1:64:R:GLU:HA	5	0.6	0.02	0.59
(1,2096)	1:64:R:GLU:HB3	1:64:R:GLU:HA	5	0.6	0.02	0.59
(1,2229)	1:167:R:PHE:HA	1:162:R:ILE:HA	5	0.6	0.15	0.62
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG21	5	0.59	0.25	0.62
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG22	5	0.59	0.25	0.62
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG23	5	0.59	0.25	0.62
(1,2204)	1:139:R:ALA:HB1	1:153:R:CYS:HA	5	0.57	0.2	0.48
(1,2204)	1:139:R:ALA:HB2	1:153:R:CYS:HA	5	0.57	0.2	0.48
(1,2204)	1:139:R:ALA:HB3	1:153:R:CYS:HA	5	0.57	0.2	0.48
(1,1639)	1:159:R:TRP:H	1:153:R:CYS:H	5	0.56	0.27	0.63
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD11	5	0.53	0.17	0.57
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD12	5	0.53	0.17	0.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD13	5	0.53	0.17	0.57
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD21	5	0.53	0.17	0.57
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD22	5	0.53	0.17	0.57
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD23	5	0.53	0.17	0.57
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD11	5	0.53	0.17	0.57
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD12	5	0.53	0.17	0.57
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD13	5	0.53	0.17	0.57
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD21	5	0.53	0.17	0.57
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD22	5	0.53	0.17	0.57
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD23	5	0.53	0.17	0.57
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD11	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD12	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD13	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD21	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD22	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD23	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD11	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD12	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD13	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD21	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD22	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD23	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD11	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD12	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD13	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD21	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD22	5	0.53	0.02	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD23	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD11	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD12	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD13	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD11	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD12	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD13	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD11	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD12	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD13	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD11	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD12	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD13	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD11	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD12	5	0.53	0.02	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD13	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD11	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD12	5	0.53	0.02	0.52
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD13	5	0.53	0.02	0.52
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG21	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG22	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG23	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG21	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG22	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG23	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG21	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG22	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG23	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG21	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG22	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG23	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG21	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG22	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG23	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG21	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG22	5	0.51	0.29	0.44
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG23	5	0.51	0.29	0.44
(1,837)	1:41:R:PHE:H	1:41:R:PHE:HZ	5	0.5	0.17	0.57
(1,1292)	1:171:R:THR:H	1:168:R:TYR:HD1	5	0.5	0.3	0.32
(1,1292)	1:171:R:THR:H	1:168:R:TYR:HD2	5	0.5	0.3	0.32
(1,2239)	1:167:R:PHE:HB3	1:167:R:PHE:HA	5	0.5	0.04	0.52
(1,2224)	1:161:R:ALA:H	1:160:R:TYR:HA	5	0.49	0.15	0.51
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD11	5	0.49	0.11	0.52
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD12	5	0.49	0.11	0.52
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD13	5	0.49	0.11	0.52
(1,1550)	1:115:R:ILE:H	1:114:R:GLY:HA3	5	0.48	0.02	0.46
(1,2263)	1:181:R:VAL:H	1:181:R:VAL:HB	5	0.48	0.07	0.5
(1,1976)	1:83:R:ILE:HG21	1:83:R:ILE:HG13	5	0.46	0.31	0.26
(1,1976)	1:83:R:ILE:HG22	1:83:R:ILE:HG13	5	0.46	0.31	0.26
(1,1976)	1:83:R:ILE:HG23	1:83:R:ILE:HG13	5	0.46	0.31	0.26
(1,2219)	1:155:R:THR:HB	1:155:R:THR:HA	5	0.46	0.03	0.46
(1,2190)	1:150:R:VAL:HB	1:150:R:VAL:HA	5	0.45	0.01	0.45
(1,1405)	1:55:R:ALA:H	1:52:R:TRP:HA	5	0.45	0.03	0.46
(1,1805)	1:110:R:LEU:HA	1:110:R:LEU:HG	5	0.44	0.08	0.45
(1,1389)	1:47:R:ASN:H	1:47:R:ASN:HB3	5	0.43	0.04	0.43
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG11	5	0.43	0.17	0.36
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG12	5	0.43	0.17	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG13	5	0.43	0.17	0.36
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD11	5	0.42	0.08	0.42
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD12	5	0.42	0.08	0.42
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD13	5	0.42	0.08	0.42
(1,2099)	1:70:R:TRP:HA	1:70:R:TRP:HB3	5	0.42	0.02	0.41
(1,723)	1:168:R:TYR:H	1:162:R:ILE:H	5	0.41	0.12	0.39
(1,1591)	1:137:R:PHE:H	1:181:R:VAL:H	5	0.4	0.1	0.4
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG21	5	0.4	0.25	0.35
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG22	5	0.4	0.25	0.35
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG23	5	0.4	0.25	0.35
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG21	5	0.4	0.25	0.35
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG22	5	0.4	0.25	0.35
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG23	5	0.4	0.25	0.35
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG21	5	0.4	0.25	0.35
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG22	5	0.4	0.25	0.35
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG23	5	0.4	0.25	0.35
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB1	5	0.4	0.21	0.43
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB2	5	0.4	0.21	0.43
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB3	5	0.4	0.21	0.43
(1,1522)	1:108:R:LYS:H	1:109:R:HIS:H	5	0.39	0.03	0.38
(1,1524)	1:109:R:HIS:H	1:108:R:LYS:H	5	0.39	0.03	0.38
(1,2110)	1:73:R:SER:H	1:73:R:SER:HB2	5	0.39	0.06	0.41
(1,1965)	1:70:R:TRP:HB3	1:70:R:TRP:HA	5	0.38	0.02	0.39
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB1	5	0.37	0.03	0.38
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB2	5	0.37	0.03	0.38
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB3	5	0.37	0.03	0.38
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB1	5	0.37	0.03	0.38
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB2	5	0.37	0.03	0.38
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB3	5	0.37	0.03	0.38
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB1	5	0.37	0.03	0.38
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB2	5	0.37	0.03	0.38
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB3	5	0.37	0.03	0.38
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG21	5	0.37	0.17	0.37
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG22	5	0.37	0.17	0.37
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG23	5	0.37	0.17	0.37
(1,1652)	1:163:R:ASP:H	1:166:R:ASP:H	5	0.36	0.05	0.33
(1,2120)	1:89:R:LEU:HA	1:89:R:LEU:HG	5	0.36	0.07	0.37
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG21	5	0.36	0.13	0.41
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG22	5	0.36	0.13	0.41
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG23	5	0.36	0.13	0.41
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG21	5	0.36	0.13	0.41
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG22	5	0.36	0.13	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG23	5	0.36	0.13	0.41
(2,99)	1:103:R:VAL:H	1:99:R:PRO:O	5	0.36	0.07	0.36
(1,1399)	1:52:R:TRP:H	1:51:R:ALA:HA	5	0.36	0.01	0.36
(1,2257)	1:180:R:PHE:HB3	1:180:R:PHE:HA	5	0.35	0.04	0.35
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB1	5	0.35	0.04	0.36
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB2	5	0.35	0.04	0.36
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB3	5	0.35	0.04	0.36
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB1	5	0.35	0.04	0.36
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB2	5	0.35	0.04	0.36
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB3	5	0.35	0.04	0.36
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB1	5	0.35	0.04	0.36
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB2	5	0.35	0.04	0.36
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB3	5	0.35	0.04	0.36
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB1	5	0.35	0.04	0.36
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB2	5	0.35	0.04	0.36
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB3	5	0.35	0.04	0.36
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB1	5	0.35	0.04	0.36
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB2	5	0.35	0.04	0.36
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB3	5	0.35	0.04	0.36
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB1	5	0.35	0.04	0.36
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB2	5	0.35	0.04	0.36
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB3	5	0.35	0.04	0.36
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG21	5	0.34	0.08	0.36
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG22	5	0.34	0.08	0.36
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG23	5	0.34	0.08	0.36
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG21	5	0.34	0.08	0.36
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG22	5	0.34	0.08	0.36
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG23	5	0.34	0.08	0.36
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG21	5	0.34	0.08	0.36
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG22	5	0.34	0.08	0.36
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG23	5	0.34	0.08	0.36
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD11	5	0.33	0.02	0.32
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD12	5	0.33	0.02	0.32
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD13	5	0.33	0.02	0.32
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD21	5	0.33	0.02	0.32
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD22	5	0.33	0.02	0.32
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD23	5	0.33	0.02	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD11	5	0.33	0.02	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD12	5	0.33	0.02	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD13	5	0.33	0.02	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD21	5	0.33	0.02	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD22	5	0.33	0.02	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD23	5	0.33	0.02	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD11	5	0.33	0.02	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD12	5	0.33	0.02	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD13	5	0.33	0.02	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD21	5	0.33	0.02	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD22	5	0.33	0.02	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD23	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD11	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD12	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD13	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD11	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD12	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD13	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD11	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD12	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD13	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD11	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD12	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD13	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD11	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD12	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD13	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD11	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD12	5	0.33	0.02	0.32
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD13	5	0.33	0.02	0.32
(1,126)	1:157:R:ASN:H	1:155:R:THR:CG2	5	0.33	0.02	0.33
(1,830)	1:40:R:THR:H	1:38:R:LYS:HA	5	0.33	0.15	0.36
(1,2255)	1:140:R:GLY:HA2	1:180:R:PHE:HA	5	0.33	0.14	0.24
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG11	5	0.33	0.04	0.33
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG12	5	0.33	0.04	0.33
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG13	5	0.33	0.04	0.33
(1,1425)	1:62:R:TYR:H	1:61:R:ARG:HA	5	0.32	0.03	0.31
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG21	5	0.31	0.09	0.31
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG22	5	0.31	0.09	0.31
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG23	5	0.31	0.09	0.31
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG21	5	0.31	0.09	0.31
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG22	5	0.31	0.09	0.31
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG23	5	0.31	0.09	0.31
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG21	5	0.31	0.09	0.31
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG22	5	0.31	0.09	0.31
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG23	5	0.31	0.09	0.31
(1,2023)	1:134:R:LEU:HB2	1:134:R:LEU:HA	5	0.31	0.02	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2023)	1:134:R:LEU:HB3	1:134:R:LEU:HA	5	0.31	0.02	0.31
(1,2181)	1:134:R:LEU:H	1:134:R:LEU:HA	5	0.31	0.16	0.25
(1,1390)	1:47:R:ASN:H	1:47:R:ASN:HB2	5	0.3	0.02	0.31
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB1	5	0.28	0.14	0.25
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB2	5	0.28	0.14	0.25
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB3	5	0.28	0.14	0.25
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG11	5	0.28	0.04	0.27
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG12	5	0.28	0.04	0.27
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG13	5	0.28	0.04	0.27
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG11	5	0.28	0.04	0.27
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG12	5	0.28	0.04	0.27
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG13	5	0.28	0.04	0.27
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG21	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG22	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG23	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG21	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG22	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG23	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG21	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG22	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG23	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG21	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG22	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG23	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG21	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG22	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG23	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG21	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG22	5	0.28	0.03	0.27
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG23	5	0.28	0.03	0.27
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD11	5	0.27	0.13	0.24
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD12	5	0.27	0.13	0.24
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD13	5	0.27	0.13	0.24
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD11	5	0.27	0.13	0.24
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD12	5	0.27	0.13	0.24
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD13	5	0.27	0.13	0.24
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD11	5	0.27	0.13	0.24
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD12	5	0.27	0.13	0.24
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD13	5	0.27	0.13	0.24
(1,2246)	1:170:R:TRP:H	1:170:R:TRP:HB2	5	0.27	0.07	0.24
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG11	5	0.26	0.06	0.26
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG12	5	0.26	0.06	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG13	5	0.26	0.06	0.26
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG11	5	0.26	0.06	0.26
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG12	5	0.26	0.06	0.26
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG13	5	0.26	0.06	0.26
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG11	5	0.26	0.06	0.26
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG12	5	0.26	0.06	0.26
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG13	5	0.26	0.06	0.26
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG11	5	0.26	0.06	0.26
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG12	5	0.26	0.06	0.26
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG13	5	0.26	0.06	0.26
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG11	5	0.26	0.06	0.26
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG12	5	0.26	0.06	0.26
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG13	5	0.26	0.06	0.26
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG11	5	0.26	0.06	0.26
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG12	5	0.26	0.06	0.26
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG13	5	0.26	0.06	0.26
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD11	5	0.26	0.04	0.25
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD12	5	0.26	0.04	0.25
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD13	5	0.26	0.04	0.25
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD11	5	0.26	0.04	0.25
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD12	5	0.26	0.04	0.25
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD13	5	0.26	0.04	0.25
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD11	5	0.26	0.04	0.25
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD12	5	0.26	0.04	0.25
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD13	5	0.26	0.04	0.25
(1,1728)	1:57:R:LEU:HD11	1:57:R:LEU:HA	5	0.25	0.08	0.22
(1,1728)	1:57:R:LEU:HD12	1:57:R:LEU:HA	5	0.25	0.08	0.22
(1,1728)	1:57:R:LEU:HD13	1:57:R:LEU:HA	5	0.25	0.08	0.22
(1,1728)	1:57:R:LEU:HD21	1:57:R:LEU:HA	5	0.25	0.08	0.22
(1,1728)	1:57:R:LEU:HD22	1:57:R:LEU:HA	5	0.25	0.08	0.22
(1,1728)	1:57:R:LEU:HD23	1:57:R:LEU:HA	5	0.25	0.08	0.22
(1,1410)	1:59:R:LEU:H	1:57:R:LEU:H	5	0.25	0.08	0.25
(1,1523)	1:109:R:HIS:H	1:108:R:LYS:HA	5	0.25	0.01	0.25
(1,1904)	1:162:R:ILE:HG12	1:162:R:ILE:HG13	5	0.24	0.01	0.24
(1,1760)	1:83:R:ILE:HG13	1:83:R:ILE:HG12	5	0.24	0.01	0.23
(1,1761)	1:83:R:ILE:HG12	1:83:R:ILE:HG13	5	0.24	0.01	0.23
(2,54)	1:116:R:GLY:N	1:124:R:VAL:O	5	0.24	0.12	0.16
(1,1939)	1:40:R:THR:HB	1:40:R:THR:HG23	5	0.23	0.02	0.24
(1,1939)	1:40:R:THR:HB	1:40:R:THR:HG22	5	0.23	0.02	0.24
(1,1939)	1:40:R:THR:HB	1:40:R:THR:HG21	5	0.23	0.02	0.24
(1,1889)	1:159:R:TRP:HB2	1:159:R:TRP:HB3	5	0.23	0.0	0.23
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG21	5	0.22	0.07	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG22	5	0.22	0.07	0.19
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG23	5	0.22	0.07	0.19
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG11	5	0.22	0.03	0.22
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG12	5	0.22	0.03	0.22
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG13	5	0.22	0.03	0.22
(1,1831)	1:125:R:CYS:HB3	1:125:R:CYS:HB2	5	0.21	0.01	0.21
(1,1832)	1:125:R:CYS:HB2	1:125:R:CYS:HB3	5	0.21	0.01	0.21
(1,1765)	1:85:R:GLN:HB3	1:85:R:GLN:HB2	5	0.21	0.0	0.21
(1,1766)	1:85:R:GLN:HB2	1:85:R:GLN:HB3	5	0.21	0.0	0.21
(1,1824)	1:122:R:SER:HB3	1:122:R:SER:HB2	5	0.21	0.0	0.21
(1,1825)	1:122:R:SER:HB2	1:122:R:SER:HB3	5	0.21	0.0	0.21
(1,1887)	1:156:R:SER:HB3	1:156:R:SER:HB2	5	0.21	0.0	0.21
(1,1888)	1:156:R:SER:HB2	1:156:R:SER:HB3	5	0.21	0.0	0.21
(1,1914)	1:170:R:TRP:HB3	1:170:R:TRP:HB2	5	0.21	0.0	0.21
(1,1982)	1:90:R:THR:HB	1:90:R:THR:HG22	5	0.2	0.05	0.19
(1,1982)	1:90:R:THR:HB	1:90:R:THR:HG21	5	0.2	0.05	0.19
(1,968)	1:80:R:LEU:H	1:81:R:GLU:HA	5	0.2	0.01	0.2
(1,1963)	1:64:R:GLU:HB2	1:64:R:GLU:HA	5	0.2	0.02	0.21
(1,1963)	1:64:R:GLU:HB3	1:64:R:GLU:HA	5	0.2	0.02	0.21
(1,2136)	1:95:R:HIS:H	1:95:R:HIS:HA	5	0.2	0.03	0.2
(1,2221)	1:156:R:SER:H	1:155:R:THR:HA	5	0.2	0.07	0.2
(1,1482)	1:85:R:GLN:H	1:83:R:ILE:HA	5	0.18	0.03	0.17
(1,1964)	1:64:R:GLU:HA	1:64:R:GLU:HG3	5	0.18	0.02	0.17
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB1	5	0.17	0.03	0.18
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB2	5	0.17	0.03	0.18
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB3	5	0.17	0.03	0.18
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB1	5	0.17	0.03	0.18
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB2	5	0.17	0.03	0.18
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB3	5	0.17	0.03	0.18
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB1	5	0.17	0.03	0.18
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB2	5	0.17	0.03	0.18
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB3	5	0.17	0.03	0.18
(2,4)	1:57:R:LEU:N	1:53:R:LEU:O	5	0.17	0.06	0.15
(1,1742)	1:70:R:TRP:HB3	1:70:R:TRP:HB2	5	0.16	0.0	0.16
(1,1743)	1:70:R:TRP:HB2	1:70:R:TRP:HB3	5	0.16	0.0	0.16
(1,2116)	1:87:R:GLU:H	1:87:R:GLU:HA	5	0.15	0.02	0.14
(1,2078)	1:52:R:TRP:H	1:52:R:TRP:HA	5	0.14	0.01	0.14
(1,1732)	1:63:R:VAL:HG11	1:63:R:VAL:HB	5	0.11	0.0	0.11
(1,1732)	1:63:R:VAL:HG12	1:63:R:VAL:HB	5	0.11	0.0	0.11
(1,1732)	1:63:R:VAL:HG13	1:63:R:VAL:HB	5	0.11	0.0	0.11
(1,1732)	1:63:R:VAL:HG21	1:63:R:VAL:HB	5	0.11	0.0	0.11
(1,1732)	1:63:R:VAL:HG22	1:63:R:VAL:HB	5	0.11	0.0	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1732)	1:63:R:VAL:HG23	1:63:R:VAL:HB	5	0.11	0.0	0.11
(1,1783)	1:100:R:PRO:CB	1:100:R:PRO:HG2	5	0.11	0.0	0.11
(1,1783)	1:100:R:PRO:CB	1:100:R:PRO:HG3	5	0.11	0.0	0.11
(1,1893)	1:170:R:TRP:HB3	1:171:R:THR:HG1	4	1.42	0.75	1.38
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD11	4	1.27	0.16	1.28
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD12	4	1.27	0.16	1.28
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD13	4	1.27	0.16	1.28
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD21	4	1.27	0.16	1.28
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD22	4	1.27	0.16	1.28
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD23	4	1.27	0.16	1.28
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD11	4	1.03	0.12	1.06
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD12	4	1.03	0.12	1.06
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD13	4	1.03	0.12	1.06
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD21	4	1.03	0.12	1.06
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD22	4	1.03	0.12	1.06
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD23	4	1.03	0.12	1.06
(1,2242)	1:161:R:ALA:HB1	1:170:R:TRP:HB3	4	0.96	0.13	0.91
(1,2242)	1:161:R:ALA:HB2	1:170:R:TRP:HB3	4	0.96	0.13	0.91
(1,2242)	1:161:R:ALA:HB3	1:170:R:TRP:HB3	4	0.96	0.13	0.91
(1,1593)	1:138:R:HIS:H	1:181:R:VAL:HG11	4	0.93	0.11	0.97
(1,1593)	1:138:R:HIS:H	1:181:R:VAL:HG12	4	0.93	0.11	0.97
(1,1593)	1:138:R:HIS:H	1:181:R:VAL:HG13	4	0.93	0.11	0.97
(1,1546)	1:114:R:GLY:H	1:115:R:ILE:HD11	4	0.92	0.33	0.82
(1,1546)	1:114:R:GLY:H	1:115:R:ILE:HD12	4	0.92	0.33	0.82
(1,1546)	1:114:R:GLY:H	1:115:R:ILE:HD13	4	0.92	0.33	0.82
(1,2020)	1:127:R:VAL:HA	1:127:R:VAL:HG21	4	0.88	0.03	0.88
(1,2020)	1:127:R:VAL:HA	1:127:R:VAL:HG22	4	0.88	0.03	0.88
(1,2020)	1:127:R:VAL:HA	1:127:R:VAL:HG23	4	0.88	0.03	0.88
(1,418)	1:91:R:GLY:H	1:89:R:LEU:HB2	4	0.87	0.06	0.86
(1,1258)	1:161:R:ALA:H	1:162:R:ILE:HG13	4	0.78	0.42	0.72
(1,2016)	1:127:R:VAL:H	1:126:R:VAL:HG21	4	0.77	0.45	0.78
(1,2016)	1:127:R:VAL:H	1:126:R:VAL:HG22	4	0.77	0.45	0.78
(1,2016)	1:127:R:VAL:H	1:126:R:VAL:HG23	4	0.77	0.45	0.78
(1,851)	1:46:R:ASN:H	1:165:R:GLU:H	4	0.71	0.46	0.6
(1,1592)	1:138:R:HIS:H	1:154:R:VAL:HG21	4	0.7	0.39	0.68
(1,1592)	1:138:R:HIS:H	1:154:R:VAL:HG22	4	0.7	0.39	0.68
(1,1592)	1:138:R:HIS:H	1:154:R:VAL:HG23	4	0.7	0.39	0.68
(1,882)	1:56:R:ILE:H	1:56:R:ILE:HD11	4	0.69	0.14	0.67
(1,882)	1:56:R:ILE:H	1:56:R:ILE:HD12	4	0.69	0.14	0.67
(1,882)	1:56:R:ILE:H	1:56:R:ILE:HD13	4	0.69	0.14	0.67
(2,57)	1:127:R:VAL:H	1:178:R:LEU:O	4	0.67	0.45	0.46
(1,1949)	1:56:R:ILE:HB	1:56:R:ILE:HD11	4	0.67	0.23	0.77

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1949)	1:56:R:ILE:HB	1:56:R:ILE:HD12	4	0.67	0.23	0.77
(1,1949)	1:56:R:ILE:HB	1:56:R:ILE:HD13	4	0.67	0.23	0.77
(1,1955)	1:56:R:ILE:HG12	1:56:R:ILE:HG21	4	0.66	0.24	0.76
(1,1955)	1:56:R:ILE:HG12	1:56:R:ILE:HG22	4	0.66	0.24	0.76
(1,1955)	1:56:R:ILE:HG12	1:56:R:ILE:HG23	4	0.66	0.24	0.76
(1,2172)	1:124:R:VAL:H	1:124:R:VAL:HG11	4	0.58	0.08	0.57
(1,2172)	1:124:R:VAL:H	1:124:R:VAL:HG12	4	0.58	0.08	0.57
(1,2172)	1:124:R:VAL:H	1:124:R:VAL:HG13	4	0.58	0.08	0.57
(1,1082)	1:112:R:HIS:H	1:111:R:LEU:HD11	4	0.58	0.17	0.58
(1,1082)	1:112:R:HIS:H	1:111:R:LEU:HD12	4	0.58	0.17	0.58
(1,1082)	1:112:R:HIS:H	1:111:R:LEU:HD13	4	0.58	0.17	0.58
(1,2103)	1:72:R:TYR:H	1:71:R:VAL:HG11	4	0.57	0.24	0.52
(1,2103)	1:72:R:TYR:H	1:71:R:VAL:HG12	4	0.57	0.24	0.52
(1,2103)	1:72:R:TYR:H	1:71:R:VAL:HG13	4	0.57	0.24	0.52
(1,1787)	1:102:R:LEU:H	1:101:R:ALA:HB1	4	0.56	0.0	0.56
(1,1787)	1:102:R:LEU:H	1:101:R:ALA:HB2	4	0.56	0.0	0.56
(1,1787)	1:102:R:LEU:H	1:101:R:ALA:HB3	4	0.56	0.0	0.56
(2,117)	1:44:R:ARG:H	1:164:R:ASP:O	4	0.54	0.44	0.32
(1,2247)	1:134:R:LEU:HD11	1:171:R:THR:HA	4	0.51	0.44	0.34
(1,2247)	1:134:R:LEU:HD12	1:171:R:THR:HA	4	0.51	0.44	0.34
(1,2247)	1:134:R:LEU:HD13	1:171:R:THR:HA	4	0.51	0.44	0.34
(1,2247)	1:134:R:LEU:HD21	1:171:R:THR:HA	4	0.51	0.44	0.34
(1,2247)	1:134:R:LEU:HD22	1:171:R:THR:HA	4	0.51	0.44	0.34
(1,2247)	1:134:R:LEU:HD23	1:171:R:THR:HA	4	0.51	0.44	0.34
(1,1724)	1:56:R:ILE:HD11	1:56:R:ILE:HG21	4	0.48	0.12	0.48
(1,1724)	1:56:R:ILE:HD11	1:56:R:ILE:HG22	4	0.48	0.12	0.48
(1,1724)	1:56:R:ILE:HD11	1:56:R:ILE:HG23	4	0.48	0.12	0.48
(1,1724)	1:56:R:ILE:HD12	1:56:R:ILE:HG21	4	0.48	0.12	0.48
(1,1724)	1:56:R:ILE:HD12	1:56:R:ILE:HG22	4	0.48	0.12	0.48
(1,1724)	1:56:R:ILE:HD12	1:56:R:ILE:HG23	4	0.48	0.12	0.48
(1,1724)	1:56:R:ILE:HD13	1:56:R:ILE:HG21	4	0.48	0.12	0.48
(1,1724)	1:56:R:ILE:HD13	1:56:R:ILE:HG22	4	0.48	0.12	0.48
(1,1724)	1:56:R:ILE:HD13	1:56:R:ILE:HG23	4	0.48	0.12	0.48
(1,1915)	1:159:R:TRP:HB2	1:171:R:THR:HA	4	0.48	0.41	0.3
(1,1048)	1:105:R:TRP:H	1:101:R:ALA:HA	4	0.46	0.1	0.47
(1,1841)	1:178:R:LEU:HD11	1:127:R:VAL:HG21	4	0.43	0.07	0.44
(1,1841)	1:178:R:LEU:HD11	1:127:R:VAL:HG22	4	0.43	0.07	0.44
(1,1841)	1:178:R:LEU:HD11	1:127:R:VAL:HG23	4	0.43	0.07	0.44
(1,1841)	1:178:R:LEU:HD12	1:127:R:VAL:HG21	4	0.43	0.07	0.44
(1,1841)	1:178:R:LEU:HD12	1:127:R:VAL:HG22	4	0.43	0.07	0.44
(1,1841)	1:178:R:LEU:HD12	1:127:R:VAL:HG23	4	0.43	0.07	0.44
(1,1841)	1:178:R:LEU:HD13	1:127:R:VAL:HG21	4	0.43	0.07	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1841)	1:178:R:LEU:HD13	1:127:R:VAL:HG22	4	0.43	0.07	0.44
(1,1841)	1:178:R:LEU:HD13	1:127:R:VAL:HG23	4	0.43	0.07	0.44
(1,1841)	1:178:R:LEU:HD21	1:127:R:VAL:HG21	4	0.43	0.07	0.44
(1,1841)	1:178:R:LEU:HD21	1:127:R:VAL:HG22	4	0.43	0.07	0.44
(1,1841)	1:178:R:LEU:HD21	1:127:R:VAL:HG23	4	0.43	0.07	0.44
(1,1841)	1:178:R:LEU:HD22	1:127:R:VAL:HG21	4	0.43	0.07	0.44
(1,1841)	1:178:R:LEU:HD22	1:127:R:VAL:HG22	4	0.43	0.07	0.44
(1,1841)	1:178:R:LEU:HD22	1:127:R:VAL:HG23	4	0.43	0.07	0.44
(1,1841)	1:178:R:LEU:HD23	1:127:R:VAL:HG21	4	0.43	0.07	0.44
(1,1841)	1:178:R:LEU:HD23	1:127:R:VAL:HG22	4	0.43	0.07	0.44
(1,1841)	1:178:R:LEU:HD23	1:127:R:VAL:HG23	4	0.43	0.07	0.44
(1,2158)	1:112:R:HIS:HA	1:112:R:HIS:HB2	4	0.42	0.06	0.44
(1,2165)	1:126:R:VAL:H	1:117:R:THR:HA	4	0.42	0.05	0.42
(1,1382)	1:43:R:SER:H	1:42:R:TYR:HD1	4	0.4	0.17	0.46
(1,1382)	1:43:R:SER:H	1:42:R:TYR:HD2	4	0.4	0.17	0.46
(1,2206)	1:153:R:CYS:HB2	1:153:R:CYS:HA	4	0.4	0.05	0.4
(1,1358)	1:34:R:TYR:H	1:155:R:THR:HA	4	0.38	0.01	0.38
(1,2160)	1:112:R:HIS:H	1:112:R:HIS:HB2	4	0.38	0.14	0.44
(1,1530)	1:110:R:LEU:H	1:109:R:HIS:HB2	4	0.36	0.02	0.37
(1,1858)	1:181:R:VAL:HG11	1:139:R:ALA:HB1	4	0.36	0.03	0.36
(1,1858)	1:181:R:VAL:HG11	1:139:R:ALA:HB2	4	0.36	0.03	0.36
(1,1858)	1:181:R:VAL:HG11	1:139:R:ALA:HB3	4	0.36	0.03	0.36
(1,1858)	1:181:R:VAL:HG12	1:139:R:ALA:HB1	4	0.36	0.03	0.36
(1,1858)	1:181:R:VAL:HG12	1:139:R:ALA:HB2	4	0.36	0.03	0.36
(1,1858)	1:181:R:VAL:HG12	1:139:R:ALA:HB3	4	0.36	0.03	0.36
(1,1858)	1:181:R:VAL:HG13	1:139:R:ALA:HB1	4	0.36	0.03	0.36
(1,1858)	1:181:R:VAL:HG13	1:139:R:ALA:HB2	4	0.36	0.03	0.36
(1,1858)	1:181:R:VAL:HG13	1:139:R:ALA:HB3	4	0.36	0.03	0.36
(1,1654)	1:164:R:ASP:H	1:163:R:ASP:HB3	4	0.34	0.05	0.34
(1,2050)	1:41:R:PHE:HE1	1:162:R:ILE:HD11	4	0.33	0.18	0.24
(1,2050)	1:41:R:PHE:HE1	1:162:R:ILE:HD12	4	0.33	0.18	0.24
(1,2050)	1:41:R:PHE:HE1	1:162:R:ILE:HD13	4	0.33	0.18	0.24
(1,2050)	1:41:R:PHE:HE2	1:162:R:ILE:HD11	4	0.33	0.18	0.24
(1,2050)	1:41:R:PHE:HE2	1:162:R:ILE:HD12	4	0.33	0.18	0.24
(1,2050)	1:41:R:PHE:HE2	1:162:R:ILE:HD13	4	0.33	0.18	0.24
(1,660)	1:153:R:CYS:H	1:155:R:THR:H	4	0.33	0.22	0.28
(1,1511)	1:105:R:TRP:H	1:103:R:VAL:H	4	0.33	0.02	0.32
(1,1440)	1:70:R:TRP:H	1:68:R:PHE:HA	4	0.33	0.08	0.3
(1,2004)	1:113:R:THR:HG1	1:113:R:THR:HA	4	0.33	0.14	0.34
(1,2004)	1:113:R:THR:HG22	1:113:R:THR:HA	4	0.33	0.14	0.34
(1,2153)	1:111:R:LEU:HB2	1:111:R:LEU:HA	4	0.32	0.01	0.32
(1,105)	1:137:R:PHE:H	1:138:R:HIS:H	4	0.32	0.02	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2109)	1:73:R:SER:H	1:73:R:SER:HB3	4	0.32	0.06	0.32
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD11	4	0.31	0.16	0.24
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD12	4	0.31	0.16	0.24
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD13	4	0.31	0.16	0.24
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD21	4	0.31	0.16	0.24
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD22	4	0.31	0.16	0.24
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD23	4	0.31	0.16	0.24
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD11	4	0.31	0.16	0.24
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD12	4	0.31	0.16	0.24
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD13	4	0.31	0.16	0.24
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD21	4	0.31	0.16	0.24
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD22	4	0.31	0.16	0.24
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD23	4	0.31	0.16	0.24
(1,42)	1:89:R:LEU:H	1:89:R:LEU:HG	4	0.31	0.01	0.31
(1,1727)	1:56:R:ILE:H	1:56:R:ILE:HG21	4	0.31	0.1	0.31
(1,1727)	1:56:R:ILE:H	1:56:R:ILE:HG22	4	0.31	0.1	0.31
(1,1727)	1:56:R:ILE:H	1:56:R:ILE:HG23	4	0.31	0.1	0.31
(1,2174)	1:125:R:CYS:H	1:125:R:CYS:HB3	4	0.3	0.13	0.3
(1,1128)	1:124:R:VAL:H	1:181:R:VAL:HA	4	0.29	0.16	0.24
(1,2122)	1:89:R:LEU:HB2	1:89:R:LEU:HG	4	0.29	0.01	0.29
(1,2312)	1:103:R:VAL:H	1:99:R:PRO:C	4	0.29	0.05	0.28
(1,1857)	1:181:R:VAL:HB	1:139:R:ALA:HB1	4	0.29	0.05	0.3
(1,1857)	1:181:R:VAL:HB	1:139:R:ALA:HB2	4	0.29	0.05	0.3
(1,1857)	1:181:R:VAL:HB	1:139:R:ALA:HB3	4	0.29	0.05	0.3
(1,1739)	1:69:R:ASP:H	1:68:R:PHE:HA	4	0.27	0.1	0.25
(1,1813)	1:115:R:ILE:HD11	1:115:R:ILE:HA	4	0.26	0.07	0.26
(1,1813)	1:115:R:ILE:HD12	1:115:R:ILE:HA	4	0.26	0.07	0.26
(1,1813)	1:115:R:ILE:HD13	1:115:R:ILE:HA	4	0.26	0.07	0.26
(1,850)	1:46:R:ASN:H	1:49:R:ASP:H	4	0.26	0.07	0.22
(1,1472)	1:82:R:ALA:H	1:71:R:VAL:HG21	4	0.25	0.14	0.2
(1,1472)	1:82:R:ALA:H	1:71:R:VAL:HG22	4	0.25	0.14	0.2
(1,1472)	1:82:R:ALA:H	1:71:R:VAL:HG23	4	0.25	0.14	0.2
(1,1817)	1:124:R:VAL:HG21	1:115:R:ILE:HG21	4	0.25	0.05	0.27
(1,1817)	1:124:R:VAL:HG21	1:115:R:ILE:HG22	4	0.25	0.05	0.27
(1,1817)	1:124:R:VAL:HG21	1:115:R:ILE:HG23	4	0.25	0.05	0.27
(1,1817)	1:124:R:VAL:HG22	1:115:R:ILE:HG21	4	0.25	0.05	0.27
(1,1817)	1:124:R:VAL:HG22	1:115:R:ILE:HG22	4	0.25	0.05	0.27
(1,1817)	1:124:R:VAL:HG22	1:115:R:ILE:HG23	4	0.25	0.05	0.27
(1,1817)	1:124:R:VAL:HG23	1:115:R:ILE:HG21	4	0.25	0.05	0.27
(1,1817)	1:124:R:VAL:HG23	1:115:R:ILE:HG22	4	0.25	0.05	0.27
(1,1817)	1:124:R:VAL:HG23	1:115:R:ILE:HG23	4	0.25	0.05	0.27
(1,1177)	1:141:R:ILE:H	1:180:R:PHE:HB2	4	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)
(1,1468)	1:81:R:GLU:H	1:79:R:THR:HB	4	0.24	0.04	0.24
(2,97)	1:104:R:ILE:H	1:100:R:PRO:O	4	0.24	0.08	0.22
(1,2019)	1:178:R:LEU:HD11	1:127:R:VAL:HG21	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD11	1:127:R:VAL:HG22	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD11	1:127:R:VAL:HG23	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD12	1:127:R:VAL:HG21	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD12	1:127:R:VAL:HG22	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD12	1:127:R:VAL:HG23	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD13	1:127:R:VAL:HG21	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD13	1:127:R:VAL:HG22	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD13	1:127:R:VAL:HG23	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD21	1:127:R:VAL:HG21	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD21	1:127:R:VAL:HG22	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD21	1:127:R:VAL:HG23	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD22	1:127:R:VAL:HG21	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD22	1:127:R:VAL:HG22	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD22	1:127:R:VAL:HG23	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD23	1:127:R:VAL:HG21	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD23	1:127:R:VAL:HG22	4	0.23	0.07	0.24
(1,2019)	1:178:R:LEU:HD23	1:127:R:VAL:HG23	4	0.23	0.07	0.24
(2,85)	1:52:R:TRP:O	1:56:R:ILE:H	4	0.22	0.07	0.24
(1,2142)	1:103:R:VAL:H	1:103:R:VAL:HB	4	0.22	0.04	0.21
(2,98)	1:104:R:ILE:N	1:100:R:PRO:O	4	0.21	0.07	0.22
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD11	4	0.21	0.07	0.22
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD12	4	0.21	0.07	0.22
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD13	4	0.21	0.07	0.22
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD21	4	0.21	0.07	0.22
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD22	4	0.21	0.07	0.22
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD23	4	0.21	0.07	0.22
(1,1729)	1:59:R:LEU:HA	1:59:R:LEU:HD11	4	0.21	0.05	0.22
(1,1729)	1:59:R:LEU:HA	1:59:R:LEU:HD12	4	0.21	0.05	0.22
(1,1729)	1:59:R:LEU:HA	1:59:R:LEU:HD13	4	0.21	0.05	0.22
(1,2319)	1:142:R:PHE:C	1:150:R:VAL:H	4	0.2	0.09	0.16
(1,1703)	1:149:R:ALA:HB1	1:51:R:ALA:HB1	4	0.2	0.01	0.2
(1,1703)	1:149:R:ALA:HB1	1:51:R:ALA:HB2	4	0.2	0.01	0.2
(1,1703)	1:149:R:ALA:HB1	1:51:R:ALA:HB3	4	0.2	0.01	0.2
(1,1703)	1:149:R:ALA:HB2	1:51:R:ALA:HB1	4	0.2	0.01	0.2
(1,1703)	1:149:R:ALA:HB2	1:51:R:ALA:HB2	4	0.2	0.01	0.2
(1,1703)	1:149:R:ALA:HB2	1:51:R:ALA:HB3	4	0.2	0.01	0.2
(1,1703)	1:149:R:ALA:HB3	1:51:R:ALA:HB1	4	0.2	0.01	0.2
(1,1703)	1:149:R:ALA:HB3	1:51:R:ALA:HB2	4	0.2	0.01	0.2
(1,1703)	1:149:R:ALA:HB3	1:51:R:ALA:HB3	4	0.2	0.01	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1859)	1:51:R:ALA:HB1	1:149:R:ALA:HB1	4	0.2	0.01	0.2
(1,1859)	1:51:R:ALA:HB1	1:149:R:ALA:HB2	4	0.2	0.01	0.2
(1,1859)	1:51:R:ALA:HB1	1:149:R:ALA:HB3	4	0.2	0.01	0.2
(1,1859)	1:51:R:ALA:HB2	1:149:R:ALA:HB1	4	0.2	0.01	0.2
(1,1859)	1:51:R:ALA:HB2	1:149:R:ALA:HB2	4	0.2	0.01	0.2
(1,1859)	1:51:R:ALA:HB2	1:149:R:ALA:HB3	4	0.2	0.01	0.2
(1,1859)	1:51:R:ALA:HB3	1:149:R:ALA:HB1	4	0.2	0.01	0.2
(1,1859)	1:51:R:ALA:HB3	1:149:R:ALA:HB2	4	0.2	0.01	0.2
(1,1859)	1:51:R:ALA:HB3	1:149:R:ALA:HB3	4	0.2	0.01	0.2
(1,1043)	1:104:R:ILE:H	1:101:R:ALA:HA	4	0.19	0.01	0.2
(1,2305)	1:52:R:TRP:C	1:56:R:ILE:H	4	0.19	0.03	0.2
(1,1990)	1:103:R:VAL:HG21	1:103:R:VAL:HA	4	0.19	0.06	0.18
(1,1990)	1:103:R:VAL:HG22	1:103:R:VAL:HA	4	0.19	0.06	0.18
(1,1990)	1:103:R:VAL:HG23	1:103:R:VAL:HA	4	0.19	0.06	0.18
(1,1995)	1:103:R:VAL:HA	1:103:R:VAL:HG21	4	0.19	0.06	0.18
(1,1995)	1:103:R:VAL:HA	1:103:R:VAL:HG22	4	0.19	0.06	0.18
(1,1995)	1:103:R:VAL:HA	1:103:R:VAL:HG23	4	0.19	0.06	0.18
(1,1352)	1:33:R:LEU:H	1:37:R:GLU:H	4	0.18	0.04	0.17
(1,1486)	1:87:R:GLU:H	1:83:R:ILE:HA	4	0.17	0.03	0.18
(1,2044)	1:155:R:THR:HG22	1:155:R:THR:HA	4	0.17	0.03	0.18
(1,2044)	1:155:R:THR:HG23	1:155:R:THR:HA	4	0.17	0.03	0.18
(1,2044)	1:155:R:THR:HG21	1:155:R:THR:HA	4	0.17	0.03	0.18
(2,10)	1:60:R:PHE:N	1:56:R:ILE:O	4	0.17	0.02	0.16
(1,1580)	1:126:R:VAL:H	1:118:R:ALA:H	4	0.16	0.02	0.16
(1,2036)	1:161:R:ALA:HB1	1:152:R:ALA:HB1	4	0.16	0.01	0.16
(1,2036)	1:161:R:ALA:HB1	1:152:R:ALA:HB2	4	0.16	0.01	0.16
(1,2036)	1:161:R:ALA:HB1	1:152:R:ALA:HB3	4	0.16	0.01	0.16
(1,2036)	1:161:R:ALA:HB2	1:152:R:ALA:HB1	4	0.16	0.01	0.16
(1,2036)	1:161:R:ALA:HB2	1:152:R:ALA:HB2	4	0.16	0.01	0.16
(1,2036)	1:161:R:ALA:HB2	1:152:R:ALA:HB3	4	0.16	0.01	0.16
(1,2036)	1:161:R:ALA:HB3	1:152:R:ALA:HB1	4	0.16	0.01	0.16
(1,2036)	1:161:R:ALA:HB3	1:152:R:ALA:HB2	4	0.16	0.01	0.16
(1,2036)	1:161:R:ALA:HB3	1:152:R:ALA:HB3	4	0.16	0.01	0.16
(1,2046)	1:152:R:ALA:HB1	1:161:R:ALA:HB1	4	0.16	0.01	0.16
(1,2046)	1:152:R:ALA:HB1	1:161:R:ALA:HB2	4	0.16	0.01	0.16
(1,2046)	1:152:R:ALA:HB1	1:161:R:ALA:HB3	4	0.16	0.01	0.16
(1,2046)	1:152:R:ALA:HB2	1:161:R:ALA:HB1	4	0.16	0.01	0.16
(1,2046)	1:152:R:ALA:HB2	1:161:R:ALA:HB2	4	0.16	0.01	0.16
(1,2046)	1:152:R:ALA:HB2	1:161:R:ALA:HB3	4	0.16	0.01	0.16
(1,2046)	1:152:R:ALA:HB3	1:161:R:ALA:HB1	4	0.16	0.01	0.16
(1,2046)	1:152:R:ALA:HB3	1:161:R:ALA:HB2	4	0.16	0.01	0.16
(1,2046)	1:152:R:ALA:HB3	1:161:R:ALA:HB3	4	0.16	0.01	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,33)	1:88:R:ASP:H	1:84:R:LYS:O	4	0.16	0.03	0.16
(1,1894)	1:170:R:TRP:HB2	1:161:R:ALA:HB1	4	0.16	0.06	0.15
(1,1894)	1:170:R:TRP:HB2	1:161:R:ALA:HB2	4	0.16	0.06	0.15
(1,1894)	1:170:R:TRP:HB2	1:161:R:ALA:HB3	4	0.16	0.06	0.15
(1,1913)	1:161:R:ALA:HB1	1:170:R:TRP:HB2	4	0.16	0.06	0.15
(1,1913)	1:161:R:ALA:HB2	1:170:R:TRP:HB2	4	0.16	0.06	0.15
(1,1913)	1:161:R:ALA:HB3	1:170:R:TRP:HB2	4	0.16	0.06	0.15
(1,2060)	1:177:R:VAL:H	1:177:R:VAL:HG11	4	0.14	0.03	0.14
(1,2060)	1:177:R:VAL:H	1:177:R:VAL:HG12	4	0.14	0.03	0.14
(1,2060)	1:177:R:VAL:H	1:177:R:VAL:HG13	4	0.14	0.03	0.14
(1,2265)	1:57:R:LEU:H	1:53:R:LEU:C	4	0.14	0.02	0.13
(1,1827)	1:124:R:VAL:HG21	1:124:R:VAL:HA	4	0.12	0.02	0.12
(1,1827)	1:124:R:VAL:HG22	1:124:R:VAL:HA	4	0.12	0.02	0.12
(1,1827)	1:124:R:VAL:HG23	1:124:R:VAL:HA	4	0.12	0.02	0.12
(1,1852)	1:134:R:LEU:HD11	1:134:R:LEU:HG	4	0.12	0.0	0.12
(1,1852)	1:134:R:LEU:HD12	1:134:R:LEU:HG	4	0.12	0.0	0.12
(1,1852)	1:134:R:LEU:HD13	1:134:R:LEU:HG	4	0.12	0.0	0.12
(1,1852)	1:134:R:LEU:HD21	1:134:R:LEU:HG	4	0.12	0.0	0.12
(1,1852)	1:134:R:LEU:HD22	1:134:R:LEU:HG	4	0.12	0.0	0.12
(1,1852)	1:134:R:LEU:HD23	1:134:R:LEU:HG	4	0.12	0.0	0.12
(1,1713)	1:53:R:LEU:HB2	1:53:R:LEU:HD21	4	0.11	0.01	0.12
(1,1713)	1:53:R:LEU:HB2	1:53:R:LEU:HD22	4	0.11	0.01	0.12
(1,1713)	1:53:R:LEU:HB2	1:53:R:LEU:HD23	4	0.11	0.01	0.12
(1,1646)	1:161:R:ALA:H	1:168:R:TYR:HD1	3	1.16	0.18	1.07
(1,1646)	1:161:R:ALA:H	1:168:R:TYR:HD2	3	1.16	0.18	1.07
(1,1895)	1:162:R:ILE:HD11	1:162:R:ILE:HA	3	0.9	0.09	0.95
(1,1895)	1:162:R:ILE:HD12	1:162:R:ILE:HA	3	0.9	0.09	0.95
(1,1895)	1:162:R:ILE:HD13	1:162:R:ILE:HA	3	0.9	0.09	0.95
(1,1384)	1:44:R:ARG:H	1:42:R:TYR:H	3	0.9	0.45	0.78
(1,1501)	1:97:R:GLY:H	1:94:R:LEU:HD11	3	0.86	0.13	0.85
(1,1501)	1:97:R:GLY:H	1:94:R:LEU:HD12	3	0.86	0.13	0.85
(1,1501)	1:97:R:GLY:H	1:94:R:LEU:HD13	3	0.86	0.13	0.85
(1,1956)	1:56:R:ILE:H	1:56:R:ILE:HG21	3	0.81	0.44	1.02
(1,1956)	1:56:R:ILE:H	1:56:R:ILE:HG22	3	0.81	0.44	1.02
(1,1956)	1:56:R:ILE:H	1:56:R:ILE:HG23	3	0.81	0.44	1.02
(1,2178)	1:126:R:VAL:H	1:126:R:VAL:HG11	3	0.74	0.27	0.89
(1,2178)	1:126:R:VAL:H	1:126:R:VAL:HG12	3	0.74	0.27	0.89
(1,2178)	1:126:R:VAL:H	1:126:R:VAL:HG13	3	0.74	0.27	0.89
(1,1303)	1:127:R:VAL:H	1:127:R:VAL:HG21	3	0.67	0.01	0.67
(1,1303)	1:127:R:VAL:H	1:127:R:VAL:HG22	3	0.67	0.01	0.67
(1,1303)	1:127:R:VAL:H	1:127:R:VAL:HG23	3	0.67	0.01	0.67
(1,1317)	1:179:R:VAL:H	1:180:R:PHE:HB2	3	0.65	0.36	0.85

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD11	3	0.62	0.58	0.24
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD12	3	0.62	0.58	0.24
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD13	3	0.62	0.58	0.24
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD21	3	0.62	0.58	0.24
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD22	3	0.62	0.58	0.24
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD23	3	0.62	0.58	0.24
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD11	3	0.6	0.18	0.64
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD12	3	0.6	0.18	0.64
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD13	3	0.6	0.18	0.64
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD21	3	0.6	0.18	0.64
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD22	3	0.6	0.18	0.64
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD23	3	0.6	0.18	0.64
(1,1715)	1:56:R:ILE:HA	1:56:R:ILE:HD11	3	0.58	0.23	0.45
(1,1715)	1:56:R:ILE:HA	1:56:R:ILE:HD12	3	0.58	0.23	0.45
(1,1715)	1:56:R:ILE:HA	1:56:R:ILE:HD13	3	0.58	0.23	0.45
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD11	3	0.57	0.13	0.57
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD12	3	0.57	0.13	0.57
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD13	3	0.57	0.13	0.57
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD21	3	0.57	0.13	0.57
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD22	3	0.57	0.13	0.57
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD23	3	0.57	0.13	0.57
(1,1285)	1:168:R:TYR:H	1:168:R:TYR:HD1	3	0.56	0.22	0.71
(1,1285)	1:168:R:TYR:H	1:168:R:TYR:HD2	3	0.56	0.22	0.71
(1,2161)	1:113:R:THR:HB	1:113:R:THR:HA	3	0.52	0.03	0.51
(1,2234)	1:162:R:ILE:H	1:162:R:ILE:HG13	3	0.52	0.25	0.38
(1,823)	1:37:R:GLU:H	1:35:R:ASN:HB3	3	0.51	0.06	0.49
(1,2089)	1:56:R:ILE:HG21	1:56:R:ILE:HG12	3	0.47	0.28	0.54
(1,2089)	1:56:R:ILE:HG22	1:56:R:ILE:HG12	3	0.47	0.28	0.54
(1,2089)	1:56:R:ILE:HG23	1:56:R:ILE:HG12	3	0.47	0.28	0.54
(1,2226)	1:162:R:ILE:HG13	1:162:R:ILE:HA	3	0.46	0.25	0.55
(1,2233)	1:162:R:ILE:HA	1:162:R:ILE:HG13	3	0.46	0.25	0.55
(1,1954)	1:56:R:ILE:HG13	1:56:R:ILE:HG21	3	0.45	0.27	0.45
(1,1954)	1:56:R:ILE:HG13	1:56:R:ILE:HG22	3	0.45	0.27	0.45
(1,1954)	1:56:R:ILE:HG13	1:56:R:ILE:HG23	3	0.45	0.27	0.45
(1,2225)	1:162:R:ILE:HB	1:162:R:ILE:HA	3	0.44	0.09	0.45
(1,824)	1:37:R:GLU:H	1:35:R:ASN:HB2	3	0.43	0.14	0.34
(1,1536)	1:111:R:LEU:H	1:112:R:HIS:H	3	0.43	0.06	0.4
(1,1539)	1:112:R:HIS:H	1:111:R:LEU:H	3	0.43	0.06	0.4
(1,2200)	1:151:R:PHE:HB3	1:151:R:PHE:HA	3	0.41	0.13	0.43
(1,2156)	1:111:R:LEU:HB2	1:112:R:HIS:HB3	3	0.4	0.2	0.47
(1,1675)	1:175:R:SER:H	1:142:R:PHE:HE1	3	0.36	0.15	0.29
(1,1675)	1:175:R:SER:H	1:142:R:PHE:HE2	3	0.36	0.15	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1667)	1:170:R:TRP:H	1:152:R:ALA:HB1	3	0.36	0.24	0.31
(1,1667)	1:170:R:TRP:H	1:152:R:ALA:HB2	3	0.36	0.24	0.31
(1,1667)	1:170:R:TRP:H	1:152:R:ALA:HB3	3	0.36	0.24	0.31
(2,58)	1:127:R:VAL:N	1:178:R:LEU:O	3	0.35	0.08	0.36
(1,1657)	1:164:R:ASP:H	1:165:R:GLU:H	3	0.32	0.11	0.28
(1,1661)	1:165:R:GLU:H	1:164:R:ASP:H	3	0.32	0.11	0.28
(1,849)	1:46:R:ASN:H	1:44:R:ARG:H	3	0.32	0.21	0.2
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD11	3	0.32	0.15	0.34
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD12	3	0.32	0.15	0.34
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD13	3	0.32	0.15	0.34
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD21	3	0.32	0.15	0.34
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD22	3	0.32	0.15	0.34
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD23	3	0.32	0.15	0.34
(1,1383)	1:43:R:SER:H	1:43:R:SER:HB3	3	0.32	0.07	0.27
(1,2047)	1:161:R:ALA:H	1:161:R:ALA:HB1	3	0.31	0.08	0.34
(1,2047)	1:161:R:ALA:H	1:161:R:ALA:HB2	3	0.31	0.08	0.34
(1,2047)	1:161:R:ALA:H	1:161:R:ALA:HB3	3	0.31	0.08	0.34
(1,1600)	1:139:R:ALA:H	1:180:R:PHE:HB2	3	0.31	0.13	0.3
(1,1711)	1:83:R:ILE:HG13	1:53:R:LEU:HD11	3	0.31	0.05	0.32
(1,1711)	1:83:R:ILE:HG13	1:53:R:LEU:HD12	3	0.31	0.05	0.32
(1,1711)	1:83:R:ILE:HG13	1:53:R:LEU:HD13	3	0.31	0.05	0.32
(1,1865)	1:142:R:PHE:HB2	1:150:R:VAL:HG21	3	0.31	0.01	0.31
(1,1865)	1:142:R:PHE:HB2	1:150:R:VAL:HG22	3	0.31	0.01	0.31
(1,1865)	1:142:R:PHE:HB2	1:150:R:VAL:HG23	3	0.31	0.01	0.31
(1,2321)	1:44:R:ARG:H	1:164:R:ASP:C	3	0.3	0.08	0.32
(1,1029)	1:97:R:GLY:H	1:49:R:ASP:HB2	3	0.29	0.1	0.34
(1,1475)	1:82:R:ALA:H	1:83:R:ILE:HD11	3	0.29	0.04	0.3
(1,1475)	1:82:R:ALA:H	1:83:R:ILE:HD12	3	0.29	0.04	0.3
(1,1475)	1:82:R:ALA:H	1:83:R:ILE:HD13	3	0.29	0.04	0.3
(1,1544)	1:114:R:GLY:H	1:113:R:THR:HB	3	0.29	0.13	0.24
(1,2288)	1:33:R:LEU:H	1:37:R:GLU:C	3	0.29	0.06	0.27
(1,2248)	1:171:R:THR:HB	1:171:R:THR:HA	3	0.28	0.04	0.26
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD11	3	0.27	0.14	0.23
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD12	3	0.27	0.14	0.23
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD13	3	0.27	0.14	0.23
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD21	3	0.27	0.14	0.23
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD22	3	0.27	0.14	0.23
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD23	3	0.27	0.14	0.23
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD11	3	0.27	0.14	0.23
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD12	3	0.27	0.14	0.23
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD13	3	0.27	0.14	0.23
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD21	3	0.27	0.14	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD22	3	0.27	0.14	0.23
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD23	3	0.27	0.14	0.23
(1,1819)	1:126:R:VAL:HG21	1:117:R:THR:HA	3	0.27	0.01	0.27
(1,1819)	1:126:R:VAL:HG22	1:117:R:THR:HA	3	0.27	0.01	0.27
(1,1819)	1:126:R:VAL:HG23	1:117:R:THR:HA	3	0.27	0.01	0.27
(1,1835)	1:117:R:THR:HA	1:126:R:VAL:HG21	3	0.27	0.01	0.27
(1,1835)	1:117:R:THR:HA	1:126:R:VAL:HG22	3	0.27	0.01	0.27
(1,1835)	1:117:R:THR:HA	1:126:R:VAL:HG23	3	0.27	0.01	0.27
(1,2298)	1:160:R:TYR:H	1:153:R:CYS:C	3	0.26	0.04	0.26
(1,959)	1:78:R:LEU:H	1:78:R:LEU:HB2	3	0.26	0.07	0.22
(1,959)	1:78:R:LEU:H	1:78:R:LEU:HB3	3	0.26	0.07	0.22
(1,659)	1:153:R:CYS:H	1:155:R:THR:CG2	3	0.25	0.13	0.16
(1,1719)	1:56:R:ILE:H	1:56:R:ILE:HD11	3	0.25	0.12	0.2
(1,1719)	1:56:R:ILE:H	1:56:R:ILE:HD12	3	0.25	0.12	0.2
(1,1719)	1:56:R:ILE:H	1:56:R:ILE:HD13	3	0.25	0.12	0.2
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD11	3	0.25	0.12	0.21
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD12	3	0.25	0.12	0.21
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD13	3	0.25	0.12	0.21
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD21	3	0.25	0.12	0.21
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD22	3	0.25	0.12	0.21
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD23	3	0.25	0.12	0.21
(1,1714)	1:83:R:ILE:HG21	1:53:R:LEU:HD21	3	0.25	0.09	0.2
(1,1714)	1:83:R:ILE:HG21	1:53:R:LEU:HD22	3	0.25	0.09	0.2
(1,1714)	1:83:R:ILE:HG21	1:53:R:LEU:HD23	3	0.25	0.09	0.2
(1,1714)	1:83:R:ILE:HG22	1:53:R:LEU:HD21	3	0.25	0.09	0.2
(1,1714)	1:83:R:ILE:HG22	1:53:R:LEU:HD22	3	0.25	0.09	0.2
(1,1714)	1:83:R:ILE:HG22	1:53:R:LEU:HD23	3	0.25	0.09	0.2
(1,1714)	1:83:R:ILE:HG23	1:53:R:LEU:HD21	3	0.25	0.09	0.2
(1,1714)	1:83:R:ILE:HG23	1:53:R:LEU:HD22	3	0.25	0.09	0.2
(1,1714)	1:83:R:ILE:HG23	1:53:R:LEU:HD23	3	0.25	0.09	0.2
(1,1777)	1:83:R:ILE:HD11	1:95:R:HIS:HA	3	0.24	0.06	0.26
(1,1777)	1:83:R:ILE:HD12	1:95:R:HIS:HA	3	0.24	0.06	0.26
(1,1777)	1:83:R:ILE:HD13	1:95:R:HIS:HA	3	0.24	0.06	0.26
(1,2071)	1:31:R:LEU:H	1:31:R:LEU:HG	3	0.24	0.06	0.28
(1,1429)	1:65:R:GLU:H	1:63:R:VAL:HB	3	0.24	0.05	0.22
(1,535)	1:117:R:THR:H	1:122:R:SER:H	3	0.23	0.07	0.22
(1,970)	1:80:R:LEU:H	1:83:R:ILE:HG13	3	0.23	0.05	0.26
(2,61)	1:178:R:LEU:H	1:141:R:ILE:O	3	0.22	0.04	0.2
(1,2244)	1:170:R:TRP:HA	1:170:R:TRP:HB2	3	0.22	0.1	0.2
(1,2266)	1:54:R:ASN:C	1:58:R:GLN:H	3	0.22	0.06	0.18
(2,91)	1:66:R:PRO:O	1:69:R:ASP:H	3	0.22	0.02	0.22
(1,1807)	1:111:R:LEU:HD21	1:111:R:LEU:HA	3	0.21	0.01	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1807)	1:111:R:LEU:HD22	1:111:R:LEU:HA	3	0.21	0.01	0.21
(1,1807)	1:111:R:LEU:HD23	1:111:R:LEU:HA	3	0.21	0.01	0.21
(1,1808)	1:111:R:LEU:HA	1:111:R:LEU:HD21	3	0.21	0.01	0.21
(1,1808)	1:111:R:LEU:HA	1:111:R:LEU:HD22	3	0.21	0.01	0.21
(1,1808)	1:111:R:LEU:HA	1:111:R:LEU:HD23	3	0.21	0.01	0.21
(1,2293)	1:178:R:LEU:H	1:141:R:ILE:C	3	0.21	0.04	0.19
(1,1626)	1:153:R:CYS:H	1:139:R:ALA:H	3	0.21	0.09	0.14
(1,1962)	1:124:R:VAL:HG11	1:63:R:VAL:HG21	3	0.21	0.04	0.2
(1,1962)	1:124:R:VAL:HG11	1:63:R:VAL:HG22	3	0.21	0.04	0.2
(1,1962)	1:124:R:VAL:HG11	1:63:R:VAL:HG23	3	0.21	0.04	0.2
(1,1962)	1:124:R:VAL:HG12	1:63:R:VAL:HG21	3	0.21	0.04	0.2
(1,1962)	1:124:R:VAL:HG12	1:63:R:VAL:HG22	3	0.21	0.04	0.2
(1,1962)	1:124:R:VAL:HG12	1:63:R:VAL:HG23	3	0.21	0.04	0.2
(1,1962)	1:124:R:VAL:HG13	1:63:R:VAL:HG21	3	0.21	0.04	0.2
(1,1962)	1:124:R:VAL:HG13	1:63:R:VAL:HG22	3	0.21	0.04	0.2
(1,1962)	1:124:R:VAL:HG13	1:63:R:VAL:HG23	3	0.21	0.04	0.2
(1,2195)	1:150:R:VAL:H	1:150:R:VAL:HG11	3	0.21	0.05	0.18
(1,2195)	1:150:R:VAL:H	1:150:R:VAL:HG12	3	0.21	0.05	0.18
(1,2195)	1:150:R:VAL:H	1:150:R:VAL:HG13	3	0.21	0.05	0.18
(2,36)	1:85:R:GLN:O	1:89:R:LEU:N	3	0.21	0.08	0.24
(1,2308)	1:66:R:PRO:C	1:69:R:ASP:H	3	0.2	0.01	0.19
(1,2301)	1:163:R:ASP:C	1:166:R:ASP:H	3	0.2	0.06	0.23
(1,156)	1:179:R:VAL:H	1:141:R:ILE:HB	3	0.19	0.06	0.21
(1,1363)	1:35:R:ASN:H	1:155:R:THR:HA	3	0.19	0.06	0.18
(1,2271)	1:68:R:PHE:C	1:72:R:TYR:H	3	0.19	0.01	0.2
(1,1059)	1:107:R:ILE:H	1:105:R:TRP:HB2	3	0.19	0.05	0.18
(1,2137)	1:95:R:HIS:H	1:95:R:HIS:HB3	3	0.19	0.05	0.19
(1,2320)	1:143:R:LEU:H	1:176:R:ASP:C	3	0.19	0.01	0.19
(1,140)	1:166:R:ASP:H	1:163:R:ASP:HB2	3	0.18	0.04	0.16
(1,982)	1:83:R:ILE:H	1:53:R:LEU:HD11	3	0.18	0.07	0.14
(1,982)	1:83:R:ILE:H	1:53:R:LEU:HD12	3	0.18	0.07	0.14
(1,982)	1:83:R:ILE:H	1:53:R:LEU:HD13	3	0.18	0.07	0.14
(1,389)	1:84:R:LYS:H	1:83:R:ILE:HG12	3	0.18	0.02	0.18
(2,55)	1:180:R:PHE:O	1:125:R:CYS:N	3	0.18	0.05	0.16
(1,1503)	1:103:R:VAL:H	1:94:R:LEU:HD21	3	0.17	0.01	0.17
(1,1503)	1:103:R:VAL:H	1:94:R:LEU:HD22	3	0.17	0.01	0.17
(1,1503)	1:103:R:VAL:H	1:94:R:LEU:HD23	3	0.17	0.01	0.17
(1,1994)	1:94:R:LEU:HD21	1:103:R:VAL:HG21	3	0.17	0.05	0.18
(1,1994)	1:94:R:LEU:HD21	1:103:R:VAL:HG22	3	0.17	0.05	0.18
(1,1994)	1:94:R:LEU:HD21	1:103:R:VAL:HG23	3	0.17	0.05	0.18
(1,1994)	1:94:R:LEU:HD22	1:103:R:VAL:HG21	3	0.17	0.05	0.18
(1,1994)	1:94:R:LEU:HD22	1:103:R:VAL:HG22	3	0.17	0.05	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1994)	1:94:R:LEU:HD22	1:103:R:VAL:HG23	3	0.17	0.05	0.18
(1,1994)	1:94:R:LEU:HD23	1:103:R:VAL:HG21	3	0.17	0.05	0.18
(1,1994)	1:94:R:LEU:HD23	1:103:R:VAL:HG22	3	0.17	0.05	0.18
(1,1994)	1:94:R:LEU:HD23	1:103:R:VAL:HG23	3	0.17	0.05	0.18
(1,1707)	1:53:R:LEU:HD21	1:53:R:LEU:HD11	3	0.17	0.02	0.16
(1,1707)	1:53:R:LEU:HD21	1:53:R:LEU:HD12	3	0.17	0.02	0.16
(1,1707)	1:53:R:LEU:HD21	1:53:R:LEU:HD13	3	0.17	0.02	0.16
(1,1707)	1:53:R:LEU:HD22	1:53:R:LEU:HD11	3	0.17	0.02	0.16
(1,1707)	1:53:R:LEU:HD22	1:53:R:LEU:HD12	3	0.17	0.02	0.16
(1,1707)	1:53:R:LEU:HD22	1:53:R:LEU:HD13	3	0.17	0.02	0.16
(1,1707)	1:53:R:LEU:HD23	1:53:R:LEU:HD11	3	0.17	0.02	0.16
(1,1707)	1:53:R:LEU:HD23	1:53:R:LEU:HD12	3	0.17	0.02	0.16
(1,1707)	1:53:R:LEU:HD23	1:53:R:LEU:HD13	3	0.17	0.02	0.16
(2,86)	1:52:R:TRP:O	1:56:R:ILE:N	3	0.17	0.02	0.16
(1,1529)	1:110:R:LEU:H	1:109:R:HIS:HB3	3	0.16	0.03	0.18
(1,2243)	1:170:R:TRP:HA	1:170:R:TRP:HB3	3	0.16	0.04	0.16
(1,594)	1:131:R:ASP:H	1:132:R:MET:H	3	0.16	0.02	0.17
(1,1997)	1:110:R:LEU:HD11	1:110:R:LEU:HA	3	0.16	0.02	0.17
(1,1997)	1:110:R:LEU:HD12	1:110:R:LEU:HA	3	0.16	0.02	0.17
(1,1997)	1:110:R:LEU:HD13	1:110:R:LEU:HA	3	0.16	0.02	0.17
(1,1794)	1:107:R:ILE:HD11	1:103:R:VAL:HG11	3	0.16	0.05	0.13
(1,1794)	1:107:R:ILE:HD11	1:103:R:VAL:HG12	3	0.16	0.05	0.13
(1,1794)	1:107:R:ILE:HD11	1:103:R:VAL:HG13	3	0.16	0.05	0.13
(1,1794)	1:107:R:ILE:HD12	1:103:R:VAL:HG11	3	0.16	0.05	0.13
(1,1794)	1:107:R:ILE:HD12	1:103:R:VAL:HG12	3	0.16	0.05	0.13
(1,1794)	1:107:R:ILE:HD12	1:103:R:VAL:HG13	3	0.16	0.05	0.13
(1,1794)	1:107:R:ILE:HD13	1:103:R:VAL:HG11	3	0.16	0.05	0.13
(1,1794)	1:107:R:ILE:HD13	1:103:R:VAL:HG12	3	0.16	0.05	0.13
(1,1794)	1:107:R:ILE:HD13	1:103:R:VAL:HG13	3	0.16	0.05	0.13
(2,11)	1:61:R:ARG:H	1:57:R:LEU:O	3	0.16	0.06	0.13
(1,1848)	1:134:R:LEU:HD21	1:134:R:LEU:HA	3	0.15	0.04	0.13
(1,1848)	1:134:R:LEU:HD22	1:134:R:LEU:HA	3	0.15	0.04	0.13
(1,1848)	1:134:R:LEU:HD23	1:134:R:LEU:HA	3	0.15	0.04	0.13
(1,1004)	1:90:R:THR:H	1:89:R:LEU:HB3	3	0.15	0.03	0.16
(1,194)	1:37:R:GLU:H	1:38:R:LYS:H	3	0.14	0.05	0.11
(1,196)	1:38:R:LYS:H	1:37:R:GLU:H	3	0.14	0.05	0.11
(1,2307)	1:50:R:ASN:C	1:54:R:ASN:H	3	0.14	0.03	0.13
(2,3)	1:57:R:LEU:H	1:53:R:LEU:O	3	0.14	0.01	0.13
(1,1484)	1:85:R:GLN:H	1:87:R:GLU:H	3	0.13	0.01	0.13
(1,1487)	1:87:R:GLU:H	1:85:R:GLN:H	3	0.13	0.01	0.13
(1,2031)	1:181:R:VAL:HB	1:139:R:ALA:HB1	3	0.12	0.02	0.1
(1,2031)	1:181:R:VAL:HB	1:139:R:ALA:HB2	3	0.12	0.02	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2031)	1:181:R:VAL:HB	1:139:R:ALA:HB3	3	0.12	0.02	0.1
(1,424)	1:92:R:LEU:H	1:90:R:THR:HA	3	0.11	0.01	0.1
(1,2021)	1:127:R:VAL:H	1:127:R:VAL:HG21	2	1.0	0.3	1.0
(1,2021)	1:127:R:VAL:H	1:127:R:VAL:HG22	2	1.0	0.3	1.0
(1,2021)	1:127:R:VAL:H	1:127:R:VAL:HG23	2	1.0	0.3	1.0
(1,1585)	1:128:R:ASP:H	1:126:R:VAL:HG21	2	0.94	0.0	0.94
(1,1585)	1:128:R:ASP:H	1:126:R:VAL:HG22	2	0.94	0.0	0.94
(1,1585)	1:128:R:ASP:H	1:126:R:VAL:HG23	2	0.94	0.0	0.94
(1,1385)	1:44:R:ARG:H	1:43:R:SER:H	2	0.9	0.3	0.9
(1,2132)	1:83:R:ILE:HD11	1:94:R:LEU:HD11	2	0.85	0.15	0.85
(1,2132)	1:83:R:ILE:HD11	1:94:R:LEU:HD12	2	0.85	0.15	0.85
(1,2132)	1:83:R:ILE:HD11	1:94:R:LEU:HD13	2	0.85	0.15	0.85
(1,2132)	1:83:R:ILE:HD12	1:94:R:LEU:HD11	2	0.85	0.15	0.85
(1,2132)	1:83:R:ILE:HD12	1:94:R:LEU:HD12	2	0.85	0.15	0.85
(1,2132)	1:83:R:ILE:HD12	1:94:R:LEU:HD13	2	0.85	0.15	0.85
(1,2132)	1:83:R:ILE:HD13	1:94:R:LEU:HD11	2	0.85	0.15	0.85
(1,2132)	1:83:R:ILE:HD13	1:94:R:LEU:HD12	2	0.85	0.15	0.85
(1,2132)	1:83:R:ILE:HD13	1:94:R:LEU:HD13	2	0.85	0.15	0.85
(1,757)	1:179:R:VAL:H	1:177:R:VAL:HA	2	0.73	0.09	0.73
(1,2232)	1:31:R:LEU:HD11	1:162:R:ILE:HG13	2	0.72	0.15	0.72
(1,2232)	1:31:R:LEU:HD12	1:162:R:ILE:HG13	2	0.72	0.15	0.72
(1,2232)	1:31:R:LEU:HD13	1:162:R:ILE:HG13	2	0.72	0.15	0.72
(1,2232)	1:31:R:LEU:HD21	1:162:R:ILE:HG13	2	0.72	0.15	0.72
(1,2232)	1:31:R:LEU:HD22	1:162:R:ILE:HG13	2	0.72	0.15	0.72
(1,2232)	1:31:R:LEU:HD23	1:162:R:ILE:HG13	2	0.72	0.15	0.72
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD11	2	0.69	0.45	0.69
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD12	2	0.69	0.45	0.69
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD13	2	0.69	0.45	0.69
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD21	2	0.69	0.45	0.69
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD22	2	0.69	0.45	0.69
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD23	2	0.69	0.45	0.69
(1,2107)	1:72:R:TYR:HB2	1:72:R:TYR:HA	2	0.62	0.01	0.62
(1,2201)	1:151:R:PHE:HB2	1:151:R:PHE:HA	2	0.6	0.04	0.6
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD11	2	0.6	0.08	0.6
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD12	2	0.6	0.08	0.6
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD13	2	0.6	0.08	0.6
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD21	2	0.6	0.08	0.6
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD22	2	0.6	0.08	0.6
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD23	2	0.6	0.08	0.6
(1,1660)	1:165:R:GLU:H	1:46:R:ASN:H	2	0.59	0.34	0.59
(1,918)	1:67:R:PHE:H	1:65:R:GLU:HA	2	0.59	0.0	0.59
(1,2143)	1:94:R:LEU:HD21	1:103:R:VAL:HG11	2	0.59	0.35	0.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2143)	1:94:R:LEU:HD21	1:103:R:VAL:HG12	2	0.59	0.35	0.59
(1,2143)	1:94:R:LEU:HD21	1:103:R:VAL:HG13	2	0.59	0.35	0.59
(1,2143)	1:94:R:LEU:HD22	1:103:R:VAL:HG11	2	0.59	0.35	0.59
(1,2143)	1:94:R:LEU:HD22	1:103:R:VAL:HG12	2	0.59	0.35	0.59
(1,2143)	1:94:R:LEU:HD22	1:103:R:VAL:HG13	2	0.59	0.35	0.59
(1,2143)	1:94:R:LEU:HD23	1:103:R:VAL:HG11	2	0.59	0.35	0.59
(1,2143)	1:94:R:LEU:HD23	1:103:R:VAL:HG12	2	0.59	0.35	0.59
(1,2143)	1:94:R:LEU:HD23	1:103:R:VAL:HG13	2	0.59	0.35	0.59
(1,778)	1:183:R:TYR:H	1:137:R:PHE:HA	2	0.57	0.46	0.57
(1,1315)	1:179:R:VAL:H	1:142:R:PHE:HA	2	0.57	0.11	0.57
(1,1909)	1:162:R:ILE:H	1:162:R:ILE:HG21	2	0.55	0.13	0.55
(1,1909)	1:162:R:ILE:H	1:162:R:ILE:HG22	2	0.55	0.13	0.55
(1,1909)	1:162:R:ILE:H	1:162:R:ILE:HG23	2	0.55	0.13	0.55
(1,2241)	1:180:R:PHE:HE1	1:125:R:CYS:HB3	2	0.55	0.21	0.55
(1,2241)	1:180:R:PHE:HE2	1:125:R:CYS:HB3	2	0.55	0.21	0.55
(1,894)	1:60:R:PHE:H	1:56:R:ILE:HD11	2	0.54	0.05	0.54
(1,894)	1:60:R:PHE:H	1:56:R:ILE:HD12	2	0.54	0.05	0.54
(1,894)	1:60:R:PHE:H	1:56:R:ILE:HD13	2	0.54	0.05	0.54
(1,2157)	1:112:R:HIS:HA	1:112:R:HIS:HB3	2	0.42	0.03	0.42
(1,1680)	1:179:R:VAL:H	1:180:R:PHE:HB2	2	0.4	0.06	0.4
(1,1838)	1:127:R:VAL:H	1:126:R:VAL:HG21	2	0.4	0.08	0.4
(1,1838)	1:127:R:VAL:H	1:126:R:VAL:HG22	2	0.4	0.08	0.4
(1,1838)	1:127:R:VAL:H	1:126:R:VAL:HG23	2	0.4	0.08	0.4
(1,1837)	1:126:R:VAL:H	1:126:R:VAL:HG21	2	0.37	0.23	0.37
(1,1837)	1:126:R:VAL:H	1:126:R:VAL:HG22	2	0.37	0.23	0.37
(1,1837)	1:126:R:VAL:H	1:126:R:VAL:HG23	2	0.37	0.23	0.37
(2,52)	1:33:R:LEU:H	1:37:R:GLU:O	2	0.36	0.16	0.36
(1,902)	1:61:R:ARG:H	1:41:R:PHE:HZ	2	0.36	0.03	0.36
(1,1671)	1:171:R:THR:H	1:168:R:TYR:HD1	2	0.36	0.08	0.36
(1,1671)	1:171:R:THR:H	1:168:R:TYR:HD2	2	0.36	0.08	0.36
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD11	2	0.35	0.03	0.35
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD12	2	0.35	0.03	0.35
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD13	2	0.35	0.03	0.35
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD21	2	0.35	0.03	0.35
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD22	2	0.35	0.03	0.35
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD23	2	0.35	0.03	0.35
(1,915)	1:65:R:GLU:H	1:63:R:VAL:HB	2	0.34	0.05	0.34
(1,1669)	1:170:R:TRP:H	1:168:R:TYR:HD1	2	0.34	0.24	0.34
(1,1669)	1:170:R:TRP:H	1:168:R:TYR:HD2	2	0.34	0.24	0.34
(2,53)	1:116:R:GLY:H	1:124:R:VAL:O	2	0.34	0.1	0.34
(1,856)	1:48:R:HIS:H	1:49:R:ASP:HB2	2	0.33	0.14	0.33
(1,2177)	1:117:R:THR:HA	1:126:R:VAL:HG11	2	0.32	0.01	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2177)	1:117:R:THR:HA	1:126:R:VAL:HG12	2	0.32	0.01	0.32
(1,2177)	1:117:R:THR:HA	1:126:R:VAL:HG13	2	0.32	0.01	0.32
(1,1427)	1:63:R:VAL:H	1:181:R:VAL:HG21	2	0.31	0.08	0.31
(1,1427)	1:63:R:VAL:H	1:181:R:VAL:HG22	2	0.31	0.08	0.31
(1,1427)	1:63:R:VAL:H	1:181:R:VAL:HG23	2	0.31	0.08	0.31
(1,1950)	1:56:R:ILE:H	1:56:R:ILE:HD11	2	0.31	0.1	0.31
(1,1950)	1:56:R:ILE:H	1:56:R:ILE:HD12	2	0.31	0.1	0.31
(1,1950)	1:56:R:ILE:H	1:56:R:ILE:HD13	2	0.31	0.1	0.31
(1,2249)	1:171:R:THR:H	1:171:R:THR:HA	2	0.3	0.07	0.3
(1,941)	1:72:R:TYR:H	1:71:R:VAL:HG11	2	0.3	0.12	0.3
(1,941)	1:72:R:TYR:H	1:71:R:VAL:HG12	2	0.3	0.12	0.3
(1,941)	1:72:R:TYR:H	1:71:R:VAL:HG13	2	0.3	0.12	0.3
(2,118)	1:44:R:ARG:N	1:164:R:ASP:O	2	0.29	0.06	0.29
(1,1537)	1:111:R:LEU:H	1:113:R:THR:HB	2	0.28	0.08	0.28
(1,1181)	1:142:R:PHE:H	1:150:R:VAL:HG21	2	0.28	0.02	0.28
(1,1181)	1:142:R:PHE:H	1:150:R:VAL:HG22	2	0.28	0.02	0.28
(1,1181)	1:142:R:PHE:H	1:150:R:VAL:HG23	2	0.28	0.02	0.28
(1,1499)	1:95:R:HIS:H	1:97:R:GLY:H	2	0.27	0.14	0.27
(1,2205)	1:153:R:CYS:HB3	1:153:R:CYS:HA	2	0.27	0.13	0.27
(1,2306)	1:60:R:PHE:C	1:65:R:GLU:H	2	0.27	0.05	0.27
(1,829)	1:39:R:LYS:H	1:37:R:GLU:HA	2	0.26	0.02	0.26
(1,1497)	1:94:R:LEU:H	1:93:R:GLU:H	2	0.26	0.15	0.26
(1,2235)	1:162:R:ILE:H	1:162:R:ILE:HG12	2	0.26	0.15	0.26
(1,700)	1:161:R:ALA:H	1:167:R:PHE:HA	2	0.24	0.08	0.24
(1,1488)	1:87:R:GLU:H	1:94:R:LEU:HD21	2	0.24	0.1	0.24
(1,1488)	1:87:R:GLU:H	1:94:R:LEU:HD22	2	0.24	0.1	0.24
(1,1488)	1:87:R:GLU:H	1:94:R:LEU:HD23	2	0.24	0.1	0.24
(1,1141)	1:127:R:VAL:H	1:128:R:ASP:H	2	0.24	0.03	0.24
(1,510)	1:113:R:THR:H	1:111:R:LEU:HD21	2	0.23	0.03	0.23
(1,510)	1:113:R:THR:H	1:111:R:LEU:HD22	2	0.23	0.03	0.23
(1,510)	1:113:R:THR:H	1:111:R:LEU:HD23	2	0.23	0.03	0.23
(1,1945)	1:83:R:ILE:HD11	1:53:R:LEU:HD11	2	0.22	0.01	0.22
(1,1945)	1:83:R:ILE:HD11	1:53:R:LEU:HD12	2	0.22	0.01	0.22
(1,1945)	1:83:R:ILE:HD11	1:53:R:LEU:HD13	2	0.22	0.01	0.22
(1,1945)	1:83:R:ILE:HD12	1:53:R:LEU:HD11	2	0.22	0.01	0.22
(1,1945)	1:83:R:ILE:HD12	1:53:R:LEU:HD12	2	0.22	0.01	0.22
(1,1945)	1:83:R:ILE:HD12	1:53:R:LEU:HD13	2	0.22	0.01	0.22
(1,1945)	1:83:R:ILE:HD13	1:53:R:LEU:HD11	2	0.22	0.01	0.22
(1,1945)	1:83:R:ILE:HD13	1:53:R:LEU:HD12	2	0.22	0.01	0.22
(1,1945)	1:83:R:ILE:HD13	1:53:R:LEU:HD13	2	0.22	0.01	0.22
(1,1366)	1:36:R:GLY:H	1:34:R:TYR:HA	2	0.22	0.02	0.22
(1,1843)	1:128:R:ASP:H	1:127:R:VAL:HG21	2	0.22	0.06	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1843)	1:128:R:ASP:H	1:127:R:VAL:HG22	2	0.22	0.06	0.22
(1,1843)	1:128:R:ASP:H	1:127:R:VAL:HG23	2	0.22	0.06	0.22
(1,2300)	1:163:R:ASP:H	1:166:R:ASP:C	2	0.22	0.02	0.22
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD11	2	0.22	0.07	0.22
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD12	2	0.22	0.07	0.22
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD13	2	0.22	0.07	0.22
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD21	2	0.22	0.07	0.22
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD22	2	0.22	0.07	0.22
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD23	2	0.22	0.07	0.22
(1,2169)	1:122:R:SER:HB2	1:122:R:SER:HA	2	0.21	0.03	0.21
(2,76)	1:163:R:ASP:H	1:166:R:ASP:O	2	0.21	0.0	0.21
(1,2133)	1:94:R:LEU:HB2	1:94:R:LEU:HG	2	0.2	0.08	0.2
(1,1608)	1:143:R:LEU:H	1:150:R:VAL:HG21	2	0.2	0.03	0.2
(1,1608)	1:143:R:LEU:H	1:150:R:VAL:HG22	2	0.2	0.03	0.2
(1,1608)	1:143:R:LEU:H	1:150:R:VAL:HG23	2	0.2	0.03	0.2
(1,1641)	1:160:R:TYR:H	1:154:R:VAL:HG21	2	0.19	0.05	0.19
(1,1641)	1:160:R:TYR:H	1:154:R:VAL:HG22	2	0.19	0.05	0.19
(1,1641)	1:160:R:TYR:H	1:154:R:VAL:HG23	2	0.19	0.05	0.19
(1,1583)	1:127:R:VAL:H	1:180:R:PHE:H	2	0.18	0.04	0.18
(1,2175)	1:125:R:CYS:H	1:125:R:CYS:HB2	2	0.18	0.02	0.18
(1,1775)	1:94:R:LEU:HD21	1:94:R:LEU:HD11	2	0.18	0.0	0.18
(1,1775)	1:94:R:LEU:HD21	1:94:R:LEU:HD12	2	0.18	0.0	0.18
(1,1775)	1:94:R:LEU:HD21	1:94:R:LEU:HD13	2	0.18	0.0	0.18
(1,1775)	1:94:R:LEU:HD22	1:94:R:LEU:HD11	2	0.18	0.0	0.18
(1,1775)	1:94:R:LEU:HD22	1:94:R:LEU:HD12	2	0.18	0.0	0.18
(1,1775)	1:94:R:LEU:HD22	1:94:R:LEU:HD13	2	0.18	0.0	0.18
(1,1775)	1:94:R:LEU:HD23	1:94:R:LEU:HD11	2	0.18	0.0	0.18
(1,1775)	1:94:R:LEU:HD23	1:94:R:LEU:HD12	2	0.18	0.0	0.18
(1,1775)	1:94:R:LEU:HD23	1:94:R:LEU:HD13	2	0.18	0.0	0.18
(1,1948)	1:57:R:LEU:HD11	1:53:R:LEU:HD21	2	0.18	0.08	0.18
(1,1948)	1:57:R:LEU:HD11	1:53:R:LEU:HD22	2	0.18	0.08	0.18
(1,1948)	1:57:R:LEU:HD11	1:53:R:LEU:HD23	2	0.18	0.08	0.18
(1,1948)	1:57:R:LEU:HD12	1:53:R:LEU:HD21	2	0.18	0.08	0.18
(1,1948)	1:57:R:LEU:HD12	1:53:R:LEU:HD22	2	0.18	0.08	0.18
(1,1948)	1:57:R:LEU:HD12	1:53:R:LEU:HD23	2	0.18	0.08	0.18
(1,1948)	1:57:R:LEU:HD13	1:53:R:LEU:HD21	2	0.18	0.08	0.18
(1,1948)	1:57:R:LEU:HD13	1:53:R:LEU:HD22	2	0.18	0.08	0.18
(1,1948)	1:57:R:LEU:HD13	1:53:R:LEU:HD23	2	0.18	0.08	0.18
(1,1948)	1:57:R:LEU:HD21	1:53:R:LEU:HD21	2	0.18	0.08	0.18
(1,1948)	1:57:R:LEU:HD21	1:53:R:LEU:HD22	2	0.18	0.08	0.18
(1,1948)	1:57:R:LEU:HD21	1:53:R:LEU:HD23	2	0.18	0.08	0.18
(1,1948)	1:57:R:LEU:HD22	1:53:R:LEU:HD21	2	0.18	0.08	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1948)	1:57:R:LEU:HD22	1:53:R:LEU:HD22	2	0.18	0.08	0.18
(1,1948)	1:57:R:LEU:HD22	1:53:R:LEU:HD23	2	0.18	0.08	0.18
(1,1948)	1:57:R:LEU:HD23	1:53:R:LEU:HD21	2	0.18	0.08	0.18
(1,1948)	1:57:R:LEU:HD23	1:53:R:LEU:HD22	2	0.18	0.08	0.18
(1,1948)	1:57:R:LEU:HD23	1:53:R:LEU:HD23	2	0.18	0.08	0.18
(2,75)	1:163:R:ASP:N	1:166:R:ASP:O	2	0.18	0.05	0.18
(1,1025)	1:95:R:HIS:H	1:94:R:LEU:HD11	2	0.18	0.03	0.18
(1,1025)	1:95:R:HIS:H	1:94:R:LEU:HD12	2	0.18	0.03	0.18
(1,1025)	1:95:R:HIS:H	1:94:R:LEU:HD13	2	0.18	0.03	0.18
(1,439)	1:95:R:HIS:H	1:94:R:LEU:HD21	2	0.17	0.0	0.17
(1,439)	1:95:R:HIS:H	1:94:R:LEU:HD22	2	0.17	0.0	0.17
(1,439)	1:95:R:HIS:H	1:94:R:LEU:HD23	2	0.17	0.0	0.17
(1,2058)	1:142:R:PHE:HD1	1:177:R:VAL:HG11	2	0.17	0.05	0.17
(1,2058)	1:142:R:PHE:HD1	1:177:R:VAL:HG12	2	0.17	0.05	0.17
(1,2058)	1:142:R:PHE:HD1	1:177:R:VAL:HG13	2	0.17	0.05	0.17
(1,2058)	1:142:R:PHE:HD2	1:177:R:VAL:HG11	2	0.17	0.05	0.17
(1,2058)	1:142:R:PHE:HD2	1:177:R:VAL:HG12	2	0.17	0.05	0.17
(1,2058)	1:142:R:PHE:HD2	1:177:R:VAL:HG13	2	0.17	0.05	0.17
(1,1720)	1:103:R:VAL:HG21	1:56:R:ILE:HD11	2	0.16	0.02	0.16
(1,1720)	1:103:R:VAL:HG21	1:56:R:ILE:HD12	2	0.16	0.02	0.16
(1,1720)	1:103:R:VAL:HG21	1:56:R:ILE:HD13	2	0.16	0.02	0.16
(1,1720)	1:103:R:VAL:HG22	1:56:R:ILE:HD11	2	0.16	0.02	0.16
(1,1720)	1:103:R:VAL:HG22	1:56:R:ILE:HD12	2	0.16	0.02	0.16
(1,1720)	1:103:R:VAL:HG22	1:56:R:ILE:HD13	2	0.16	0.02	0.16
(1,1720)	1:103:R:VAL:HG23	1:56:R:ILE:HD11	2	0.16	0.02	0.16
(1,1720)	1:103:R:VAL:HG23	1:56:R:ILE:HD12	2	0.16	0.02	0.16
(1,1720)	1:103:R:VAL:HG23	1:56:R:ILE:HD13	2	0.16	0.02	0.16
(1,2316)	1:139:R:ALA:C	1:181:R:VAL:H	2	0.16	0.05	0.16
(2,78)	1:163:R:ASP:O	1:166:R:ASP:H	2	0.16	0.02	0.16
(1,2228)	1:162:R:ILE:H	1:162:R:ILE:HA	2	0.15	0.02	0.15
(2,20)	1:69:R:ASP:O	1:73:R:SER:N	2	0.15	0.02	0.15
(1,1788)	1:103:R:VAL:HG11	1:103:R:VAL:HA	2	0.15	0.03	0.15
(1,1788)	1:103:R:VAL:HG12	1:103:R:VAL:HA	2	0.15	0.03	0.15
(1,1788)	1:103:R:VAL:HG13	1:103:R:VAL:HA	2	0.15	0.03	0.15
(1,1792)	1:103:R:VAL:HA	1:103:R:VAL:HG11	2	0.15	0.03	0.15
(1,1792)	1:103:R:VAL:HA	1:103:R:VAL:HG12	2	0.15	0.03	0.15
(1,1792)	1:103:R:VAL:HA	1:103:R:VAL:HG13	2	0.15	0.03	0.15
(2,18)	1:68:R:PHE:O	1:72:R:TYR:N	2	0.15	0.0	0.15
(2,29)	1:82:R:ALA:O	1:86:R:LEU:H	2	0.15	0.0	0.15
(1,1297)	1:173:R:ASP:H	1:176:R:ASP:H	2	0.14	0.04	0.14
(1,2164)	1:117:R:THR:H	1:117:R:THR:HA	2	0.14	0.03	0.14
(1,2299)	1:162:R:ILE:H	1:151:R:PHE:C	2	0.14	0.03	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,958)	1:78:R:LEU:H	1:78:R:LEU:HA	2	0.14	0.02	0.14
(1,1346)	1:32:R:THR:H	1:38:R:LYS:HA	2	0.14	0.01	0.14
(1,1491)	1:90:R:THR:H	1:89:R:LEU:HG	2	0.14	0.02	0.14
(2,35)	1:85:R:GLN:O	1:89:R:LEU:H	2	0.14	0.02	0.14
(1,192)	1:37:R:GLU:H	1:35:R:ASN:H	2	0.13	0.0	0.13
(1,583)	1:129:R:GLY:H	1:128:R:ASP:HB2	2	0.13	0.02	0.13
(1,689)	1:159:R:TRP:H	1:155:R:THR:H	2	0.13	0.01	0.13
(1,1401)	1:54:R:ASN:H	1:52:R:TRP:H	2	0.13	0.01	0.13
(1,1757)	1:82:R:ALA:H	1:82:R:ALA:HB1	2	0.13	0.02	0.13
(1,1757)	1:82:R:ALA:H	1:82:R:ALA:HB2	2	0.13	0.02	0.13
(1,1757)	1:82:R:ALA:H	1:82:R:ALA:HB3	2	0.13	0.02	0.13
(1,1908)	1:162:R:ILE:HG12	1:162:R:ILE:HG21	2	0.13	0.03	0.13
(1,1908)	1:162:R:ILE:HG12	1:162:R:ILE:HG22	2	0.13	0.03	0.13
(1,1908)	1:162:R:ILE:HG12	1:162:R:ILE:HG23	2	0.13	0.03	0.13
(1,2041)	1:34:R:TYR:HB2	1:154:R:VAL:HG11	2	0.13	0.0	0.13
(1,2041)	1:34:R:TYR:HB2	1:154:R:VAL:HG12	2	0.13	0.0	0.13
(1,2041)	1:34:R:TYR:HB2	1:154:R:VAL:HG13	2	0.13	0.0	0.13
(1,2041)	1:34:R:TYR:HB3	1:154:R:VAL:HG11	2	0.13	0.0	0.13
(1,2041)	1:34:R:TYR:HB3	1:154:R:VAL:HG12	2	0.13	0.0	0.13
(1,2041)	1:34:R:TYR:HB3	1:154:R:VAL:HG13	2	0.13	0.0	0.13
(2,60)	1:141:R:ILE:N	1:179:R:VAL:O	2	0.13	0.0	0.13
(1,695)	1:160:R:TYR:H	1:158:R:GLY:HA2	2	0.12	0.02	0.12
(1,695)	1:160:R:TYR:H	1:158:R:GLY:HA3	2	0.12	0.02	0.12
(1,773)	1:181:R:VAL:H	1:180:R:PHE:HE1	2	0.12	0.02	0.12
(1,773)	1:181:R:VAL:H	1:180:R:PHE:HE2	2	0.12	0.02	0.12
(1,2268)	1:61:R:ARG:H	1:57:R:LEU:C	2	0.12	0.01	0.12
(1,2294)	1:140:R:GLY:H	1:152:R:ALA:C	2	0.12	0.01	0.12
(1,2317)	1:140:R:GLY:H	1:152:R:ALA:C	2	0.12	0.01	0.12
(2,12)	1:61:R:ARG:N	1:57:R:LEU:O	2	0.12	0.01	0.12
(2,87)	1:60:R:PHE:O	1:65:R:GLU:H	2	0.12	0.02	0.12
(1,2287)	1:31:R:LEU:C	1:39:R:LYS:H	2	0.12	0.01	0.12
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD11	2	0.11	0.0	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD12	2	0.11	0.0	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD13	2	0.11	0.0	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD21	2	0.11	0.0	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD22	2	0.11	0.0	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD23	2	0.11	0.0	0.11
(1,1770)	1:89:R:LEU:HD11	1:89:R:LEU:HG	2	0.11	0.0	0.11
(1,1770)	1:89:R:LEU:HD12	1:89:R:LEU:HG	2	0.11	0.0	0.11
(1,1770)	1:89:R:LEU:HD13	1:89:R:LEU:HG	2	0.11	0.0	0.11
(1,1770)	1:89:R:LEU:HD21	1:89:R:LEU:HG	2	0.11	0.0	0.11
(1,1770)	1:89:R:LEU:HD22	1:89:R:LEU:HG	2	0.11	0.0	0.11

Continued on next page...

Continued from previous page...

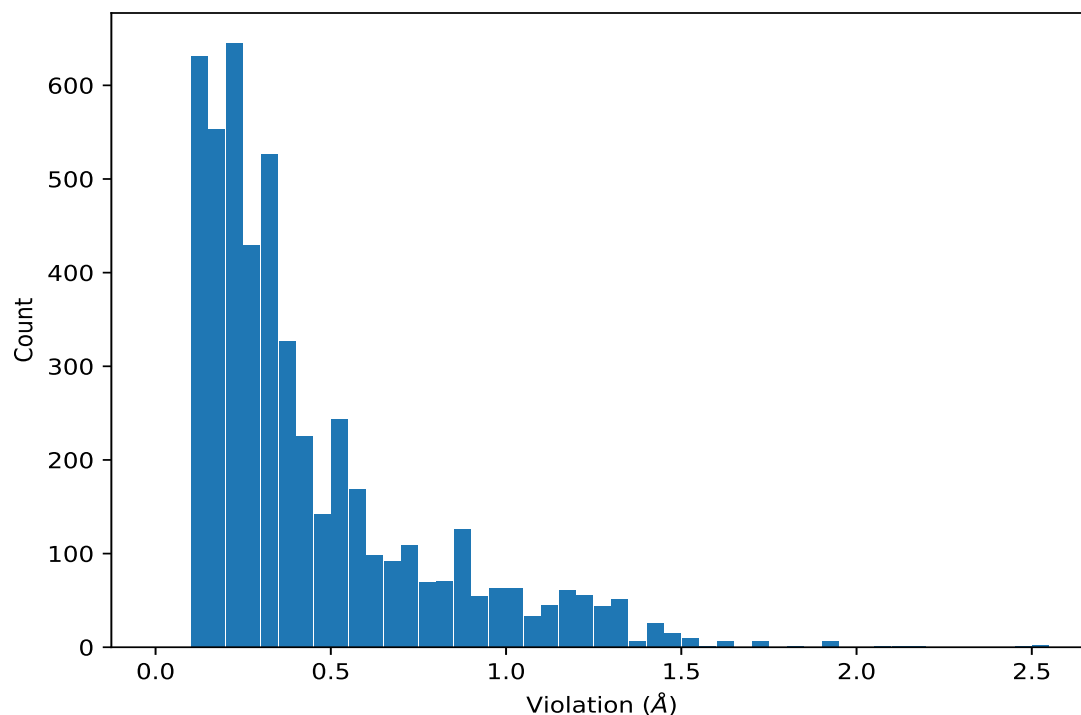
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1770)	1:89:R:LEU:HD23	1:89:R:LEU:HG	2	0.11	0.0	0.11
(1,1944)	1:82:R:ALA:HB1	1:53:R:LEU:HD11	2	0.11	0.01	0.11
(1,1944)	1:82:R:ALA:HB1	1:53:R:LEU:HD12	2	0.11	0.01	0.11
(1,1944)	1:82:R:ALA:HB1	1:53:R:LEU:HD13	2	0.11	0.01	0.11
(1,1944)	1:82:R:ALA:HB2	1:53:R:LEU:HD11	2	0.11	0.01	0.11
(1,1944)	1:82:R:ALA:HB2	1:53:R:LEU:HD12	2	0.11	0.01	0.11
(1,1944)	1:82:R:ALA:HB2	1:53:R:LEU:HD13	2	0.11	0.01	0.11
(1,1944)	1:82:R:ALA:HB3	1:53:R:LEU:HD11	2	0.11	0.01	0.11
(1,1944)	1:82:R:ALA:HB3	1:53:R:LEU:HD12	2	0.11	0.01	0.11
(1,1944)	1:82:R:ALA:HB3	1:53:R:LEU:HD13	2	0.11	0.01	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:153:R:CYS:H	1:158:R:GLY:HA3	1	2.54
(1,1893)	1:170:R:TRP:HB3	1:171:R:THR:HG1	5	2.51
(1,1222)	1:153:R:CYS:H	1:158:R:GLY:HA3	5	2.48
(1,1222)	1:153:R:CYS:H	1:158:R:GLY:HA3	4	2.15
(1,1222)	1:153:R:CYS:H	1:158:R:GLY:HA3	3	2.14
(1,1222)	1:153:R:CYS:H	1:158:R:GLY:HA3	2	2.09
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD11	1	1.91
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD12	1	1.91
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD13	1	1.91
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD21	1	1.91
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD22	1	1.91
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD23	1	1.91
(1,606)	1:139:R:ALA:H	1:180:R:PHE:HB3	3	1.82
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD11	2	1.71
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD12	2	1.71
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD13	2	1.71
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD21	2	1.71
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD22	2	1.71
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD23	2	1.71
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD11	3	1.62
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD12	3	1.62
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD13	3	1.62
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD21	3	1.62
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD22	3	1.62
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD23	3	1.62
(1,1893)	1:170:R:TRP:HB3	1:171:R:THR:HG1	1	1.58
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG21	2	1.54
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG22	2	1.54
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG23	2	1.54
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD11	5	1.53
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD12	5	1.53
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD13	5	1.53
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD21	5	1.53
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD22	5	1.53
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD23	5	1.53
(1,1384)	1:44:R:ARG:H	1:42:R:TYR:H	5	1.5
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD11	4	1.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD12	4	1.46
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD13	4	1.46
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD21	4	1.46
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD22	4	1.46
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD23	4	1.46
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD11	4	1.46
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD12	4	1.46
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD13	4	1.46
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD21	4	1.46
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD22	4	1.46
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD23	4	1.46
(1,1546)	1:114:R:GLY:H	1:115:R:ILE:HD11	5	1.45
(1,1546)	1:114:R:GLY:H	1:115:R:ILE:HD12	5	1.45
(1,1546)	1:114:R:GLY:H	1:115:R:ILE:HD13	5	1.45
(2,57)	1:127:R:VAL:H	1:178:R:LEU:O	4	1.44
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD11	2	1.44
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD12	2	1.44
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD13	2	1.44
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD21	2	1.44
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD22	2	1.44
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD23	2	1.44
(1,2291)	1:127:R:VAL:H	1:178:R:LEU:C	4	1.43
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD11	1	1.43
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD12	1	1.43
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD13	1	1.43
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD21	1	1.43
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD22	1	1.43
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD23	1	1.43
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD11	3	1.43
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD12	3	1.43
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD13	3	1.43
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD21	3	1.43
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD22	3	1.43
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD23	3	1.43
(1,851)	1:46:R:ASN:H	1:165:R:GLU:H	5	1.43
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG21	5	1.42
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG22	5	1.42
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG23	5	1.42
(1,1646)	1:161:R:ALA:H	1:168:R:TYR:HD1	1	1.42
(1,1646)	1:161:R:ALA:H	1:168:R:TYR:HD2	1	1.42
(1,1698)	1:42:R:TYR:HE1	1:42:R:TYR:HA	1	1.39
(1,1698)	1:42:R:TYR:HE2	1:42:R:TYR:HA	1	1.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2112)	1:53:R:LEU:HD11	1:83:R:ILE:HG13	1	1.37
(1,2112)	1:53:R:LEU:HD12	1:83:R:ILE:HG13	1	1.37
(1,2112)	1:53:R:LEU:HD13	1:83:R:ILE:HG13	1	1.37
(1,1258)	1:161:R:ALA:H	1:162:R:ILE:HG13	3	1.35
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG21	4	1.34
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG22	4	1.34
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG23	4	1.34
(1,29)	1:79:R:THR:H	1:80:R:LEU:HA	4	1.34
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD11	2	1.33
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD12	2	1.33
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD13	2	1.33
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD21	2	1.33
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD22	2	1.33
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD23	2	1.33
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD11	2	1.33
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD12	2	1.33
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD13	2	1.33
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD21	2	1.33
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD22	2	1.33
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD23	2	1.33
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD11	2	1.33
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD12	2	1.33
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD13	2	1.33
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD21	2	1.33
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD22	2	1.33
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD23	2	1.33
(1,1698)	1:42:R:TYR:HE1	1:42:R:TYR:HA	2	1.33
(1,1698)	1:42:R:TYR:HE2	1:42:R:TYR:HA	2	1.33
(1,29)	1:79:R:THR:H	1:80:R:LEU:HA	5	1.33
(1,2112)	1:53:R:LEU:HD11	1:83:R:ILE:HG13	5	1.32
(1,2112)	1:53:R:LEU:HD12	1:83:R:ILE:HG13	5	1.32
(1,2112)	1:53:R:LEU:HD13	1:83:R:ILE:HG13	5	1.32
(1,29)	1:79:R:THR:H	1:80:R:LEU:HA	2	1.32
(2,117)	1:44:R:ARG:H	1:164:R:ASP:O	5	1.3
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD11	1	1.3
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD12	1	1.3
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD13	1	1.3
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD21	1	1.3
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD22	1	1.3
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD23	1	1.3
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD11	1	1.3
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD12	1	1.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD13	1	1.3
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD21	1	1.3
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD22	1	1.3
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD23	1	1.3
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD11	1	1.3
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD12	1	1.3
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD13	1	1.3
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD21	1	1.3
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD22	1	1.3
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD23	1	1.3
(1,2021)	1:127:R:VAL:H	1:127:R:VAL:HG21	1	1.3
(1,2021)	1:127:R:VAL:H	1:127:R:VAL:HG22	1	1.3
(1,2021)	1:127:R:VAL:H	1:127:R:VAL:HG23	1	1.3
(1,2016)	1:127:R:VAL:H	1:126:R:VAL:HG21	5	1.28
(1,2016)	1:127:R:VAL:H	1:126:R:VAL:HG22	5	1.28
(1,2016)	1:127:R:VAL:H	1:126:R:VAL:HG23	5	1.28
(1,1698)	1:42:R:TYR:HE1	1:42:R:TYR:HA	3	1.28
(1,1698)	1:42:R:TYR:HE2	1:42:R:TYR:HA	3	1.28
(1,1575)	1:125:R:CYS:H	1:180:R:PHE:HD1	4	1.28
(1,1575)	1:125:R:CYS:H	1:180:R:PHE:HD2	4	1.28
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD11	5	1.27
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD12	5	1.27
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD13	5	1.27
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD21	5	1.27
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD22	5	1.27
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD23	5	1.27
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD11	5	1.27
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD12	5	1.27
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD13	5	1.27
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD21	5	1.27
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD22	5	1.27
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD23	5	1.27
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD11	5	1.27
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD12	5	1.27
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD13	5	1.27
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD21	5	1.27
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD22	5	1.27
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD23	5	1.27
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD11	3	1.25
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD12	3	1.25
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD13	3	1.25
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD21	3	1.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD22	3	1.25
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD23	3	1.25
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD11	3	1.25
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD12	3	1.25
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD13	3	1.25
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD21	3	1.25
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD22	3	1.25
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD23	3	1.25
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD11	3	1.25
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD12	3	1.25
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD13	3	1.25
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD21	3	1.25
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD22	3	1.25
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD23	3	1.25
(1,29)	1:79:R:THR:H	1:80:R:LEU:HA	3	1.25
(1,2247)	1:134:R:LEU:HD11	1:171:R:THR:HA	2	1.24
(1,2247)	1:134:R:LEU:HD12	1:171:R:THR:HA	2	1.24
(1,2247)	1:134:R:LEU:HD13	1:171:R:THR:HA	2	1.24
(1,2247)	1:134:R:LEU:HD21	1:171:R:THR:HA	2	1.24
(1,2247)	1:134:R:LEU:HD22	1:171:R:THR:HA	2	1.24
(1,2247)	1:134:R:LEU:HD23	1:171:R:THR:HA	2	1.24
(1,2112)	1:53:R:LEU:HD11	1:83:R:ILE:HG13	2	1.24
(1,2112)	1:53:R:LEU:HD12	1:83:R:ILE:HG13	2	1.24
(1,2112)	1:53:R:LEU:HD13	1:83:R:ILE:HG13	2	1.24
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD11	4	1.24
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD12	4	1.24
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD13	4	1.24
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD21	4	1.24
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD22	4	1.24
(1,2091)	1:71:R:VAL:HG21	1:57:R:LEU:HD23	4	1.24
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD11	4	1.24
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD12	4	1.24
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD13	4	1.24
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD21	4	1.24
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD22	4	1.24
(1,2091)	1:71:R:VAL:HG22	1:57:R:LEU:HD23	4	1.24
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD11	4	1.24
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD12	4	1.24
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD13	4	1.24
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD21	4	1.24
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD22	4	1.24
(1,2091)	1:71:R:VAL:HG23	1:57:R:LEU:HD23	4	1.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2118)	1:89:R:LEU:H	1:89:R:LEU:HD11	3	1.23
(1,2118)	1:89:R:LEU:H	1:89:R:LEU:HD12	3	1.23
(1,2118)	1:89:R:LEU:H	1:89:R:LEU:HD13	3	1.23
(1,2118)	1:89:R:LEU:H	1:89:R:LEU:HD21	3	1.23
(1,2118)	1:89:R:LEU:H	1:89:R:LEU:HD22	3	1.23
(1,2118)	1:89:R:LEU:H	1:89:R:LEU:HD23	3	1.23
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD11	5	1.23
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD12	5	1.23
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD13	5	1.23
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD21	5	1.23
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD22	5	1.23
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD23	5	1.23
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD11	5	1.23
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD12	5	1.23
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD13	5	1.23
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD21	5	1.23
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD22	5	1.23
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD23	5	1.23
(1,29)	1:79:R:THR:H	1:80:R:LEU:HA	1	1.23
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG21	3	1.22
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG22	3	1.22
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG23	3	1.22
(1,1956)	1:56:R:ILE:H	1:56:R:ILE:HG21	4	1.21
(1,1956)	1:56:R:ILE:H	1:56:R:ILE:HG22	4	1.21
(1,1956)	1:56:R:ILE:H	1:56:R:ILE:HG23	4	1.21
(1,1592)	1:138:R:HIS:H	1:154:R:VAL:HG21	3	1.21
(1,1592)	1:138:R:HIS:H	1:154:R:VAL:HG22	3	1.21
(1,1592)	1:138:R:HIS:H	1:154:R:VAL:HG23	3	1.21
(1,1385)	1:44:R:ARG:H	1:43:R:SER:H	3	1.2
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD11	4	1.19
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD12	4	1.19
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD13	4	1.19
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD21	4	1.19
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD22	4	1.19
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD23	4	1.19
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD11	4	1.19
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD12	4	1.19
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD13	4	1.19
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD21	4	1.19
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD22	4	1.19
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD23	4	1.19
(1,2076)	1:49:R:ASP:HB2	1:49:R:ASP:HB3	1	1.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1915)	1:159:R:TRP:HB2	1:171:R:THR:HA	3	1.18
(1,2242)	1:161:R:ALA:HB1	1:170:R:TRP:HB3	3	1.17
(1,2242)	1:161:R:ALA:HB2	1:170:R:TRP:HB3	3	1.17
(1,2242)	1:161:R:ALA:HB3	1:170:R:TRP:HB3	3	1.17
(1,2210)	1:153:R:CYS:HB2	1:153:R:CYS:HB3	1	1.17
(1,2210)	1:153:R:CYS:HB2	1:153:R:CYS:HB3	2	1.17
(1,2210)	1:153:R:CYS:HB2	1:153:R:CYS:HB3	3	1.17
(1,2088)	1:56:R:ILE:HG13	1:56:R:ILE:HG12	1	1.17
(1,2088)	1:56:R:ILE:HG13	1:56:R:ILE:HG12	2	1.17
(1,2088)	1:56:R:ILE:HG13	1:56:R:ILE:HG12	3	1.17
(1,2088)	1:56:R:ILE:HG13	1:56:R:ILE:HG12	5	1.17
(1,2081)	1:52:R:TRP:HB3	1:52:R:TRP:HB2	1	1.17
(1,2081)	1:52:R:TRP:HB3	1:52:R:TRP:HB2	2	1.17
(1,2081)	1:52:R:TRP:HB3	1:52:R:TRP:HB2	3	1.17
(1,2081)	1:52:R:TRP:HB3	1:52:R:TRP:HB2	4	1.17
(1,2081)	1:52:R:TRP:HB3	1:52:R:TRP:HB2	5	1.17
(1,2076)	1:49:R:ASP:HB2	1:49:R:ASP:HB3	2	1.17
(1,2076)	1:49:R:ASP:HB2	1:49:R:ASP:HB3	3	1.17
(1,2076)	1:49:R:ASP:HB2	1:49:R:ASP:HB3	4	1.17
(1,2076)	1:49:R:ASP:HB2	1:49:R:ASP:HB3	5	1.17
(1,1893)	1:170:R:TRP:HB3	1:171:R:THR:HG1	4	1.17
(1,1698)	1:42:R:TYR:HE1	1:42:R:TYR:HA	4	1.17
(1,1698)	1:42:R:TYR:HE2	1:42:R:TYR:HA	4	1.17
(1,1698)	1:42:R:TYR:HE1	1:42:R:TYR:HA	5	1.17
(1,1698)	1:42:R:TYR:HE2	1:42:R:TYR:HA	5	1.17
(1,2210)	1:153:R:CYS:HB2	1:153:R:CYS:HB3	4	1.16
(1,2210)	1:153:R:CYS:HB2	1:153:R:CYS:HB3	5	1.16
(1,2101)	1:70:R:TRP:HB2	1:70:R:TRP:HB3	1	1.16
(1,2101)	1:70:R:TRP:HB2	1:70:R:TRP:HB3	2	1.16
(1,2101)	1:70:R:TRP:HB2	1:70:R:TRP:HB3	3	1.16
(1,2101)	1:70:R:TRP:HB2	1:70:R:TRP:HB3	4	1.16
(1,2101)	1:70:R:TRP:HB2	1:70:R:TRP:HB3	5	1.16
(1,2088)	1:56:R:ILE:HG13	1:56:R:ILE:HG12	4	1.16
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD11	1	1.15
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD12	1	1.15
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD13	1	1.15
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD21	1	1.15
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD22	1	1.15
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD23	1	1.15
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD11	4	1.15
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD12	4	1.15
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD13	4	1.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD21	4	1.15
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD22	4	1.15
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD23	4	1.15
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB1	5	1.15
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB2	5	1.15
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB3	5	1.15
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD11	2	1.14
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD12	2	1.14
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD13	2	1.14
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD21	2	1.14
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD22	2	1.14
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD23	2	1.14
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD11	5	1.14
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD12	5	1.14
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD13	5	1.14
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD21	5	1.14
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD22	5	1.14
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD23	5	1.14
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD11	2	1.13
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD12	2	1.13
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD13	2	1.13
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD21	2	1.13
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD22	2	1.13
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD23	2	1.13
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD11	2	1.13
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD12	2	1.13
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD13	2	1.13
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD21	2	1.13
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD22	2	1.13
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD23	2	1.13
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD11	4	1.13
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD12	4	1.13
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD13	4	1.13
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD21	4	1.13
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD22	4	1.13
(1,1374)	1:41:R:PHE:H	1:31:R:LEU:HD23	4	1.13
(1,2016)	1:127:R:VAL:H	1:126:R:VAL:HG21	3	1.12
(1,2016)	1:127:R:VAL:H	1:126:R:VAL:HG22	3	1.12
(1,2016)	1:127:R:VAL:H	1:126:R:VAL:HG23	3	1.12
(1,1170)	1:139:R:ALA:H	1:181:R:VAL:HG11	3	1.12
(1,1170)	1:139:R:ALA:H	1:181:R:VAL:HG12	3	1.12
(1,1170)	1:139:R:ALA:H	1:181:R:VAL:HG13	3	1.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG21	1	1.11
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG22	1	1.11
(1,1968)	1:53:R:LEU:HB2	1:71:R:VAL:HG23	1	1.11
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD11	4	1.1
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD12	4	1.1
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD13	4	1.1
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD21	4	1.1
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD22	4	1.1
(1,1364)	1:36:R:GLY:H	1:33:R:LEU:HD23	4	1.1
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD21	5	1.09
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD22	5	1.09
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD23	5	1.09
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD11	3	1.09
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD12	3	1.09
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD13	3	1.09
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD21	3	1.09
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD22	3	1.09
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD23	3	1.09
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD11	3	1.09
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD12	3	1.09
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD13	3	1.09
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD21	3	1.09
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD22	3	1.09
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD23	3	1.09
(1,1646)	1:161:R:ALA:H	1:168:R:TYR:HD1	5	1.07
(1,1646)	1:161:R:ALA:H	1:168:R:TYR:HD2	5	1.07
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD11	5	1.06
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD12	5	1.06
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD13	5	1.06
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD21	5	1.06
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD22	5	1.06
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD23	5	1.06
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD11	5	1.06
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD12	5	1.06
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD13	5	1.06
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD21	5	1.06
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD22	5	1.06
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD23	5	1.06
(1,606)	1:139:R:ALA:H	1:180:R:PHE:HB3	1	1.06
(1,2212)	1:34:R:TYR:HB2	1:154:R:VAL:HB	3	1.05
(1,2212)	1:34:R:TYR:HB3	1:154:R:VAL:HB	3	1.05
(1,606)	1:139:R:ALA:H	1:180:R:PHE:HB3	4	1.05

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD11	2	1.04
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD12	2	1.04
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD13	2	1.04
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD21	2	1.04
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD22	2	1.04
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD23	2	1.04
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD11	2	1.04
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD12	2	1.04
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD13	2	1.04
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD21	2	1.04
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD22	2	1.04
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD23	2	1.04
(1,1593)	1:138:R:HIS:H	1:181:R:VAL:HG11	1	1.04
(1,1593)	1:138:R:HIS:H	1:181:R:VAL:HG12	1	1.04
(1,1593)	1:138:R:HIS:H	1:181:R:VAL:HG13	1	1.04
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD21	2	1.03
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD22	2	1.03
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD23	2	1.03
(1,2130)	1:94:R:LEU:H	1:94:R:LEU:HD21	3	1.03
(1,2130)	1:94:R:LEU:H	1:94:R:LEU:HD22	3	1.03
(1,2130)	1:94:R:LEU:H	1:94:R:LEU:HD23	3	1.03
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD21	4	1.03
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD22	4	1.03
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD23	4	1.03
(1,778)	1:183:R:TYR:H	1:137:R:PHE:HA	3	1.03
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD11	1	1.02
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD12	1	1.02
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD13	1	1.02
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD21	1	1.02
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD22	1	1.02
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD23	1	1.02
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD11	1	1.02
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD12	1	1.02
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD13	1	1.02
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD21	1	1.02
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD22	1	1.02
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD23	1	1.02
(1,1956)	1:56:R:ILE:H	1:56:R:ILE:HG21	1	1.02
(1,1956)	1:56:R:ILE:H	1:56:R:ILE:HG22	1	1.02
(1,1956)	1:56:R:ILE:H	1:56:R:ILE:HG23	1	1.02
(1,1593)	1:138:R:HIS:H	1:181:R:VAL:HG11	5	1.02
(1,1593)	1:138:R:HIS:H	1:181:R:VAL:HG12	5	1.02

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1593)	1:138:R:HIS:H	1:181:R:VAL:HG13	5	1.02
(1,1501)	1:97:R:GLY:H	1:94:R:LEU:HD11	4	1.02
(1,1501)	1:97:R:GLY:H	1:94:R:LEU:HD12	4	1.02
(1,1501)	1:97:R:GLY:H	1:94:R:LEU:HD13	4	1.02
(1,1258)	1:161:R:ALA:H	1:162:R:ILE:HG13	2	1.02
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG21	3	1.02
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG22	3	1.02
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG23	3	1.02
(1,180)	1:33:R:LEU:H	1:36:R:GLY:HA3	1	1.01
(1,2132)	1:83:R:ILE:HD11	1:94:R:LEU:HD11	4	1.0
(1,2132)	1:83:R:ILE:HD11	1:94:R:LEU:HD12	4	1.0
(1,2132)	1:83:R:ILE:HD11	1:94:R:LEU:HD13	4	1.0
(1,2132)	1:83:R:ILE:HD12	1:94:R:LEU:HD11	4	1.0
(1,2132)	1:83:R:ILE:HD12	1:94:R:LEU:HD12	4	1.0
(1,2132)	1:83:R:ILE:HD12	1:94:R:LEU:HD13	4	1.0
(1,2132)	1:83:R:ILE:HD13	1:94:R:LEU:HD11	4	1.0
(1,2132)	1:83:R:ILE:HD13	1:94:R:LEU:HD12	4	1.0
(1,2132)	1:83:R:ILE:HD13	1:94:R:LEU:HD13	4	1.0
(1,1646)	1:161:R:ALA:H	1:168:R:TYR:HD1	2	1.0
(1,1646)	1:161:R:ALA:H	1:168:R:TYR:HD2	2	1.0
(1,180)	1:33:R:LEU:H	1:36:R:GLY:HA3	3	1.0
(1,1639)	1:159:R:TRP:H	1:153:R:CYS:H	4	0.99
(1,1495)	1:94:R:LEU:H	1:83:R:ILE:HD11	3	0.99
(1,1495)	1:94:R:LEU:H	1:83:R:ILE:HD12	3	0.99
(1,1495)	1:94:R:LEU:H	1:83:R:ILE:HD13	3	0.99
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD21	3	0.98
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD22	3	0.98
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD23	3	0.98
(1,1951)	1:103:R:VAL:HG21	1:56:R:ILE:HD11	5	0.98
(1,1951)	1:103:R:VAL:HG21	1:56:R:ILE:HD12	5	0.98
(1,1951)	1:103:R:VAL:HG21	1:56:R:ILE:HD13	5	0.98
(1,1951)	1:103:R:VAL:HG22	1:56:R:ILE:HD11	5	0.98
(1,1951)	1:103:R:VAL:HG22	1:56:R:ILE:HD12	5	0.98
(1,1951)	1:103:R:VAL:HG22	1:56:R:ILE:HD13	5	0.98
(1,1951)	1:103:R:VAL:HG23	1:56:R:ILE:HD11	5	0.98
(1,1951)	1:103:R:VAL:HG23	1:56:R:ILE:HD12	5	0.98
(1,1951)	1:103:R:VAL:HG23	1:56:R:ILE:HD13	5	0.98
(1,1895)	1:162:R:ILE:HD11	1:162:R:ILE:HA	4	0.98
(1,1895)	1:162:R:ILE:HD12	1:162:R:ILE:HA	4	0.98
(1,1895)	1:162:R:ILE:HD13	1:162:R:ILE:HA	4	0.98
(1,2242)	1:161:R:ALA:HB1	1:170:R:TRP:HB3	4	0.97
(1,2242)	1:161:R:ALA:HB2	1:170:R:TRP:HB3	4	0.97

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2242)	1:161:R:ALA:HB3	1:170:R:TRP:HB3	4	0.97
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD11	5	0.97
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD12	5	0.97
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD13	5	0.97
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD21	5	0.97
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD22	5	0.97
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD23	5	0.97
(1,2178)	1:126:R:VAL:H	1:126:R:VAL:HG11	2	0.96
(1,2178)	1:126:R:VAL:H	1:126:R:VAL:HG12	2	0.96
(1,2178)	1:126:R:VAL:H	1:126:R:VAL:HG13	2	0.96
(1,1317)	1:179:R:VAL:H	1:180:R:PHE:HB2	4	0.96
(1,418)	1:91:R:GLY:H	1:89:R:LEU:HB2	5	0.96
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG21	5	0.95
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG22	5	0.95
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG23	5	0.95
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG21	5	0.95
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG22	5	0.95
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG23	5	0.95
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG21	5	0.95
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG22	5	0.95
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG23	5	0.95
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG21	5	0.95
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG22	5	0.95
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG23	5	0.95
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG21	5	0.95
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG22	5	0.95
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG23	5	0.95
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG21	5	0.95
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG22	5	0.95
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG23	5	0.95
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG21	5	0.95
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG22	5	0.95
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG23	5	0.95
(1,1895)	1:162:R:ILE:HD11	1:162:R:ILE:HA	3	0.95
(1,1895)	1:162:R:ILE:HD12	1:162:R:ILE:HA	3	0.95
(1,1895)	1:162:R:ILE:HD13	1:162:R:ILE:HA	3	0.95
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD21	2	0.95
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD22	2	0.95
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD23	2	0.95
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD21	3	0.95
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD22	3	0.95
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD23	3	0.95

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD21	4	0.94
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD22	4	0.94
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD23	4	0.94
(1,2143)	1:94:R:LEU:HD21	1:103:R:VAL:HG11	5	0.94
(1,2143)	1:94:R:LEU:HD21	1:103:R:VAL:HG12	5	0.94
(1,2143)	1:94:R:LEU:HD21	1:103:R:VAL:HG13	5	0.94
(1,2143)	1:94:R:LEU:HD22	1:103:R:VAL:HG11	5	0.94
(1,2143)	1:94:R:LEU:HD22	1:103:R:VAL:HG12	5	0.94
(1,2143)	1:94:R:LEU:HD22	1:103:R:VAL:HG13	5	0.94
(1,2143)	1:94:R:LEU:HD23	1:103:R:VAL:HG11	5	0.94
(1,2143)	1:94:R:LEU:HD23	1:103:R:VAL:HG12	5	0.94
(1,2143)	1:94:R:LEU:HD23	1:103:R:VAL:HG13	5	0.94
(1,1585)	1:128:R:ASP:H	1:126:R:VAL:HG21	2	0.94
(1,1585)	1:128:R:ASP:H	1:126:R:VAL:HG22	2	0.94
(1,1585)	1:128:R:ASP:H	1:126:R:VAL:HG23	2	0.94
(1,1585)	1:128:R:ASP:H	1:126:R:VAL:HG21	3	0.94
(1,1585)	1:128:R:ASP:H	1:126:R:VAL:HG22	3	0.94
(1,1585)	1:128:R:ASP:H	1:126:R:VAL:HG23	3	0.94
(1,1292)	1:171:R:THR:H	1:168:R:TYR:HD1	2	0.94
(1,1292)	1:171:R:THR:H	1:168:R:TYR:HD2	2	0.94
(1,1676)	1:176:R:ASP:H	1:142:R:PHE:HE1	1	0.93
(1,1676)	1:176:R:ASP:H	1:142:R:PHE:HE2	1	0.93
(1,1660)	1:165:R:GLU:H	1:46:R:ASN:H	5	0.93
(1,2179)	1:128:R:ASP:H	1:127:R:VAL:HG11	1	0.92
(1,2179)	1:128:R:ASP:H	1:127:R:VAL:HG12	1	0.92
(1,2179)	1:128:R:ASP:H	1:127:R:VAL:HG13	1	0.92
(1,2134)	1:94:R:LEU:HD21	1:94:R:LEU:HG	4	0.92
(1,2134)	1:94:R:LEU:HD22	1:94:R:LEU:HG	4	0.92
(1,2134)	1:94:R:LEU:HD23	1:94:R:LEU:HG	4	0.92
(1,2103)	1:72:R:TYR:H	1:71:R:VAL:HG11	2	0.92
(1,2103)	1:72:R:TYR:H	1:71:R:VAL:HG12	2	0.92
(1,2103)	1:72:R:TYR:H	1:71:R:VAL:HG13	2	0.92
(1,2020)	1:127:R:VAL:HA	1:127:R:VAL:HG21	5	0.92
(1,2020)	1:127:R:VAL:HA	1:127:R:VAL:HG22	5	0.92
(1,2020)	1:127:R:VAL:HA	1:127:R:VAL:HG23	5	0.92
(1,2134)	1:94:R:LEU:HD21	1:94:R:LEU:HG	2	0.91
(1,2134)	1:94:R:LEU:HD22	1:94:R:LEU:HG	2	0.91
(1,2134)	1:94:R:LEU:HD23	1:94:R:LEU:HG	2	0.91
(1,1715)	1:56:R:ILE:HA	1:56:R:ILE:HD11	3	0.91
(1,1715)	1:56:R:ILE:HA	1:56:R:ILE:HD12	3	0.91
(1,1715)	1:56:R:ILE:HA	1:56:R:ILE:HD13	3	0.91
(1,1593)	1:138:R:HIS:H	1:181:R:VAL:HG11	2	0.91

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1593)	1:138:R:HIS:H	1:181:R:VAL:HG12	2	0.91
(1,1593)	1:138:R:HIS:H	1:181:R:VAL:HG13	2	0.91
(1,882)	1:56:R:ILE:H	1:56:R:ILE:HD11	2	0.91
(1,882)	1:56:R:ILE:H	1:56:R:ILE:HD12	2	0.91
(1,882)	1:56:R:ILE:H	1:56:R:ILE:HD13	2	0.91
(1,2020)	1:127:R:VAL:HA	1:127:R:VAL:HG21	2	0.9
(1,2020)	1:127:R:VAL:HA	1:127:R:VAL:HG22	2	0.9
(1,2020)	1:127:R:VAL:HA	1:127:R:VAL:HG23	2	0.9
(1,1592)	1:138:R:HIS:H	1:154:R:VAL:HG21	2	0.9
(1,1592)	1:138:R:HIS:H	1:154:R:VAL:HG22	2	0.9
(1,1592)	1:138:R:HIS:H	1:154:R:VAL:HG23	2	0.9
(1,606)	1:139:R:ALA:H	1:180:R:PHE:HB3	5	0.9
(1,2204)	1:139:R:ALA:HB1	1:153:R:CYS:HA	2	0.89
(1,2204)	1:139:R:ALA:HB2	1:153:R:CYS:HA	2	0.89
(1,2204)	1:139:R:ALA:HB3	1:153:R:CYS:HA	2	0.89
(1,2178)	1:126:R:VAL:H	1:126:R:VAL:HG11	1	0.89
(1,2178)	1:126:R:VAL:H	1:126:R:VAL:HG12	1	0.89
(1,2178)	1:126:R:VAL:H	1:126:R:VAL:HG13	1	0.89
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG21	2	0.89
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG22	2	0.89
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG23	2	0.89
(1,2134)	1:94:R:LEU:HD21	1:94:R:LEU:HG	5	0.89
(1,2134)	1:94:R:LEU:HD22	1:94:R:LEU:HG	5	0.89
(1,2134)	1:94:R:LEU:HD23	1:94:R:LEU:HG	5	0.89
(1,1546)	1:114:R:GLY:H	1:115:R:ILE:HD11	2	0.89
(1,1546)	1:114:R:GLY:H	1:115:R:ILE:HD12	2	0.89
(1,1546)	1:114:R:GLY:H	1:115:R:ILE:HD13	2	0.89
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB1	1	0.89
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB2	1	0.89
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB3	1	0.89
(1,2154)	1:111:R:LEU:HD21	1:111:R:LEU:HG	2	0.88
(1,2154)	1:111:R:LEU:HD22	1:111:R:LEU:HG	2	0.88
(1,2154)	1:111:R:LEU:HD23	1:111:R:LEU:HG	2	0.88
(1,2154)	1:111:R:LEU:HD21	1:111:R:LEU:HG	4	0.88
(1,2154)	1:111:R:LEU:HD22	1:111:R:LEU:HG	4	0.88
(1,2154)	1:111:R:LEU:HD23	1:111:R:LEU:HG	4	0.88
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD21	3	0.88
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD22	3	0.88
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD23	3	0.88
(1,2134)	1:94:R:LEU:HD21	1:94:R:LEU:HG	1	0.88
(1,2134)	1:94:R:LEU:HD22	1:94:R:LEU:HG	1	0.88
(1,2134)	1:94:R:LEU:HD23	1:94:R:LEU:HG	1	0.88

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2134)	1:94:R:LEU:HD21	1:94:R:LEU:HG	3	0.88
(1,2134)	1:94:R:LEU:HD22	1:94:R:LEU:HG	3	0.88
(1,2134)	1:94:R:LEU:HD23	1:94:R:LEU:HG	3	0.88
(1,2234)	1:162:R:ILE:H	1:162:R:ILE:HG13	4	0.87
(1,2154)	1:111:R:LEU:HD21	1:111:R:LEU:HG	3	0.87
(1,2154)	1:111:R:LEU:HD22	1:111:R:LEU:HG	3	0.87
(1,2154)	1:111:R:LEU:HD23	1:111:R:LEU:HG	3	0.87
(1,2086)	1:56:R:ILE:HD11	1:56:R:ILE:HG13	2	0.87
(1,2086)	1:56:R:ILE:HD12	1:56:R:ILE:HG13	2	0.87
(1,2086)	1:56:R:ILE:HD13	1:56:R:ILE:HG13	2	0.87
(1,2020)	1:127:R:VAL:HA	1:127:R:VAL:HG21	3	0.87
(1,2020)	1:127:R:VAL:HA	1:127:R:VAL:HG22	3	0.87
(1,2020)	1:127:R:VAL:HA	1:127:R:VAL:HG23	3	0.87
(1,2002)	1:111:R:LEU:HB2	1:111:R:LEU:HD21	3	0.87
(1,2002)	1:111:R:LEU:HB2	1:111:R:LEU:HD22	3	0.87
(1,2002)	1:111:R:LEU:HB2	1:111:R:LEU:HD23	3	0.87
(1,1361)	1:35:R:ASN:H	1:36:R:GLY:H	1	0.87
(1,418)	1:91:R:GLY:H	1:89:R:LEU:HB2	4	0.87
(1,2232)	1:31:R:LEU:HD11	1:162:R:ILE:HG13	5	0.86
(1,2232)	1:31:R:LEU:HD12	1:162:R:ILE:HG13	5	0.86
(1,2232)	1:31:R:LEU:HD13	1:162:R:ILE:HG13	5	0.86
(1,2232)	1:31:R:LEU:HD21	1:162:R:ILE:HG13	5	0.86
(1,2232)	1:31:R:LEU:HD22	1:162:R:ILE:HG13	5	0.86
(1,2232)	1:31:R:LEU:HD23	1:162:R:ILE:HG13	5	0.86
(1,2154)	1:111:R:LEU:HD21	1:111:R:LEU:HG	1	0.86
(1,2154)	1:111:R:LEU:HD22	1:111:R:LEU:HG	1	0.86
(1,2154)	1:111:R:LEU:HD23	1:111:R:LEU:HG	1	0.86
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD11	3	0.86
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD12	3	0.86
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD13	3	0.86
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD21	3	0.86
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD22	3	0.86
(1,2090)	1:57:R:LEU:H	1:57:R:LEU:HD23	3	0.86
(1,2087)	1:56:R:ILE:HD11	1:56:R:ILE:HG12	2	0.86
(1,2087)	1:56:R:ILE:HD12	1:56:R:ILE:HG12	2	0.86
(1,2087)	1:56:R:ILE:HD13	1:56:R:ILE:HG12	2	0.86
(1,2086)	1:56:R:ILE:HD11	1:56:R:ILE:HG13	1	0.86
(1,2086)	1:56:R:ILE:HD12	1:56:R:ILE:HG13	1	0.86
(1,2086)	1:56:R:ILE:HD13	1:56:R:ILE:HG13	1	0.86
(1,2086)	1:56:R:ILE:HD11	1:56:R:ILE:HG13	3	0.86
(1,2086)	1:56:R:ILE:HD12	1:56:R:ILE:HG13	3	0.86
(1,2086)	1:56:R:ILE:HD13	1:56:R:ILE:HG13	3	0.86

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG21	4	0.86
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG22	4	0.86
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG23	4	0.86
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG21	4	0.86
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG22	4	0.86
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG23	4	0.86
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG21	4	0.86
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG22	4	0.86
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG23	4	0.86
(1,1949)	1:56:R:ILE:HB	1:56:R:ILE:HD11	1	0.86
(1,1949)	1:56:R:ILE:HB	1:56:R:ILE:HD12	1	0.86
(1,1949)	1:56:R:ILE:HB	1:56:R:ILE:HD13	1	0.86
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB1	2	0.86
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB2	2	0.86
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB3	2	0.86
(1,2242)	1:161:R:ALA:HB1	1:170:R:TRP:HB3	1	0.85
(1,2242)	1:161:R:ALA:HB2	1:170:R:TRP:HB3	1	0.85
(1,2242)	1:161:R:ALA:HB3	1:170:R:TRP:HB3	1	0.85
(1,2242)	1:161:R:ALA:HB1	1:170:R:TRP:HB3	5	0.85
(1,2242)	1:161:R:ALA:HB2	1:170:R:TRP:HB3	5	0.85
(1,2242)	1:161:R:ALA:HB3	1:170:R:TRP:HB3	5	0.85
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB1	1	0.85
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB2	1	0.85
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB3	1	0.85
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB1	2	0.85
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB2	2	0.85
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB3	2	0.85
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB1	3	0.85
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB2	3	0.85
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB3	3	0.85
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB1	5	0.85
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB2	5	0.85
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB3	5	0.85
(1,2154)	1:111:R:LEU:HD21	1:111:R:LEU:HG	5	0.85
(1,2154)	1:111:R:LEU:HD22	1:111:R:LEU:HG	5	0.85
(1,2154)	1:111:R:LEU:HD23	1:111:R:LEU:HG	5	0.85
(1,2087)	1:56:R:ILE:HD11	1:56:R:ILE:HG12	3	0.85
(1,2087)	1:56:R:ILE:HD12	1:56:R:ILE:HG12	3	0.85
(1,2087)	1:56:R:ILE:HD13	1:56:R:ILE:HG12	3	0.85
(1,2086)	1:56:R:ILE:HD11	1:56:R:ILE:HG13	5	0.85
(1,2086)	1:56:R:ILE:HD12	1:56:R:ILE:HG13	5	0.85
(1,2086)	1:56:R:ILE:HD13	1:56:R:ILE:HG13	5	0.85

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1976)	1:83:R:ILE:HG21	1:83:R:ILE:HG13	3	0.85
(1,1976)	1:83:R:ILE:HG22	1:83:R:ILE:HG13	3	0.85
(1,1976)	1:83:R:ILE:HG23	1:83:R:ILE:HG13	3	0.85
(1,1955)	1:56:R:ILE:HG12	1:56:R:ILE:HG21	2	0.85
(1,1955)	1:56:R:ILE:HG12	1:56:R:ILE:HG22	2	0.85
(1,1955)	1:56:R:ILE:HG12	1:56:R:ILE:HG23	2	0.85
(1,1501)	1:97:R:GLY:H	1:94:R:LEU:HD11	2	0.85
(1,1501)	1:97:R:GLY:H	1:94:R:LEU:HD12	2	0.85
(1,1501)	1:97:R:GLY:H	1:94:R:LEU:HD13	2	0.85
(1,1361)	1:35:R:ASN:H	1:36:R:GLY:H	3	0.85
(1,1317)	1:179:R:VAL:H	1:180:R:PHE:HB2	5	0.85
(1,418)	1:91:R:GLY:H	1:89:R:LEU:HB2	1	0.85
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB1	4	0.84
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB2	4	0.84
(1,2187)	1:149:R:ALA:HA	1:149:R:ALA:HB3	4	0.84
(1,2020)	1:127:R:VAL:HA	1:127:R:VAL:HG21	4	0.84
(1,2020)	1:127:R:VAL:HA	1:127:R:VAL:HG22	4	0.84
(1,2020)	1:127:R:VAL:HA	1:127:R:VAL:HG23	4	0.84
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD21	1	0.83
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD22	1	0.83
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD23	1	0.83
(1,2087)	1:56:R:ILE:HD11	1:56:R:ILE:HG12	1	0.83
(1,2087)	1:56:R:ILE:HD12	1:56:R:ILE:HG12	1	0.83
(1,2087)	1:56:R:ILE:HD13	1:56:R:ILE:HG12	1	0.83
(1,2087)	1:56:R:ILE:HD11	1:56:R:ILE:HG12	4	0.83
(1,2087)	1:56:R:ILE:HD12	1:56:R:ILE:HG12	4	0.83
(1,2087)	1:56:R:ILE:HD13	1:56:R:ILE:HG12	4	0.83
(1,2087)	1:56:R:ILE:HD11	1:56:R:ILE:HG12	5	0.83
(1,2087)	1:56:R:ILE:HD12	1:56:R:ILE:HG12	5	0.83
(1,2087)	1:56:R:ILE:HD13	1:56:R:ILE:HG12	5	0.83
(1,2086)	1:56:R:ILE:HD11	1:56:R:ILE:HG13	4	0.83
(1,2086)	1:56:R:ILE:HD12	1:56:R:ILE:HG13	4	0.83
(1,2086)	1:56:R:ILE:HD13	1:56:R:ILE:HG13	4	0.83
(1,1976)	1:83:R:ILE:HG21	1:83:R:ILE:HG13	4	0.83
(1,1976)	1:83:R:ILE:HG22	1:83:R:ILE:HG13	4	0.83
(1,1976)	1:83:R:ILE:HG23	1:83:R:ILE:HG13	4	0.83
(1,1022)	1:94:R:LEU:H	1:94:R:LEU:HD11	1	0.83
(1,1022)	1:94:R:LEU:H	1:94:R:LEU:HD12	1	0.83
(1,1022)	1:94:R:LEU:H	1:94:R:LEU:HD13	1	0.83
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB1	3	0.83
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB2	3	0.83
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB3	3	0.83

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG21	5	0.82
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG22	5	0.82
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG23	5	0.82
(1,1955)	1:56:R:ILE:HG12	1:56:R:ILE:HG21	1	0.82
(1,1955)	1:56:R:ILE:HG12	1:56:R:ILE:HG22	1	0.82
(1,1955)	1:56:R:ILE:HG12	1:56:R:ILE:HG23	1	0.82
(1,1949)	1:56:R:ILE:HB	1:56:R:ILE:HD11	2	0.82
(1,1949)	1:56:R:ILE:HB	1:56:R:ILE:HD12	2	0.82
(1,1949)	1:56:R:ILE:HB	1:56:R:ILE:HD13	2	0.82
(1,1470)	1:81:R:GLU:H	1:80:R:LEU:H	4	0.82
(1,1168)	1:139:R:ALA:H	1:180:R:PHE:HB3	3	0.82
(1,757)	1:179:R:VAL:H	1:177:R:VAL:HA	4	0.82
(1,2212)	1:34:R:TYR:HB2	1:154:R:VAL:HB	4	0.81
(1,2212)	1:34:R:TYR:HB3	1:154:R:VAL:HB	4	0.81
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD21	4	0.81
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD22	4	0.81
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD23	4	0.81
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD21	5	0.81
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD22	5	0.81
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD23	5	0.81
(1,1966)	1:70:R:TRP:HB2	1:70:R:TRP:HA	2	0.81
(1,964)	1:79:R:THR:H	1:78:R:LEU:HB2	2	0.81
(1,964)	1:79:R:THR:H	1:78:R:LEU:HB3	2	0.81
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG21	3	0.8
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG22	3	0.8
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG23	3	0.8
(1,1966)	1:70:R:TRP:HB2	1:70:R:TRP:HA	1	0.8
(1,1966)	1:70:R:TRP:HB2	1:70:R:TRP:HA	3	0.8
(1,1966)	1:70:R:TRP:HB2	1:70:R:TRP:HA	4	0.8
(1,1966)	1:70:R:TRP:HB2	1:70:R:TRP:HA	5	0.8
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD11	2	0.8
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD12	2	0.8
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD13	2	0.8
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD21	2	0.8
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD22	2	0.8
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD23	2	0.8
(1,1137)	1:126:R:VAL:H	1:124:R:VAL:HA	1	0.8
(1,1082)	1:112:R:HIS:H	1:111:R:LEU:HD11	2	0.8
(1,1082)	1:112:R:HIS:H	1:111:R:LEU:HD12	2	0.8
(1,1082)	1:112:R:HIS:H	1:111:R:LEU:HD13	2	0.8
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD21	2	0.79
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD22	2	0.79

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2147)	1:110:R:LEU:HB2	1:110:R:LEU:HD23	2	0.79
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD11	3	0.79
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD12	3	0.79
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD13	3	0.79
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD21	3	0.79
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD22	3	0.79
(1,2069)	1:41:R:PHE:HD1	1:31:R:LEU:HD23	3	0.79
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD11	3	0.79
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD12	3	0.79
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD13	3	0.79
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD21	3	0.79
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD22	3	0.79
(1,2069)	1:41:R:PHE:HD2	1:31:R:LEU:HD23	3	0.79
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD11	2	0.79
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD12	2	0.79
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD13	2	0.79
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD11	5	0.79
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD12	5	0.79
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD13	5	0.79
(1,418)	1:91:R:GLY:H	1:89:R:LEU:HB2	2	0.79
(1,1954)	1:56:R:ILE:HG13	1:56:R:ILE:HG21	3	0.78
(1,1954)	1:56:R:ILE:HG13	1:56:R:ILE:HG22	3	0.78
(1,1954)	1:56:R:ILE:HG13	1:56:R:ILE:HG23	3	0.78
(1,1895)	1:162:R:ILE:HD11	1:162:R:ILE:HA	1	0.78
(1,1895)	1:162:R:ILE:HD12	1:162:R:ILE:HA	1	0.78
(1,1895)	1:162:R:ILE:HD13	1:162:R:ILE:HA	1	0.78
(1,1470)	1:81:R:GLU:H	1:80:R:LEU:H	1	0.78
(1,1470)	1:81:R:GLU:H	1:80:R:LEU:H	5	0.78
(1,1384)	1:44:R:ARG:H	1:42:R:TYR:H	3	0.78
(1,901)	1:61:R:ARG:H	1:41:R:PHE:HD1	2	0.78
(1,901)	1:61:R:ARG:H	1:41:R:PHE:HD2	2	0.78
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG21	4	0.77
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG22	4	0.77
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG23	4	0.77
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG21	4	0.77
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG22	4	0.77
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG23	4	0.77
(1,2089)	1:56:R:ILE:HG21	1:56:R:ILE:HG12	4	0.77
(1,2089)	1:56:R:ILE:HG22	1:56:R:ILE:HG12	4	0.77
(1,2089)	1:56:R:ILE:HG23	1:56:R:ILE:HG12	4	0.77
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD11	4	0.77
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD12	4	0.77

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD13	4	0.77
(1,1292)	1:171:R:THR:H	1:168:R:TYR:HD1	5	0.77
(1,1292)	1:171:R:THR:H	1:168:R:TYR:HD2	5	0.77
(1,1137)	1:126:R:VAL:H	1:124:R:VAL:HA	5	0.77
(1,2241)	1:180:R:PHE:HE1	1:125:R:CYS:HB3	3	0.76
(1,2241)	1:180:R:PHE:HE2	1:125:R:CYS:HB3	3	0.76
(1,1593)	1:138:R:HIS:H	1:181:R:VAL:HG11	4	0.76
(1,1593)	1:138:R:HIS:H	1:181:R:VAL:HG12	4	0.76
(1,1593)	1:138:R:HIS:H	1:181:R:VAL:HG13	4	0.76
(1,1470)	1:81:R:GLU:H	1:80:R:LEU:H	3	0.76
(1,1361)	1:35:R:ASN:H	1:36:R:GLY:H	2	0.76
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB1	4	0.76
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB2	4	0.76
(1,532)	1:117:R:THR:H	1:118:R:ALA:HB3	4	0.76
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD21	1	0.75
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD22	1	0.75
(1,2148)	1:110:R:LEU:H	1:110:R:LEU:HD23	1	0.75
(1,1546)	1:114:R:GLY:H	1:115:R:ILE:HD11	1	0.75
(1,1546)	1:114:R:GLY:H	1:115:R:ILE:HD12	1	0.75
(1,1546)	1:114:R:GLY:H	1:115:R:ILE:HD13	1	0.75
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD21	5	0.75
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD22	5	0.75
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD23	5	0.75
(1,1470)	1:81:R:GLU:H	1:80:R:LEU:H	2	0.75
(1,851)	1:46:R:ASN:H	1:165:R:GLU:H	4	0.75
(1,2229)	1:167:R:PHE:HA	1:162:R:ILE:HA	2	0.74
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG21	1	0.74
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG22	1	0.74
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG23	1	0.74
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG21	3	0.74
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG22	3	0.74
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG23	3	0.74
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB1	2	0.74
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB2	2	0.74
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB3	2	0.74
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB1	5	0.73
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB2	5	0.73
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB3	5	0.73
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD11	1	0.73
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD12	1	0.73
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD13	1	0.73
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD21	1	0.73

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD22	1	0.73
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD23	1	0.73
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG21	2	0.72
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG22	2	0.72
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG23	2	0.72
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG21	2	0.72
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG22	2	0.72
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG23	2	0.72
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG21	2	0.72
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG22	2	0.72
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG23	2	0.72
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG21	2	0.72
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG22	2	0.72
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG23	2	0.72
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG21	2	0.72
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG22	2	0.72
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG23	2	0.72
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG21	2	0.72
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG22	2	0.72
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG23	2	0.72
(1,2229)	1:167:R:PHE:HA	1:162:R:ILE:HA	1	0.72
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG11	1	0.72
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG12	1	0.72
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG13	1	0.72
(1,2191)	1:150:R:VAL:HG11	1:150:R:VAL:HA	1	0.72
(1,2191)	1:150:R:VAL:HG12	1:150:R:VAL:HA	1	0.72
(1,2191)	1:150:R:VAL:HG13	1:150:R:VAL:HA	1	0.72
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB1	4	0.72
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB2	4	0.72
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB3	4	0.72
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB1	4	0.72
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB2	4	0.72
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB3	4	0.72
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD11	2	0.72
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD12	2	0.72
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD13	2	0.72
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD21	2	0.72
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD22	2	0.72
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD23	2	0.72
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD11	2	0.72
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD12	2	0.72
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD13	2	0.72

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD21	2	0.72
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD22	2	0.72
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD23	2	0.72
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD11	3	0.72
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD12	3	0.72
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD13	3	0.72
(1,1949)	1:56:R:ILE:HB	1:56:R:ILE:HD11	5	0.72
(1,1949)	1:56:R:ILE:HB	1:56:R:ILE:HD12	5	0.72
(1,1949)	1:56:R:ILE:HB	1:56:R:ILE:HD13	5	0.72
(1,2233)	1:162:R:ILE:HA	1:162:R:ILE:HG13	5	0.71
(1,2226)	1:162:R:ILE:HG13	1:162:R:ILE:HA	5	0.71
(1,2021)	1:127:R:VAL:H	1:127:R:VAL:HG21	4	0.71
(1,2021)	1:127:R:VAL:H	1:127:R:VAL:HG22	4	0.71
(1,2021)	1:127:R:VAL:H	1:127:R:VAL:HG23	4	0.71
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD11	1	0.71
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD12	1	0.71
(1,1999)	1:110:R:LEU:HB2	1:110:R:LEU:HD13	1	0.71
(1,1501)	1:97:R:GLY:H	1:94:R:LEU:HD11	3	0.71
(1,1501)	1:97:R:GLY:H	1:94:R:LEU:HD12	3	0.71
(1,1501)	1:97:R:GLY:H	1:94:R:LEU:HD13	3	0.71
(1,1285)	1:168:R:TYR:H	1:168:R:TYR:HD1	2	0.71
(1,1285)	1:168:R:TYR:H	1:168:R:TYR:HD2	2	0.71
(1,1285)	1:168:R:TYR:H	1:168:R:TYR:HD1	5	0.71
(1,1285)	1:168:R:TYR:H	1:168:R:TYR:HD2	5	0.71
(1,603)	1:138:R:HIS:H	1:139:R:ALA:HA	4	0.71
(1,2204)	1:139:R:ALA:HB1	1:153:R:CYS:HA	5	0.7
(1,2204)	1:139:R:ALA:HB2	1:153:R:CYS:HA	5	0.7
(1,2204)	1:139:R:ALA:HB3	1:153:R:CYS:HA	5	0.7
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG11	3	0.7
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG12	3	0.7
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG13	3	0.7
(1,2191)	1:150:R:VAL:HG11	1:150:R:VAL:HA	3	0.7
(1,2191)	1:150:R:VAL:HG12	1:150:R:VAL:HA	3	0.7
(1,2191)	1:150:R:VAL:HG13	1:150:R:VAL:HA	3	0.7
(1,2132)	1:83:R:ILE:HD11	1:94:R:LEU:HD11	2	0.7
(1,2132)	1:83:R:ILE:HD11	1:94:R:LEU:HD12	2	0.7
(1,2132)	1:83:R:ILE:HD11	1:94:R:LEU:HD13	2	0.7
(1,2132)	1:83:R:ILE:HD12	1:94:R:LEU:HD11	2	0.7
(1,2132)	1:83:R:ILE:HD12	1:94:R:LEU:HD12	2	0.7
(1,2132)	1:83:R:ILE:HD12	1:94:R:LEU:HD13	2	0.7
(1,2132)	1:83:R:ILE:HD13	1:94:R:LEU:HD11	2	0.7
(1,2132)	1:83:R:ILE:HD13	1:94:R:LEU:HD12	2	0.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2132)	1:83:R:ILE:HD13	1:94:R:LEU:HD13	2	0.7
(1,1955)	1:56:R:ILE:HG12	1:56:R:ILE:HG21	5	0.7
(1,1955)	1:56:R:ILE:HG12	1:56:R:ILE:HG22	5	0.7
(1,1955)	1:56:R:ILE:HG12	1:56:R:ILE:HG23	5	0.7
(1,882)	1:56:R:ILE:H	1:56:R:ILE:HD11	5	0.7
(1,882)	1:56:R:ILE:H	1:56:R:ILE:HD12	5	0.7
(1,882)	1:56:R:ILE:H	1:56:R:ILE:HD13	5	0.7
(1,603)	1:138:R:HIS:H	1:139:R:ALA:HA	1	0.7
(1,2208)	1:154:R:VAL:H	1:153:R:CYS:HA	3	0.69
(1,2203)	1:152:R:ALA:H	1:151:R:PHE:HA	4	0.69
(1,2172)	1:124:R:VAL:H	1:124:R:VAL:HG11	1	0.69
(1,2172)	1:124:R:VAL:H	1:124:R:VAL:HG12	1	0.69
(1,2172)	1:124:R:VAL:H	1:124:R:VAL:HG13	1	0.69
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB1	3	0.69
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB2	3	0.69
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB3	3	0.69
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB1	1	0.69
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB2	1	0.69
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB3	1	0.69
(1,1315)	1:179:R:VAL:H	1:142:R:PHE:HA	5	0.69
(1,1303)	1:127:R:VAL:H	1:127:R:VAL:HG21	5	0.69
(1,1303)	1:127:R:VAL:H	1:127:R:VAL:HG22	5	0.69
(1,1303)	1:127:R:VAL:H	1:127:R:VAL:HG23	5	0.69
(1,2208)	1:154:R:VAL:H	1:153:R:CYS:HA	5	0.68
(1,2203)	1:152:R:ALA:H	1:151:R:PHE:HA	3	0.68
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG21	2	0.68
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG22	2	0.68
(1,2105)	1:71:R:VAL:H	1:71:R:VAL:HG23	2	0.68
(1,1909)	1:162:R:ILE:H	1:162:R:ILE:HG21	1	0.68
(1,1909)	1:162:R:ILE:H	1:162:R:ILE:HG22	1	0.68
(1,1909)	1:162:R:ILE:H	1:162:R:ILE:HG23	1	0.68
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB1	3	0.68
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB2	3	0.68
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB3	3	0.68
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD11	1	0.68
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD12	1	0.68
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD13	1	0.68
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD21	1	0.68
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD22	1	0.68
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD23	1	0.68
(1,2252)	1:178:R:LEU:H	1:177:R:VAL:HA	4	0.67
(1,2203)	1:152:R:ALA:H	1:151:R:PHE:HA	5	0.67

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2103)	1:72:R:TYR:H	1:71:R:VAL:HG11	1	0.67
(1,2103)	1:72:R:TYR:H	1:71:R:VAL:HG12	1	0.67
(1,2103)	1:72:R:TYR:H	1:71:R:VAL:HG13	1	0.67
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB1	1	0.67
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB2	1	0.67
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB3	1	0.67
(1,1667)	1:170:R:TRP:H	1:152:R:ALA:HB1	2	0.67
(1,1667)	1:170:R:TRP:H	1:152:R:ALA:HB2	2	0.67
(1,1667)	1:170:R:TRP:H	1:152:R:ALA:HB3	2	0.67
(1,1303)	1:127:R:VAL:H	1:127:R:VAL:HG21	3	0.67
(1,1303)	1:127:R:VAL:H	1:127:R:VAL:HG22	3	0.67
(1,1303)	1:127:R:VAL:H	1:127:R:VAL:HG23	3	0.67
(1,1122)	1:123:R:GLU:H	1:114:R:GLY:H	5	0.67
(1,1096)	1:114:R:GLY:H	1:123:R:GLU:H	5	0.67
(1,837)	1:41:R:PHE:H	1:41:R:PHE:HZ	2	0.67
(1,660)	1:153:R:CYS:H	1:155:R:THR:H	2	0.67
(1,603)	1:138:R:HIS:H	1:139:R:ALA:HA	5	0.67
(1,2258)	1:180:R:PHE:HB2	1:180:R:PHE:HA	4	0.66
(1,2208)	1:154:R:VAL:H	1:153:R:CYS:HA	1	0.66
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG11	2	0.66
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG12	2	0.66
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG13	2	0.66
(1,2191)	1:150:R:VAL:HG11	1:150:R:VAL:HA	2	0.66
(1,2191)	1:150:R:VAL:HG12	1:150:R:VAL:HA	2	0.66
(1,2191)	1:150:R:VAL:HG13	1:150:R:VAL:HA	2	0.66
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB1	2	0.66
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB2	2	0.66
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB3	2	0.66
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB1	4	0.66
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB2	4	0.66
(1,1870)	1:153:R:CYS:HA	1:152:R:ALA:HB3	4	0.66
(1,1359)	1:35:R:ASN:H	1:34:R:TYR:H	5	0.66
(1,1356)	1:34:R:TYR:H	1:35:R:ASN:H	5	0.66
(1,1303)	1:127:R:VAL:H	1:127:R:VAL:HG21	2	0.66
(1,1303)	1:127:R:VAL:H	1:127:R:VAL:HG22	2	0.66
(1,1303)	1:127:R:VAL:H	1:127:R:VAL:HG23	2	0.66
(1,2252)	1:178:R:LEU:H	1:177:R:VAL:HA	3	0.65
(1,2224)	1:161:R:ALA:H	1:160:R:TYR:HA	3	0.65
(1,2215)	1:154:R:VAL:H	1:154:R:VAL:HB	5	0.65
(1,2208)	1:154:R:VAL:H	1:153:R:CYS:HA	2	0.65
(1,2203)	1:152:R:ALA:H	1:151:R:PHE:HA	1	0.65
(1,2201)	1:151:R:PHE:HB2	1:151:R:PHE:HA	4	0.65

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD11	1	0.65
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD12	1	0.65
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD13	1	0.65
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD11	2	0.65
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD12	2	0.65
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD13	2	0.65
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD11	3	0.65
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD12	3	0.65
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD13	3	0.65
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG11	2	0.65
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG12	2	0.65
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG13	2	0.65
(1,1639)	1:159:R:TRP:H	1:153:R:CYS:H	1	0.65
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG21	1	0.65
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG22	1	0.65
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG23	1	0.65
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD11	4	0.64
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD12	4	0.64
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD13	4	0.64
(1,2050)	1:41:R:PHE:HE1	1:162:R:ILE:HD11	4	0.64
(1,2050)	1:41:R:PHE:HE1	1:162:R:ILE:HD12	4	0.64
(1,2050)	1:41:R:PHE:HE1	1:162:R:ILE:HD13	4	0.64
(1,2050)	1:41:R:PHE:HE2	1:162:R:ILE:HD11	4	0.64
(1,2050)	1:41:R:PHE:HE2	1:162:R:ILE:HD12	4	0.64
(1,2050)	1:41:R:PHE:HE2	1:162:R:ILE:HD13	4	0.64
(1,1724)	1:56:R:ILE:HD11	1:56:R:ILE:HG21	5	0.64
(1,1724)	1:56:R:ILE:HD11	1:56:R:ILE:HG22	5	0.64
(1,1724)	1:56:R:ILE:HD11	1:56:R:ILE:HG23	5	0.64
(1,1724)	1:56:R:ILE:HD12	1:56:R:ILE:HG21	5	0.64
(1,1724)	1:56:R:ILE:HD12	1:56:R:ILE:HG22	5	0.64
(1,1724)	1:56:R:ILE:HD12	1:56:R:ILE:HG23	5	0.64
(1,1724)	1:56:R:ILE:HD13	1:56:R:ILE:HG21	5	0.64
(1,1724)	1:56:R:ILE:HD13	1:56:R:ILE:HG22	5	0.64
(1,1724)	1:56:R:ILE:HD13	1:56:R:ILE:HG23	5	0.64
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD11	5	0.64
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD12	5	0.64
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD13	5	0.64
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD21	5	0.64
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD22	5	0.64
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD23	5	0.64
(1,882)	1:56:R:ILE:H	1:56:R:ILE:HD11	4	0.64
(1,882)	1:56:R:ILE:H	1:56:R:ILE:HD12	4	0.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,882)	1:56:R:ILE:H	1:56:R:ILE:HD13	4	0.64
(1,757)	1:179:R:VAL:H	1:177:R:VAL:HA	5	0.64
(1,2258)	1:180:R:PHE:HB2	1:180:R:PHE:HA	2	0.63
(1,2172)	1:124:R:VAL:H	1:124:R:VAL:HG11	4	0.63
(1,2172)	1:124:R:VAL:H	1:124:R:VAL:HG12	4	0.63
(1,2172)	1:124:R:VAL:H	1:124:R:VAL:HG13	4	0.63
(1,2107)	1:72:R:TYR:HB2	1:72:R:TYR:HA	5	0.63
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD11	1	0.63
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD12	1	0.63
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD13	1	0.63
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD21	1	0.63
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD22	1	0.63
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD23	1	0.63
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD11	1	0.63
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD12	1	0.63
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD13	1	0.63
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD21	1	0.63
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD22	1	0.63
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD23	1	0.63
(1,1639)	1:159:R:TRP:H	1:153:R:CYS:H	5	0.63
(1,1359)	1:35:R:ASN:H	1:34:R:TYR:H	4	0.63
(1,1356)	1:34:R:TYR:H	1:35:R:ASN:H	4	0.63
(1,808)	1:34:R:TYR:H	1:33:R:LEU:HD11	2	0.63
(1,808)	1:34:R:TYR:H	1:33:R:LEU:HD12	2	0.63
(1,808)	1:34:R:TYR:H	1:33:R:LEU:HD13	2	0.63
(1,808)	1:34:R:TYR:H	1:33:R:LEU:HD21	2	0.63
(1,808)	1:34:R:TYR:H	1:33:R:LEU:HD22	2	0.63
(1,808)	1:34:R:TYR:H	1:33:R:LEU:HD23	2	0.63
(1,2258)	1:180:R:PHE:HB2	1:180:R:PHE:HA	5	0.62
(1,2252)	1:178:R:LEU:H	1:177:R:VAL:HA	5	0.62
(1,2229)	1:167:R:PHE:HA	1:162:R:ILE:HA	4	0.62
(1,2203)	1:152:R:ALA:H	1:151:R:PHE:HA	2	0.62
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG21	1	0.62
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG22	1	0.62
(1,2162)	1:116:R:GLY:H	1:115:R:ILE:HG23	1	0.62
(1,2107)	1:72:R:TYR:HB2	1:72:R:TYR:HA	3	0.62
(1,2096)	1:64:R:GLU:HB2	1:64:R:GLU:HA	1	0.62
(1,2096)	1:64:R:GLU:HB3	1:64:R:GLU:HA	1	0.62
(1,2096)	1:64:R:GLU:HB2	1:64:R:GLU:HA	3	0.62
(1,2096)	1:64:R:GLU:HB3	1:64:R:GLU:HA	3	0.62
(1,849)	1:46:R:ASN:H	1:44:R:ARG:H	3	0.62
(1,824)	1:37:R:GLU:H	1:35:R:ASN:HB2	2	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG21	2	0.62
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG22	2	0.62
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG23	2	0.62
(1,603)	1:138:R:HIS:H	1:139:R:ALA:HA	2	0.62
(1,2258)	1:180:R:PHE:HB2	1:180:R:PHE:HA	3	0.61
(1,2252)	1:178:R:LEU:H	1:177:R:VAL:HA	1	0.61
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD11	1	0.61
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD12	1	0.61
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD13	1	0.61
(1,1137)	1:126:R:VAL:H	1:124:R:VAL:HA	4	0.61
(1,1082)	1:112:R:HIS:H	1:111:R:LEU:HD11	5	0.61
(1,1082)	1:112:R:HIS:H	1:111:R:LEU:HD12	5	0.61
(1,1082)	1:112:R:HIS:H	1:111:R:LEU:HD13	5	0.61
(1,2224)	1:161:R:ALA:H	1:160:R:TYR:HA	1	0.6
(1,2215)	1:154:R:VAL:H	1:154:R:VAL:HB	3	0.6
(1,2156)	1:111:R:LEU:HB2	1:112:R:HIS:HB3	5	0.6
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG21	3	0.6
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG22	3	0.6
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG23	3	0.6
(1,1837)	1:126:R:VAL:H	1:126:R:VAL:HG21	4	0.6
(1,1837)	1:126:R:VAL:H	1:126:R:VAL:HG22	4	0.6
(1,1837)	1:126:R:VAL:H	1:126:R:VAL:HG23	4	0.6
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG11	1	0.6
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG12	1	0.6
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG13	1	0.6
(1,1314)	1:179:R:VAL:H	1:126:R:VAL:HA	4	0.6
(1,884)	1:57:R:LEU:H	1:56:R:ILE:HD11	2	0.6
(1,884)	1:57:R:LEU:H	1:56:R:ILE:HD12	2	0.6
(1,884)	1:57:R:LEU:H	1:56:R:ILE:HD13	2	0.6
(1,823)	1:37:R:GLU:H	1:35:R:ASN:HB3	2	0.6
(1,2258)	1:180:R:PHE:HB2	1:180:R:PHE:HA	1	0.59
(1,2229)	1:167:R:PHE:HA	1:162:R:ILE:HA	3	0.59
(1,2215)	1:154:R:VAL:H	1:154:R:VAL:HB	1	0.59
(1,2215)	1:154:R:VAL:H	1:154:R:VAL:HB	2	0.59
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG11	4	0.59
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG12	4	0.59
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG13	4	0.59
(1,2191)	1:150:R:VAL:HG11	1:150:R:VAL:HA	4	0.59
(1,2191)	1:150:R:VAL:HG12	1:150:R:VAL:HA	4	0.59
(1,2191)	1:150:R:VAL:HG13	1:150:R:VAL:HA	4	0.59
(1,2096)	1:64:R:GLU:HB2	1:64:R:GLU:HA	4	0.59
(1,2096)	1:64:R:GLU:HB3	1:64:R:GLU:HA	4	0.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2096)	1:64:R:GLU:HB2	1:64:R:GLU:HA	5	0.59
(1,2096)	1:64:R:GLU:HB3	1:64:R:GLU:HA	5	0.59
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD11	5	0.59
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD12	5	0.59
(1,2083)	1:53:R:LEU:HB2	1:53:R:LEU:HD13	5	0.59
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD11	3	0.59
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD12	3	0.59
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD13	3	0.59
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD21	3	0.59
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD22	3	0.59
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD23	3	0.59
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD11	3	0.59
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD12	3	0.59
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD13	3	0.59
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD21	3	0.59
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD22	3	0.59
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD23	3	0.59
(1,1669)	1:170:R:TRP:H	1:168:R:TYR:HD1	1	0.59
(1,1669)	1:170:R:TRP:H	1:168:R:TYR:HD2	1	0.59
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD11	3	0.59
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD12	3	0.59
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD13	3	0.59
(1,1385)	1:44:R:ARG:H	1:43:R:SER:H	4	0.59
(1,1137)	1:126:R:VAL:H	1:124:R:VAL:HA	3	0.59
(1,1048)	1:105:R:TRP:H	1:101:R:ALA:HA	5	0.59
(1,918)	1:67:R:PHE:H	1:65:R:GLU:HA	1	0.59
(1,918)	1:67:R:PHE:H	1:65:R:GLU:HA	3	0.59
(1,894)	1:60:R:PHE:H	1:56:R:ILE:HD11	5	0.59
(1,894)	1:60:R:PHE:H	1:56:R:ILE:HD12	5	0.59
(1,894)	1:60:R:PHE:H	1:56:R:ILE:HD13	5	0.59
(1,2252)	1:178:R:LEU:H	1:177:R:VAL:HA	2	0.58
(1,2215)	1:154:R:VAL:H	1:154:R:VAL:HB	4	0.58
(1,2212)	1:34:R:TYR:HB2	1:154:R:VAL:HB	5	0.58
(1,2212)	1:34:R:TYR:HB3	1:154:R:VAL:HB	5	0.58
(1,2096)	1:64:R:GLU:HB2	1:64:R:GLU:HA	2	0.58
(1,2096)	1:64:R:GLU:HB3	1:64:R:GLU:HA	2	0.58
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD11	5	0.58
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD12	5	0.58
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD13	5	0.58
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD11	5	0.58
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD12	5	0.58
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD13	5	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD11	5	0.58
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD12	5	0.58
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD13	5	0.58
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD11	5	0.58
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD12	5	0.58
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD13	5	0.58
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD11	5	0.58
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD12	5	0.58
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD13	5	0.58
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD11	5	0.58
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD12	5	0.58
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD13	5	0.58
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD11	5	0.58
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD12	5	0.58
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD13	5	0.58
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD21	5	0.58
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD22	5	0.58
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD23	5	0.58
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD11	5	0.58
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD12	5	0.58
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD13	5	0.58
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD21	5	0.58
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD22	5	0.58
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD23	5	0.58
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD11	5	0.58
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD12	5	0.58
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD13	5	0.58
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD21	5	0.58
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD22	5	0.58
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD23	5	0.58
(1,1546)	1:114:R:GLY:H	1:115:R:ILE:HD11	4	0.58
(1,1546)	1:114:R:GLY:H	1:115:R:ILE:HD12	4	0.58
(1,1546)	1:114:R:GLY:H	1:115:R:ILE:HD13	4	0.58
(1,1359)	1:35:R:ASN:H	1:34:R:TYR:H	1	0.58
(1,1359)	1:35:R:ASN:H	1:34:R:TYR:H	3	0.58
(1,1356)	1:34:R:TYR:H	1:35:R:ASN:H	1	0.58
(1,1356)	1:34:R:TYR:H	1:35:R:ASN:H	3	0.58
(1,1137)	1:126:R:VAL:H	1:124:R:VAL:HA	2	0.58
(1,837)	1:41:R:PHE:H	1:41:R:PHE:HZ	5	0.58
(1,2232)	1:31:R:LEU:HD11	1:162:R:ILE:HG13	1	0.57
(1,2232)	1:31:R:LEU:HD12	1:162:R:ILE:HG13	1	0.57
(1,2232)	1:31:R:LEU:HD13	1:162:R:ILE:HG13	1	0.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2232)	1:31:R:LEU:HD21	1:162:R:ILE:HG13	1	0.57
(1,2232)	1:31:R:LEU:HD22	1:162:R:ILE:HG13	1	0.57
(1,2232)	1:31:R:LEU:HD23	1:162:R:ILE:HG13	1	0.57
(1,2161)	1:113:R:THR:HB	1:113:R:THR:HA	5	0.57
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD11	4	0.57
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD12	4	0.57
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD13	4	0.57
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD21	4	0.57
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD22	4	0.57
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD23	4	0.57
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD11	4	0.57
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD12	4	0.57
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD13	4	0.57
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD21	4	0.57
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD22	4	0.57
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD23	4	0.57
(1,1787)	1:102:R:LEU:H	1:101:R:ALA:HB1	3	0.57
(1,1787)	1:102:R:LEU:H	1:101:R:ALA:HB2	3	0.57
(1,1787)	1:102:R:LEU:H	1:101:R:ALA:HB3	3	0.57
(1,1675)	1:175:R:SER:H	1:142:R:PHE:HE1	1	0.57
(1,1675)	1:175:R:SER:H	1:142:R:PHE:HE2	1	0.57
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD11	5	0.57
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD12	5	0.57
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD13	5	0.57
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD21	5	0.57
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD22	5	0.57
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD23	5	0.57
(1,837)	1:41:R:PHE:H	1:41:R:PHE:HZ	4	0.57
(1,2255)	1:140:R:GLY:HA2	1:180:R:PHE:HA	3	0.56
(1,2201)	1:151:R:PHE:HB2	1:151:R:PHE:HA	2	0.56
(1,2200)	1:151:R:PHE:HB3	1:151:R:PHE:HA	5	0.56
(1,2181)	1:134:R:LEU:H	1:134:R:LEU:HA	5	0.56
(1,1787)	1:102:R:LEU:H	1:101:R:ALA:HB1	1	0.56
(1,1787)	1:102:R:LEU:H	1:101:R:ALA:HB2	1	0.56
(1,1787)	1:102:R:LEU:H	1:101:R:ALA:HB3	1	0.56
(1,1787)	1:102:R:LEU:H	1:101:R:ALA:HB1	4	0.56
(1,1787)	1:102:R:LEU:H	1:101:R:ALA:HB2	4	0.56
(1,1787)	1:102:R:LEU:H	1:101:R:ALA:HB3	4	0.56
(1,1787)	1:102:R:LEU:H	1:101:R:ALA:HB1	5	0.56
(1,1787)	1:102:R:LEU:H	1:101:R:ALA:HB2	5	0.56
(1,1787)	1:102:R:LEU:H	1:101:R:ALA:HB3	5	0.56
(1,1382)	1:43:R:SER:H	1:42:R:TYR:HD1	5	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1382)	1:43:R:SER:H	1:42:R:TYR:HD2	5	0.56
(1,1359)	1:35:R:ASN:H	1:34:R:TYR:H	2	0.56
(1,1356)	1:34:R:TYR:H	1:35:R:ASN:H	2	0.56
(1,1082)	1:112:R:HIS:H	1:111:R:LEU:HD11	4	0.56
(1,1082)	1:112:R:HIS:H	1:111:R:LEU:HD12	4	0.56
(1,1082)	1:112:R:HIS:H	1:111:R:LEU:HD13	4	0.56
(1,2263)	1:181:R:VAL:H	1:181:R:VAL:HB	3	0.55
(1,2233)	1:162:R:ILE:HA	1:162:R:ILE:HG13	2	0.55
(1,2226)	1:162:R:ILE:HG13	1:162:R:ILE:HA	2	0.55
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG11	5	0.55
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG12	5	0.55
(1,2194)	1:150:R:VAL:HA	1:150:R:VAL:HG13	5	0.55
(1,2191)	1:150:R:VAL:HG11	1:150:R:VAL:HA	5	0.55
(1,2191)	1:150:R:VAL:HG12	1:150:R:VAL:HA	5	0.55
(1,2191)	1:150:R:VAL:HG13	1:150:R:VAL:HA	5	0.55
(1,2108)	1:73:R:SER:HA	1:73:R:SER:HB3	4	0.55
(1,1724)	1:56:R:ILE:HD11	1:56:R:ILE:HG21	3	0.55
(1,1724)	1:56:R:ILE:HD11	1:56:R:ILE:HG22	3	0.55
(1,1724)	1:56:R:ILE:HD11	1:56:R:ILE:HG23	3	0.55
(1,1724)	1:56:R:ILE:HD12	1:56:R:ILE:HG21	3	0.55
(1,1724)	1:56:R:ILE:HD12	1:56:R:ILE:HG22	3	0.55
(1,1724)	1:56:R:ILE:HD12	1:56:R:ILE:HG23	3	0.55
(1,1724)	1:56:R:ILE:HD13	1:56:R:ILE:HG21	3	0.55
(1,1724)	1:56:R:ILE:HD13	1:56:R:ILE:HG22	3	0.55
(1,1724)	1:56:R:ILE:HD13	1:56:R:ILE:HG23	3	0.55
(1,1591)	1:137:R:PHE:H	1:181:R:VAL:H	5	0.55
(1,1382)	1:43:R:SER:H	1:42:R:TYR:HD1	3	0.55
(1,1382)	1:43:R:SER:H	1:42:R:TYR:HD2	3	0.55
(1,1128)	1:124:R:VAL:H	1:181:R:VAL:HA	5	0.55
(1,830)	1:40:R:THR:H	1:38:R:LYS:HA	4	0.55
(1,723)	1:168:R:TYR:H	1:162:R:ILE:H	5	0.55
(1,2225)	1:162:R:ILE:HB	1:162:R:ILE:HA	3	0.54
(1,2089)	1:56:R:ILE:HG21	1:56:R:ILE:HG12	3	0.54
(1,2089)	1:56:R:ILE:HG22	1:56:R:ILE:HG12	3	0.54
(1,2089)	1:56:R:ILE:HG23	1:56:R:ILE:HG12	3	0.54
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD11	5	0.54
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD12	5	0.54
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD13	5	0.54
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD21	5	0.54
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD22	5	0.54
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD23	5	0.54
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD11	5	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD12	5	0.54
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD13	5	0.54
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD21	5	0.54
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD22	5	0.54
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD23	5	0.54
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB1	3	0.54
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB2	3	0.54
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB3	3	0.54
(1,606)	1:139:R:ALA:H	1:180:R:PHE:HB3	2	0.54
(1,2263)	1:181:R:VAL:H	1:181:R:VAL:HB	1	0.53
(1,2239)	1:167:R:PHE:HB3	1:167:R:PHE:HA	1	0.53
(1,2239)	1:167:R:PHE:HB3	1:167:R:PHE:HA	3	0.53
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD11	2	0.53
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD12	2	0.53
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD13	2	0.53
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD11	2	0.53
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD12	2	0.53
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD13	2	0.53
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD11	2	0.53
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD12	2	0.53
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD13	2	0.53
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD11	2	0.53
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD12	2	0.53
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD13	2	0.53
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD11	2	0.53
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD12	2	0.53
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD13	2	0.53
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD11	2	0.53
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD12	2	0.53
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD13	2	0.53
(1,1805)	1:110:R:LEU:HA	1:110:R:LEU:HG	5	0.53
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD11	2	0.53
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD12	2	0.53
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD13	2	0.53
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD21	2	0.53
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD22	2	0.53
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD23	2	0.53
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD11	2	0.53
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD12	2	0.53
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD13	2	0.53
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD21	2	0.53
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD22	2	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD23	2	0.53
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD11	2	0.53
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD12	2	0.53
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD13	2	0.53
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD21	2	0.53
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD22	2	0.53
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD23	2	0.53
(1,1023)	1:94:R:LEU:H	1:94:R:LEU:HD21	3	0.53
(1,1023)	1:94:R:LEU:H	1:94:R:LEU:HD22	3	0.53
(1,1023)	1:94:R:LEU:H	1:94:R:LEU:HD23	3	0.53
(2,52)	1:33:R:LEU:H	1:37:R:GLU:O	2	0.52
(1,2239)	1:167:R:PHE:HB3	1:167:R:PHE:HA	5	0.52
(1,2172)	1:124:R:VAL:H	1:124:R:VAL:HG11	2	0.52
(1,2172)	1:124:R:VAL:H	1:124:R:VAL:HG12	2	0.52
(1,2172)	1:124:R:VAL:H	1:124:R:VAL:HG13	2	0.52
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB1	5	0.52
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB2	5	0.52
(1,2077)	1:52:R:TRP:H	1:51:R:ALA:HB3	5	0.52
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD11	3	0.52
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD12	3	0.52
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD13	3	0.52
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD11	1	0.52
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD12	1	0.52
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD13	1	0.52
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD11	1	0.52
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD12	1	0.52
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD13	1	0.52
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD11	1	0.52
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD12	1	0.52
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD13	1	0.52
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD11	1	0.52
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD12	1	0.52
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD13	1	0.52
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD11	1	0.52
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD12	1	0.52
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD13	1	0.52
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD11	1	0.52
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD12	1	0.52
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD13	1	0.52
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD11	4	0.52
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD12	4	0.52
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD13	4	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD11	4	0.52
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD12	4	0.52
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD13	4	0.52
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD11	4	0.52
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD12	4	0.52
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD13	4	0.52
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD11	4	0.52
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD12	4	0.52
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD13	4	0.52
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD11	4	0.52
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD12	4	0.52
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD13	4	0.52
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD11	4	0.52
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD12	4	0.52
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD13	4	0.52
(1,1841)	1:178:R:LEU:HD11	1:127:R:VAL:HG21	1	0.52
(1,1841)	1:178:R:LEU:HD11	1:127:R:VAL:HG22	1	0.52
(1,1841)	1:178:R:LEU:HD11	1:127:R:VAL:HG23	1	0.52
(1,1841)	1:178:R:LEU:HD12	1:127:R:VAL:HG21	1	0.52
(1,1841)	1:178:R:LEU:HD12	1:127:R:VAL:HG22	1	0.52
(1,1841)	1:178:R:LEU:HD12	1:127:R:VAL:HG23	1	0.52
(1,1841)	1:178:R:LEU:HD13	1:127:R:VAL:HG21	1	0.52
(1,1841)	1:178:R:LEU:HD13	1:127:R:VAL:HG22	1	0.52
(1,1841)	1:178:R:LEU:HD13	1:127:R:VAL:HG23	1	0.52
(1,1841)	1:178:R:LEU:HD21	1:127:R:VAL:HG21	1	0.52
(1,1841)	1:178:R:LEU:HD21	1:127:R:VAL:HG22	1	0.52
(1,1841)	1:178:R:LEU:HD21	1:127:R:VAL:HG23	1	0.52
(1,1841)	1:178:R:LEU:HD22	1:127:R:VAL:HG21	1	0.52
(1,1841)	1:178:R:LEU:HD22	1:127:R:VAL:HG22	1	0.52
(1,1841)	1:178:R:LEU:HD22	1:127:R:VAL:HG23	1	0.52
(1,1841)	1:178:R:LEU:HD23	1:127:R:VAL:HG21	1	0.52
(1,1841)	1:178:R:LEU:HD23	1:127:R:VAL:HG22	1	0.52
(1,1841)	1:178:R:LEU:HD23	1:127:R:VAL:HG23	1	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD11	1	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD12	1	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD13	1	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD21	1	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD22	1	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD23	1	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD11	1	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD12	1	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD13	1	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD21	1	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD22	1	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD23	1	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD11	1	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD12	1	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD13	1	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD21	1	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD22	1	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD23	1	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD11	4	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD12	4	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD13	4	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD21	4	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD22	4	0.52
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD23	4	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD11	4	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD12	4	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD13	4	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD21	4	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD22	4	0.52
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD23	4	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD11	4	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD12	4	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD13	4	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD21	4	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD22	4	0.52
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD23	4	0.52
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD11	4	0.52
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD12	4	0.52
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD13	4	0.52
(1,1159)	1:138:R:HIS:H	1:181:R:VAL:HB	3	0.52
(1,960)	1:78:R:LEU:H	1:78:R:LEU:HD11	2	0.52
(1,960)	1:78:R:LEU:H	1:78:R:LEU:HD12	2	0.52
(1,960)	1:78:R:LEU:H	1:78:R:LEU:HD13	2	0.52
(1,960)	1:78:R:LEU:H	1:78:R:LEU:HD21	2	0.52
(1,960)	1:78:R:LEU:H	1:78:R:LEU:HD22	2	0.52
(1,960)	1:78:R:LEU:H	1:78:R:LEU:HD23	2	0.52
(1,882)	1:56:R:ILE:H	1:56:R:ILE:HD11	1	0.52
(1,882)	1:56:R:ILE:H	1:56:R:ILE:HD12	1	0.52
(1,882)	1:56:R:ILE:H	1:56:R:ILE:HD13	1	0.52
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD11	3	0.52
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD12	3	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD13	3	0.52
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD21	3	0.52
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD22	3	0.52
(1,821)	1:37:R:GLU:H	1:33:R:LEU:HD23	3	0.52
(1,723)	1:168:R:TYR:H	1:162:R:ILE:H	1	0.52
(1,2224)	1:161:R:ALA:H	1:160:R:TYR:HA	2	0.51
(1,2161)	1:113:R:THR:HB	1:113:R:THR:HA	2	0.51
(1,2004)	1:113:R:THR:HG1	1:113:R:THR:HA	5	0.51
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD11	3	0.51
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD12	3	0.51
(1,1896)	1:31:R:LEU:HD11	1:162:R:ILE:HD13	3	0.51
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD11	3	0.51
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD12	3	0.51
(1,1896)	1:31:R:LEU:HD12	1:162:R:ILE:HD13	3	0.51
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD11	3	0.51
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD12	3	0.51
(1,1896)	1:31:R:LEU:HD13	1:162:R:ILE:HD13	3	0.51
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD11	3	0.51
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD12	3	0.51
(1,1896)	1:31:R:LEU:HD21	1:162:R:ILE:HD13	3	0.51
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD11	3	0.51
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD12	3	0.51
(1,1896)	1:31:R:LEU:HD22	1:162:R:ILE:HD13	3	0.51
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD11	3	0.51
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD12	3	0.51
(1,1896)	1:31:R:LEU:HD23	1:162:R:ILE:HD13	3	0.51
(1,1805)	1:110:R:LEU:HA	1:110:R:LEU:HG	2	0.51
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD11	3	0.51
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD12	3	0.51
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD13	3	0.51
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD21	3	0.51
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD22	3	0.51
(1,1693)	1:162:R:ILE:HD11	1:31:R:LEU:HD23	3	0.51
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD11	3	0.51
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD12	3	0.51
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD13	3	0.51
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD21	3	0.51
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD22	3	0.51
(1,1693)	1:162:R:ILE:HD12	1:31:R:LEU:HD23	3	0.51
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD11	3	0.51
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD12	3	0.51
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD13	3	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD21	3	0.51
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD22	3	0.51
(1,1693)	1:162:R:ILE:HD13	1:31:R:LEU:HD23	3	0.51
(1,1539)	1:112:R:HIS:H	1:111:R:LEU:H	1	0.51
(1,1536)	1:111:R:LEU:H	1:112:R:HIS:H	1	0.51
(1,837)	1:41:R:PHE:H	1:41:R:PHE:HZ	1	0.51
(2,57)	1:127:R:VAL:H	1:178:R:LEU:O	1	0.5
(1,2263)	1:181:R:VAL:H	1:181:R:VAL:HB	2	0.5
(1,2239)	1:167:R:PHE:HB3	1:167:R:PHE:HA	4	0.5
(1,2172)	1:124:R:VAL:H	1:124:R:VAL:HG11	3	0.5
(1,2172)	1:124:R:VAL:H	1:124:R:VAL:HG12	3	0.5
(1,2172)	1:124:R:VAL:H	1:124:R:VAL:HG13	3	0.5
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB1	3	0.5
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB2	3	0.5
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB3	3	0.5
(1,2165)	1:126:R:VAL:H	1:117:R:THR:HA	1	0.5
(1,2160)	1:112:R:HIS:H	1:112:R:HIS:HB2	2	0.5
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG21	5	0.5
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG22	5	0.5
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG23	5	0.5
(1,1550)	1:115:R:ILE:H	1:114:R:GLY:HA3	1	0.5
(1,1550)	1:115:R:ILE:H	1:114:R:GLY:HA3	4	0.5
(1,2219)	1:155:R:THR:HB	1:155:R:THR:HA	3	0.49
(1,2208)	1:154:R:VAL:H	1:153:R:CYS:HA	4	0.49
(1,2161)	1:113:R:THR:HB	1:113:R:THR:HA	1	0.49
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD11	1	0.49
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD12	1	0.49
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD13	1	0.49
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG21	5	0.49
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG22	5	0.49
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG23	5	0.49
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG21	5	0.49
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG22	5	0.49
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG23	5	0.49
(1,1405)	1:55:R:ALA:H	1:52:R:TRP:HA	5	0.49
(1,1086)	1:113:R:THR:H	1:111:R:LEU:HD11	4	0.49
(1,1086)	1:113:R:THR:H	1:111:R:LEU:HD12	4	0.49
(1,1086)	1:113:R:THR:H	1:111:R:LEU:HD13	4	0.49
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD11	3	0.49
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD12	3	0.49
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD13	3	0.49
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD21	3	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD22	3	0.49
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD23	3	0.49
(1,894)	1:60:R:PHE:H	1:56:R:ILE:HD11	3	0.49
(1,894)	1:60:R:PHE:H	1:56:R:ILE:HD12	3	0.49
(1,894)	1:60:R:PHE:H	1:56:R:ILE:HD13	3	0.49
(1,823)	1:37:R:GLU:H	1:35:R:ASN:HB3	4	0.49
(1,2247)	1:134:R:LEU:HD11	1:171:R:THR:HA	1	0.48
(1,2247)	1:134:R:LEU:HD12	1:171:R:THR:HA	1	0.48
(1,2247)	1:134:R:LEU:HD13	1:171:R:THR:HA	1	0.48
(1,2247)	1:134:R:LEU:HD21	1:171:R:THR:HA	1	0.48
(1,2247)	1:134:R:LEU:HD22	1:171:R:THR:HA	1	0.48
(1,2247)	1:134:R:LEU:HD23	1:171:R:THR:HA	1	0.48
(1,2224)	1:161:R:ALA:H	1:160:R:TYR:HA	4	0.48
(1,2219)	1:155:R:THR:HB	1:155:R:THR:HA	1	0.48
(1,2204)	1:139:R:ALA:HB1	1:153:R:CYS:HA	3	0.48
(1,2204)	1:139:R:ALA:HB2	1:153:R:CYS:HA	3	0.48
(1,2204)	1:139:R:ALA:HB3	1:153:R:CYS:HA	3	0.48
(1,2158)	1:112:R:HIS:HA	1:112:R:HIS:HB2	4	0.48
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG21	2	0.48
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG22	2	0.48
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG23	2	0.48
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG21	2	0.48
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG22	2	0.48
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG23	2	0.48
(1,1838)	1:127:R:VAL:H	1:126:R:VAL:HG21	5	0.48
(1,1838)	1:127:R:VAL:H	1:126:R:VAL:HG22	5	0.48
(1,1838)	1:127:R:VAL:H	1:126:R:VAL:HG23	5	0.48
(1,1600)	1:139:R:ALA:H	1:180:R:PHE:HB2	2	0.48
(1,1472)	1:82:R:ALA:H	1:71:R:VAL:HG21	2	0.48
(1,1472)	1:82:R:ALA:H	1:71:R:VAL:HG22	2	0.48
(1,1472)	1:82:R:ALA:H	1:71:R:VAL:HG23	2	0.48
(1,1389)	1:47:R:ASN:H	1:47:R:ASN:HB3	1	0.48
(2,99)	1:103:R:VAL:H	1:99:R:PRO:O	3	0.47
(1,2230)	1:162:R:ILE:HA	1:162:R:ILE:HD11	2	0.47
(1,2230)	1:162:R:ILE:HA	1:162:R:ILE:HD12	2	0.47
(1,2230)	1:162:R:ILE:HA	1:162:R:ILE:HD13	2	0.47
(1,2204)	1:139:R:ALA:HB1	1:153:R:CYS:HA	1	0.47
(1,2204)	1:139:R:ALA:HB2	1:153:R:CYS:HA	1	0.47
(1,2204)	1:139:R:ALA:HB3	1:153:R:CYS:HA	1	0.47
(1,2156)	1:111:R:LEU:HB2	1:112:R:HIS:HB3	4	0.47
(1,1661)	1:165:R:GLU:H	1:164:R:ASP:H	2	0.47
(1,1657)	1:164:R:ASP:H	1:165:R:GLU:H	2	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1592)	1:138:R:HIS:H	1:154:R:VAL:HG21	4	0.47
(1,1592)	1:138:R:HIS:H	1:154:R:VAL:HG22	4	0.47
(1,1592)	1:138:R:HIS:H	1:154:R:VAL:HG23	4	0.47
(1,1544)	1:114:R:GLY:H	1:113:R:THR:HB	5	0.47
(1,1048)	1:105:R:TRP:H	1:101:R:ALA:HA	1	0.47
(1,1048)	1:105:R:TRP:H	1:101:R:ALA:HA	4	0.47
(1,856)	1:48:R:HIS:H	1:49:R:ASP:HB2	4	0.47
(1,2219)	1:155:R:THR:HB	1:155:R:THR:HA	4	0.46
(1,2206)	1:153:R:CYS:HB2	1:153:R:CYS:HA	4	0.46
(1,2190)	1:150:R:VAL:HB	1:150:R:VAL:HA	3	0.46
(1,2190)	1:150:R:VAL:HB	1:150:R:VAL:HA	5	0.46
(1,1841)	1:178:R:LEU:HD11	1:127:R:VAL:HG21	2	0.46
(1,1841)	1:178:R:LEU:HD11	1:127:R:VAL:HG22	2	0.46
(1,1841)	1:178:R:LEU:HD11	1:127:R:VAL:HG23	2	0.46
(1,1841)	1:178:R:LEU:HD12	1:127:R:VAL:HG21	2	0.46
(1,1841)	1:178:R:LEU:HD12	1:127:R:VAL:HG22	2	0.46
(1,1841)	1:178:R:LEU:HD12	1:127:R:VAL:HG23	2	0.46
(1,1841)	1:178:R:LEU:HD13	1:127:R:VAL:HG21	2	0.46
(1,1841)	1:178:R:LEU:HD13	1:127:R:VAL:HG22	2	0.46
(1,1841)	1:178:R:LEU:HD13	1:127:R:VAL:HG23	2	0.46
(1,1841)	1:178:R:LEU:HD21	1:127:R:VAL:HG21	2	0.46
(1,1841)	1:178:R:LEU:HD21	1:127:R:VAL:HG22	2	0.46
(1,1841)	1:178:R:LEU:HD21	1:127:R:VAL:HG23	2	0.46
(1,1841)	1:178:R:LEU:HD22	1:127:R:VAL:HG21	2	0.46
(1,1841)	1:178:R:LEU:HD22	1:127:R:VAL:HG22	2	0.46
(1,1841)	1:178:R:LEU:HD22	1:127:R:VAL:HG23	2	0.46
(1,1841)	1:178:R:LEU:HD23	1:127:R:VAL:HG21	2	0.46
(1,1841)	1:178:R:LEU:HD23	1:127:R:VAL:HG22	2	0.46
(1,1841)	1:178:R:LEU:HD23	1:127:R:VAL:HG23	2	0.46
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG21	2	0.46
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG22	2	0.46
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG23	2	0.46
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG21	2	0.46
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG22	2	0.46
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG23	2	0.46
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG21	2	0.46
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG22	2	0.46
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG23	2	0.46
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD11	4	0.46
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD12	4	0.46
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD13	4	0.46
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD21	4	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD22	4	0.46
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD23	4	0.46
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD11	4	0.46
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD12	4	0.46
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD13	4	0.46
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD21	4	0.46
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD22	4	0.46
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD23	4	0.46
(1,1687)	1:184:R:ASP:H	1:183:R:TYR:HE1	5	0.46
(1,1687)	1:184:R:ASP:H	1:183:R:TYR:HE2	5	0.46
(1,1680)	1:179:R:VAL:H	1:180:R:PHE:HB2	4	0.46
(1,1550)	1:115:R:ILE:H	1:114:R:GLY:HA3	2	0.46
(1,1550)	1:115:R:ILE:H	1:114:R:GLY:HA3	3	0.46
(1,1550)	1:115:R:ILE:H	1:114:R:GLY:HA3	5	0.46
(1,1440)	1:70:R:TRP:H	1:68:R:PHE:HA	5	0.46
(1,1405)	1:55:R:ALA:H	1:52:R:TRP:HA	1	0.46
(1,1405)	1:55:R:ALA:H	1:52:R:TRP:HA	2	0.46
(1,1315)	1:179:R:VAL:H	1:142:R:PHE:HA	4	0.46
(2,58)	1:127:R:VAL:N	1:178:R:LEU:O	2	0.45
(1,2225)	1:162:R:ILE:HB	1:162:R:ILE:HA	4	0.45
(1,2190)	1:150:R:VAL:HB	1:150:R:VAL:HA	1	0.45
(1,2190)	1:150:R:VAL:HB	1:150:R:VAL:HA	2	0.45
(1,2174)	1:125:R:CYS:H	1:125:R:CYS:HB3	2	0.45
(1,2160)	1:112:R:HIS:H	1:112:R:HIS:HB2	1	0.45
(1,2158)	1:112:R:HIS:HA	1:112:R:HIS:HB2	1	0.45
(1,2157)	1:112:R:HIS:HA	1:112:R:HIS:HB3	4	0.45
(1,2099)	1:70:R:TRP:HA	1:70:R:TRP:HB3	2	0.45
(1,1954)	1:56:R:ILE:HG13	1:56:R:ILE:HG21	5	0.45
(1,1954)	1:56:R:ILE:HG13	1:56:R:ILE:HG22	5	0.45
(1,1954)	1:56:R:ILE:HG13	1:56:R:ILE:HG23	5	0.45
(1,1805)	1:110:R:LEU:HA	1:110:R:LEU:HG	4	0.45
(1,1715)	1:56:R:ILE:HA	1:56:R:ILE:HD11	2	0.45
(1,1715)	1:56:R:ILE:HA	1:56:R:ILE:HD12	2	0.45
(1,1715)	1:56:R:ILE:HA	1:56:R:ILE:HD13	2	0.45
(1,1652)	1:163:R:ASP:H	1:166:R:ASP:H	3	0.45
(1,1389)	1:47:R:ASN:H	1:47:R:ASN:HB3	2	0.45
(1,851)	1:46:R:ASN:H	1:165:R:GLU:H	3	0.45
(1,823)	1:37:R:GLU:H	1:35:R:ASN:HB3	5	0.45
(2,53)	1:116:R:GLY:H	1:124:R:VAL:O	5	0.44
(1,2263)	1:181:R:VAL:H	1:181:R:VAL:HB	5	0.44
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG21	4	0.44
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG22	4	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG23	4	0.44
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG21	4	0.44
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG22	4	0.44
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG23	4	0.44
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG21	4	0.44
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG22	4	0.44
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG23	4	0.44
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG21	4	0.44
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG22	4	0.44
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG23	4	0.44
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG21	4	0.44
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG22	4	0.44
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG23	4	0.44
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG21	4	0.44
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG22	4	0.44
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG23	4	0.44
(1,2219)	1:155:R:THR:HB	1:155:R:THR:HA	5	0.44
(1,2212)	1:34:R:TYR:HB2	1:154:R:VAL:HB	2	0.44
(1,2212)	1:34:R:TYR:HB3	1:154:R:VAL:HB	2	0.44
(1,2190)	1:150:R:VAL:HB	1:150:R:VAL:HA	4	0.44
(1,2158)	1:112:R:HIS:HA	1:112:R:HIS:HB2	2	0.44
(1,2120)	1:89:R:LEU:HA	1:89:R:LEU:HG	2	0.44
(1,2120)	1:89:R:LEU:HA	1:89:R:LEU:HG	5	0.44
(1,2110)	1:73:R:SER:H	1:73:R:SER:HB2	1	0.44
(1,2016)	1:127:R:VAL:H	1:126:R:VAL:HG21	2	0.44
(1,2016)	1:127:R:VAL:H	1:126:R:VAL:HG22	2	0.44
(1,2016)	1:127:R:VAL:H	1:126:R:VAL:HG23	2	0.44
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG21	5	0.44
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG22	5	0.44
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG23	5	0.44
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG21	5	0.44
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG22	5	0.44
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG23	5	0.44
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG21	5	0.44
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG22	5	0.44
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG23	5	0.44
(1,1671)	1:171:R:THR:H	1:168:R:TYR:HD1	2	0.44
(1,1671)	1:171:R:THR:H	1:168:R:TYR:HD2	2	0.44
(1,1463)	1:79:R:THR:H	1:71:R:VAL:HG11	2	0.44
(1,1463)	1:79:R:THR:H	1:71:R:VAL:HG12	2	0.44
(1,1463)	1:79:R:THR:H	1:71:R:VAL:HG13	2	0.44
(1,659)	1:153:R:CYS:H	1:155:R:THR:CG2	2	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,57)	1:127:R:VAL:H	1:178:R:LEU:O	2	0.43
(1,2206)	1:153:R:CYS:HB2	1:153:R:CYS:HA	5	0.43
(1,2200)	1:151:R:PHE:HB3	1:151:R:PHE:HA	1	0.43
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB1	1	0.43
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB2	1	0.43
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB3	1	0.43
(1,2165)	1:126:R:VAL:H	1:117:R:THR:HA	5	0.43
(1,2160)	1:112:R:HIS:H	1:112:R:HIS:HB2	5	0.43
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG21	3	0.43
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG22	3	0.43
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG23	3	0.43
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG21	3	0.43
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG22	3	0.43
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG23	3	0.43
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG21	3	0.43
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG22	3	0.43
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG23	3	0.43
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD11	2	0.43
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD12	2	0.43
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD13	2	0.43
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD11	2	0.43
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD12	2	0.43
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD13	2	0.43
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD11	2	0.43
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD12	2	0.43
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD13	2	0.43
(1,1591)	1:137:R:PHE:H	1:181:R:VAL:H	2	0.43
(1,1524)	1:109:R:HIS:H	1:108:R:LYS:H	5	0.43
(1,1522)	1:108:R:LYS:H	1:109:R:HIS:H	5	0.43
(1,1405)	1:55:R:ALA:H	1:52:R:TRP:HA	4	0.43
(1,1389)	1:47:R:ASN:H	1:47:R:ASN:HB3	4	0.43
(1,1389)	1:47:R:ASN:H	1:47:R:ASN:HB3	5	0.43
(2,54)	1:116:R:GLY:N	1:124:R:VAL:O	5	0.42
(1,2262)	1:139:R:ALA:H	1:181:R:VAL:HB	3	0.42
(1,2239)	1:167:R:PHE:HB3	1:167:R:PHE:HA	2	0.42
(1,2219)	1:155:R:THR:HB	1:155:R:THR:HA	2	0.42
(1,2110)	1:73:R:SER:H	1:73:R:SER:HB2	2	0.42
(1,2099)	1:70:R:TRP:HA	1:70:R:TRP:HB3	1	0.42
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD11	4	0.42
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD12	4	0.42
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD13	4	0.42
(1,1909)	1:162:R:ILE:H	1:162:R:ILE:HG21	5	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1909)	1:162:R:ILE:H	1:162:R:ILE:HG22	5	0.42
(1,1909)	1:162:R:ILE:H	1:162:R:ILE:HG23	5	0.42
(1,1893)	1:170:R:TRP:HB3	1:171:R:THR:HG1	3	0.42
(1,1811)	1:114:R:GLY:H	1:113:R:THR:HA	5	0.42
(1,1739)	1:69:R:ASP:H	1:68:R:PHE:HA	1	0.42
(1,1724)	1:56:R:ILE:HD11	1:56:R:ILE:HG21	2	0.42
(1,1724)	1:56:R:ILE:HD11	1:56:R:ILE:HG22	2	0.42
(1,1724)	1:56:R:ILE:HD11	1:56:R:ILE:HG23	2	0.42
(1,1724)	1:56:R:ILE:HD12	1:56:R:ILE:HG21	2	0.42
(1,1724)	1:56:R:ILE:HD12	1:56:R:ILE:HG22	2	0.42
(1,1724)	1:56:R:ILE:HD12	1:56:R:ILE:HG23	2	0.42
(1,1724)	1:56:R:ILE:HD13	1:56:R:ILE:HG21	2	0.42
(1,1724)	1:56:R:ILE:HD13	1:56:R:ILE:HG22	2	0.42
(1,1724)	1:56:R:ILE:HD13	1:56:R:ILE:HG23	2	0.42
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD11	5	0.42
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD12	5	0.42
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD13	5	0.42
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD11	5	0.42
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD12	5	0.42
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD13	5	0.42
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD11	5	0.42
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD12	5	0.42
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD13	5	0.42
(1,1383)	1:43:R:SER:H	1:43:R:SER:HB3	5	0.42
(1,1258)	1:161:R:ALA:H	1:162:R:ILE:HG13	5	0.42
(1,941)	1:72:R:TYR:H	1:71:R:VAL:HG11	2	0.42
(1,941)	1:72:R:TYR:H	1:71:R:VAL:HG12	2	0.42
(1,941)	1:72:R:TYR:H	1:71:R:VAL:HG13	2	0.42
(1,2255)	1:140:R:GLY:HA2	1:180:R:PHE:HA	1	0.41
(1,2181)	1:134:R:LEU:H	1:134:R:LEU:HA	2	0.41
(1,2174)	1:125:R:CYS:H	1:125:R:CYS:HB3	5	0.41
(1,2110)	1:73:R:SER:H	1:73:R:SER:HB2	5	0.41
(1,2099)	1:70:R:TRP:HA	1:70:R:TRP:HB3	3	0.41
(1,2099)	1:70:R:TRP:HA	1:70:R:TRP:HB3	4	0.41
(1,2099)	1:70:R:TRP:HA	1:70:R:TRP:HB3	5	0.41
(1,2084)	1:56:R:ILE:HA	1:56:R:ILE:HG13	4	0.41
(1,1950)	1:56:R:ILE:H	1:56:R:ILE:HD11	3	0.41
(1,1950)	1:56:R:ILE:H	1:56:R:ILE:HD12	3	0.41
(1,1950)	1:56:R:ILE:H	1:56:R:ILE:HD13	3	0.41
(1,1915)	1:159:R:TRP:HB2	1:171:R:THR:HA	2	0.41
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG21	1	0.41
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG22	1	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG23	1	0.41
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG21	1	0.41
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG22	1	0.41
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG23	1	0.41
(1,1841)	1:178:R:LEU:HD11	1:127:R:VAL:HG21	3	0.41
(1,1841)	1:178:R:LEU:HD11	1:127:R:VAL:HG22	3	0.41
(1,1841)	1:178:R:LEU:HD11	1:127:R:VAL:HG23	3	0.41
(1,1841)	1:178:R:LEU:HD12	1:127:R:VAL:HG21	3	0.41
(1,1841)	1:178:R:LEU:HD12	1:127:R:VAL:HG22	3	0.41
(1,1841)	1:178:R:LEU:HD12	1:127:R:VAL:HG23	3	0.41
(1,1841)	1:178:R:LEU:HD13	1:127:R:VAL:HG21	3	0.41
(1,1841)	1:178:R:LEU:HD13	1:127:R:VAL:HG22	3	0.41
(1,1841)	1:178:R:LEU:HD13	1:127:R:VAL:HG23	3	0.41
(1,1841)	1:178:R:LEU:HD21	1:127:R:VAL:HG21	3	0.41
(1,1841)	1:178:R:LEU:HD21	1:127:R:VAL:HG22	3	0.41
(1,1841)	1:178:R:LEU:HD21	1:127:R:VAL:HG23	3	0.41
(1,1841)	1:178:R:LEU:HD22	1:127:R:VAL:HG21	3	0.41
(1,1841)	1:178:R:LEU:HD22	1:127:R:VAL:HG22	3	0.41
(1,1841)	1:178:R:LEU:HD22	1:127:R:VAL:HG23	3	0.41
(1,1841)	1:178:R:LEU:HD23	1:127:R:VAL:HG21	3	0.41
(1,1841)	1:178:R:LEU:HD23	1:127:R:VAL:HG22	3	0.41
(1,1841)	1:178:R:LEU:HD23	1:127:R:VAL:HG23	3	0.41
(1,1728)	1:57:R:LEU:HD11	1:57:R:LEU:HA	2	0.41
(1,1728)	1:57:R:LEU:HD12	1:57:R:LEU:HA	2	0.41
(1,1728)	1:57:R:LEU:HD13	1:57:R:LEU:HA	2	0.41
(1,1728)	1:57:R:LEU:HD21	1:57:R:LEU:HA	2	0.41
(1,1728)	1:57:R:LEU:HD22	1:57:R:LEU:HA	2	0.41
(1,1728)	1:57:R:LEU:HD23	1:57:R:LEU:HA	2	0.41
(1,1727)	1:56:R:ILE:H	1:56:R:ILE:HG21	4	0.41
(1,1727)	1:56:R:ILE:H	1:56:R:ILE:HG22	4	0.41
(1,1727)	1:56:R:ILE:H	1:56:R:ILE:HG23	4	0.41
(1,1719)	1:56:R:ILE:H	1:56:R:ILE:HD11	2	0.41
(1,1719)	1:56:R:ILE:H	1:56:R:ILE:HD12	2	0.41
(1,1719)	1:56:R:ILE:H	1:56:R:ILE:HD13	2	0.41
(1,1499)	1:95:R:HIS:H	1:97:R:GLY:H	5	0.41
(1,1497)	1:94:R:LEU:H	1:93:R:GLU:H	2	0.41
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD11	2	0.41
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD12	2	0.41
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD13	2	0.41
(1,1384)	1:44:R:ARG:H	1:42:R:TYR:H	4	0.41
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD11	1	0.41
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD12	1	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD13	1	0.41
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD21	1	0.41
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD22	1	0.41
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD23	1	0.41
(1,830)	1:40:R:THR:H	1:38:R:LYS:HA	1	0.41
(1,2257)	1:180:R:PHE:HB3	1:180:R:PHE:HA	3	0.4
(1,2235)	1:162:R:ILE:H	1:162:R:ILE:HG12	3	0.4
(1,2205)	1:153:R:CYS:HB3	1:153:R:CYS:HA	4	0.4
(1,2165)	1:126:R:VAL:H	1:117:R:THR:HA	2	0.4
(1,2047)	1:161:R:ALA:H	1:161:R:ALA:HB1	5	0.4
(1,2047)	1:161:R:ALA:H	1:161:R:ALA:HB2	5	0.4
(1,2047)	1:161:R:ALA:H	1:161:R:ALA:HB3	5	0.4
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB1	3	0.4
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB2	3	0.4
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB3	3	0.4
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB1	3	0.4
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB2	3	0.4
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB3	3	0.4
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB1	3	0.4
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB2	3	0.4
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB3	3	0.4
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG21	3	0.4
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG22	3	0.4
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG23	3	0.4
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG21	3	0.4
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG22	3	0.4
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG23	3	0.4
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG21	3	0.4
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG22	3	0.4
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG23	3	0.4
(1,1727)	1:56:R:ILE:H	1:56:R:ILE:HG21	2	0.4
(1,1727)	1:56:R:ILE:H	1:56:R:ILE:HG22	2	0.4
(1,1727)	1:56:R:ILE:H	1:56:R:ILE:HG23	2	0.4
(1,1591)	1:137:R:PHE:H	1:181:R:VAL:H	4	0.4
(1,1539)	1:112:R:HIS:H	1:111:R:LEU:H	2	0.4
(1,1536)	1:111:R:LEU:H	1:112:R:HIS:H	2	0.4
(1,1524)	1:109:R:HIS:H	1:108:R:LYS:H	1	0.4
(1,1522)	1:108:R:LYS:H	1:109:R:HIS:H	1	0.4
(1,1464)	1:79:R:THR:H	1:71:R:VAL:HG21	2	0.4
(1,1464)	1:79:R:THR:H	1:71:R:VAL:HG22	2	0.4
(1,1464)	1:79:R:THR:H	1:71:R:VAL:HG23	2	0.4
(1,1361)	1:35:R:ASN:H	1:36:R:GLY:H	4	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1361)	1:35:R:ASN:H	1:36:R:GLY:H	5	0.4
(1,1358)	1:34:R:TYR:H	1:155:R:THR:HA	5	0.4
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD11	4	0.4
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD12	4	0.4
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD13	4	0.4
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD21	4	0.4
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD22	4	0.4
(1,973)	1:81:R:GLU:H	1:80:R:LEU:HD23	4	0.4
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG21	5	0.4
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG22	5	0.4
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG23	5	0.4
(1,2321)	1:44:R:ARG:H	1:164:R:ASP:C	5	0.39
(1,2231)	1:162:R:ILE:H	1:162:R:ILE:HD11	5	0.39
(1,2231)	1:162:R:ILE:H	1:162:R:ILE:HD12	5	0.39
(1,2231)	1:162:R:ILE:H	1:162:R:ILE:HD13	5	0.39
(1,2157)	1:112:R:HIS:HA	1:112:R:HIS:HB3	5	0.39
(1,2110)	1:73:R:SER:H	1:73:R:SER:HB2	3	0.39
(1,2073)	1:167:R:PHE:HD1	1:31:R:LEU:HG	1	0.39
(1,2073)	1:167:R:PHE:HD2	1:31:R:LEU:HG	1	0.39
(1,1965)	1:70:R:TRP:HB3	1:70:R:TRP:HA	3	0.39
(1,1965)	1:70:R:TRP:HB3	1:70:R:TRP:HA	4	0.39
(1,1965)	1:70:R:TRP:HB3	1:70:R:TRP:HA	5	0.39
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG11	2	0.39
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG12	2	0.39
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG13	2	0.39
(1,1858)	1:181:R:VAL:HG11	1:139:R:ALA:HB1	2	0.39
(1,1858)	1:181:R:VAL:HG11	1:139:R:ALA:HB2	2	0.39
(1,1858)	1:181:R:VAL:HG11	1:139:R:ALA:HB3	2	0.39
(1,1858)	1:181:R:VAL:HG12	1:139:R:ALA:HB1	2	0.39
(1,1858)	1:181:R:VAL:HG12	1:139:R:ALA:HB2	2	0.39
(1,1858)	1:181:R:VAL:HG12	1:139:R:ALA:HB3	2	0.39
(1,1858)	1:181:R:VAL:HG13	1:139:R:ALA:HB1	2	0.39
(1,1858)	1:181:R:VAL:HG13	1:139:R:ALA:HB2	2	0.39
(1,1858)	1:181:R:VAL:HG13	1:139:R:ALA:HB3	2	0.39
(1,1858)	1:181:R:VAL:HG11	1:139:R:ALA:HB1	4	0.39
(1,1858)	1:181:R:VAL:HG11	1:139:R:ALA:HB2	4	0.39
(1,1858)	1:181:R:VAL:HG11	1:139:R:ALA:HB3	4	0.39
(1,1858)	1:181:R:VAL:HG12	1:139:R:ALA:HB1	4	0.39
(1,1858)	1:181:R:VAL:HG12	1:139:R:ALA:HB2	4	0.39
(1,1858)	1:181:R:VAL:HG12	1:139:R:ALA:HB3	4	0.39
(1,1858)	1:181:R:VAL:HG13	1:139:R:ALA:HB1	4	0.39
(1,1858)	1:181:R:VAL:HG13	1:139:R:ALA:HB2	4	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1858)	1:181:R:VAL:HG13	1:139:R:ALA:HB3	4	0.39
(1,1805)	1:110:R:LEU:HA	1:110:R:LEU:HG	1	0.39
(1,1715)	1:56:R:ILE:HA	1:56:R:ILE:HD11	5	0.39
(1,1715)	1:56:R:ILE:HA	1:56:R:ILE:HD12	5	0.39
(1,1715)	1:56:R:ILE:HA	1:56:R:ILE:HD13	5	0.39
(1,1654)	1:164:R:ASP:H	1:163:R:ASP:HB3	2	0.39
(1,1654)	1:164:R:ASP:H	1:163:R:ASP:HB3	4	0.39
(1,1652)	1:163:R:ASP:H	1:166:R:ASP:H	2	0.39
(1,1591)	1:137:R:PHE:H	1:181:R:VAL:H	3	0.39
(1,1427)	1:63:R:VAL:H	1:181:R:VAL:HG21	4	0.39
(1,1427)	1:63:R:VAL:H	1:181:R:VAL:HG22	4	0.39
(1,1427)	1:63:R:VAL:H	1:181:R:VAL:HG23	4	0.39
(1,1405)	1:55:R:ALA:H	1:52:R:TRP:HA	3	0.39
(1,915)	1:65:R:GLU:H	1:63:R:VAL:HB	1	0.39
(1,902)	1:61:R:ARG:H	1:41:R:PHE:HZ	4	0.39
(1,723)	1:168:R:TYR:H	1:162:R:ILE:H	4	0.39
(2,99)	1:103:R:VAL:H	1:99:R:PRO:O	1	0.38
(1,2288)	1:33:R:LEU:H	1:37:R:GLU:C	5	0.38
(1,2257)	1:180:R:PHE:HB3	1:180:R:PHE:HA	1	0.38
(1,2246)	1:170:R:TRP:H	1:170:R:TRP:HB2	2	0.38
(1,2234)	1:162:R:ILE:H	1:162:R:ILE:HG13	3	0.38
(1,2206)	1:153:R:CYS:HB2	1:153:R:CYS:HA	1	0.38
(1,2109)	1:73:R:SER:H	1:73:R:SER:HB3	5	0.38
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD11	5	0.38
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD12	5	0.38
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD13	5	0.38
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD11	5	0.38
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD12	5	0.38
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD13	5	0.38
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD11	5	0.38
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD12	5	0.38
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD13	5	0.38
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD11	5	0.38
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD12	5	0.38
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD13	5	0.38
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD11	5	0.38
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD12	5	0.38
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD13	5	0.38
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD11	5	0.38
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD12	5	0.38
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD13	5	0.38
(1,2025)	1:134:R:LEU:HA	1:134:R:LEU:HD11	2	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2025)	1:134:R:LEU:HA	1:134:R:LEU:HD12	2	0.38
(1,2025)	1:134:R:LEU:HA	1:134:R:LEU:HD13	2	0.38
(1,1965)	1:70:R:TRP:HB3	1:70:R:TRP:HA	1	0.38
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD11	5	0.38
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD12	5	0.38
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD13	5	0.38
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD21	5	0.38
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD22	5	0.38
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD23	5	0.38
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD11	5	0.38
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD12	5	0.38
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD13	5	0.38
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD21	5	0.38
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD22	5	0.38
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD23	5	0.38
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD11	5	0.38
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD12	5	0.38
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD13	5	0.38
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD21	5	0.38
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD22	5	0.38
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD23	5	0.38
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB1	4	0.38
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB2	4	0.38
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB3	4	0.38
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB1	4	0.38
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB2	4	0.38
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB3	4	0.38
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB1	4	0.38
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB2	4	0.38
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB3	4	0.38
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB1	4	0.38
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB2	4	0.38
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB3	4	0.38
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB1	4	0.38
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB2	4	0.38
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB3	4	0.38
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB1	4	0.38
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB2	4	0.38
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB3	4	0.38
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG21	5	0.38
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG22	5	0.38
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG23	5	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG21	5	0.38
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG22	5	0.38
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG23	5	0.38
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG21	5	0.38
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG22	5	0.38
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG23	5	0.38
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB1	1	0.38
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB2	1	0.38
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB3	1	0.38
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB1	1	0.38
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB2	1	0.38
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB3	1	0.38
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB1	1	0.38
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB2	1	0.38
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB3	1	0.38
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB1	2	0.38
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB2	2	0.38
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB3	2	0.38
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB1	2	0.38
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB2	2	0.38
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB3	2	0.38
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB1	2	0.38
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB2	2	0.38
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB3	2	0.38
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB1	5	0.38
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB2	5	0.38
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB3	5	0.38
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB1	5	0.38
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB2	5	0.38
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB3	5	0.38
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB1	5	0.38
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB2	5	0.38
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB3	5	0.38
(1,1530)	1:110:R:LEU:H	1:109:R:HIS:HB2	5	0.38
(1,1524)	1:109:R:HIS:H	1:108:R:LYS:H	3	0.38
(1,1524)	1:109:R:HIS:H	1:108:R:LYS:H	4	0.38
(1,1522)	1:108:R:LYS:H	1:109:R:HIS:H	3	0.38
(1,1522)	1:108:R:LYS:H	1:109:R:HIS:H	4	0.38
(1,1425)	1:62:R:TYR:H	1:61:R:ARG:HA	4	0.38
(1,1358)	1:34:R:TYR:H	1:155:R:THR:HA	1	0.38
(1,1358)	1:34:R:TYR:H	1:155:R:THR:HA	4	0.38
(1,1250)	1:159:R:TRP:H	1:170:R:TRP:H	4	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1029)	1:97:R:GLY:H	1:49:R:ASP:HB2	4	0.38
(1,850)	1:46:R:ASN:H	1:49:R:ASP:H	2	0.38
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD11	3	0.38
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD12	3	0.38
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD13	3	0.38
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD21	3	0.38
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD22	3	0.38
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD23	3	0.38
(1,660)	1:153:R:CYS:H	1:155:R:THR:H	3	0.38
(1,180)	1:33:R:LEU:H	1:36:R:GLY:HA3	2	0.38
(1,2312)	1:103:R:VAL:H	1:99:R:PRO:C	3	0.37
(1,2249)	1:171:R:THR:H	1:171:R:THR:HA	3	0.37
(1,2212)	1:34:R:TYR:HB2	1:154:R:VAL:HB	1	0.37
(1,2212)	1:34:R:TYR:HB3	1:154:R:VAL:HB	1	0.37
(1,2165)	1:126:R:VAL:H	1:117:R:THR:HA	3	0.37
(1,2120)	1:89:R:LEU:HA	1:89:R:LEU:HG	4	0.37
(1,2109)	1:73:R:SER:H	1:73:R:SER:HB3	3	0.37
(1,2103)	1:72:R:TYR:H	1:71:R:VAL:HG11	3	0.37
(1,2103)	1:72:R:TYR:H	1:71:R:VAL:HG12	3	0.37
(1,2103)	1:72:R:TYR:H	1:71:R:VAL:HG13	3	0.37
(1,2048)	1:170:R:TRP:HB2	1:161:R:ALA:HB1	2	0.37
(1,2048)	1:170:R:TRP:HB2	1:161:R:ALA:HB2	2	0.37
(1,2048)	1:170:R:TRP:HB2	1:161:R:ALA:HB3	2	0.37
(1,2004)	1:113:R:THR:HG22	1:113:R:THR:HA	3	0.37
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG21	1	0.37
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG22	1	0.37
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG23	1	0.37
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB1	3	0.37
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB2	3	0.37
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB3	3	0.37
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB1	3	0.37
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB2	3	0.37
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB3	3	0.37
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB1	3	0.37
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB2	3	0.37
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB3	3	0.37
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB1	3	0.37
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB2	3	0.37
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB3	3	0.37
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB1	3	0.37
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB2	3	0.37
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB3	3	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB1	3	0.37
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB2	3	0.37
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB3	3	0.37
(1,1714)	1:83:R:ILE:HG21	1:53:R:LEU:HD21	4	0.37
(1,1714)	1:83:R:ILE:HG21	1:53:R:LEU:HD22	4	0.37
(1,1714)	1:83:R:ILE:HG21	1:53:R:LEU:HD23	4	0.37
(1,1714)	1:83:R:ILE:HG22	1:53:R:LEU:HD21	4	0.37
(1,1714)	1:83:R:ILE:HG22	1:53:R:LEU:HD22	4	0.37
(1,1714)	1:83:R:ILE:HG22	1:53:R:LEU:HD23	4	0.37
(1,1714)	1:83:R:ILE:HG23	1:53:R:LEU:HD21	4	0.37
(1,1714)	1:83:R:ILE:HG23	1:53:R:LEU:HD22	4	0.37
(1,1714)	1:83:R:ILE:HG23	1:53:R:LEU:HD23	4	0.37
(1,1711)	1:83:R:ILE:HG13	1:53:R:LEU:HD11	1	0.37
(1,1711)	1:83:R:ILE:HG13	1:53:R:LEU:HD12	1	0.37
(1,1711)	1:83:R:ILE:HG13	1:53:R:LEU:HD13	1	0.37
(1,1539)	1:112:R:HIS:H	1:111:R:LEU:H	5	0.37
(1,1536)	1:111:R:LEU:H	1:112:R:HIS:H	5	0.37
(1,1530)	1:110:R:LEU:H	1:109:R:HIS:HB2	2	0.37
(1,1530)	1:110:R:LEU:H	1:109:R:HIS:HB2	3	0.37
(1,1511)	1:105:R:TRP:H	1:103:R:VAL:H	5	0.37
(1,1399)	1:52:R:TRP:H	1:51:R:ALA:HA	5	0.37
(1,1389)	1:47:R:ASN:H	1:47:R:ASN:HB3	3	0.37
(1,1358)	1:34:R:TYR:H	1:155:R:THR:HA	3	0.37
(2,99)	1:103:R:VAL:H	1:99:R:PRO:O	4	0.36
(2,97)	1:104:R:ILE:H	1:100:R:PRO:O	3	0.36
(2,58)	1:127:R:VAL:N	1:178:R:LEU:O	3	0.36
(1,2319)	1:142:R:PHE:C	1:150:R:VAL:H	3	0.36
(1,2263)	1:181:R:VAL:H	1:181:R:VAL:HB	4	0.36
(1,2227)	1:162:R:ILE:HG12	1:162:R:ILE:HA	1	0.36
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG21	2	0.36
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG22	2	0.36
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG23	2	0.36
(1,2178)	1:126:R:VAL:H	1:126:R:VAL:HG11	3	0.36
(1,2178)	1:126:R:VAL:H	1:126:R:VAL:HG12	3	0.36
(1,2178)	1:126:R:VAL:H	1:126:R:VAL:HG13	3	0.36
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB1	1	0.36
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB2	1	0.36
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB3	1	0.36
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB1	1	0.36
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB2	1	0.36
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB3	1	0.36
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB1	1	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB2	1	0.36
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB3	1	0.36
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB1	1	0.36
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB2	1	0.36
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB3	1	0.36
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB1	1	0.36
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB2	1	0.36
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB3	1	0.36
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB1	1	0.36
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB2	1	0.36
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB3	1	0.36
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG11	3	0.36
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG12	3	0.36
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG13	3	0.36
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG21	1	0.36
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG22	1	0.36
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG23	1	0.36
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG21	1	0.36
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG22	1	0.36
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG23	1	0.36
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG21	1	0.36
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG22	1	0.36
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG23	1	0.36
(1,1659)	1:165:R:GLU:H	1:44:R:ARG:H	5	0.36
(1,1541)	1:112:R:HIS:H	1:113:R:THR:HG22	4	0.36
(1,1537)	1:111:R:LEU:H	1:113:R:THR:HB	4	0.36
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD11	4	0.36
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD12	4	0.36
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD13	4	0.36
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD21	4	0.36
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD22	4	0.36
(1,1432)	1:68:R:PHE:H	1:57:R:LEU:HD23	4	0.36
(1,1399)	1:52:R:TRP:H	1:51:R:ALA:HA	1	0.36
(1,1399)	1:52:R:TRP:H	1:51:R:ALA:HA	3	0.36
(1,1399)	1:52:R:TRP:H	1:51:R:ALA:HA	4	0.36
(1,1386)	1:44:R:ARG:H	1:165:R:GLU:H	5	0.36
(1,1382)	1:43:R:SER:H	1:42:R:TYR:HD1	4	0.36
(1,1382)	1:43:R:SER:H	1:42:R:TYR:HD2	4	0.36
(1,959)	1:78:R:LEU:H	1:78:R:LEU:HB2	4	0.36
(1,959)	1:78:R:LEU:H	1:78:R:LEU:HB3	4	0.36
(1,830)	1:40:R:THR:H	1:38:R:LYS:HA	5	0.36
(1,126)	1:157:R:ASN:H	1:155:R:THR:CG2	1	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2257)	1:180:R:PHE:HB3	1:180:R:PHE:HA	2	0.35
(1,2244)	1:170:R:TRP:HA	1:170:R:TRP:HB2	3	0.35
(1,2129)	1:94:R:LEU:HB3	1:94:R:LEU:HD11	3	0.35
(1,2129)	1:94:R:LEU:HB3	1:94:R:LEU:HD12	3	0.35
(1,2129)	1:94:R:LEU:HB3	1:94:R:LEU:HD13	3	0.35
(1,1965)	1:70:R:TRP:HB3	1:70:R:TRP:HA	2	0.35
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG21	3	0.35
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG22	3	0.35
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG23	3	0.35
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG21	3	0.35
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG22	3	0.35
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG23	3	0.35
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG21	3	0.35
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG22	3	0.35
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG23	3	0.35
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB1	5	0.35
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB2	5	0.35
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB3	5	0.35
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB1	5	0.35
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB2	5	0.35
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB3	5	0.35
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB1	5	0.35
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB2	5	0.35
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB3	5	0.35
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB1	5	0.35
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB2	5	0.35
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB3	5	0.35
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB1	5	0.35
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB2	5	0.35
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB3	5	0.35
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB1	5	0.35
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB2	5	0.35
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB3	5	0.35
(1,1857)	1:181:R:VAL:HB	1:139:R:ALA:HB1	5	0.35
(1,1857)	1:181:R:VAL:HB	1:139:R:ALA:HB2	5	0.35
(1,1857)	1:181:R:VAL:HB	1:139:R:ALA:HB3	5	0.35
(1,1846)	1:131:R:ASP:H	1:130:R:THR:HG21	1	0.35
(1,1680)	1:179:R:VAL:H	1:180:R:PHE:HB2	5	0.35
(1,1488)	1:87:R:GLU:H	1:94:R:LEU:HD21	1	0.35
(1,1488)	1:87:R:GLU:H	1:94:R:LEU:HD22	1	0.35
(1,1488)	1:87:R:GLU:H	1:94:R:LEU:HD23	1	0.35
(1,1410)	1:59:R:LEU:H	1:57:R:LEU:H	5	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,723)	1:168:R:TYR:H	1:162:R:ILE:H	3	0.35
(1,105)	1:137:R:PHE:H	1:138:R:HIS:H	2	0.35
(2,118)	1:44:R:ARG:N	1:164:R:ASP:O	5	0.34
(2,117)	1:44:R:ARG:H	1:164:R:ASP:O	4	0.34
(2,99)	1:103:R:VAL:H	1:99:R:PRO:O	5	0.34
(1,2248)	1:171:R:THR:HB	1:171:R:THR:HA	1	0.34
(1,2241)	1:180:R:PHE:HE1	1:125:R:CYS:HB3	5	0.34
(1,2241)	1:180:R:PHE:HE2	1:125:R:CYS:HB3	5	0.34
(1,2153)	1:111:R:LEU:HB2	1:111:R:LEU:HA	4	0.34
(1,2047)	1:161:R:ALA:H	1:161:R:ALA:HB1	2	0.34
(1,2047)	1:161:R:ALA:H	1:161:R:ALA:HB2	2	0.34
(1,2047)	1:161:R:ALA:H	1:161:R:ALA:HB3	2	0.34
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD11	2	0.34
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD12	2	0.34
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD13	2	0.34
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG11	5	0.34
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG12	5	0.34
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG13	5	0.34
(1,1841)	1:178:R:LEU:HD11	1:127:R:VAL:HG21	4	0.34
(1,1841)	1:178:R:LEU:HD11	1:127:R:VAL:HG22	4	0.34
(1,1841)	1:178:R:LEU:HD11	1:127:R:VAL:HG23	4	0.34
(1,1841)	1:178:R:LEU:HD12	1:127:R:VAL:HG21	4	0.34
(1,1841)	1:178:R:LEU:HD12	1:127:R:VAL:HG22	4	0.34
(1,1841)	1:178:R:LEU:HD12	1:127:R:VAL:HG23	4	0.34
(1,1841)	1:178:R:LEU:HD13	1:127:R:VAL:HG21	4	0.34
(1,1841)	1:178:R:LEU:HD13	1:127:R:VAL:HG22	4	0.34
(1,1841)	1:178:R:LEU:HD13	1:127:R:VAL:HG23	4	0.34
(1,1841)	1:178:R:LEU:HD21	1:127:R:VAL:HG21	4	0.34
(1,1841)	1:178:R:LEU:HD21	1:127:R:VAL:HG22	4	0.34
(1,1841)	1:178:R:LEU:HD21	1:127:R:VAL:HG23	4	0.34
(1,1841)	1:178:R:LEU:HD22	1:127:R:VAL:HG21	4	0.34
(1,1841)	1:178:R:LEU:HD22	1:127:R:VAL:HG22	4	0.34
(1,1841)	1:178:R:LEU:HD22	1:127:R:VAL:HG23	4	0.34
(1,1841)	1:178:R:LEU:HD23	1:127:R:VAL:HG21	4	0.34
(1,1841)	1:178:R:LEU:HD23	1:127:R:VAL:HG22	4	0.34
(1,1841)	1:178:R:LEU:HD23	1:127:R:VAL:HG23	4	0.34
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG11	4	0.34
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG12	4	0.34
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG13	4	0.34
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG11	4	0.34
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG12	4	0.34
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG13	4	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG11	4	0.34
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG12	4	0.34
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG13	4	0.34
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG11	4	0.34
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG12	4	0.34
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG13	4	0.34
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG11	4	0.34
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG12	4	0.34
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG13	4	0.34
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG11	4	0.34
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG12	4	0.34
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG13	4	0.34
(1,1626)	1:153:R:CYS:H	1:139:R:ALA:H	3	0.34
(1,1524)	1:109:R:HIS:H	1:108:R:LYS:H	2	0.34
(1,1522)	1:108:R:LYS:H	1:109:R:HIS:H	2	0.34
(1,1475)	1:82:R:ALA:H	1:83:R:ILE:HD11	5	0.34
(1,1475)	1:82:R:ALA:H	1:83:R:ILE:HD12	5	0.34
(1,1475)	1:82:R:ALA:H	1:83:R:ILE:HD13	5	0.34
(1,1425)	1:62:R:TYR:H	1:61:R:ARG:HA	5	0.34
(1,1399)	1:52:R:TRP:H	1:51:R:ALA:HA	2	0.34
(1,1288)	1:170:R:TRP:H	1:161:R:ALA:HB1	2	0.34
(1,1288)	1:170:R:TRP:H	1:161:R:ALA:HB2	2	0.34
(1,1288)	1:170:R:TRP:H	1:161:R:ALA:HB3	2	0.34
(1,1258)	1:161:R:ALA:H	1:162:R:ILE:HG13	4	0.34
(1,1133)	1:126:R:VAL:H	1:116:R:GLY:H	4	0.34
(1,1029)	1:97:R:GLY:H	1:49:R:ASP:HB2	5	0.34
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD11	5	0.34
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD12	5	0.34
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD13	5	0.34
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD21	5	0.34
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD22	5	0.34
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD23	5	0.34
(1,824)	1:37:R:GLU:H	1:35:R:ASN:HB2	4	0.34
(1,126)	1:157:R:ASN:H	1:155:R:THR:CG2	2	0.34
(2,93)	1:78:R:LEU:H	1:76:R:GLU:O	2	0.33
(2,54)	1:116:R:GLY:N	1:124:R:VAL:O	4	0.33
(1,2257)	1:180:R:PHE:HB3	1:180:R:PHE:HA	5	0.33
(1,2225)	1:162:R:ILE:HB	1:162:R:ILE:HA	2	0.33
(1,2221)	1:156:R:SER:H	1:155:R:THR:HA	2	0.33
(1,2177)	1:117:R:THR:HA	1:126:R:VAL:HG11	2	0.33
(1,2177)	1:117:R:THR:HA	1:126:R:VAL:HG12	2	0.33
(1,2177)	1:117:R:THR:HA	1:126:R:VAL:HG13	2	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2158)	1:112:R:HIS:HA	1:112:R:HIS:HB2	3	0.33
(1,2153)	1:111:R:LEU:HB2	1:111:R:LEU:HA	2	0.33
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD11	2	0.33
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD12	2	0.33
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD13	2	0.33
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD11	2	0.33
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD12	2	0.33
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD13	2	0.33
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD11	2	0.33
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD12	2	0.33
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD13	2	0.33
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD11	2	0.33
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD12	2	0.33
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD13	2	0.33
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD11	2	0.33
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD12	2	0.33
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD13	2	0.33
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD11	2	0.33
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD12	2	0.33
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD13	2	0.33
(1,2023)	1:134:R:LEU:HB2	1:134:R:LEU:HA	4	0.33
(1,2023)	1:134:R:LEU:HB3	1:134:R:LEU:HA	4	0.33
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD11	5	0.33
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD12	5	0.33
(1,1998)	1:110:R:LEU:HB3	1:110:R:LEU:HD13	5	0.33
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD11	2	0.33
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD12	2	0.33
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD13	2	0.33
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD21	2	0.33
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD22	2	0.33
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD23	2	0.33
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD11	2	0.33
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD12	2	0.33
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD13	2	0.33
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD21	2	0.33
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD22	2	0.33
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD23	2	0.33
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD11	2	0.33
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD12	2	0.33
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD13	2	0.33
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD21	2	0.33
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD22	2	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD23	2	0.33
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG11	4	0.33
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG12	4	0.33
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG13	4	0.33
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG11	1	0.33
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG12	1	0.33
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG13	1	0.33
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG11	1	0.33
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG12	1	0.33
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG13	1	0.33
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG11	2	0.33
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG12	2	0.33
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG13	2	0.33
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG11	2	0.33
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG12	2	0.33
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG13	2	0.33
(1,1858)	1:181:R:VAL:HG11	1:139:R:ALA:HB1	1	0.33
(1,1858)	1:181:R:VAL:HG11	1:139:R:ALA:HB2	1	0.33
(1,1858)	1:181:R:VAL:HG11	1:139:R:ALA:HB3	1	0.33
(1,1858)	1:181:R:VAL:HG12	1:139:R:ALA:HB1	1	0.33
(1,1858)	1:181:R:VAL:HG12	1:139:R:ALA:HB2	1	0.33
(1,1858)	1:181:R:VAL:HG12	1:139:R:ALA:HB3	1	0.33
(1,1858)	1:181:R:VAL:HG13	1:139:R:ALA:HB1	1	0.33
(1,1858)	1:181:R:VAL:HG13	1:139:R:ALA:HB2	1	0.33
(1,1858)	1:181:R:VAL:HG13	1:139:R:ALA:HB3	1	0.33
(1,1858)	1:181:R:VAL:HG11	1:139:R:ALA:HB1	5	0.33
(1,1858)	1:181:R:VAL:HG11	1:139:R:ALA:HB2	5	0.33
(1,1858)	1:181:R:VAL:HG11	1:139:R:ALA:HB3	5	0.33
(1,1858)	1:181:R:VAL:HG12	1:139:R:ALA:HB1	5	0.33
(1,1858)	1:181:R:VAL:HG12	1:139:R:ALA:HB2	5	0.33
(1,1858)	1:181:R:VAL:HG12	1:139:R:ALA:HB3	5	0.33
(1,1858)	1:181:R:VAL:HG13	1:139:R:ALA:HB1	5	0.33
(1,1858)	1:181:R:VAL:HG13	1:139:R:ALA:HB2	5	0.33
(1,1858)	1:181:R:VAL:HG13	1:139:R:ALA:HB3	5	0.33
(1,1813)	1:115:R:ILE:HD11	1:115:R:ILE:HA	2	0.33
(1,1813)	1:115:R:ILE:HD12	1:115:R:ILE:HA	2	0.33
(1,1813)	1:115:R:ILE:HD13	1:115:R:ILE:HA	2	0.33
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG21	2	0.33
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG22	2	0.33
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG23	2	0.33
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG21	2	0.33
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG22	2	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG23	2	0.33
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG21	2	0.33
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG22	2	0.33
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG23	2	0.33
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG21	2	0.33
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG22	2	0.33
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG23	2	0.33
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG21	2	0.33
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG22	2	0.33
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG23	2	0.33
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG21	2	0.33
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG22	2	0.33
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG23	2	0.33
(1,1724)	1:56:R:ILE:HD11	1:56:R:ILE:HG21	1	0.33
(1,1724)	1:56:R:ILE:HD11	1:56:R:ILE:HG22	1	0.33
(1,1724)	1:56:R:ILE:HD11	1:56:R:ILE:HG23	1	0.33
(1,1724)	1:56:R:ILE:HD12	1:56:R:ILE:HG21	1	0.33
(1,1724)	1:56:R:ILE:HD12	1:56:R:ILE:HG22	1	0.33
(1,1724)	1:56:R:ILE:HD12	1:56:R:ILE:HG23	1	0.33
(1,1724)	1:56:R:ILE:HD13	1:56:R:ILE:HG21	1	0.33
(1,1724)	1:56:R:ILE:HD13	1:56:R:ILE:HG22	1	0.33
(1,1724)	1:56:R:ILE:HD13	1:56:R:ILE:HG23	1	0.33
(1,1652)	1:163:R:ASP:H	1:166:R:ASP:H	1	0.33
(1,1652)	1:163:R:ASP:H	1:166:R:ASP:H	4	0.33
(1,1530)	1:110:R:LEU:H	1:109:R:HIS:HB2	4	0.33
(1,1440)	1:70:R:TRP:H	1:68:R:PHE:HA	4	0.33
(1,1390)	1:47:R:ASN:H	1:47:R:ASN:HB2	2	0.33
(1,1293)	1:171:R:THR:H	1:170:R:TRP:H	2	0.33
(1,1082)	1:112:R:HIS:H	1:111:R:LEU:HD11	1	0.33
(1,1082)	1:112:R:HIS:H	1:111:R:LEU:HD12	1	0.33
(1,1082)	1:112:R:HIS:H	1:111:R:LEU:HD13	1	0.33
(1,902)	1:61:R:ARG:H	1:41:R:PHE:HZ	3	0.33
(1,126)	1:157:R:ASN:H	1:155:R:THR:CG2	5	0.33
(1,42)	1:89:R:LEU:H	1:89:R:LEU:HG	2	0.33
(2,57)	1:127:R:VAL:H	1:178:R:LEU:O	3	0.32
(1,2321)	1:44:R:ARG:H	1:164:R:ASP:C	2	0.32
(1,2306)	1:60:R:PHE:C	1:65:R:GLU:H	3	0.32
(1,2234)	1:162:R:ILE:H	1:162:R:ILE:HG13	1	0.32
(1,2206)	1:153:R:CYS:HB2	1:153:R:CYS:HA	3	0.32
(1,2204)	1:139:R:ALA:HB1	1:153:R:CYS:HA	4	0.32
(1,2204)	1:139:R:ALA:HB2	1:153:R:CYS:HA	4	0.32
(1,2204)	1:139:R:ALA:HB3	1:153:R:CYS:HA	4	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2177)	1:117:R:THR:HA	1:126:R:VAL:HG11	1	0.32
(1,2177)	1:117:R:THR:HA	1:126:R:VAL:HG12	1	0.32
(1,2177)	1:117:R:THR:HA	1:126:R:VAL:HG13	1	0.32
(1,2153)	1:111:R:LEU:HB2	1:111:R:LEU:HA	1	0.32
(1,2121)	1:89:R:LEU:HB3	1:89:R:LEU:HG	3	0.32
(1,2120)	1:89:R:LEU:HA	1:89:R:LEU:HG	1	0.32
(1,2103)	1:72:R:TYR:H	1:71:R:VAL:HG11	4	0.32
(1,2103)	1:72:R:TYR:H	1:71:R:VAL:HG12	4	0.32
(1,2103)	1:72:R:TYR:H	1:71:R:VAL:HG13	4	0.32
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD11	1	0.32
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD12	1	0.32
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD13	1	0.32
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD11	1	0.32
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD12	1	0.32
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD13	1	0.32
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD11	1	0.32
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD12	1	0.32
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD13	1	0.32
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD11	1	0.32
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD12	1	0.32
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD13	1	0.32
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD11	1	0.32
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD12	1	0.32
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD13	1	0.32
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD11	1	0.32
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD12	1	0.32
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD13	1	0.32
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD11	4	0.32
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD12	4	0.32
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD13	4	0.32
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD11	4	0.32
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD12	4	0.32
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD13	4	0.32
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD11	4	0.32
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD12	4	0.32
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD13	4	0.32
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD11	4	0.32
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD12	4	0.32
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD13	4	0.32
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD11	4	0.32
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD12	4	0.32
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD13	4	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD11	4	0.32
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD12	4	0.32
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD13	4	0.32
(1,2019)	1:178:R:LEU:HD11	1:127:R:VAL:HG21	1	0.32
(1,2019)	1:178:R:LEU:HD11	1:127:R:VAL:HG22	1	0.32
(1,2019)	1:178:R:LEU:HD11	1:127:R:VAL:HG23	1	0.32
(1,2019)	1:178:R:LEU:HD12	1:127:R:VAL:HG21	1	0.32
(1,2019)	1:178:R:LEU:HD12	1:127:R:VAL:HG22	1	0.32
(1,2019)	1:178:R:LEU:HD12	1:127:R:VAL:HG23	1	0.32
(1,2019)	1:178:R:LEU:HD13	1:127:R:VAL:HG21	1	0.32
(1,2019)	1:178:R:LEU:HD13	1:127:R:VAL:HG22	1	0.32
(1,2019)	1:178:R:LEU:HD13	1:127:R:VAL:HG23	1	0.32
(1,2019)	1:178:R:LEU:HD21	1:127:R:VAL:HG21	1	0.32
(1,2019)	1:178:R:LEU:HD21	1:127:R:VAL:HG22	1	0.32
(1,2019)	1:178:R:LEU:HD21	1:127:R:VAL:HG23	1	0.32
(1,2019)	1:178:R:LEU:HD22	1:127:R:VAL:HG21	1	0.32
(1,2019)	1:178:R:LEU:HD22	1:127:R:VAL:HG22	1	0.32
(1,2019)	1:178:R:LEU:HD22	1:127:R:VAL:HG23	1	0.32
(1,2019)	1:178:R:LEU:HD23	1:127:R:VAL:HG21	1	0.32
(1,2019)	1:178:R:LEU:HD23	1:127:R:VAL:HG22	1	0.32
(1,2019)	1:178:R:LEU:HD23	1:127:R:VAL:HG23	1	0.32
(1,2004)	1:113:R:THR:HG1	1:113:R:THR:HA	4	0.32
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD11	1	0.32
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD12	1	0.32
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD13	1	0.32
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD21	1	0.32
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD22	1	0.32
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD23	1	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD11	1	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD12	1	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD13	1	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD21	1	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD22	1	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD23	1	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD11	1	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD12	1	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD13	1	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD21	1	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD22	1	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD23	1	0.32
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD11	4	0.32
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD12	4	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD13	4	0.32
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD21	4	0.32
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD22	4	0.32
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD23	4	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD11	4	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD12	4	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD13	4	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD21	4	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD22	4	0.32
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD23	4	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD11	4	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD12	4	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD13	4	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD21	4	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD22	4	0.32
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD23	4	0.32
(1,1865)	1:142:R:PHE:HB2	1:150:R:VAL:HG21	1	0.32
(1,1865)	1:142:R:PHE:HB2	1:150:R:VAL:HG22	1	0.32
(1,1865)	1:142:R:PHE:HB2	1:150:R:VAL:HG23	1	0.32
(1,1838)	1:127:R:VAL:H	1:126:R:VAL:HG21	3	0.32
(1,1838)	1:127:R:VAL:H	1:126:R:VAL:HG22	3	0.32
(1,1838)	1:127:R:VAL:H	1:126:R:VAL:HG23	3	0.32
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG11	4	0.32
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG12	4	0.32
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG13	4	0.32
(1,1813)	1:115:R:ILE:HD11	1:115:R:ILE:HA	1	0.32
(1,1813)	1:115:R:ILE:HD12	1:115:R:ILE:HA	1	0.32
(1,1813)	1:115:R:ILE:HD13	1:115:R:ILE:HA	1	0.32
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB1	4	0.32
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB2	4	0.32
(1,1756)	1:71:R:VAL:HG21	1:82:R:ALA:HB3	4	0.32
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB1	4	0.32
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB2	4	0.32
(1,1756)	1:71:R:VAL:HG22	1:82:R:ALA:HB3	4	0.32
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB1	4	0.32
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB2	4	0.32
(1,1756)	1:71:R:VAL:HG23	1:82:R:ALA:HB3	4	0.32
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG11	5	0.32
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG12	5	0.32
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG13	5	0.32
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG11	5	0.32
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG12	5	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG13	5	0.32
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG11	5	0.32
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG12	5	0.32
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG13	5	0.32
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG11	5	0.32
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG12	5	0.32
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG13	5	0.32
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG11	5	0.32
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG12	5	0.32
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG13	5	0.32
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG11	5	0.32
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG12	5	0.32
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG13	5	0.32
(1,1711)	1:83:R:ILE:HG13	1:53:R:LEU:HD11	5	0.32
(1,1711)	1:83:R:ILE:HG13	1:53:R:LEU:HD12	5	0.32
(1,1711)	1:83:R:ILE:HG13	1:53:R:LEU:HD13	5	0.32
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD11	1	0.32
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD12	1	0.32
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD13	1	0.32
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD11	1	0.32
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD12	1	0.32
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD13	1	0.32
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD11	1	0.32
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD12	1	0.32
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD13	1	0.32
(1,1652)	1:163:R:ASP:H	1:166:R:ASP:H	5	0.32
(1,1511)	1:105:R:TRP:H	1:103:R:VAL:H	1	0.32
(1,1511)	1:105:R:TRP:H	1:103:R:VAL:H	4	0.32
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD11	5	0.32
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD12	5	0.32
(1,1471)	1:82:R:ALA:H	1:53:R:LEU:HD13	5	0.32
(1,1390)	1:47:R:ASN:H	1:47:R:ASN:HB2	5	0.32
(1,1378)	1:41:R:PHE:H	1:162:R:ILE:HD11	4	0.32
(1,1378)	1:41:R:PHE:H	1:162:R:ILE:HD12	4	0.32
(1,1378)	1:41:R:PHE:H	1:162:R:ILE:HD13	4	0.32
(1,1347)	1:32:R:THR:H	1:155:R:THR:HA	2	0.32
(1,1292)	1:171:R:THR:H	1:168:R:TYR:HD1	4	0.32
(1,1292)	1:171:R:THR:H	1:168:R:TYR:HD2	4	0.32
(1,1048)	1:105:R:TRP:H	1:101:R:ALA:HA	3	0.32
(1,824)	1:37:R:GLU:H	1:35:R:ASN:HB2	5	0.32
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD11	1	0.32
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD12	1	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD13	1	0.32
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD21	1	0.32
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD22	1	0.32
(1,810)	1:35:R:ASN:H	1:33:R:LEU:HD23	1	0.32
(1,700)	1:161:R:ALA:H	1:167:R:PHE:HA	3	0.32
(1,603)	1:138:R:HIS:H	1:139:R:ALA:HA	3	0.32
(1,180)	1:33:R:LEU:H	1:36:R:GLY:HA3	4	0.32
(1,180)	1:33:R:LEU:H	1:36:R:GLY:HA3	5	0.32
(1,126)	1:157:R:ASN:H	1:155:R:THR:CG2	3	0.32
(1,105)	1:137:R:PHE:H	1:138:R:HIS:H	1	0.32
(1,105)	1:137:R:PHE:H	1:138:R:HIS:H	4	0.32
(1,2298)	1:160:R:TYR:H	1:153:R:CYS:C	5	0.31
(1,2229)	1:167:R:PHE:HA	1:162:R:ILE:HA	5	0.31
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD11	3	0.31
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD12	3	0.31
(1,2049)	1:31:R:LEU:HD11	1:162:R:ILE:HD13	3	0.31
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD11	3	0.31
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD12	3	0.31
(1,2049)	1:31:R:LEU:HD12	1:162:R:ILE:HD13	3	0.31
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD11	3	0.31
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD12	3	0.31
(1,2049)	1:31:R:LEU:HD13	1:162:R:ILE:HD13	3	0.31
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD11	3	0.31
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD12	3	0.31
(1,2049)	1:31:R:LEU:HD21	1:162:R:ILE:HD13	3	0.31
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD11	3	0.31
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD12	3	0.31
(1,2049)	1:31:R:LEU:HD22	1:162:R:ILE:HD13	3	0.31
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD11	3	0.31
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD12	3	0.31
(1,2049)	1:31:R:LEU:HD23	1:162:R:ILE:HD13	3	0.31
(1,2023)	1:134:R:LEU:HB2	1:134:R:LEU:HA	1	0.31
(1,2023)	1:134:R:LEU:HB3	1:134:R:LEU:HA	1	0.31
(1,2023)	1:134:R:LEU:HB2	1:134:R:LEU:HA	3	0.31
(1,2023)	1:134:R:LEU:HB3	1:134:R:LEU:HA	3	0.31
(1,2023)	1:134:R:LEU:HB2	1:134:R:LEU:HA	5	0.31
(1,2023)	1:134:R:LEU:HB3	1:134:R:LEU:HA	5	0.31
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD11	3	0.31
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD12	3	0.31
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD13	3	0.31
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD21	3	0.31
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD22	3	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1934)	1:162:R:ILE:HD11	1:31:R:LEU:HD23	3	0.31
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD11	3	0.31
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD12	3	0.31
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD13	3	0.31
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD21	3	0.31
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD22	3	0.31
(1,1934)	1:162:R:ILE:HD12	1:31:R:LEU:HD23	3	0.31
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD11	3	0.31
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD12	3	0.31
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD13	3	0.31
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD21	3	0.31
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD22	3	0.31
(1,1934)	1:162:R:ILE:HD13	1:31:R:LEU:HD23	3	0.31
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG11	1	0.31
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG12	1	0.31
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG13	1	0.31
(1,1865)	1:142:R:PHE:HB2	1:150:R:VAL:HG21	4	0.31
(1,1865)	1:142:R:PHE:HB2	1:150:R:VAL:HG22	4	0.31
(1,1865)	1:142:R:PHE:HB2	1:150:R:VAL:HG23	4	0.31
(1,1805)	1:110:R:LEU:HA	1:110:R:LEU:HG	3	0.31
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG21	4	0.31
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG22	4	0.31
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG23	4	0.31
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG21	4	0.31
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG22	4	0.31
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG23	4	0.31
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG21	4	0.31
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG22	4	0.31
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG23	4	0.31
(1,1777)	1:83:R:ILE:HD11	1:95:R:HIS:HA	2	0.31
(1,1777)	1:83:R:ILE:HD12	1:95:R:HIS:HA	2	0.31
(1,1777)	1:83:R:ILE:HD13	1:95:R:HIS:HA	2	0.31
(1,1667)	1:170:R:TRP:H	1:152:R:ALA:HB1	1	0.31
(1,1667)	1:170:R:TRP:H	1:152:R:ALA:HB2	1	0.31
(1,1667)	1:170:R:TRP:H	1:152:R:ALA:HB3	1	0.31
(1,1511)	1:105:R:TRP:H	1:103:R:VAL:H	3	0.31
(1,1429)	1:65:R:GLU:H	1:63:R:VAL:HB	5	0.31
(1,1425)	1:62:R:TYR:H	1:61:R:ARG:HA	2	0.31
(1,1410)	1:59:R:LEU:H	1:57:R:LEU:H	1	0.31
(1,1390)	1:47:R:ASN:H	1:47:R:ASN:HB2	3	0.31
(1,1177)	1:141:R:ILE:H	1:180:R:PHE:HB2	1	0.31
(1,1132)	1:125:R:CYS:H	1:181:R:VAL:HB	4	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1124)	1:124:R:VAL:H	1:114:R:GLY:H	5	0.31
(1,535)	1:117:R:THR:H	1:122:R:SER:H	2	0.31
(1,42)	1:89:R:LEU:H	1:89:R:LEU:HG	4	0.31
(1,42)	1:89:R:LEU:H	1:89:R:LEU:HG	5	0.31
(1,2266)	1:54:R:ASN:C	1:58:R:GLN:H	4	0.3
(1,2257)	1:180:R:PHE:HB3	1:180:R:PHE:HA	4	0.3
(1,2153)	1:111:R:LEU:HB2	1:111:R:LEU:HA	5	0.3
(1,2122)	1:89:R:LEU:HB2	1:89:R:LEU:HG	1	0.3
(1,2122)	1:89:R:LEU:HB2	1:89:R:LEU:HG	4	0.3
(1,1857)	1:181:R:VAL:HB	1:139:R:ALA:HB1	1	0.3
(1,1857)	1:181:R:VAL:HB	1:139:R:ALA:HB2	1	0.3
(1,1857)	1:181:R:VAL:HB	1:139:R:ALA:HB3	1	0.3
(1,1857)	1:181:R:VAL:HB	1:139:R:ALA:HB1	4	0.3
(1,1857)	1:181:R:VAL:HB	1:139:R:ALA:HB2	4	0.3
(1,1857)	1:181:R:VAL:HB	1:139:R:ALA:HB3	4	0.3
(1,1817)	1:124:R:VAL:HG21	1:115:R:ILE:HG21	3	0.3
(1,1817)	1:124:R:VAL:HG21	1:115:R:ILE:HG22	3	0.3
(1,1817)	1:124:R:VAL:HG21	1:115:R:ILE:HG23	3	0.3
(1,1817)	1:124:R:VAL:HG22	1:115:R:ILE:HG21	3	0.3
(1,1817)	1:124:R:VAL:HG22	1:115:R:ILE:HG22	3	0.3
(1,1817)	1:124:R:VAL:HG22	1:115:R:ILE:HG23	3	0.3
(1,1817)	1:124:R:VAL:HG23	1:115:R:ILE:HG21	3	0.3
(1,1817)	1:124:R:VAL:HG23	1:115:R:ILE:HG22	3	0.3
(1,1817)	1:124:R:VAL:HG23	1:115:R:ILE:HG23	3	0.3
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG21	1	0.3
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG22	1	0.3
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG23	1	0.3
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG21	1	0.3
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG22	1	0.3
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG23	1	0.3
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG21	1	0.3
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG22	1	0.3
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG23	1	0.3
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG21	1	0.3
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG22	1	0.3
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG23	1	0.3
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG21	1	0.3
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG22	1	0.3
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG23	1	0.3
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG21	1	0.3
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG22	1	0.3
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG23	1	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD11	3	0.3
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD12	3	0.3
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD13	3	0.3
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD11	3	0.3
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD12	3	0.3
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD13	3	0.3
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD11	3	0.3
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD12	3	0.3
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD13	3	0.3
(1,1654)	1:164:R:ASP:H	1:163:R:ASP:HB3	3	0.3
(1,1600)	1:139:R:ALA:H	1:180:R:PHE:HB2	5	0.3
(1,1475)	1:82:R:ALA:H	1:83:R:ILE:HD11	1	0.3
(1,1475)	1:82:R:ALA:H	1:83:R:ILE:HD12	1	0.3
(1,1475)	1:82:R:ALA:H	1:83:R:ILE:HD13	1	0.3
(1,1448)	1:71:R:VAL:H	1:78:R:LEU:HB2	2	0.3
(1,1448)	1:71:R:VAL:H	1:78:R:LEU:HB3	2	0.3
(1,1425)	1:62:R:TYR:H	1:61:R:ARG:HA	1	0.3
(1,1181)	1:142:R:PHE:H	1:150:R:VAL:HG21	4	0.3
(1,1181)	1:142:R:PHE:H	1:150:R:VAL:HG22	4	0.3
(1,1181)	1:142:R:PHE:H	1:150:R:VAL:HG23	4	0.3
(1,1088)	1:113:R:THR:H	1:111:R:LEU:H	1	0.3
(1,1081)	1:111:R:LEU:H	1:113:R:THR:H	1	0.3
(1,916)	1:65:R:GLU:H	1:63:R:VAL:H	1	0.3
(1,915)	1:65:R:GLU:H	1:63:R:VAL:HB	3	0.3
(2,117)	1:44:R:ARG:H	1:164:R:ASP:O	2	0.29
(2,85)	1:52:R:TRP:O	1:56:R:ILE:H	4	0.29
(1,2312)	1:103:R:VAL:H	1:99:R:PRO:C	4	0.29
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG21	3	0.29
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG22	3	0.29
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG23	3	0.29
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG21	3	0.29
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG22	3	0.29
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG23	3	0.29
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG21	3	0.29
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG22	3	0.29
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG23	3	0.29
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG21	3	0.29
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG22	3	0.29
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG23	3	0.29
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG21	3	0.29
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG22	3	0.29
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG23	3	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG21	3	0.29
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG22	3	0.29
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG23	3	0.29
(1,2246)	1:170:R:TRP:H	1:170:R:TRP:HB2	1	0.29
(1,2071)	1:31:R:LEU:H	1:31:R:LEU:HG	3	0.29
(1,2050)	1:41:R:PHE:HE1	1:162:R:ILE:HD11	2	0.29
(1,2050)	1:41:R:PHE:HE1	1:162:R:ILE:HD12	2	0.29
(1,2050)	1:41:R:PHE:HE1	1:162:R:ILE:HD13	2	0.29
(1,2050)	1:41:R:PHE:HE2	1:162:R:ILE:HD11	2	0.29
(1,2050)	1:41:R:PHE:HE2	1:162:R:ILE:HD12	2	0.29
(1,2050)	1:41:R:PHE:HE2	1:162:R:ILE:HD13	2	0.29
(1,1865)	1:142:R:PHE:HB2	1:150:R:VAL:HG21	2	0.29
(1,1865)	1:142:R:PHE:HB2	1:150:R:VAL:HG22	2	0.29
(1,1865)	1:142:R:PHE:HB2	1:150:R:VAL:HG23	2	0.29
(1,1835)	1:117:R:THR:HA	1:126:R:VAL:HG21	2	0.29
(1,1835)	1:117:R:THR:HA	1:126:R:VAL:HG22	2	0.29
(1,1835)	1:117:R:THR:HA	1:126:R:VAL:HG23	2	0.29
(1,1819)	1:126:R:VAL:HG21	1:117:R:THR:HA	2	0.29
(1,1819)	1:126:R:VAL:HG22	1:117:R:THR:HA	2	0.29
(1,1819)	1:126:R:VAL:HG23	1:117:R:THR:HA	2	0.29
(1,1739)	1:69:R:ASP:H	1:68:R:PHE:HA	3	0.29
(1,1675)	1:175:R:SER:H	1:142:R:PHE:HE1	3	0.29
(1,1675)	1:175:R:SER:H	1:142:R:PHE:HE2	3	0.29
(1,1639)	1:159:R:TRP:H	1:153:R:CYS:H	2	0.29
(1,1436)	1:69:R:ASP:H	1:68:R:PHE:HB3	1	0.29
(1,1425)	1:62:R:TYR:H	1:61:R:ARG:HA	3	0.29
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD11	3	0.29
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD12	3	0.29
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD13	3	0.29
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD21	3	0.29
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD22	3	0.29
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD23	3	0.29
(1,1390)	1:47:R:ASN:H	1:47:R:ASN:HB2	4	0.29
(1,1292)	1:171:R:THR:H	1:168:R:TYR:HD1	1	0.29
(1,1292)	1:171:R:THR:H	1:168:R:TYR:HD2	1	0.29
(1,126)	1:157:R:ASN:H	1:155:R:THR:CG2	4	0.29
(1,42)	1:89:R:LEU:H	1:89:R:LEU:HG	1	0.29
(2,98)	1:104:R:ILE:N	1:100:R:PRO:O	3	0.28
(2,61)	1:178:R:LEU:H	1:141:R:ILE:O	3	0.28
(2,36)	1:85:R:GLN:O	1:89:R:LEU:N	3	0.28
(2,4)	1:57:R:LEU:N	1:53:R:LEU:O	2	0.28
(1,2217)	1:159:R:TRP:HE1	1:154:R:VAL:HG21	1	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2217)	1:159:R:TRP:HE1	1:154:R:VAL:HG22	1	0.28
(1,2217)	1:159:R:TRP:HE1	1:154:R:VAL:HG23	1	0.28
(1,2195)	1:150:R:VAL:H	1:150:R:VAL:HG11	5	0.28
(1,2195)	1:150:R:VAL:H	1:150:R:VAL:HG12	5	0.28
(1,2195)	1:150:R:VAL:H	1:150:R:VAL:HG13	5	0.28
(1,2142)	1:103:R:VAL:H	1:103:R:VAL:HB	3	0.28
(1,2133)	1:94:R:LEU:HB2	1:94:R:LEU:HG	3	0.28
(1,2122)	1:89:R:LEU:HB2	1:89:R:LEU:HG	2	0.28
(1,2122)	1:89:R:LEU:HB2	1:89:R:LEU:HG	5	0.28
(1,2112)	1:53:R:LEU:HD11	1:83:R:ILE:HG13	4	0.28
(1,2112)	1:53:R:LEU:HD12	1:83:R:ILE:HG13	4	0.28
(1,2112)	1:53:R:LEU:HD13	1:83:R:ILE:HG13	4	0.28
(1,2071)	1:31:R:LEU:H	1:31:R:LEU:HG	5	0.28
(1,2023)	1:134:R:LEU:HB2	1:134:R:LEU:HA	2	0.28
(1,2023)	1:134:R:LEU:HB3	1:134:R:LEU:HA	2	0.28
(1,1949)	1:56:R:ILE:HB	1:56:R:ILE:HD11	3	0.28
(1,1949)	1:56:R:ILE:HB	1:56:R:ILE:HD12	3	0.28
(1,1949)	1:56:R:ILE:HB	1:56:R:ILE:HD13	3	0.28
(1,1817)	1:124:R:VAL:HG21	1:115:R:ILE:HG21	2	0.28
(1,1817)	1:124:R:VAL:HG21	1:115:R:ILE:HG22	2	0.28
(1,1817)	1:124:R:VAL:HG21	1:115:R:ILE:HG23	2	0.28
(1,1817)	1:124:R:VAL:HG22	1:115:R:ILE:HG21	2	0.28
(1,1817)	1:124:R:VAL:HG22	1:115:R:ILE:HG22	2	0.28
(1,1817)	1:124:R:VAL:HG22	1:115:R:ILE:HG23	2	0.28
(1,1817)	1:124:R:VAL:HG23	1:115:R:ILE:HG21	2	0.28
(1,1817)	1:124:R:VAL:HG23	1:115:R:ILE:HG22	2	0.28
(1,1817)	1:124:R:VAL:HG23	1:115:R:ILE:HG23	2	0.28
(1,1661)	1:165:R:GLU:H	1:164:R:ASP:H	5	0.28
(1,1657)	1:164:R:ASP:H	1:165:R:GLU:H	5	0.28
(1,1654)	1:164:R:ASP:H	1:163:R:ASP:HB3	5	0.28
(1,1587)	1:129:R:GLY:H	1:128:R:ASP:HB3	1	0.28
(1,1468)	1:81:R:GLU:H	1:79:R:THR:HB	2	0.28
(1,1417)	1:61:R:ARG:H	1:41:R:PHE:HD1	2	0.28
(1,1417)	1:61:R:ARG:H	1:41:R:PHE:HD2	2	0.28
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD11	4	0.28
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD12	4	0.28
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD13	4	0.28
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD21	4	0.28
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD22	4	0.28
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD23	4	0.28
(1,982)	1:83:R:ILE:H	1:53:R:LEU:HD11	3	0.28
(1,982)	1:83:R:ILE:H	1:53:R:LEU:HD12	3	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,982)	1:83:R:ILE:H	1:53:R:LEU:HD13	3	0.28
(1,829)	1:39:R:LYS:H	1:37:R:GLU:HA	1	0.28
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG21	4	0.28
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG22	4	0.28
(1,768)	1:181:R:VAL:H	1:177:R:VAL:HG23	4	0.28
(1,105)	1:137:R:PHE:H	1:138:R:HIS:H	5	0.28
(2,98)	1:104:R:ILE:N	1:100:R:PRO:O	5	0.27
(1,2288)	1:33:R:LEU:H	1:37:R:GLU:C	4	0.27
(1,2110)	1:73:R:SER:H	1:73:R:SER:HB2	4	0.27
(1,1995)	1:103:R:VAL:HA	1:103:R:VAL:HG21	5	0.27
(1,1995)	1:103:R:VAL:HA	1:103:R:VAL:HG22	5	0.27
(1,1995)	1:103:R:VAL:HA	1:103:R:VAL:HG23	5	0.27
(1,1990)	1:103:R:VAL:HG21	1:103:R:VAL:HA	5	0.27
(1,1990)	1:103:R:VAL:HG22	1:103:R:VAL:HA	5	0.27
(1,1990)	1:103:R:VAL:HG23	1:103:R:VAL:HA	5	0.27
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB1	2	0.27
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB2	2	0.27
(1,1890)	1:152:R:ALA:HB1	1:161:R:ALA:HB3	2	0.27
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB1	2	0.27
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB2	2	0.27
(1,1890)	1:152:R:ALA:HB2	1:161:R:ALA:HB3	2	0.27
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB1	2	0.27
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB2	2	0.27
(1,1890)	1:152:R:ALA:HB3	1:161:R:ALA:HB3	2	0.27
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG11	4	0.27
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG12	4	0.27
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG13	4	0.27
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG11	4	0.27
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG12	4	0.27
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG13	4	0.27
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB1	2	0.27
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB2	2	0.27
(1,1872)	1:161:R:ALA:HB1	1:152:R:ALA:HB3	2	0.27
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB1	2	0.27
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB2	2	0.27
(1,1872)	1:161:R:ALA:HB2	1:152:R:ALA:HB3	2	0.27
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB1	2	0.27
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB2	2	0.27
(1,1872)	1:161:R:ALA:HB3	1:152:R:ALA:HB3	2	0.27
(1,1843)	1:128:R:ASP:H	1:127:R:VAL:HG21	1	0.27
(1,1843)	1:128:R:ASP:H	1:127:R:VAL:HG22	1	0.27
(1,1843)	1:128:R:ASP:H	1:127:R:VAL:HG23	1	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1835)	1:117:R:THR:HA	1:126:R:VAL:HG21	3	0.27
(1,1835)	1:117:R:THR:HA	1:126:R:VAL:HG22	3	0.27
(1,1835)	1:117:R:THR:HA	1:126:R:VAL:HG23	3	0.27
(1,1819)	1:126:R:VAL:HG21	1:117:R:THR:HA	3	0.27
(1,1819)	1:126:R:VAL:HG22	1:117:R:THR:HA	3	0.27
(1,1819)	1:126:R:VAL:HG23	1:117:R:THR:HA	3	0.27
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG21	5	0.27
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG22	5	0.27
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG23	5	0.27
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG21	5	0.27
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG22	5	0.27
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG23	5	0.27
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG21	5	0.27
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG22	5	0.27
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG23	5	0.27
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG21	5	0.27
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG22	5	0.27
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG23	5	0.27
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG21	5	0.27
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG22	5	0.27
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG23	5	0.27
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG21	5	0.27
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG22	5	0.27
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG23	5	0.27
(1,1729)	1:59:R:LEU:HA	1:59:R:LEU:HD11	4	0.27
(1,1729)	1:59:R:LEU:HA	1:59:R:LEU:HD12	4	0.27
(1,1729)	1:59:R:LEU:HA	1:59:R:LEU:HD13	4	0.27
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB1	1	0.27
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB2	1	0.27
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB3	1	0.27
(1,1671)	1:171:R:THR:H	1:168:R:TYR:HD1	5	0.27
(1,1671)	1:171:R:THR:H	1:168:R:TYR:HD2	5	0.27
(1,1468)	1:81:R:GLU:H	1:79:R:THR:HB	3	0.27
(1,1440)	1:70:R:TRP:H	1:68:R:PHE:HA	2	0.27
(1,1383)	1:43:R:SER:H	1:43:R:SER:HB3	2	0.27
(1,1363)	1:35:R:ASN:H	1:155:R:THR:HA	2	0.27
(1,1177)	1:141:R:ILE:H	1:180:R:PHE:HB2	2	0.27
(1,1141)	1:127:R:VAL:H	1:128:R:ASP:H	3	0.27
(1,1134)	1:126:R:VAL:H	1:117:R:THR:H	4	0.27
(1,1113)	1:117:R:THR:H	1:126:R:VAL:H	4	0.27
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD11	1	0.27
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD12	1	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD13	1	0.27
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD21	1	0.27
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD22	1	0.27
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD23	1	0.27
(2,99)	1:103:R:VAL:H	1:99:R:PRO:O	2	0.26
(2,5)	1:54:R:ASN:O	1:58:R:GLN:H	2	0.26
(1,2312)	1:103:R:VAL:H	1:99:R:PRO:C	1	0.26
(1,2298)	1:160:R:TYR:H	1:153:R:CYS:C	1	0.26
(1,2293)	1:178:R:LEU:H	1:141:R:ILE:C	3	0.26
(1,2248)	1:171:R:THR:HB	1:171:R:THR:HA	4	0.26
(1,2109)	1:73:R:SER:H	1:73:R:SER:HB3	1	0.26
(1,2019)	1:178:R:LEU:HD11	1:127:R:VAL:HG21	2	0.26
(1,2019)	1:178:R:LEU:HD11	1:127:R:VAL:HG22	2	0.26
(1,2019)	1:178:R:LEU:HD11	1:127:R:VAL:HG23	2	0.26
(1,2019)	1:178:R:LEU:HD12	1:127:R:VAL:HG21	2	0.26
(1,2019)	1:178:R:LEU:HD12	1:127:R:VAL:HG22	2	0.26
(1,2019)	1:178:R:LEU:HD12	1:127:R:VAL:HG23	2	0.26
(1,2019)	1:178:R:LEU:HD13	1:127:R:VAL:HG21	2	0.26
(1,2019)	1:178:R:LEU:HD13	1:127:R:VAL:HG22	2	0.26
(1,2019)	1:178:R:LEU:HD13	1:127:R:VAL:HG23	2	0.26
(1,2019)	1:178:R:LEU:HD21	1:127:R:VAL:HG21	2	0.26
(1,2019)	1:178:R:LEU:HD21	1:127:R:VAL:HG22	2	0.26
(1,2019)	1:178:R:LEU:HD21	1:127:R:VAL:HG23	2	0.26
(1,2019)	1:178:R:LEU:HD22	1:127:R:VAL:HG21	2	0.26
(1,2019)	1:178:R:LEU:HD22	1:127:R:VAL:HG22	2	0.26
(1,2019)	1:178:R:LEU:HD22	1:127:R:VAL:HG23	2	0.26
(1,2019)	1:178:R:LEU:HD23	1:127:R:VAL:HG21	2	0.26
(1,2019)	1:178:R:LEU:HD23	1:127:R:VAL:HG22	2	0.26
(1,2019)	1:178:R:LEU:HD23	1:127:R:VAL:HG23	2	0.26
(1,1982)	1:90:R:THR:HB	1:90:R:THR:HG21	3	0.26
(1,1982)	1:90:R:THR:HB	1:90:R:THR:HG21	5	0.26
(1,1976)	1:83:R:ILE:HG21	1:83:R:ILE:HG13	2	0.26
(1,1976)	1:83:R:ILE:HG22	1:83:R:ILE:HG13	2	0.26
(1,1976)	1:83:R:ILE:HG23	1:83:R:ILE:HG13	2	0.26
(1,1962)	1:124:R:VAL:HG11	1:63:R:VAL:HG21	2	0.26
(1,1962)	1:124:R:VAL:HG11	1:63:R:VAL:HG22	2	0.26
(1,1962)	1:124:R:VAL:HG11	1:63:R:VAL:HG23	2	0.26
(1,1962)	1:124:R:VAL:HG12	1:63:R:VAL:HG21	2	0.26
(1,1962)	1:124:R:VAL:HG12	1:63:R:VAL:HG22	2	0.26
(1,1962)	1:124:R:VAL:HG12	1:63:R:VAL:HG23	2	0.26
(1,1962)	1:124:R:VAL:HG13	1:63:R:VAL:HG21	2	0.26
(1,1962)	1:124:R:VAL:HG13	1:63:R:VAL:HG22	2	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1962)	1:124:R:VAL:HG13	1:63:R:VAL:HG23	2	0.26
(1,1955)	1:56:R:ILE:HG12	1:56:R:ILE:HG21	3	0.26
(1,1955)	1:56:R:ILE:HG12	1:56:R:ILE:HG22	3	0.26
(1,1955)	1:56:R:ILE:HG12	1:56:R:ILE:HG23	3	0.26
(1,1948)	1:57:R:LEU:HD11	1:53:R:LEU:HD21	4	0.26
(1,1948)	1:57:R:LEU:HD11	1:53:R:LEU:HD22	4	0.26
(1,1948)	1:57:R:LEU:HD11	1:53:R:LEU:HD23	4	0.26
(1,1948)	1:57:R:LEU:HD12	1:53:R:LEU:HD21	4	0.26
(1,1948)	1:57:R:LEU:HD12	1:53:R:LEU:HD22	4	0.26
(1,1948)	1:57:R:LEU:HD12	1:53:R:LEU:HD23	4	0.26
(1,1948)	1:57:R:LEU:HD13	1:53:R:LEU:HD21	4	0.26
(1,1948)	1:57:R:LEU:HD13	1:53:R:LEU:HD22	4	0.26
(1,1948)	1:57:R:LEU:HD13	1:53:R:LEU:HD23	4	0.26
(1,1948)	1:57:R:LEU:HD21	1:53:R:LEU:HD21	4	0.26
(1,1948)	1:57:R:LEU:HD21	1:53:R:LEU:HD22	4	0.26
(1,1948)	1:57:R:LEU:HD21	1:53:R:LEU:HD23	4	0.26
(1,1948)	1:57:R:LEU:HD22	1:53:R:LEU:HD21	4	0.26
(1,1948)	1:57:R:LEU:HD22	1:53:R:LEU:HD22	4	0.26
(1,1948)	1:57:R:LEU:HD22	1:53:R:LEU:HD23	4	0.26
(1,1948)	1:57:R:LEU:HD23	1:53:R:LEU:HD21	4	0.26
(1,1948)	1:57:R:LEU:HD23	1:53:R:LEU:HD22	4	0.26
(1,1948)	1:57:R:LEU:HD23	1:53:R:LEU:HD23	4	0.26
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD11	5	0.26
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD12	5	0.26
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD13	5	0.26
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD21	5	0.26
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD22	5	0.26
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD23	5	0.26
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD11	5	0.26
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD12	5	0.26
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD13	5	0.26
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD21	5	0.26
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD22	5	0.26
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD23	5	0.26
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG11	3	0.26
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG12	3	0.26
(1,1924)	1:177:R:VAL:H	1:177:R:VAL:HG13	3	0.26
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG21	4	0.26
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG22	4	0.26
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG23	4	0.26
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG21	4	0.26
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG22	4	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG23	4	0.26
(1,1835)	1:117:R:THR:HA	1:126:R:VAL:HG21	1	0.26
(1,1835)	1:117:R:THR:HA	1:126:R:VAL:HG22	1	0.26
(1,1835)	1:117:R:THR:HA	1:126:R:VAL:HG23	1	0.26
(1,1819)	1:126:R:VAL:HG21	1:117:R:THR:HA	1	0.26
(1,1819)	1:126:R:VAL:HG22	1:117:R:THR:HA	1	0.26
(1,1819)	1:126:R:VAL:HG23	1:117:R:THR:HA	1	0.26
(1,1817)	1:124:R:VAL:HG21	1:115:R:ILE:HG21	4	0.26
(1,1817)	1:124:R:VAL:HG21	1:115:R:ILE:HG22	4	0.26
(1,1817)	1:124:R:VAL:HG21	1:115:R:ILE:HG23	4	0.26
(1,1817)	1:124:R:VAL:HG22	1:115:R:ILE:HG21	4	0.26
(1,1817)	1:124:R:VAL:HG22	1:115:R:ILE:HG22	4	0.26
(1,1817)	1:124:R:VAL:HG22	1:115:R:ILE:HG23	4	0.26
(1,1817)	1:124:R:VAL:HG23	1:115:R:ILE:HG21	4	0.26
(1,1817)	1:124:R:VAL:HG23	1:115:R:ILE:HG22	4	0.26
(1,1817)	1:124:R:VAL:HG23	1:115:R:ILE:HG23	4	0.26
(1,1777)	1:83:R:ILE:HD11	1:95:R:HIS:HA	1	0.26
(1,1777)	1:83:R:ILE:HD12	1:95:R:HIS:HA	1	0.26
(1,1777)	1:83:R:ILE:HD13	1:95:R:HIS:HA	1	0.26
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG11	1	0.26
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG12	1	0.26
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG13	1	0.26
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG11	1	0.26
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG12	1	0.26
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG13	1	0.26
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG11	1	0.26
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG12	1	0.26
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG13	1	0.26
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG11	1	0.26
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG12	1	0.26
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG13	1	0.26
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG11	1	0.26
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG12	1	0.26
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG13	1	0.26
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG11	1	0.26
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG12	1	0.26
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG13	1	0.26
(1,1523)	1:109:R:HIS:H	1:108:R:LYS:HA	1	0.26
(1,1523)	1:109:R:HIS:H	1:108:R:LYS:HA	3	0.26
(1,1390)	1:47:R:ASN:H	1:47:R:ASN:HB2	1	0.26
(1,1383)	1:43:R:SER:H	1:43:R:SER:HB3	1	0.26
(1,1181)	1:142:R:PHE:H	1:150:R:VAL:HG21	1	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1181)	1:142:R:PHE:H	1:150:R:VAL:HG22	1	0.26
(1,1181)	1:142:R:PHE:H	1:150:R:VAL:HG23	1	0.26
(1,970)	1:80:R:LEU:H	1:83:R:ILE:HG13	1	0.26
(1,970)	1:80:R:LEU:H	1:83:R:ILE:HG13	2	0.26
(1,961)	1:78:R:LEU:H	1:79:R:THR:HA	2	0.26
(1,510)	1:113:R:THR:H	1:111:R:LEU:HD21	4	0.26
(1,510)	1:113:R:THR:H	1:111:R:LEU:HD22	4	0.26
(1,510)	1:113:R:THR:H	1:111:R:LEU:HD23	4	0.26
(1,156)	1:179:R:VAL:H	1:141:R:ILE:HB	3	0.26
(1,138)	1:162:R:ILE:H	1:162:R:ILE:HG13	2	0.26
(2,105)	1:154:R:VAL:H	1:138:R:HIS:O	3	0.25
(2,85)	1:52:R:TRP:O	1:56:R:ILE:H	1	0.25
(2,58)	1:127:R:VAL:N	1:178:R:LEU:O	4	0.25
(2,53)	1:116:R:GLY:H	1:124:R:VAL:O	4	0.25
(1,2301)	1:163:R:ASP:C	1:166:R:ASP:H	4	0.25
(1,2200)	1:151:R:PHE:HB3	1:151:R:PHE:HA	3	0.25
(1,2182)	1:137:R:PHE:HD1	1:134:R:LEU:HA	2	0.25
(1,2182)	1:137:R:PHE:HD2	1:134:R:LEU:HA	2	0.25
(1,2181)	1:134:R:LEU:H	1:134:R:LEU:HA	1	0.25
(1,2137)	1:95:R:HIS:H	1:95:R:HIS:HB3	4	0.25
(1,2120)	1:89:R:LEU:HA	1:89:R:LEU:HG	3	0.25
(1,2112)	1:53:R:LEU:HD11	1:83:R:ILE:HG13	3	0.25
(1,2112)	1:53:R:LEU:HD12	1:83:R:ILE:HG13	3	0.25
(1,2112)	1:53:R:LEU:HD13	1:83:R:ILE:HG13	3	0.25
(1,2109)	1:73:R:SER:H	1:73:R:SER:HB3	2	0.25
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG11	2	0.25
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG12	2	0.25
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG13	2	0.25
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG11	5	0.25
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG12	5	0.25
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG13	5	0.25
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG21	2	0.25
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG22	2	0.25
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG23	2	0.25
(1,1913)	1:161:R:ALA:HB1	1:170:R:TRP:HB2	1	0.25
(1,1913)	1:161:R:ALA:HB2	1:170:R:TRP:HB2	1	0.25
(1,1913)	1:161:R:ALA:HB3	1:170:R:TRP:HB2	1	0.25
(1,1904)	1:162:R:ILE:HG12	1:162:R:ILE:HG13	4	0.25
(1,1904)	1:162:R:ILE:HG12	1:162:R:ILE:HG13	5	0.25
(1,1894)	1:170:R:TRP:HB2	1:161:R:ALA:HB1	1	0.25
(1,1894)	1:170:R:TRP:HB2	1:161:R:ALA:HB2	1	0.25
(1,1894)	1:170:R:TRP:HB2	1:161:R:ALA:HB3	1	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG11	5	0.25
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG12	5	0.25
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG13	5	0.25
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG11	5	0.25
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG12	5	0.25
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG13	5	0.25
(1,1761)	1:83:R:ILE:HG12	1:83:R:ILE:HG13	3	0.25
(1,1761)	1:83:R:ILE:HG12	1:83:R:ILE:HG13	4	0.25
(1,1760)	1:83:R:ILE:HG13	1:83:R:ILE:HG12	3	0.25
(1,1760)	1:83:R:ILE:HG13	1:83:R:ILE:HG12	4	0.25
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG21	3	0.25
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG22	3	0.25
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG23	3	0.25
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG21	3	0.25
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG22	3	0.25
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG23	3	0.25
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG21	3	0.25
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG22	3	0.25
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG23	3	0.25
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG21	3	0.25
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG22	3	0.25
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG23	3	0.25
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG21	3	0.25
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG22	3	0.25
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG23	3	0.25
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG21	3	0.25
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG22	3	0.25
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG23	3	0.25
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG21	4	0.25
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG22	4	0.25
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG23	4	0.25
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG21	4	0.25
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG22	4	0.25
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG23	4	0.25
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG21	4	0.25
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG22	4	0.25
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG23	4	0.25
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG21	5	0.25
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG22	5	0.25
(1,1735)	1:124:R:VAL:HG11	1:63:R:VAL:HG23	5	0.25
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG21	5	0.25
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG22	5	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1735)	1:124:R:VAL:HG12	1:63:R:VAL:HG23	5	0.25
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG21	5	0.25
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG22	5	0.25
(1,1735)	1:124:R:VAL:HG13	1:63:R:VAL:HG23	5	0.25
(1,1728)	1:57:R:LEU:HD11	1:57:R:LEU:HA	4	0.25
(1,1728)	1:57:R:LEU:HD12	1:57:R:LEU:HA	4	0.25
(1,1728)	1:57:R:LEU:HD13	1:57:R:LEU:HA	4	0.25
(1,1728)	1:57:R:LEU:HD21	1:57:R:LEU:HA	4	0.25
(1,1728)	1:57:R:LEU:HD22	1:57:R:LEU:HA	4	0.25
(1,1728)	1:57:R:LEU:HD23	1:57:R:LEU:HA	4	0.25
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD11	4	0.25
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD12	4	0.25
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD13	4	0.25
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD11	4	0.25
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD12	4	0.25
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD13	4	0.25
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD11	4	0.25
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD12	4	0.25
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD13	4	0.25
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB1	5	0.25
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB2	5	0.25
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB3	5	0.25
(1,1660)	1:165:R:GLU:H	1:46:R:ASN:H	4	0.25
(1,1639)	1:159:R:TRP:H	1:153:R:CYS:H	3	0.25
(1,1545)	1:114:R:GLY:H	1:113:R:THR:H	5	0.25
(1,1543)	1:113:R:THR:H	1:114:R:GLY:H	5	0.25
(1,1523)	1:109:R:HIS:H	1:108:R:LYS:HA	4	0.25
(1,1440)	1:70:R:TRP:H	1:68:R:PHE:HA	3	0.25
(1,1410)	1:59:R:LEU:H	1:57:R:LEU:H	3	0.25
(1,1285)	1:168:R:TYR:H	1:168:R:TYR:HD1	4	0.25
(1,1285)	1:168:R:TYR:H	1:168:R:TYR:HD2	4	0.25
(1,1128)	1:124:R:VAL:H	1:181:R:VAL:HA	2	0.25
(1,1059)	1:107:R:ILE:H	1:105:R:TRP:HB2	4	0.25
(2,97)	1:104:R:ILE:H	1:100:R:PRO:O	5	0.24
(2,91)	1:66:R:PRO:O	1:69:R:ASP:H	2	0.24
(2,71)	1:160:R:TYR:N	1:153:R:CYS:O	2	0.24
(2,55)	1:180:R:PHE:O	1:125:R:CYS:N	5	0.24
(2,36)	1:85:R:GLN:O	1:89:R:LEU:N	5	0.24
(2,11)	1:61:R:ARG:H	1:57:R:LEU:O	2	0.24
(2,2)	1:51:R:ALA:O	1:55:R:ALA:N	3	0.24
(1,2312)	1:103:R:VAL:H	1:99:R:PRO:C	5	0.24
(1,2255)	1:140:R:GLY:HA2	1:180:R:PHE:HA	4	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2255)	1:140:R:GLY:HA2	1:180:R:PHE:HA	5	0.24
(1,2248)	1:171:R:THR:HB	1:171:R:THR:HA	2	0.24
(1,2246)	1:170:R:TRP:H	1:170:R:TRP:HB2	5	0.24
(1,2169)	1:122:R:SER:HB2	1:122:R:SER:HA	3	0.24
(1,2143)	1:94:R:LEU:HD21	1:103:R:VAL:HG11	4	0.24
(1,2143)	1:94:R:LEU:HD21	1:103:R:VAL:HG12	4	0.24
(1,2143)	1:94:R:LEU:HD21	1:103:R:VAL:HG13	4	0.24
(1,2143)	1:94:R:LEU:HD22	1:103:R:VAL:HG11	4	0.24
(1,2143)	1:94:R:LEU:HD22	1:103:R:VAL:HG12	4	0.24
(1,2143)	1:94:R:LEU:HD22	1:103:R:VAL:HG13	4	0.24
(1,2143)	1:94:R:LEU:HD23	1:103:R:VAL:HG11	4	0.24
(1,2143)	1:94:R:LEU:HD23	1:103:R:VAL:HG12	4	0.24
(1,2143)	1:94:R:LEU:HD23	1:103:R:VAL:HG13	4	0.24
(1,2136)	1:95:R:HIS:H	1:95:R:HIS:HA	2	0.24
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD11	1	0.24
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD12	1	0.24
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD13	1	0.24
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD21	1	0.24
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD22	1	0.24
(1,2067)	1:31:R:LEU:HA	1:31:R:LEU:HD23	1	0.24
(1,2018)	1:127:R:VAL:H	1:127:R:VAL:HG11	1	0.24
(1,2018)	1:127:R:VAL:H	1:127:R:VAL:HG12	1	0.24
(1,2018)	1:127:R:VAL:H	1:127:R:VAL:HG13	1	0.24
(1,1939)	1:40:R:THR:HB	1:40:R:THR:HG23	3	0.24
(1,1939)	1:40:R:THR:HB	1:40:R:THR:HG23	4	0.24
(1,1939)	1:40:R:THR:HB	1:40:R:THR:HG21	5	0.24
(1,1904)	1:162:R:ILE:HG12	1:162:R:ILE:HG13	1	0.24
(1,1904)	1:162:R:ILE:HG12	1:162:R:ILE:HG13	2	0.24
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG21	4	0.24
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG22	4	0.24
(1,1749)	1:57:R:LEU:HD11	1:71:R:VAL:HG23	4	0.24
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG21	4	0.24
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG22	4	0.24
(1,1749)	1:57:R:LEU:HD12	1:71:R:VAL:HG23	4	0.24
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG21	4	0.24
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG22	4	0.24
(1,1749)	1:57:R:LEU:HD13	1:71:R:VAL:HG23	4	0.24
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG21	4	0.24
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG22	4	0.24
(1,1749)	1:57:R:LEU:HD21	1:71:R:VAL:HG23	4	0.24
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG21	4	0.24
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG22	4	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1749)	1:57:R:LEU:HD22	1:71:R:VAL:HG23	4	0.24
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG21	4	0.24
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG22	4	0.24
(1,1749)	1:57:R:LEU:HD23	1:71:R:VAL:HG23	4	0.24
(1,1711)	1:83:R:ILE:HG13	1:53:R:LEU:HD11	2	0.24
(1,1711)	1:83:R:ILE:HG13	1:53:R:LEU:HD12	2	0.24
(1,1711)	1:83:R:ILE:HG13	1:53:R:LEU:HD13	2	0.24
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD11	4	0.24
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD12	4	0.24
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD13	4	0.24
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD11	4	0.24
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD12	4	0.24
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD13	4	0.24
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD11	4	0.24
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD12	4	0.24
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD13	4	0.24
(1,1647)	1:162:R:ILE:H	1:151:R:PHE:H	2	0.24
(1,1641)	1:160:R:TYR:H	1:154:R:VAL:HG21	5	0.24
(1,1641)	1:160:R:TYR:H	1:154:R:VAL:HG22	5	0.24
(1,1641)	1:160:R:TYR:H	1:154:R:VAL:HG23	5	0.24
(1,1591)	1:137:R:PHE:H	1:181:R:VAL:H	1	0.24
(1,1544)	1:114:R:GLY:H	1:113:R:THR:HB	2	0.24
(1,1523)	1:109:R:HIS:H	1:108:R:LYS:HA	2	0.24
(1,1523)	1:109:R:HIS:H	1:108:R:LYS:HA	5	0.24
(1,1482)	1:85:R:GLN:H	1:83:R:ILE:HA	2	0.24
(1,1475)	1:82:R:ALA:H	1:83:R:ILE:HD11	2	0.24
(1,1475)	1:82:R:ALA:H	1:83:R:ILE:HD12	2	0.24
(1,1475)	1:82:R:ALA:H	1:83:R:ILE:HD13	2	0.24
(1,1460)	1:78:R:LEU:H	1:71:R:VAL:HG11	5	0.24
(1,1460)	1:78:R:LEU:H	1:71:R:VAL:HG12	5	0.24
(1,1460)	1:78:R:LEU:H	1:71:R:VAL:HG13	5	0.24
(1,1380)	1:42:R:TYR:H	1:41:R:PHE:HE1	1	0.24
(1,1380)	1:42:R:TYR:H	1:41:R:PHE:HE2	1	0.24
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD11	1	0.24
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD12	1	0.24
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD13	1	0.24
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD21	1	0.24
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD22	1	0.24
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD23	1	0.24
(1,1366)	1:36:R:GLY:H	1:34:R:TYR:HA	1	0.24
(1,1128)	1:124:R:VAL:H	1:181:R:VAL:HA	1	0.24
(1,829)	1:39:R:LYS:H	1:37:R:GLU:HA	3	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,802)	1:32:R:THR:H	1:38:R:LYS:HA	2	0.24
(2,118)	1:44:R:ARG:N	1:164:R:ASP:O	3	0.23
(2,85)	1:52:R:TRP:O	1:56:R:ILE:H	2	0.23
(2,75)	1:163:R:ASP:N	1:166:R:ASP:O	4	0.23
(1,2305)	1:52:R:TRP:C	1:56:R:ILE:H	2	0.23
(1,2301)	1:163:R:ASP:C	1:166:R:ASP:H	3	0.23
(1,2300)	1:163:R:ASP:H	1:166:R:ASP:C	4	0.23
(1,2288)	1:33:R:LEU:H	1:37:R:GLU:C	2	0.23
(1,2249)	1:171:R:THR:H	1:171:R:THR:HA	2	0.23
(1,2246)	1:170:R:TRP:H	1:170:R:TRP:HB2	4	0.23
(1,2224)	1:161:R:ALA:H	1:160:R:TYR:HA	5	0.23
(1,2119)	1:89:R:LEU:H	1:89:R:LEU:HG	3	0.23
(1,1994)	1:94:R:LEU:HD21	1:103:R:VAL:HG21	3	0.23
(1,1994)	1:94:R:LEU:HD21	1:103:R:VAL:HG22	3	0.23
(1,1994)	1:94:R:LEU:HD21	1:103:R:VAL:HG23	3	0.23
(1,1994)	1:94:R:LEU:HD22	1:103:R:VAL:HG21	3	0.23
(1,1994)	1:94:R:LEU:HD22	1:103:R:VAL:HG22	3	0.23
(1,1994)	1:94:R:LEU:HD22	1:103:R:VAL:HG23	3	0.23
(1,1994)	1:94:R:LEU:HD23	1:103:R:VAL:HG21	3	0.23
(1,1994)	1:94:R:LEU:HD23	1:103:R:VAL:HG22	3	0.23
(1,1994)	1:94:R:LEU:HD23	1:103:R:VAL:HG23	3	0.23
(1,1976)	1:83:R:ILE:HG21	1:83:R:ILE:HG13	1	0.23
(1,1976)	1:83:R:ILE:HG22	1:83:R:ILE:HG13	1	0.23
(1,1976)	1:83:R:ILE:HG23	1:83:R:ILE:HG13	1	0.23
(1,1945)	1:83:R:ILE:HD11	1:53:R:LEU:HD11	2	0.23
(1,1945)	1:83:R:ILE:HD11	1:53:R:LEU:HD12	2	0.23
(1,1945)	1:83:R:ILE:HD11	1:53:R:LEU:HD13	2	0.23
(1,1945)	1:83:R:ILE:HD12	1:53:R:LEU:HD11	2	0.23
(1,1945)	1:83:R:ILE:HD12	1:53:R:LEU:HD12	2	0.23
(1,1945)	1:83:R:ILE:HD12	1:53:R:LEU:HD13	2	0.23
(1,1945)	1:83:R:ILE:HD13	1:53:R:LEU:HD11	2	0.23
(1,1945)	1:83:R:ILE:HD13	1:53:R:LEU:HD12	2	0.23
(1,1945)	1:83:R:ILE:HD13	1:53:R:LEU:HD13	2	0.23
(1,1939)	1:40:R:THR:HB	1:40:R:THR:HG23	1	0.23
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD11	4	0.23
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD12	4	0.23
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD13	4	0.23
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD21	4	0.23
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD22	4	0.23
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD23	4	0.23
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD11	4	0.23
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD12	4	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD13	4	0.23
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD21	4	0.23
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD22	4	0.23
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD23	4	0.23
(1,1904)	1:162:R:ILE:HG12	1:162:R:ILE:HG13	3	0.23
(1,1889)	1:159:R:TRP:HB2	1:159:R:TRP:HB3	1	0.23
(1,1889)	1:159:R:TRP:HB2	1:159:R:TRP:HB3	3	0.23
(1,1889)	1:159:R:TRP:HB2	1:159:R:TRP:HB3	4	0.23
(1,1889)	1:159:R:TRP:HB2	1:159:R:TRP:HB3	5	0.23
(1,1832)	1:125:R:CYS:HB2	1:125:R:CYS:HB3	4	0.23
(1,1831)	1:125:R:CYS:HB3	1:125:R:CYS:HB2	4	0.23
(1,1794)	1:107:R:ILE:HD11	1:103:R:VAL:HG11	5	0.23
(1,1794)	1:107:R:ILE:HD11	1:103:R:VAL:HG12	5	0.23
(1,1794)	1:107:R:ILE:HD11	1:103:R:VAL:HG13	5	0.23
(1,1794)	1:107:R:ILE:HD12	1:103:R:VAL:HG11	5	0.23
(1,1794)	1:107:R:ILE:HD12	1:103:R:VAL:HG12	5	0.23
(1,1794)	1:107:R:ILE:HD12	1:103:R:VAL:HG13	5	0.23
(1,1794)	1:107:R:ILE:HD13	1:103:R:VAL:HG11	5	0.23
(1,1794)	1:107:R:ILE:HD13	1:103:R:VAL:HG12	5	0.23
(1,1794)	1:107:R:ILE:HD13	1:103:R:VAL:HG13	5	0.23
(1,1761)	1:83:R:ILE:HG12	1:83:R:ILE:HG13	1	0.23
(1,1761)	1:83:R:ILE:HG12	1:83:R:ILE:HG13	2	0.23
(1,1761)	1:83:R:ILE:HG12	1:83:R:ILE:HG13	5	0.23
(1,1760)	1:83:R:ILE:HG13	1:83:R:ILE:HG12	1	0.23
(1,1760)	1:83:R:ILE:HG13	1:83:R:ILE:HG12	2	0.23
(1,1760)	1:83:R:ILE:HG13	1:83:R:ILE:HG12	5	0.23
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD11	5	0.23
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD12	5	0.23
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD13	5	0.23
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD21	5	0.23
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD22	5	0.23
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD23	5	0.23
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD11	5	0.23
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD12	5	0.23
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD13	5	0.23
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD21	5	0.23
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD22	5	0.23
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD23	5	0.23
(1,1675)	1:175:R:SER:H	1:142:R:PHE:HE1	5	0.23
(1,1675)	1:175:R:SER:H	1:142:R:PHE:HE2	5	0.23
(1,1608)	1:143:R:LEU:H	1:150:R:VAL:HG21	2	0.23
(1,1608)	1:143:R:LEU:H	1:150:R:VAL:HG22	2	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1608)	1:143:R:LEU:H	1:150:R:VAL:HG23	2	0.23
(1,1583)	1:127:R:VAL:H	1:180:R:PHE:H	5	0.23
(1,1427)	1:63:R:VAL:H	1:181:R:VAL:HG21	1	0.23
(1,1427)	1:63:R:VAL:H	1:181:R:VAL:HG22	1	0.23
(1,1427)	1:63:R:VAL:H	1:181:R:VAL:HG23	1	0.23
(1,1410)	1:59:R:LEU:H	1:57:R:LEU:H	2	0.23
(1,1352)	1:33:R:LEU:H	1:37:R:GLU:H	3	0.23
(1,1101)	1:115:R:ILE:H	1:123:R:GLU:H	5	0.23
(1,850)	1:46:R:ASN:H	1:49:R:ASP:H	3	0.23
(1,177)	1:32:R:THR:H	1:31:R:LEU:HG	2	0.23
(1,140)	1:166:R:ASP:H	1:163:R:ASP:HB2	1	0.23
(2,91)	1:66:R:PRO:O	1:69:R:ASP:H	5	0.22
(1,2308)	1:66:R:PRO:C	1:69:R:ASP:H	1	0.22
(1,2306)	1:60:R:PHE:C	1:65:R:GLU:H	1	0.22
(1,2298)	1:160:R:TYR:H	1:153:R:CYS:C	2	0.22
(1,2281)	1:86:R:LEU:C	1:90:R:THR:H	2	0.22
(1,2243)	1:170:R:TRP:HA	1:170:R:TRP:HB3	1	0.22
(1,2138)	1:95:R:HIS:H	1:95:R:HIS:HB2	3	0.22
(1,2136)	1:95:R:HIS:H	1:95:R:HIS:HA	1	0.22
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD11	1	0.22
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD12	1	0.22
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD13	1	0.22
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD21	1	0.22
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD22	1	0.22
(1,2068)	1:31:R:LEU:H	1:31:R:LEU:HD23	1	0.22
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD11	1	0.22
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD12	1	0.22
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD13	1	0.22
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD21	1	0.22
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD22	1	0.22
(1,2066)	1:31:R:LEU:H	1:31:R:LEU:HD23	1	0.22
(1,2058)	1:142:R:PHE:HD1	1:177:R:VAL:HG11	1	0.22
(1,2058)	1:142:R:PHE:HD1	1:177:R:VAL:HG12	1	0.22
(1,2058)	1:142:R:PHE:HD1	1:177:R:VAL:HG13	1	0.22
(1,2058)	1:142:R:PHE:HD2	1:177:R:VAL:HG11	1	0.22
(1,2058)	1:142:R:PHE:HD2	1:177:R:VAL:HG12	1	0.22
(1,2058)	1:142:R:PHE:HD2	1:177:R:VAL:HG13	1	0.22
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG11	3	0.22
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG12	3	0.22
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG13	3	0.22
(1,2016)	1:127:R:VAL:H	1:126:R:VAL:HG21	1	0.22
(1,2016)	1:127:R:VAL:H	1:126:R:VAL:HG22	1	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2016)	1:127:R:VAL:H	1:126:R:VAL:HG23	1	0.22
(1,1995)	1:103:R:VAL:HA	1:103:R:VAL:HG21	4	0.22
(1,1995)	1:103:R:VAL:HA	1:103:R:VAL:HG22	4	0.22
(1,1995)	1:103:R:VAL:HA	1:103:R:VAL:HG23	4	0.22
(1,1990)	1:103:R:VAL:HG21	1:103:R:VAL:HA	4	0.22
(1,1990)	1:103:R:VAL:HG22	1:103:R:VAL:HA	4	0.22
(1,1990)	1:103:R:VAL:HG23	1:103:R:VAL:HA	4	0.22
(1,1964)	1:64:R:GLU:HA	1:64:R:GLU:HG3	1	0.22
(1,1963)	1:64:R:GLU:HB2	1:64:R:GLU:HA	2	0.22
(1,1963)	1:64:R:GLU:HB3	1:64:R:GLU:HA	2	0.22
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG21	2	0.22
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG22	2	0.22
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG23	2	0.22
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG21	2	0.22
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG22	2	0.22
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG23	2	0.22
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG21	2	0.22
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG22	2	0.22
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG23	2	0.22
(1,1945)	1:83:R:ILE:HD11	1:53:R:LEU:HD11	5	0.22
(1,1945)	1:83:R:ILE:HD11	1:53:R:LEU:HD12	5	0.22
(1,1945)	1:83:R:ILE:HD11	1:53:R:LEU:HD13	5	0.22
(1,1945)	1:83:R:ILE:HD12	1:53:R:LEU:HD11	5	0.22
(1,1945)	1:83:R:ILE:HD12	1:53:R:LEU:HD12	5	0.22
(1,1945)	1:83:R:ILE:HD12	1:53:R:LEU:HD13	5	0.22
(1,1945)	1:83:R:ILE:HD13	1:53:R:LEU:HD11	5	0.22
(1,1945)	1:83:R:ILE:HD13	1:53:R:LEU:HD12	5	0.22
(1,1945)	1:83:R:ILE:HD13	1:53:R:LEU:HD13	5	0.22
(1,1889)	1:159:R:TRP:HB2	1:159:R:TRP:HB3	2	0.22
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG11	3	0.22
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG12	3	0.22
(1,1880)	1:34:R:TYR:HB2	1:154:R:VAL:HG13	3	0.22
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG11	3	0.22
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG12	3	0.22
(1,1880)	1:34:R:TYR:HB3	1:154:R:VAL:HG13	3	0.22
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG11	5	0.22
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG12	5	0.22
(1,1834)	1:127:R:VAL:H	1:126:R:VAL:HG13	5	0.22
(1,1808)	1:111:R:LEU:HA	1:111:R:LEU:HD21	5	0.22
(1,1808)	1:111:R:LEU:HA	1:111:R:LEU:HD22	5	0.22
(1,1808)	1:111:R:LEU:HA	1:111:R:LEU:HD23	5	0.22
(1,1807)	1:111:R:LEU:HD21	1:111:R:LEU:HA	5	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1807)	1:111:R:LEU:HD22	1:111:R:LEU:HA	5	0.22
(1,1807)	1:111:R:LEU:HD23	1:111:R:LEU:HA	5	0.22
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG21	1	0.22
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG22	1	0.22
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG23	1	0.22
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG21	1	0.22
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG22	1	0.22
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG23	1	0.22
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG21	1	0.22
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG22	1	0.22
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG23	1	0.22
(1,1729)	1:59:R:LEU:HA	1:59:R:LEU:HD11	5	0.22
(1,1729)	1:59:R:LEU:HA	1:59:R:LEU:HD12	5	0.22
(1,1729)	1:59:R:LEU:HA	1:59:R:LEU:HD13	5	0.22
(1,1728)	1:57:R:LEU:HD11	1:57:R:LEU:HA	5	0.22
(1,1728)	1:57:R:LEU:HD12	1:57:R:LEU:HA	5	0.22
(1,1728)	1:57:R:LEU:HD13	1:57:R:LEU:HA	5	0.22
(1,1728)	1:57:R:LEU:HD21	1:57:R:LEU:HA	5	0.22
(1,1728)	1:57:R:LEU:HD22	1:57:R:LEU:HA	5	0.22
(1,1728)	1:57:R:LEU:HD23	1:57:R:LEU:HA	5	0.22
(1,1727)	1:56:R:ILE:H	1:56:R:ILE:HG21	1	0.22
(1,1727)	1:56:R:ILE:H	1:56:R:ILE:HG22	1	0.22
(1,1727)	1:56:R:ILE:H	1:56:R:ILE:HG23	1	0.22
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD11	2	0.22
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD12	2	0.22
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD13	2	0.22
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD11	2	0.22
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD12	2	0.22
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD13	2	0.22
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD11	2	0.22
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD12	2	0.22
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD13	2	0.22
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD11	5	0.22
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD12	5	0.22
(1,1709)	1:82:R:ALA:HB1	1:53:R:LEU:HD13	5	0.22
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD11	5	0.22
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD12	5	0.22
(1,1709)	1:82:R:ALA:HB2	1:53:R:LEU:HD13	5	0.22
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD11	5	0.22
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD12	5	0.22
(1,1709)	1:82:R:ALA:HB3	1:53:R:LEU:HD13	5	0.22
(1,1666)	1:167:R:PHE:H	1:168:R:TYR:HD1	4	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1666)	1:167:R:PHE:H	1:168:R:TYR:HD2	4	0.22
(1,1661)	1:165:R:GLU:H	1:164:R:ASP:H	1	0.22
(1,1657)	1:164:R:ASP:H	1:165:R:GLU:H	1	0.22
(1,1472)	1:82:R:ALA:H	1:71:R:VAL:HG21	3	0.22
(1,1472)	1:82:R:ALA:H	1:71:R:VAL:HG22	3	0.22
(1,1472)	1:82:R:ALA:H	1:71:R:VAL:HG23	3	0.22
(1,1468)	1:81:R:GLU:H	1:79:R:THR:HB	5	0.22
(1,1450)	1:72:R:TYR:H	1:74:R:SER:H	2	0.22
(1,1429)	1:65:R:GLU:H	1:63:R:VAL:HB	4	0.22
(1,1371)	1:39:R:LYS:H	1:31:R:LEU:HD11	4	0.22
(1,1371)	1:39:R:LYS:H	1:31:R:LEU:HD12	4	0.22
(1,1371)	1:39:R:LYS:H	1:31:R:LEU:HD13	4	0.22
(1,1371)	1:39:R:LYS:H	1:31:R:LEU:HD21	4	0.22
(1,1371)	1:39:R:LYS:H	1:31:R:LEU:HD22	4	0.22
(1,1371)	1:39:R:LYS:H	1:31:R:LEU:HD23	4	0.22
(1,1177)	1:141:R:ILE:H	1:180:R:PHE:HB2	3	0.22
(1,968)	1:80:R:LEU:H	1:81:R:GLU:HA	3	0.22
(1,959)	1:78:R:LEU:H	1:78:R:LEU:HB2	5	0.22
(1,959)	1:78:R:LEU:H	1:78:R:LEU:HB3	5	0.22
(1,857)	1:48:R:HIS:H	1:50:R:ASN:H	3	0.22
(1,850)	1:46:R:ASN:H	1:49:R:ASP:H	5	0.22
(1,723)	1:168:R:TYR:H	1:162:R:ILE:H	2	0.22
(1,535)	1:117:R:THR:H	1:122:R:SER:H	1	0.22
(2,117)	1:44:R:ARG:H	1:164:R:ASP:O	3	0.21
(2,97)	1:104:R:ILE:H	1:100:R:PRO:O	4	0.21
(2,76)	1:163:R:ASP:H	1:166:R:ASP:O	3	0.21
(2,76)	1:163:R:ASP:H	1:166:R:ASP:O	4	0.21
(2,52)	1:33:R:LEU:H	1:37:R:GLU:O	4	0.21
(2,33)	1:88:R:ASP:H	1:84:R:LYS:O	3	0.21
(1,2316)	1:139:R:ALA:C	1:181:R:VAL:H	1	0.21
(1,2247)	1:134:R:LEU:HD11	1:171:R:THR:HA	4	0.21
(1,2247)	1:134:R:LEU:HD12	1:171:R:THR:HA	4	0.21
(1,2247)	1:134:R:LEU:HD13	1:171:R:THR:HA	4	0.21
(1,2247)	1:134:R:LEU:HD21	1:171:R:THR:HA	4	0.21
(1,2247)	1:134:R:LEU:HD22	1:171:R:THR:HA	4	0.21
(1,2247)	1:134:R:LEU:HD23	1:171:R:THR:HA	4	0.21
(1,2221)	1:156:R:SER:H	1:155:R:THR:HA	1	0.21
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG21	1	0.21
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG22	1	0.21
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG23	1	0.21
(1,2142)	1:103:R:VAL:H	1:103:R:VAL:HB	1	0.21
(1,2142)	1:103:R:VAL:H	1:103:R:VAL:HB	2	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD11	3	0.21
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD12	3	0.21
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD13	3	0.21
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD21	3	0.21
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD22	3	0.21
(1,2070)	1:167:R:PHE:HD1	1:31:R:LEU:HD23	3	0.21
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD11	3	0.21
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD12	3	0.21
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD13	3	0.21
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD21	3	0.21
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD22	3	0.21
(1,2070)	1:167:R:PHE:HD2	1:31:R:LEU:HD23	3	0.21
(1,2019)	1:178:R:LEU:HD11	1:127:R:VAL:HG21	3	0.21
(1,2019)	1:178:R:LEU:HD11	1:127:R:VAL:HG22	3	0.21
(1,2019)	1:178:R:LEU:HD11	1:127:R:VAL:HG23	3	0.21
(1,2019)	1:178:R:LEU:HD12	1:127:R:VAL:HG21	3	0.21
(1,2019)	1:178:R:LEU:HD12	1:127:R:VAL:HG22	3	0.21
(1,2019)	1:178:R:LEU:HD12	1:127:R:VAL:HG23	3	0.21
(1,2019)	1:178:R:LEU:HD13	1:127:R:VAL:HG21	3	0.21
(1,2019)	1:178:R:LEU:HD13	1:127:R:VAL:HG22	3	0.21
(1,2019)	1:178:R:LEU:HD13	1:127:R:VAL:HG23	3	0.21
(1,2019)	1:178:R:LEU:HD21	1:127:R:VAL:HG21	3	0.21
(1,2019)	1:178:R:LEU:HD21	1:127:R:VAL:HG22	3	0.21
(1,2019)	1:178:R:LEU:HD21	1:127:R:VAL:HG23	3	0.21
(1,2019)	1:178:R:LEU:HD22	1:127:R:VAL:HG21	3	0.21
(1,2019)	1:178:R:LEU:HD22	1:127:R:VAL:HG22	3	0.21
(1,2019)	1:178:R:LEU:HD22	1:127:R:VAL:HG23	3	0.21
(1,2019)	1:178:R:LEU:HD23	1:127:R:VAL:HG21	3	0.21
(1,2019)	1:178:R:LEU:HD23	1:127:R:VAL:HG22	3	0.21
(1,2019)	1:178:R:LEU:HD23	1:127:R:VAL:HG23	3	0.21
(1,1963)	1:64:R:GLU:HB2	1:64:R:GLU:HA	4	0.21
(1,1963)	1:64:R:GLU:HB3	1:64:R:GLU:HA	4	0.21
(1,1963)	1:64:R:GLU:HB2	1:64:R:GLU:HA	5	0.21
(1,1963)	1:64:R:GLU:HB3	1:64:R:GLU:HA	5	0.21
(1,1957)	1:57:R:LEU:HD11	1:57:R:LEU:HA	2	0.21
(1,1957)	1:57:R:LEU:HD12	1:57:R:LEU:HA	2	0.21
(1,1957)	1:57:R:LEU:HD13	1:57:R:LEU:HA	2	0.21
(1,1957)	1:57:R:LEU:HD21	1:57:R:LEU:HA	2	0.21
(1,1957)	1:57:R:LEU:HD22	1:57:R:LEU:HA	2	0.21
(1,1957)	1:57:R:LEU:HD23	1:57:R:LEU:HA	2	0.21
(1,1950)	1:56:R:ILE:H	1:56:R:ILE:HD11	2	0.21
(1,1950)	1:56:R:ILE:H	1:56:R:ILE:HD12	2	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1950)	1:56:R:ILE:H	1:56:R:ILE:HD13	2	0.21
(1,1914)	1:170:R:TRP:HB3	1:170:R:TRP:HB2	1	0.21
(1,1914)	1:170:R:TRP:HB3	1:170:R:TRP:HB2	2	0.21
(1,1914)	1:170:R:TRP:HB3	1:170:R:TRP:HB2	4	0.21
(1,1914)	1:170:R:TRP:HB3	1:170:R:TRP:HB2	5	0.21
(1,1888)	1:156:R:SER:HB2	1:156:R:SER:HB3	1	0.21
(1,1888)	1:156:R:SER:HB2	1:156:R:SER:HB3	2	0.21
(1,1888)	1:156:R:SER:HB2	1:156:R:SER:HB3	3	0.21
(1,1888)	1:156:R:SER:HB2	1:156:R:SER:HB3	4	0.21
(1,1888)	1:156:R:SER:HB2	1:156:R:SER:HB3	5	0.21
(1,1887)	1:156:R:SER:HB3	1:156:R:SER:HB2	1	0.21
(1,1887)	1:156:R:SER:HB3	1:156:R:SER:HB2	2	0.21
(1,1887)	1:156:R:SER:HB3	1:156:R:SER:HB2	3	0.21
(1,1887)	1:156:R:SER:HB3	1:156:R:SER:HB2	4	0.21
(1,1887)	1:156:R:SER:HB3	1:156:R:SER:HB2	5	0.21
(1,1859)	1:51:R:ALA:HB1	1:149:R:ALA:HB1	2	0.21
(1,1859)	1:51:R:ALA:HB1	1:149:R:ALA:HB2	2	0.21
(1,1859)	1:51:R:ALA:HB1	1:149:R:ALA:HB3	2	0.21
(1,1859)	1:51:R:ALA:HB2	1:149:R:ALA:HB1	2	0.21
(1,1859)	1:51:R:ALA:HB2	1:149:R:ALA:HB2	2	0.21
(1,1859)	1:51:R:ALA:HB2	1:149:R:ALA:HB3	2	0.21
(1,1859)	1:51:R:ALA:HB3	1:149:R:ALA:HB1	2	0.21
(1,1859)	1:51:R:ALA:HB3	1:149:R:ALA:HB2	2	0.21
(1,1859)	1:51:R:ALA:HB3	1:149:R:ALA:HB3	2	0.21
(1,1859)	1:51:R:ALA:HB1	1:149:R:ALA:HB1	4	0.21
(1,1859)	1:51:R:ALA:HB1	1:149:R:ALA:HB2	4	0.21
(1,1859)	1:51:R:ALA:HB1	1:149:R:ALA:HB3	4	0.21
(1,1859)	1:51:R:ALA:HB2	1:149:R:ALA:HB1	4	0.21
(1,1859)	1:51:R:ALA:HB2	1:149:R:ALA:HB2	4	0.21
(1,1859)	1:51:R:ALA:HB2	1:149:R:ALA:HB3	4	0.21
(1,1859)	1:51:R:ALA:HB3	1:149:R:ALA:HB1	4	0.21
(1,1859)	1:51:R:ALA:HB3	1:149:R:ALA:HB2	4	0.21
(1,1859)	1:51:R:ALA:HB3	1:149:R:ALA:HB3	4	0.21
(1,1832)	1:125:R:CYS:HB2	1:125:R:CYS:HB3	1	0.21
(1,1832)	1:125:R:CYS:HB2	1:125:R:CYS:HB3	2	0.21
(1,1832)	1:125:R:CYS:HB2	1:125:R:CYS:HB3	3	0.21
(1,1832)	1:125:R:CYS:HB2	1:125:R:CYS:HB3	5	0.21
(1,1831)	1:125:R:CYS:HB3	1:125:R:CYS:HB2	1	0.21
(1,1831)	1:125:R:CYS:HB3	1:125:R:CYS:HB2	2	0.21
(1,1831)	1:125:R:CYS:HB3	1:125:R:CYS:HB2	3	0.21
(1,1831)	1:125:R:CYS:HB3	1:125:R:CYS:HB2	5	0.21
(1,1825)	1:122:R:SER:HB2	1:122:R:SER:HB3	1	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1825)	1:122:R:SER:HB2	1:122:R:SER:HB3	2	0.21
(1,1825)	1:122:R:SER:HB2	1:122:R:SER:HB3	3	0.21
(1,1825)	1:122:R:SER:HB2	1:122:R:SER:HB3	4	0.21
(1,1825)	1:122:R:SER:HB2	1:122:R:SER:HB3	5	0.21
(1,1824)	1:122:R:SER:HB3	1:122:R:SER:HB2	1	0.21
(1,1824)	1:122:R:SER:HB3	1:122:R:SER:HB2	2	0.21
(1,1824)	1:122:R:SER:HB3	1:122:R:SER:HB2	3	0.21
(1,1824)	1:122:R:SER:HB3	1:122:R:SER:HB2	4	0.21
(1,1824)	1:122:R:SER:HB3	1:122:R:SER:HB2	5	0.21
(1,1813)	1:115:R:ILE:HD11	1:115:R:ILE:HA	4	0.21
(1,1813)	1:115:R:ILE:HD12	1:115:R:ILE:HA	4	0.21
(1,1813)	1:115:R:ILE:HD13	1:115:R:ILE:HA	4	0.21
(1,1808)	1:111:R:LEU:HA	1:111:R:LEU:HD21	2	0.21
(1,1808)	1:111:R:LEU:HA	1:111:R:LEU:HD22	2	0.21
(1,1808)	1:111:R:LEU:HA	1:111:R:LEU:HD23	2	0.21
(1,1807)	1:111:R:LEU:HD21	1:111:R:LEU:HA	2	0.21
(1,1807)	1:111:R:LEU:HD22	1:111:R:LEU:HA	2	0.21
(1,1807)	1:111:R:LEU:HD23	1:111:R:LEU:HA	2	0.21
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG21	2	0.21
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG22	2	0.21
(1,1795)	1:94:R:LEU:HD21	1:103:R:VAL:HG23	2	0.21
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG21	2	0.21
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG22	2	0.21
(1,1795)	1:94:R:LEU:HD22	1:103:R:VAL:HG23	2	0.21
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG21	2	0.21
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG22	2	0.21
(1,1795)	1:94:R:LEU:HD23	1:103:R:VAL:HG23	2	0.21
(1,1766)	1:85:R:GLN:HB2	1:85:R:GLN:HB3	1	0.21
(1,1766)	1:85:R:GLN:HB2	1:85:R:GLN:HB3	2	0.21
(1,1766)	1:85:R:GLN:HB2	1:85:R:GLN:HB3	3	0.21
(1,1766)	1:85:R:GLN:HB2	1:85:R:GLN:HB3	4	0.21
(1,1766)	1:85:R:GLN:HB2	1:85:R:GLN:HB3	5	0.21
(1,1765)	1:85:R:GLN:HB3	1:85:R:GLN:HB2	1	0.21
(1,1765)	1:85:R:GLN:HB3	1:85:R:GLN:HB2	2	0.21
(1,1765)	1:85:R:GLN:HB3	1:85:R:GLN:HB2	3	0.21
(1,1765)	1:85:R:GLN:HB3	1:85:R:GLN:HB2	4	0.21
(1,1765)	1:85:R:GLN:HB3	1:85:R:GLN:HB2	5	0.21
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG11	3	0.21
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG12	3	0.21
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG13	3	0.21
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG11	3	0.21
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG12	3	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG13	3	0.21
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG11	3	0.21
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG12	3	0.21
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG13	3	0.21
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG11	3	0.21
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG12	3	0.21
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG13	3	0.21
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG11	3	0.21
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG12	3	0.21
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG13	3	0.21
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG11	3	0.21
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG12	3	0.21
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG13	3	0.21
(1,1739)	1:69:R:ASP:H	1:68:R:PHE:HA	2	0.21
(1,1729)	1:59:R:LEU:HA	1:59:R:LEU:HD11	1	0.21
(1,1729)	1:59:R:LEU:HA	1:59:R:LEU:HD12	1	0.21
(1,1729)	1:59:R:LEU:HA	1:59:R:LEU:HD13	1	0.21
(1,1728)	1:57:R:LEU:HD11	1:57:R:LEU:HA	3	0.21
(1,1728)	1:57:R:LEU:HD12	1:57:R:LEU:HA	3	0.21
(1,1728)	1:57:R:LEU:HD13	1:57:R:LEU:HA	3	0.21
(1,1728)	1:57:R:LEU:HD21	1:57:R:LEU:HA	3	0.21
(1,1728)	1:57:R:LEU:HD22	1:57:R:LEU:HA	3	0.21
(1,1728)	1:57:R:LEU:HD23	1:57:R:LEU:HA	3	0.21
(1,1703)	1:149:R:ALA:HB1	1:51:R:ALA:HB1	2	0.21
(1,1703)	1:149:R:ALA:HB1	1:51:R:ALA:HB2	2	0.21
(1,1703)	1:149:R:ALA:HB1	1:51:R:ALA:HB3	2	0.21
(1,1703)	1:149:R:ALA:HB2	1:51:R:ALA:HB1	2	0.21
(1,1703)	1:149:R:ALA:HB2	1:51:R:ALA:HB2	2	0.21
(1,1703)	1:149:R:ALA:HB2	1:51:R:ALA:HB3	2	0.21
(1,1703)	1:149:R:ALA:HB3	1:51:R:ALA:HB1	2	0.21
(1,1703)	1:149:R:ALA:HB3	1:51:R:ALA:HB2	2	0.21
(1,1703)	1:149:R:ALA:HB3	1:51:R:ALA:HB3	2	0.21
(1,1703)	1:149:R:ALA:HB1	1:51:R:ALA:HB1	4	0.21
(1,1703)	1:149:R:ALA:HB1	1:51:R:ALA:HB2	4	0.21
(1,1703)	1:149:R:ALA:HB1	1:51:R:ALA:HB3	4	0.21
(1,1703)	1:149:R:ALA:HB2	1:51:R:ALA:HB1	4	0.21
(1,1703)	1:149:R:ALA:HB2	1:51:R:ALA:HB2	4	0.21
(1,1703)	1:149:R:ALA:HB2	1:51:R:ALA:HB3	4	0.21
(1,1703)	1:149:R:ALA:HB3	1:51:R:ALA:HB1	4	0.21
(1,1703)	1:149:R:ALA:HB3	1:51:R:ALA:HB2	4	0.21
(1,1703)	1:149:R:ALA:HB3	1:51:R:ALA:HB3	4	0.21
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB1	4	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB2	4	0.21
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB3	4	0.21
(1,1589)	1:135:R:ALA:H	1:133:R:CYS:H	3	0.21
(1,1537)	1:111:R:LEU:H	1:113:R:THR:HB	5	0.21
(1,1486)	1:87:R:GLU:H	1:83:R:ILE:HA	1	0.21
(1,1366)	1:36:R:GLY:H	1:34:R:TYR:HA	3	0.21
(1,1141)	1:127:R:VAL:H	1:128:R:ASP:H	2	0.21
(1,1025)	1:95:R:HIS:H	1:94:R:LEU:HD11	1	0.21
(1,1025)	1:95:R:HIS:H	1:94:R:LEU:HD12	1	0.21
(1,1025)	1:95:R:HIS:H	1:94:R:LEU:HD13	1	0.21
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD11	2	0.21
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD12	2	0.21
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD13	2	0.21
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD21	2	0.21
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD22	2	0.21
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD23	2	0.21
(1,703)	1:162:R:ILE:H	1:153:R:CYS:H	3	0.21
(1,662)	1:153:R:CYS:H	1:162:R:ILE:H	3	0.21
(1,196)	1:38:R:LYS:H	1:37:R:GLU:H	2	0.21
(1,194)	1:37:R:GLU:H	1:38:R:LYS:H	2	0.21
(1,156)	1:179:R:VAL:H	1:141:R:ILE:HB	1	0.21
(2,108)	1:139:R:ALA:O	1:181:R:VAL:N	3	0.2
(2,86)	1:52:R:TRP:O	1:56:R:ILE:N	4	0.2
(2,61)	1:178:R:LEU:H	1:141:R:ILE:O	1	0.2
(2,51)	1:33:R:LEU:N	1:37:R:GLU:O	4	0.2
(2,10)	1:60:R:PHE:N	1:56:R:ILE:O	5	0.2
(1,2321)	1:44:R:ARG:H	1:164:R:ASP:C	3	0.2
(1,2320)	1:143:R:LEU:H	1:176:R:ASP:C	3	0.2
(1,2305)	1:52:R:TRP:C	1:56:R:ILE:H	1	0.2
(1,2300)	1:163:R:ASP:H	1:166:R:ASP:C	3	0.2
(1,2271)	1:68:R:PHE:C	1:72:R:TYR:H	3	0.2
(1,2271)	1:68:R:PHE:C	1:72:R:TYR:H	5	0.2
(1,2244)	1:170:R:TRP:HA	1:170:R:TRP:HB2	5	0.2
(1,2221)	1:156:R:SER:H	1:155:R:THR:HA	5	0.2
(1,2175)	1:125:R:CYS:H	1:125:R:CYS:HB2	5	0.2
(1,2159)	1:112:R:HIS:H	1:112:R:HIS:HB3	3	0.2
(1,2136)	1:95:R:HIS:H	1:95:R:HIS:HA	4	0.2
(1,2050)	1:41:R:PHE:HE1	1:162:R:ILE:HD11	1	0.2
(1,2050)	1:41:R:PHE:HE1	1:162:R:ILE:HD12	1	0.2
(1,2050)	1:41:R:PHE:HE1	1:162:R:ILE:HD13	1	0.2
(1,2050)	1:41:R:PHE:HE2	1:162:R:ILE:HD11	1	0.2
(1,2050)	1:41:R:PHE:HE2	1:162:R:ILE:HD12	1	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2050)	1:41:R:PHE:HE2	1:162:R:ILE:HD13	1	0.2
(1,2050)	1:41:R:PHE:HE1	1:162:R:ILE:HD11	5	0.2
(1,2050)	1:41:R:PHE:HE1	1:162:R:ILE:HD12	5	0.2
(1,2050)	1:41:R:PHE:HE1	1:162:R:ILE:HD13	5	0.2
(1,2050)	1:41:R:PHE:HE2	1:162:R:ILE:HD11	5	0.2
(1,2050)	1:41:R:PHE:HE2	1:162:R:ILE:HD12	5	0.2
(1,2050)	1:41:R:PHE:HE2	1:162:R:ILE:HD13	5	0.2
(1,2047)	1:161:R:ALA:H	1:161:R:ALA:HB1	4	0.2
(1,2047)	1:161:R:ALA:H	1:161:R:ALA:HB2	4	0.2
(1,2047)	1:161:R:ALA:H	1:161:R:ALA:HB3	4	0.2
(1,2044)	1:155:R:THR:HG21	1:155:R:THR:HA	5	0.2
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB1	3	0.2
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB2	3	0.2
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB3	3	0.2
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB1	3	0.2
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB2	3	0.2
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB3	3	0.2
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB1	3	0.2
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB2	3	0.2
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB3	3	0.2
(1,1962)	1:124:R:VAL:HG11	1:63:R:VAL:HG21	3	0.2
(1,1962)	1:124:R:VAL:HG11	1:63:R:VAL:HG22	3	0.2
(1,1962)	1:124:R:VAL:HG11	1:63:R:VAL:HG23	3	0.2
(1,1962)	1:124:R:VAL:HG12	1:63:R:VAL:HG21	3	0.2
(1,1962)	1:124:R:VAL:HG12	1:63:R:VAL:HG22	3	0.2
(1,1962)	1:124:R:VAL:HG12	1:63:R:VAL:HG23	3	0.2
(1,1962)	1:124:R:VAL:HG13	1:63:R:VAL:HG21	3	0.2
(1,1962)	1:124:R:VAL:HG13	1:63:R:VAL:HG22	3	0.2
(1,1962)	1:124:R:VAL:HG13	1:63:R:VAL:HG23	3	0.2
(1,1956)	1:56:R:ILE:H	1:56:R:ILE:HG21	2	0.2
(1,1956)	1:56:R:ILE:H	1:56:R:ILE:HG22	2	0.2
(1,1956)	1:56:R:ILE:H	1:56:R:ILE:HG23	2	0.2
(1,1939)	1:40:R:THR:HB	1:40:R:THR:HG22	2	0.2
(1,1914)	1:170:R:TRP:HB3	1:170:R:TRP:HB2	3	0.2
(1,1857)	1:181:R:VAL:HB	1:139:R:ALA:HB1	2	0.2
(1,1857)	1:181:R:VAL:HB	1:139:R:ALA:HB2	2	0.2
(1,1857)	1:181:R:VAL:HB	1:139:R:ALA:HB3	2	0.2
(1,1848)	1:134:R:LEU:HD21	1:134:R:LEU:HA	2	0.2
(1,1848)	1:134:R:LEU:HD22	1:134:R:LEU:HA	2	0.2
(1,1848)	1:134:R:LEU:HD23	1:134:R:LEU:HA	2	0.2
(1,1808)	1:111:R:LEU:HA	1:111:R:LEU:HD21	1	0.2
(1,1808)	1:111:R:LEU:HA	1:111:R:LEU:HD22	1	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1808)	1:111:R:LEU:HA	1:111:R:LEU:HD23	1	0.2
(1,1807)	1:111:R:LEU:HD21	1:111:R:LEU:HA	1	0.2
(1,1807)	1:111:R:LEU:HD22	1:111:R:LEU:HA	1	0.2
(1,1807)	1:111:R:LEU:HD23	1:111:R:LEU:HA	1	0.2
(1,1727)	1:56:R:ILE:H	1:56:R:ILE:HG21	3	0.2
(1,1727)	1:56:R:ILE:H	1:56:R:ILE:HG22	3	0.2
(1,1727)	1:56:R:ILE:H	1:56:R:ILE:HG23	3	0.2
(1,1719)	1:56:R:ILE:H	1:56:R:ILE:HD11	5	0.2
(1,1719)	1:56:R:ILE:H	1:56:R:ILE:HD12	5	0.2
(1,1719)	1:56:R:ILE:H	1:56:R:ILE:HD13	5	0.2
(1,1714)	1:83:R:ILE:HG21	1:53:R:LEU:HD21	3	0.2
(1,1714)	1:83:R:ILE:HG21	1:53:R:LEU:HD22	3	0.2
(1,1714)	1:83:R:ILE:HG21	1:53:R:LEU:HD23	3	0.2
(1,1714)	1:83:R:ILE:HG22	1:53:R:LEU:HD21	3	0.2
(1,1714)	1:83:R:ILE:HG22	1:53:R:LEU:HD22	3	0.2
(1,1714)	1:83:R:ILE:HG22	1:53:R:LEU:HD23	3	0.2
(1,1714)	1:83:R:ILE:HG23	1:53:R:LEU:HD21	3	0.2
(1,1714)	1:83:R:ILE:HG23	1:53:R:LEU:HD22	3	0.2
(1,1714)	1:83:R:ILE:HG23	1:53:R:LEU:HD23	3	0.2
(1,1707)	1:53:R:LEU:HD21	1:53:R:LEU:HD11	2	0.2
(1,1707)	1:53:R:LEU:HD21	1:53:R:LEU:HD12	2	0.2
(1,1707)	1:53:R:LEU:HD21	1:53:R:LEU:HD13	2	0.2
(1,1707)	1:53:R:LEU:HD22	1:53:R:LEU:HD11	2	0.2
(1,1707)	1:53:R:LEU:HD22	1:53:R:LEU:HD12	2	0.2
(1,1707)	1:53:R:LEU:HD22	1:53:R:LEU:HD13	2	0.2
(1,1707)	1:53:R:LEU:HD23	1:53:R:LEU:HD11	2	0.2
(1,1707)	1:53:R:LEU:HD23	1:53:R:LEU:HD12	2	0.2
(1,1707)	1:53:R:LEU:HD23	1:53:R:LEU:HD13	2	0.2
(1,1592)	1:138:R:HIS:H	1:154:R:VAL:HG21	5	0.2
(1,1592)	1:138:R:HIS:H	1:154:R:VAL:HG22	5	0.2
(1,1592)	1:138:R:HIS:H	1:154:R:VAL:HG23	5	0.2
(1,1580)	1:126:R:VAL:H	1:118:R:ALA:H	3	0.2
(1,1482)	1:85:R:GLN:H	1:83:R:ILE:HA	1	0.2
(1,1275)	1:166:R:ASP:H	1:44:R:ARG:H	1	0.2
(1,1043)	1:104:R:ILE:H	1:101:R:ALA:HA	1	0.2
(1,1043)	1:104:R:ILE:H	1:101:R:ALA:HA	4	0.2
(1,968)	1:80:R:LEU:H	1:81:R:GLU:HA	1	0.2
(1,968)	1:80:R:LEU:H	1:81:R:GLU:HA	2	0.2
(1,968)	1:80:R:LEU:H	1:81:R:GLU:HA	5	0.2
(1,959)	1:78:R:LEU:H	1:78:R:LEU:HB2	1	0.2
(1,959)	1:78:R:LEU:H	1:78:R:LEU:HB3	1	0.2
(1,851)	1:46:R:ASN:H	1:165:R:GLU:H	2	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:46:R:ASN:H	1:44:R:ARG:H	1	0.2
(1,552)	1:122:R:SER:H	1:124:R:VAL:H	4	0.2
(1,510)	1:113:R:THR:H	1:111:R:LEU:HD21	2	0.2
(1,510)	1:113:R:THR:H	1:111:R:LEU:HD22	2	0.2
(1,510)	1:113:R:THR:H	1:111:R:LEU:HD23	2	0.2
(1,389)	1:84:R:LYS:H	1:83:R:ILE:HG12	2	0.2
(2,91)	1:66:R:PRO:O	1:69:R:ASP:H	4	0.19
(2,84)	1:159:R:TRP:O	1:170:R:TRP:H	4	0.19
(2,61)	1:178:R:LEU:H	1:141:R:ILE:O	2	0.19
(2,44)	1:133:R:CYS:O	1:136:R:ASP:N	4	0.19
(1,2320)	1:143:R:LEU:H	1:176:R:ASP:C	2	0.19
(1,2319)	1:142:R:PHE:C	1:150:R:VAL:H	5	0.19
(1,2308)	1:66:R:PRO:C	1:69:R:ASP:H	2	0.19
(1,2308)	1:66:R:PRO:C	1:69:R:ASP:H	5	0.19
(1,2305)	1:52:R:TRP:C	1:56:R:ILE:H	4	0.19
(1,2293)	1:178:R:LEU:H	1:141:R:ILE:C	1	0.19
(1,2255)	1:140:R:GLY:HA2	1:180:R:PHE:HA	2	0.19
(1,2246)	1:170:R:TRP:H	1:170:R:TRP:HB2	3	0.19
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG21	5	0.19
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG22	5	0.19
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG23	5	0.19
(1,2181)	1:134:R:LEU:H	1:134:R:LEU:HA	3	0.19
(1,2174)	1:125:R:CYS:H	1:125:R:CYS:HB3	1	0.19
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB1	2	0.19
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB2	2	0.19
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB3	2	0.19
(1,2137)	1:95:R:HIS:H	1:95:R:HIS:HB3	5	0.19
(1,2060)	1:177:R:VAL:H	1:177:R:VAL:HG11	2	0.19
(1,2060)	1:177:R:VAL:H	1:177:R:VAL:HG12	2	0.19
(1,2060)	1:177:R:VAL:H	1:177:R:VAL:HG13	2	0.19
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG11	4	0.19
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG12	4	0.19
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG13	4	0.19
(1,1982)	1:90:R:THR:HB	1:90:R:THR:HG22	1	0.19
(1,1964)	1:64:R:GLU:HA	1:64:R:GLU:HG3	3	0.19
(1,1915)	1:159:R:TRP:HB2	1:171:R:THR:HA	5	0.19
(1,1859)	1:51:R:ALA:HB1	1:149:R:ALA:HB1	1	0.19
(1,1859)	1:51:R:ALA:HB1	1:149:R:ALA:HB2	1	0.19
(1,1859)	1:51:R:ALA:HB1	1:149:R:ALA:HB3	1	0.19
(1,1859)	1:51:R:ALA:HB2	1:149:R:ALA:HB1	1	0.19
(1,1859)	1:51:R:ALA:HB2	1:149:R:ALA:HB2	1	0.19
(1,1859)	1:51:R:ALA:HB2	1:149:R:ALA:HB3	1	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1859)	1:51:R:ALA:HB3	1:149:R:ALA:HB1	1	0.19
(1,1859)	1:51:R:ALA:HB3	1:149:R:ALA:HB2	1	0.19
(1,1859)	1:51:R:ALA:HB3	1:149:R:ALA:HB3	1	0.19
(1,1859)	1:51:R:ALA:HB1	1:149:R:ALA:HB1	5	0.19
(1,1859)	1:51:R:ALA:HB1	1:149:R:ALA:HB2	5	0.19
(1,1859)	1:51:R:ALA:HB1	1:149:R:ALA:HB3	5	0.19
(1,1859)	1:51:R:ALA:HB2	1:149:R:ALA:HB1	5	0.19
(1,1859)	1:51:R:ALA:HB2	1:149:R:ALA:HB2	5	0.19
(1,1859)	1:51:R:ALA:HB2	1:149:R:ALA:HB3	5	0.19
(1,1859)	1:51:R:ALA:HB3	1:149:R:ALA:HB1	5	0.19
(1,1859)	1:51:R:ALA:HB3	1:149:R:ALA:HB2	5	0.19
(1,1859)	1:51:R:ALA:HB3	1:149:R:ALA:HB3	5	0.19
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG11	2	0.19
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG12	2	0.19
(1,1746)	1:57:R:LEU:HD11	1:71:R:VAL:HG13	2	0.19
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG11	2	0.19
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG12	2	0.19
(1,1746)	1:57:R:LEU:HD12	1:71:R:VAL:HG13	2	0.19
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG11	2	0.19
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG12	2	0.19
(1,1746)	1:57:R:LEU:HD13	1:71:R:VAL:HG13	2	0.19
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG11	2	0.19
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG12	2	0.19
(1,1746)	1:57:R:LEU:HD21	1:71:R:VAL:HG13	2	0.19
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG11	2	0.19
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG12	2	0.19
(1,1746)	1:57:R:LEU:HD22	1:71:R:VAL:HG13	2	0.19
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG11	2	0.19
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG12	2	0.19
(1,1746)	1:57:R:LEU:HD23	1:71:R:VAL:HG13	2	0.19
(1,1703)	1:149:R:ALA:HB1	1:51:R:ALA:HB1	1	0.19
(1,1703)	1:149:R:ALA:HB1	1:51:R:ALA:HB2	1	0.19
(1,1703)	1:149:R:ALA:HB1	1:51:R:ALA:HB3	1	0.19
(1,1703)	1:149:R:ALA:HB2	1:51:R:ALA:HB1	1	0.19
(1,1703)	1:149:R:ALA:HB2	1:51:R:ALA:HB2	1	0.19
(1,1703)	1:149:R:ALA:HB2	1:51:R:ALA:HB3	1	0.19
(1,1703)	1:149:R:ALA:HB3	1:51:R:ALA:HB1	1	0.19
(1,1703)	1:149:R:ALA:HB3	1:51:R:ALA:HB2	1	0.19
(1,1703)	1:149:R:ALA:HB3	1:51:R:ALA:HB3	1	0.19
(1,1703)	1:149:R:ALA:HB1	1:51:R:ALA:HB1	5	0.19
(1,1703)	1:149:R:ALA:HB1	1:51:R:ALA:HB2	5	0.19
(1,1703)	1:149:R:ALA:HB1	1:51:R:ALA:HB3	5	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1703)	1:149:R:ALA:HB2	1:51:R:ALA:HB1	5	0.19
(1,1703)	1:149:R:ALA:HB2	1:51:R:ALA:HB2	5	0.19
(1,1703)	1:149:R:ALA:HB2	1:51:R:ALA:HB3	5	0.19
(1,1703)	1:149:R:ALA:HB3	1:51:R:ALA:HB1	5	0.19
(1,1703)	1:149:R:ALA:HB3	1:51:R:ALA:HB2	5	0.19
(1,1703)	1:149:R:ALA:HB3	1:51:R:ALA:HB3	5	0.19
(1,1529)	1:110:R:LEU:H	1:109:R:HIS:HB3	5	0.19
(1,1503)	1:103:R:VAL:H	1:94:R:LEU:HD21	1	0.19
(1,1503)	1:103:R:VAL:H	1:94:R:LEU:HD22	1	0.19
(1,1503)	1:103:R:VAL:H	1:94:R:LEU:HD23	1	0.19
(1,1391)	1:48:R:HIS:H	1:48:R:HIS:HD2	5	0.19
(1,1352)	1:33:R:LEU:H	1:37:R:GLU:H	4	0.19
(1,1292)	1:171:R:THR:H	1:168:R:TYR:HD1	3	0.19
(1,1292)	1:171:R:THR:H	1:168:R:TYR:HD2	3	0.19
(1,1043)	1:104:R:ILE:H	1:101:R:ALA:HA	3	0.19
(1,1012)	1:91:R:GLY:H	1:89:R:LEU:HG	3	0.19
(1,950)	1:73:R:SER:H	1:72:R:TYR:HD1	5	0.19
(1,950)	1:73:R:SER:H	1:72:R:TYR:HD2	5	0.19
(1,856)	1:48:R:HIS:H	1:49:R:ASP:HB2	2	0.19
(1,850)	1:46:R:ASN:H	1:49:R:ASP:H	4	0.19
(2,98)	1:104:R:ILE:N	1:100:R:PRO:O	1	0.18
(1,2307)	1:50:R:ASN:C	1:54:R:ASN:H	3	0.18
(1,2293)	1:178:R:LEU:H	1:141:R:ILE:C	2	0.18
(1,2271)	1:68:R:PHE:C	1:72:R:TYR:H	1	0.18
(1,2266)	1:54:R:ASN:C	1:58:R:GLN:H	1	0.18
(1,2266)	1:54:R:ASN:C	1:58:R:GLN:H	5	0.18
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG21	4	0.18
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG22	4	0.18
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG23	4	0.18
(1,2195)	1:150:R:VAL:H	1:150:R:VAL:HG11	4	0.18
(1,2195)	1:150:R:VAL:H	1:150:R:VAL:HG12	4	0.18
(1,2195)	1:150:R:VAL:H	1:150:R:VAL:HG13	4	0.18
(1,2169)	1:122:R:SER:HB2	1:122:R:SER:HA	2	0.18
(1,2163)	1:117:R:THR:HB	1:117:R:THR:HA	4	0.18
(1,2046)	1:152:R:ALA:HB1	1:161:R:ALA:HB1	4	0.18
(1,2046)	1:152:R:ALA:HB1	1:161:R:ALA:HB2	4	0.18
(1,2046)	1:152:R:ALA:HB1	1:161:R:ALA:HB3	4	0.18
(1,2046)	1:152:R:ALA:HB2	1:161:R:ALA:HB1	4	0.18
(1,2046)	1:152:R:ALA:HB2	1:161:R:ALA:HB2	4	0.18
(1,2046)	1:152:R:ALA:HB2	1:161:R:ALA:HB3	4	0.18
(1,2046)	1:152:R:ALA:HB3	1:161:R:ALA:HB1	4	0.18
(1,2046)	1:152:R:ALA:HB3	1:161:R:ALA:HB2	4	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2046)	1:152:R:ALA:HB3	1:161:R:ALA:HB3	4	0.18
(1,2044)	1:155:R:THR:HG22	1:155:R:THR:HA	1	0.18
(1,2036)	1:161:R:ALA:HB1	1:152:R:ALA:HB1	4	0.18
(1,2036)	1:161:R:ALA:HB1	1:152:R:ALA:HB2	4	0.18
(1,2036)	1:161:R:ALA:HB1	1:152:R:ALA:HB3	4	0.18
(1,2036)	1:161:R:ALA:HB2	1:152:R:ALA:HB1	4	0.18
(1,2036)	1:161:R:ALA:HB2	1:152:R:ALA:HB2	4	0.18
(1,2036)	1:161:R:ALA:HB2	1:152:R:ALA:HB3	4	0.18
(1,2036)	1:161:R:ALA:HB3	1:152:R:ALA:HB1	4	0.18
(1,2036)	1:161:R:ALA:HB3	1:152:R:ALA:HB2	4	0.18
(1,2036)	1:161:R:ALA:HB3	1:152:R:ALA:HB3	4	0.18
(1,1994)	1:94:R:LEU:HD21	1:103:R:VAL:HG21	5	0.18
(1,1994)	1:94:R:LEU:HD21	1:103:R:VAL:HG22	5	0.18
(1,1994)	1:94:R:LEU:HD21	1:103:R:VAL:HG23	5	0.18
(1,1994)	1:94:R:LEU:HD22	1:103:R:VAL:HG21	5	0.18
(1,1994)	1:94:R:LEU:HD22	1:103:R:VAL:HG22	5	0.18
(1,1994)	1:94:R:LEU:HD22	1:103:R:VAL:HG23	5	0.18
(1,1994)	1:94:R:LEU:HD23	1:103:R:VAL:HG21	5	0.18
(1,1994)	1:94:R:LEU:HD23	1:103:R:VAL:HG22	5	0.18
(1,1994)	1:94:R:LEU:HD23	1:103:R:VAL:HG23	5	0.18
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB1	1	0.18
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB2	1	0.18
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB3	1	0.18
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB1	1	0.18
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB2	1	0.18
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB3	1	0.18
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB1	1	0.18
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB2	1	0.18
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB3	1	0.18
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB1	2	0.18
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB2	2	0.18
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB3	2	0.18
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB1	2	0.18
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB2	2	0.18
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB3	2	0.18
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB1	2	0.18
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB2	2	0.18
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB3	2	0.18
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB1	5	0.18
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB2	5	0.18
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB3	5	0.18
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB1	5	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB2	5	0.18
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB3	5	0.18
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB1	5	0.18
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB2	5	0.18
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB3	5	0.18
(1,1963)	1:64:R:GLU:HB2	1:64:R:GLU:HA	1	0.18
(1,1963)	1:64:R:GLU:HB3	1:64:R:GLU:HA	1	0.18
(1,1963)	1:64:R:GLU:HB2	1:64:R:GLU:HA	3	0.18
(1,1963)	1:64:R:GLU:HB3	1:64:R:GLU:HA	3	0.18
(1,1828)	1:115:R:ILE:HD11	1:124:R:VAL:HG11	2	0.18
(1,1828)	1:115:R:ILE:HD11	1:124:R:VAL:HG12	2	0.18
(1,1828)	1:115:R:ILE:HD11	1:124:R:VAL:HG13	2	0.18
(1,1828)	1:115:R:ILE:HD12	1:124:R:VAL:HG11	2	0.18
(1,1828)	1:115:R:ILE:HD12	1:124:R:VAL:HG12	2	0.18
(1,1828)	1:115:R:ILE:HD12	1:124:R:VAL:HG13	2	0.18
(1,1828)	1:115:R:ILE:HD13	1:124:R:VAL:HG11	2	0.18
(1,1828)	1:115:R:ILE:HD13	1:124:R:VAL:HG12	2	0.18
(1,1828)	1:115:R:ILE:HD13	1:124:R:VAL:HG13	2	0.18
(1,1813)	1:115:R:ILE:HD11	1:115:R:ILE:HA	5	0.18
(1,1813)	1:115:R:ILE:HD12	1:115:R:ILE:HA	5	0.18
(1,1813)	1:115:R:ILE:HD13	1:115:R:ILE:HA	5	0.18
(1,1775)	1:94:R:LEU:HD21	1:94:R:LEU:HD11	2	0.18
(1,1775)	1:94:R:LEU:HD21	1:94:R:LEU:HD12	2	0.18
(1,1775)	1:94:R:LEU:HD21	1:94:R:LEU:HD13	2	0.18
(1,1775)	1:94:R:LEU:HD22	1:94:R:LEU:HD11	2	0.18
(1,1775)	1:94:R:LEU:HD22	1:94:R:LEU:HD12	2	0.18
(1,1775)	1:94:R:LEU:HD22	1:94:R:LEU:HD13	2	0.18
(1,1775)	1:94:R:LEU:HD23	1:94:R:LEU:HD11	2	0.18
(1,1775)	1:94:R:LEU:HD23	1:94:R:LEU:HD12	2	0.18
(1,1775)	1:94:R:LEU:HD23	1:94:R:LEU:HD13	2	0.18
(1,1775)	1:94:R:LEU:HD21	1:94:R:LEU:HD11	4	0.18
(1,1775)	1:94:R:LEU:HD21	1:94:R:LEU:HD12	4	0.18
(1,1775)	1:94:R:LEU:HD21	1:94:R:LEU:HD13	4	0.18
(1,1775)	1:94:R:LEU:HD22	1:94:R:LEU:HD11	4	0.18
(1,1775)	1:94:R:LEU:HD22	1:94:R:LEU:HD12	4	0.18
(1,1775)	1:94:R:LEU:HD22	1:94:R:LEU:HD13	4	0.18
(1,1775)	1:94:R:LEU:HD23	1:94:R:LEU:HD11	4	0.18
(1,1775)	1:94:R:LEU:HD23	1:94:R:LEU:HD12	4	0.18
(1,1775)	1:94:R:LEU:HD23	1:94:R:LEU:HD13	4	0.18
(1,1728)	1:57:R:LEU:HD11	1:57:R:LEU:HA	1	0.18
(1,1728)	1:57:R:LEU:HD12	1:57:R:LEU:HA	1	0.18
(1,1728)	1:57:R:LEU:HD13	1:57:R:LEU:HA	1	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1728)	1:57:R:LEU:HD21	1:57:R:LEU:HA	1	0.18
(1,1728)	1:57:R:LEU:HD22	1:57:R:LEU:HA	1	0.18
(1,1728)	1:57:R:LEU:HD23	1:57:R:LEU:HA	1	0.18
(1,1720)	1:103:R:VAL:HG21	1:56:R:ILE:HD11	5	0.18
(1,1720)	1:103:R:VAL:HG21	1:56:R:ILE:HD12	5	0.18
(1,1720)	1:103:R:VAL:HG21	1:56:R:ILE:HD13	5	0.18
(1,1720)	1:103:R:VAL:HG22	1:56:R:ILE:HD11	5	0.18
(1,1720)	1:103:R:VAL:HG22	1:56:R:ILE:HD12	5	0.18
(1,1720)	1:103:R:VAL:HG22	1:56:R:ILE:HD13	5	0.18
(1,1720)	1:103:R:VAL:HG23	1:56:R:ILE:HD11	5	0.18
(1,1720)	1:103:R:VAL:HG23	1:56:R:ILE:HD12	5	0.18
(1,1720)	1:103:R:VAL:HG23	1:56:R:ILE:HD13	5	0.18
(1,1529)	1:110:R:LEU:H	1:109:R:HIS:HB3	2	0.18
(1,1486)	1:87:R:GLU:H	1:83:R:ILE:HA	3	0.18
(1,1472)	1:82:R:ALA:H	1:71:R:VAL:HG21	4	0.18
(1,1472)	1:82:R:ALA:H	1:71:R:VAL:HG22	4	0.18
(1,1472)	1:82:R:ALA:H	1:71:R:VAL:HG23	4	0.18
(1,1429)	1:65:R:GLU:H	1:63:R:VAL:HB	2	0.18
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD11	3	0.18
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD12	3	0.18
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD13	3	0.18
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD21	3	0.18
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD22	3	0.18
(1,1370)	1:38:R:LYS:H	1:33:R:LEU:HD23	3	0.18
(1,1363)	1:35:R:ASN:H	1:155:R:THR:HA	1	0.18
(1,1297)	1:173:R:ASP:H	1:176:R:ASP:H	1	0.18
(1,1059)	1:107:R:ILE:H	1:105:R:TRP:HB2	1	0.18
(1,968)	1:80:R:LEU:H	1:81:R:GLU:HA	4	0.18
(1,837)	1:41:R:PHE:H	1:41:R:PHE:HZ	3	0.18
(1,594)	1:131:R:ASP:H	1:132:R:MET:H	4	0.18
(1,389)	1:84:R:LYS:H	1:83:R:ILE:HG12	1	0.18
(2,78)	1:163:R:ASP:O	1:166:R:ASP:H	3	0.17
(2,74)	1:162:R:ILE:H	1:151:R:PHE:O	4	0.17
(2,33)	1:88:R:ASP:H	1:84:R:LYS:O	2	0.17
(2,20)	1:69:R:ASP:O	1:73:R:SER:N	3	0.17
(2,4)	1:57:R:LEU:N	1:53:R:LEU:O	5	0.17
(1,2320)	1:143:R:LEU:H	1:176:R:ASP:C	5	0.17
(1,2299)	1:162:R:ILE:H	1:151:R:PHE:C	3	0.17
(1,2228)	1:162:R:ILE:H	1:162:R:ILE:HA	2	0.17
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG21	3	0.17
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG22	3	0.17
(1,2197)	1:144:R:LYS:H	1:150:R:VAL:HG23	3	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2175)	1:125:R:CYS:H	1:125:R:CYS:HB2	1	0.17
(1,2164)	1:117:R:THR:H	1:117:R:THR:HA	4	0.17
(1,2136)	1:95:R:HIS:H	1:95:R:HIS:HA	3	0.17
(1,2136)	1:95:R:HIS:H	1:95:R:HIS:HA	5	0.17
(1,2116)	1:87:R:GLU:H	1:87:R:GLU:HA	2	0.17
(1,2046)	1:152:R:ALA:HB1	1:161:R:ALA:HB1	3	0.17
(1,2046)	1:152:R:ALA:HB1	1:161:R:ALA:HB2	3	0.17
(1,2046)	1:152:R:ALA:HB1	1:161:R:ALA:HB3	3	0.17
(1,2046)	1:152:R:ALA:HB2	1:161:R:ALA:HB1	3	0.17
(1,2046)	1:152:R:ALA:HB2	1:161:R:ALA:HB2	3	0.17
(1,2046)	1:152:R:ALA:HB2	1:161:R:ALA:HB3	3	0.17
(1,2046)	1:152:R:ALA:HB3	1:161:R:ALA:HB1	3	0.17
(1,2046)	1:152:R:ALA:HB3	1:161:R:ALA:HB2	3	0.17
(1,2046)	1:152:R:ALA:HB3	1:161:R:ALA:HB3	3	0.17
(1,2044)	1:155:R:THR:HG23	1:155:R:THR:HA	2	0.17
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG11	1	0.17
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG12	1	0.17
(1,2039)	1:154:R:VAL:HA	1:154:R:VAL:HG13	1	0.17
(1,2036)	1:161:R:ALA:HB1	1:152:R:ALA:HB1	3	0.17
(1,2036)	1:161:R:ALA:HB1	1:152:R:ALA:HB2	3	0.17
(1,2036)	1:161:R:ALA:HB1	1:152:R:ALA:HB3	3	0.17
(1,2036)	1:161:R:ALA:HB2	1:152:R:ALA:HB1	3	0.17
(1,2036)	1:161:R:ALA:HB2	1:152:R:ALA:HB2	3	0.17
(1,2036)	1:161:R:ALA:HB2	1:152:R:ALA:HB3	3	0.17
(1,2036)	1:161:R:ALA:HB3	1:152:R:ALA:HB1	3	0.17
(1,2036)	1:161:R:ALA:HB3	1:152:R:ALA:HB2	3	0.17
(1,2036)	1:161:R:ALA:HB3	1:152:R:ALA:HB3	3	0.17
(1,1997)	1:110:R:LEU:HD11	1:110:R:LEU:HA	3	0.17
(1,1997)	1:110:R:LEU:HD12	1:110:R:LEU:HA	3	0.17
(1,1997)	1:110:R:LEU:HD13	1:110:R:LEU:HA	3	0.17
(1,1997)	1:110:R:LEU:HD11	1:110:R:LEU:HA	4	0.17
(1,1997)	1:110:R:LEU:HD12	1:110:R:LEU:HA	4	0.17
(1,1997)	1:110:R:LEU:HD13	1:110:R:LEU:HA	4	0.17
(1,1964)	1:64:R:GLU:HA	1:64:R:GLU:HG3	4	0.17
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD11	1	0.17
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD12	1	0.17
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD13	1	0.17
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD21	1	0.17
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD22	1	0.17
(1,1935)	1:167:R:PHE:HD1	1:31:R:LEU:HD23	1	0.17
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD11	1	0.17
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD12	1	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD13	1	0.17
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD21	1	0.17
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD22	1	0.17
(1,1935)	1:167:R:PHE:HD2	1:31:R:LEU:HD23	1	0.17
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG21	3	0.17
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG22	3	0.17
(1,1881)	1:34:R:TYR:HB2	1:154:R:VAL:HG23	3	0.17
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG21	3	0.17
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG22	3	0.17
(1,1881)	1:34:R:TYR:HB3	1:154:R:VAL:HG23	3	0.17
(1,1792)	1:103:R:VAL:HA	1:103:R:VAL:HG11	5	0.17
(1,1792)	1:103:R:VAL:HA	1:103:R:VAL:HG12	5	0.17
(1,1792)	1:103:R:VAL:HA	1:103:R:VAL:HG13	5	0.17
(1,1788)	1:103:R:VAL:HG11	1:103:R:VAL:HA	5	0.17
(1,1788)	1:103:R:VAL:HG12	1:103:R:VAL:HA	5	0.17
(1,1788)	1:103:R:VAL:HG13	1:103:R:VAL:HA	5	0.17
(1,1714)	1:83:R:ILE:HG21	1:53:R:LEU:HD21	1	0.17
(1,1714)	1:83:R:ILE:HG21	1:53:R:LEU:HD22	1	0.17
(1,1714)	1:83:R:ILE:HG21	1:53:R:LEU:HD23	1	0.17
(1,1714)	1:83:R:ILE:HG22	1:53:R:LEU:HD21	1	0.17
(1,1714)	1:83:R:ILE:HG22	1:53:R:LEU:HD22	1	0.17
(1,1714)	1:83:R:ILE:HG22	1:53:R:LEU:HD23	1	0.17
(1,1714)	1:83:R:ILE:HG23	1:53:R:LEU:HD21	1	0.17
(1,1714)	1:83:R:ILE:HG23	1:53:R:LEU:HD22	1	0.17
(1,1714)	1:83:R:ILE:HG23	1:53:R:LEU:HD23	1	0.17
(1,1688)	1:191:R:GLU:H	1:191:R:GLU:HB3	4	0.17
(1,1608)	1:143:R:LEU:H	1:150:R:VAL:HG21	3	0.17
(1,1608)	1:143:R:LEU:H	1:150:R:VAL:HG22	3	0.17
(1,1608)	1:143:R:LEU:H	1:150:R:VAL:HG23	3	0.17
(1,1564)	1:123:R:GLU:H	1:114:R:GLY:H	5	0.17
(1,1547)	1:114:R:GLY:H	1:123:R:GLU:H	5	0.17
(1,1544)	1:114:R:GLY:H	1:113:R:THR:HB	1	0.17
(1,1503)	1:103:R:VAL:H	1:94:R:LEU:HD21	5	0.17
(1,1503)	1:103:R:VAL:H	1:94:R:LEU:HD22	5	0.17
(1,1503)	1:103:R:VAL:H	1:94:R:LEU:HD23	5	0.17
(1,1486)	1:87:R:GLU:H	1:83:R:ILE:HA	4	0.17
(1,1482)	1:85:R:GLN:H	1:83:R:ILE:HA	4	0.17
(1,1482)	1:85:R:GLN:H	1:83:R:ILE:HA	5	0.17
(1,1468)	1:81:R:GLU:H	1:79:R:THR:HB	4	0.17
(1,1421)	1:61:R:ARG:H	1:62:R:TYR:HD1	2	0.17
(1,1421)	1:61:R:ARG:H	1:62:R:TYR:HD2	2	0.17
(1,1376)	1:41:R:PHE:H	1:41:R:PHE:HZ	2	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1138)	1:126:R:VAL:H	1:126:R:VAL:HB	5	0.17
(1,1043)	1:104:R:ILE:H	1:101:R:ALA:HA	5	0.17
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD11	5	0.17
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD12	5	0.17
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD13	5	0.17
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD21	5	0.17
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD22	5	0.17
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD23	5	0.17
(1,1004)	1:90:R:THR:H	1:89:R:LEU:HB3	2	0.17
(1,941)	1:72:R:TYR:H	1:71:R:VAL:HG11	1	0.17
(1,941)	1:72:R:TYR:H	1:71:R:VAL:HG12	1	0.17
(1,941)	1:72:R:TYR:H	1:71:R:VAL:HG13	1	0.17
(1,793)	1:180:R:PHE:H	1:125:R:CYS:HB3	4	0.17
(1,700)	1:161:R:ALA:H	1:167:R:PHE:HA	1	0.17
(1,660)	1:153:R:CYS:H	1:155:R:THR:H	1	0.17
(1,594)	1:131:R:ASP:H	1:132:R:MET:H	5	0.17
(1,439)	1:95:R:HIS:H	1:94:R:LEU:HD21	1	0.17
(1,439)	1:95:R:HIS:H	1:94:R:LEU:HD22	1	0.17
(1,439)	1:95:R:HIS:H	1:94:R:LEU:HD23	1	0.17
(1,439)	1:95:R:HIS:H	1:94:R:LEU:HD21	4	0.17
(1,439)	1:95:R:HIS:H	1:94:R:LEU:HD22	4	0.17
(1,439)	1:95:R:HIS:H	1:94:R:LEU:HD23	4	0.17
(2,86)	1:52:R:TRP:O	1:56:R:ILE:N	2	0.16
(2,55)	1:180:R:PHE:O	1:125:R:CYS:N	1	0.16
(2,54)	1:116:R:GLY:N	1:124:R:VAL:O	3	0.16
(2,35)	1:85:R:GLN:O	1:89:R:LEU:H	3	0.16
(2,10)	1:60:R:PHE:N	1:56:R:ILE:O	1	0.16
(2,10)	1:60:R:PHE:N	1:56:R:ILE:O	2	0.16
(1,2315)	1:154:R:VAL:H	1:138:R:HIS:C	4	0.16
(1,2265)	1:57:R:LEU:H	1:53:R:LEU:C	4	0.16
(1,2243)	1:170:R:TRP:HA	1:170:R:TRP:HB3	4	0.16
(1,2195)	1:150:R:VAL:H	1:150:R:VAL:HG11	3	0.16
(1,2195)	1:150:R:VAL:H	1:150:R:VAL:HG12	3	0.16
(1,2195)	1:150:R:VAL:H	1:150:R:VAL:HG13	3	0.16
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB1	5	0.16
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB2	5	0.16
(1,2167)	1:119:R:SER:H	1:118:R:ALA:HB3	5	0.16
(1,2142)	1:103:R:VAL:H	1:103:R:VAL:HB	4	0.16
(1,2116)	1:87:R:GLU:H	1:87:R:GLU:HA	5	0.16
(1,2078)	1:52:R:TRP:H	1:52:R:TRP:HA	2	0.16
(1,2046)	1:152:R:ALA:HB1	1:161:R:ALA:HB1	1	0.16
(1,2046)	1:152:R:ALA:HB1	1:161:R:ALA:HB2	1	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2046)	1:152:R:ALA:HB1	1:161:R:ALA:HB3	1	0.16
(1,2046)	1:152:R:ALA:HB2	1:161:R:ALA:HB1	1	0.16
(1,2046)	1:152:R:ALA:HB2	1:161:R:ALA:HB2	1	0.16
(1,2046)	1:152:R:ALA:HB2	1:161:R:ALA:HB3	1	0.16
(1,2046)	1:152:R:ALA:HB3	1:161:R:ALA:HB1	1	0.16
(1,2046)	1:152:R:ALA:HB3	1:161:R:ALA:HB2	1	0.16
(1,2046)	1:152:R:ALA:HB3	1:161:R:ALA:HB3	1	0.16
(1,2036)	1:161:R:ALA:HB1	1:152:R:ALA:HB1	1	0.16
(1,2036)	1:161:R:ALA:HB1	1:152:R:ALA:HB2	1	0.16
(1,2036)	1:161:R:ALA:HB1	1:152:R:ALA:HB3	1	0.16
(1,2036)	1:161:R:ALA:HB2	1:152:R:ALA:HB1	1	0.16
(1,2036)	1:161:R:ALA:HB2	1:152:R:ALA:HB2	1	0.16
(1,2036)	1:161:R:ALA:HB2	1:152:R:ALA:HB3	1	0.16
(1,2036)	1:161:R:ALA:HB3	1:152:R:ALA:HB1	1	0.16
(1,2036)	1:161:R:ALA:HB3	1:152:R:ALA:HB2	1	0.16
(1,2036)	1:161:R:ALA:HB3	1:152:R:ALA:HB3	1	0.16
(1,1982)	1:90:R:THR:HB	1:90:R:THR:HG21	4	0.16
(1,1964)	1:64:R:GLU:HA	1:64:R:GLU:HG3	5	0.16
(1,1962)	1:124:R:VAL:HG11	1:63:R:VAL:HG21	1	0.16
(1,1962)	1:124:R:VAL:HG11	1:63:R:VAL:HG22	1	0.16
(1,1962)	1:124:R:VAL:HG11	1:63:R:VAL:HG23	1	0.16
(1,1962)	1:124:R:VAL:HG12	1:63:R:VAL:HG21	1	0.16
(1,1962)	1:124:R:VAL:HG12	1:63:R:VAL:HG22	1	0.16
(1,1962)	1:124:R:VAL:HG12	1:63:R:VAL:HG23	1	0.16
(1,1962)	1:124:R:VAL:HG13	1:63:R:VAL:HG21	1	0.16
(1,1962)	1:124:R:VAL:HG13	1:63:R:VAL:HG22	1	0.16
(1,1962)	1:124:R:VAL:HG13	1:63:R:VAL:HG23	1	0.16
(1,1908)	1:162:R:ILE:HG12	1:162:R:ILE:HG21	4	0.16
(1,1908)	1:162:R:ILE:HG12	1:162:R:ILE:HG22	4	0.16
(1,1908)	1:162:R:ILE:HG12	1:162:R:ILE:HG23	4	0.16
(1,1843)	1:128:R:ASP:H	1:127:R:VAL:HG21	2	0.16
(1,1843)	1:128:R:ASP:H	1:127:R:VAL:HG22	2	0.16
(1,1843)	1:128:R:ASP:H	1:127:R:VAL:HG23	2	0.16
(1,1827)	1:124:R:VAL:HG21	1:124:R:VAL:HA	3	0.16
(1,1827)	1:124:R:VAL:HG22	1:124:R:VAL:HA	3	0.16
(1,1827)	1:124:R:VAL:HG23	1:124:R:VAL:HA	3	0.16
(1,1817)	1:124:R:VAL:HG21	1:115:R:ILE:HG21	1	0.16
(1,1817)	1:124:R:VAL:HG21	1:115:R:ILE:HG22	1	0.16
(1,1817)	1:124:R:VAL:HG21	1:115:R:ILE:HG23	1	0.16
(1,1817)	1:124:R:VAL:HG22	1:115:R:ILE:HG21	1	0.16
(1,1817)	1:124:R:VAL:HG22	1:115:R:ILE:HG22	1	0.16
(1,1817)	1:124:R:VAL:HG22	1:115:R:ILE:HG23	1	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1817)	1:124:R:VAL:HG23	1:115:R:ILE:HG21	1	0.16
(1,1817)	1:124:R:VAL:HG23	1:115:R:ILE:HG22	1	0.16
(1,1817)	1:124:R:VAL:HG23	1:115:R:ILE:HG23	1	0.16
(1,1777)	1:83:R:ILE:HD11	1:95:R:HIS:HA	4	0.16
(1,1777)	1:83:R:ILE:HD12	1:95:R:HIS:HA	4	0.16
(1,1777)	1:83:R:ILE:HD13	1:95:R:HIS:HA	4	0.16
(1,1743)	1:70:R:TRP:HB2	1:70:R:TRP:HB3	1	0.16
(1,1743)	1:70:R:TRP:HB2	1:70:R:TRP:HB3	2	0.16
(1,1743)	1:70:R:TRP:HB2	1:70:R:TRP:HB3	3	0.16
(1,1743)	1:70:R:TRP:HB2	1:70:R:TRP:HB3	4	0.16
(1,1743)	1:70:R:TRP:HB2	1:70:R:TRP:HB3	5	0.16
(1,1742)	1:70:R:TRP:HB3	1:70:R:TRP:HB2	1	0.16
(1,1742)	1:70:R:TRP:HB3	1:70:R:TRP:HB2	2	0.16
(1,1742)	1:70:R:TRP:HB3	1:70:R:TRP:HB2	3	0.16
(1,1742)	1:70:R:TRP:HB3	1:70:R:TRP:HB2	4	0.16
(1,1742)	1:70:R:TRP:HB3	1:70:R:TRP:HB2	5	0.16
(1,1707)	1:53:R:LEU:HD21	1:53:R:LEU:HD11	5	0.16
(1,1707)	1:53:R:LEU:HD21	1:53:R:LEU:HD12	5	0.16
(1,1707)	1:53:R:LEU:HD21	1:53:R:LEU:HD13	5	0.16
(1,1707)	1:53:R:LEU:HD22	1:53:R:LEU:HD11	5	0.16
(1,1707)	1:53:R:LEU:HD22	1:53:R:LEU:HD12	5	0.16
(1,1707)	1:53:R:LEU:HD22	1:53:R:LEU:HD13	5	0.16
(1,1707)	1:53:R:LEU:HD23	1:53:R:LEU:HD11	5	0.16
(1,1707)	1:53:R:LEU:HD23	1:53:R:LEU:HD12	5	0.16
(1,1707)	1:53:R:LEU:HD23	1:53:R:LEU:HD13	5	0.16
(1,1580)	1:126:R:VAL:H	1:118:R:ALA:H	5	0.16
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD21	1	0.16
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD22	1	0.16
(1,1526)	1:109:R:HIS:H	1:110:R:LEU:HD23	1	0.16
(1,1503)	1:103:R:VAL:H	1:94:R:LEU:HD21	2	0.16
(1,1503)	1:103:R:VAL:H	1:94:R:LEU:HD22	2	0.16
(1,1503)	1:103:R:VAL:H	1:94:R:LEU:HD23	2	0.16
(1,1491)	1:90:R:THR:H	1:89:R:LEU:HG	1	0.16
(1,1177)	1:141:R:ILE:H	1:180:R:PHE:HB2	4	0.16
(1,1143)	1:128:R:ASP:H	1:118:R:ALA:H	1	0.16
(1,1115)	1:118:R:ALA:H	1:128:R:ASP:H	1	0.16
(1,1029)	1:97:R:GLY:H	1:49:R:ASP:HB2	1	0.16
(1,1004)	1:90:R:THR:H	1:89:R:LEU:HB3	5	0.16
(1,970)	1:80:R:LEU:H	1:83:R:ILE:HG13	5	0.16
(1,861)	1:51:R:ALA:H	1:49:R:ASP:HB2	1	0.16
(1,830)	1:40:R:THR:H	1:38:R:LYS:HA	2	0.16
(1,830)	1:40:R:THR:H	1:38:R:LYS:HA	3	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:153:R:CYS:H	1:155:R:THR:CG2	5	0.16
(1,358)	1:79:R:THR:H	1:78:R:LEU:H	2	0.16
(1,140)	1:166:R:ASP:H	1:163:R:ASP:HB2	2	0.16
(2,54)	1:116:R:GLY:N	1:124:R:VAL:O	2	0.15
(2,29)	1:82:R:ALA:O	1:86:R:LEU:H	5	0.15
(2,18)	1:68:R:PHE:O	1:72:R:TYR:N	5	0.15
(2,10)	1:60:R:PHE:N	1:56:R:ILE:O	3	0.15
(2,8)	1:59:R:LEU:N	1:55:R:ALA:O	5	0.15
(2,4)	1:57:R:LEU:N	1:53:R:LEU:O	4	0.15
(2,3)	1:57:R:LEU:H	1:53:R:LEU:O	4	0.15
(1,2245)	1:170:R:TRP:H	1:170:R:TRP:HB3	3	0.15
(1,2160)	1:112:R:HIS:H	1:112:R:HIS:HB2	3	0.15
(1,2071)	1:31:R:LEU:H	1:31:R:LEU:HG	4	0.15
(1,2046)	1:152:R:ALA:HB1	1:161:R:ALA:HB1	5	0.15
(1,2046)	1:152:R:ALA:HB1	1:161:R:ALA:HB2	5	0.15
(1,2046)	1:152:R:ALA:HB1	1:161:R:ALA:HB3	5	0.15
(1,2046)	1:152:R:ALA:HB2	1:161:R:ALA:HB1	5	0.15
(1,2046)	1:152:R:ALA:HB2	1:161:R:ALA:HB2	5	0.15
(1,2046)	1:152:R:ALA:HB2	1:161:R:ALA:HB3	5	0.15
(1,2046)	1:152:R:ALA:HB3	1:161:R:ALA:HB1	5	0.15
(1,2046)	1:152:R:ALA:HB3	1:161:R:ALA:HB2	5	0.15
(1,2046)	1:152:R:ALA:HB3	1:161:R:ALA:HB3	5	0.15
(1,2036)	1:161:R:ALA:HB1	1:152:R:ALA:HB1	5	0.15
(1,2036)	1:161:R:ALA:HB1	1:152:R:ALA:HB2	5	0.15
(1,2036)	1:161:R:ALA:HB1	1:152:R:ALA:HB3	5	0.15
(1,2036)	1:161:R:ALA:HB2	1:152:R:ALA:HB1	5	0.15
(1,2036)	1:161:R:ALA:HB2	1:152:R:ALA:HB2	5	0.15
(1,2036)	1:161:R:ALA:HB2	1:152:R:ALA:HB3	5	0.15
(1,2036)	1:161:R:ALA:HB3	1:152:R:ALA:HB1	5	0.15
(1,2036)	1:161:R:ALA:HB3	1:152:R:ALA:HB2	5	0.15
(1,2036)	1:161:R:ALA:HB3	1:152:R:ALA:HB3	5	0.15
(1,2031)	1:181:R:VAL:HB	1:139:R:ALA:HB1	5	0.15
(1,2031)	1:181:R:VAL:HB	1:139:R:ALA:HB2	5	0.15
(1,2031)	1:181:R:VAL:HB	1:139:R:ALA:HB3	5	0.15
(1,1982)	1:90:R:THR:HB	1:90:R:THR:HG21	2	0.15
(1,1976)	1:83:R:ILE:HG21	1:83:R:ILE:HG13	5	0.15
(1,1976)	1:83:R:ILE:HG22	1:83:R:ILE:HG13	5	0.15
(1,1976)	1:83:R:ILE:HG23	1:83:R:ILE:HG13	5	0.15
(1,1964)	1:64:R:GLU:HA	1:64:R:GLU:HG3	2	0.15
(1,1915)	1:159:R:TRP:HB2	1:171:R:THR:HA	4	0.15
(1,1913)	1:161:R:ALA:HB1	1:170:R:TRP:HB2	3	0.15
(1,1913)	1:161:R:ALA:HB2	1:170:R:TRP:HB2	3	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1913)	1:161:R:ALA:HB3	1:170:R:TRP:HB2	3	0.15
(1,1894)	1:170:R:TRP:HB2	1:161:R:ALA:HB1	3	0.15
(1,1894)	1:170:R:TRP:HB2	1:161:R:ALA:HB2	3	0.15
(1,1894)	1:170:R:TRP:HB2	1:161:R:ALA:HB3	3	0.15
(1,1757)	1:82:R:ALA:H	1:82:R:ALA:HB1	5	0.15
(1,1757)	1:82:R:ALA:H	1:82:R:ALA:HB2	5	0.15
(1,1757)	1:82:R:ALA:H	1:82:R:ALA:HB3	5	0.15
(1,1739)	1:69:R:ASP:H	1:68:R:PHE:HA	4	0.15
(1,1720)	1:103:R:VAL:HG21	1:56:R:ILE:HD11	2	0.15
(1,1720)	1:103:R:VAL:HG21	1:56:R:ILE:HD12	2	0.15
(1,1720)	1:103:R:VAL:HG21	1:56:R:ILE:HD13	2	0.15
(1,1720)	1:103:R:VAL:HG22	1:56:R:ILE:HD11	2	0.15
(1,1720)	1:103:R:VAL:HG22	1:56:R:ILE:HD12	2	0.15
(1,1720)	1:103:R:VAL:HG22	1:56:R:ILE:HD13	2	0.15
(1,1720)	1:103:R:VAL:HG23	1:56:R:ILE:HD11	2	0.15
(1,1720)	1:103:R:VAL:HG23	1:56:R:ILE:HD12	2	0.15
(1,1720)	1:103:R:VAL:HG23	1:56:R:ILE:HD13	2	0.15
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD11	1	0.15
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD12	1	0.15
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD13	1	0.15
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD11	1	0.15
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD12	1	0.15
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD13	1	0.15
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD11	1	0.15
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD12	1	0.15
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD13	1	0.15
(1,1707)	1:53:R:LEU:HD21	1:53:R:LEU:HD11	1	0.15
(1,1707)	1:53:R:LEU:HD21	1:53:R:LEU:HD12	1	0.15
(1,1707)	1:53:R:LEU:HD21	1:53:R:LEU:HD13	1	0.15
(1,1707)	1:53:R:LEU:HD22	1:53:R:LEU:HD11	1	0.15
(1,1707)	1:53:R:LEU:HD22	1:53:R:LEU:HD12	1	0.15
(1,1707)	1:53:R:LEU:HD22	1:53:R:LEU:HD13	1	0.15
(1,1707)	1:53:R:LEU:HD23	1:53:R:LEU:HD11	1	0.15
(1,1707)	1:53:R:LEU:HD23	1:53:R:LEU:HD12	1	0.15
(1,1707)	1:53:R:LEU:HD23	1:53:R:LEU:HD13	1	0.15
(1,1674)	1:175:R:SER:H	1:142:R:PHE:HD1	3	0.15
(1,1674)	1:175:R:SER:H	1:142:R:PHE:HD2	3	0.15
(1,1600)	1:139:R:ALA:H	1:180:R:PHE:HB2	4	0.15
(1,1595)	1:138:R:HIS:H	1:183:R:TYR:HE1	4	0.15
(1,1595)	1:138:R:HIS:H	1:183:R:TYR:HE2	4	0.15
(1,1580)	1:126:R:VAL:H	1:118:R:ALA:H	1	0.15
(1,1580)	1:126:R:VAL:H	1:118:R:ALA:H	2	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1352)	1:33:R:LEU:H	1:37:R:GLU:H	2	0.15
(1,1317)	1:179:R:VAL:H	1:180:R:PHE:HB2	3	0.15
(1,1210)	1:152:R:ALA:H	1:150:R:VAL:HB	5	0.15
(1,958)	1:78:R:LEU:H	1:78:R:LEU:HA	2	0.15
(1,840)	1:42:R:TYR:H	1:41:R:PHE:HB2	3	0.15
(1,659)	1:153:R:CYS:H	1:155:R:THR:CG2	1	0.15
(1,583)	1:129:R:GLY:H	1:128:R:ASP:HB2	4	0.15
(1,535)	1:117:R:THR:H	1:122:R:SER:H	3	0.15
(1,389)	1:84:R:LYS:H	1:83:R:ILE:HG12	5	0.15
(1,189)	1:36:R:GLY:H	1:35:R:ASN:HB3	3	0.15
(1,140)	1:166:R:ASP:H	1:163:R:ASP:HB2	5	0.15
(1,31)	1:83:R:ILE:H	1:83:R:ILE:HG12	3	0.15
(1,10)	1:43:R:SER:H	1:42:R:TYR:HB2	1	0.15
(2,87)	1:60:R:PHE:O	1:65:R:GLU:H	1	0.14
(2,86)	1:52:R:TRP:O	1:56:R:ILE:N	1	0.14
(2,78)	1:163:R:ASP:O	1:166:R:ASP:H	4	0.14
(2,34)	1:88:R:ASP:N	1:84:R:LYS:O	2	0.14
(2,33)	1:88:R:ASP:H	1:84:R:LYS:O	1	0.14
(2,29)	1:82:R:ALA:O	1:86:R:LEU:H	2	0.14
(2,18)	1:68:R:PHE:O	1:72:R:TYR:N	3	0.14
(2,4)	1:57:R:LEU:N	1:53:R:LEU:O	1	0.14
(1,2319)	1:142:R:PHE:C	1:150:R:VAL:H	1	0.14
(1,2305)	1:52:R:TRP:C	1:56:R:ILE:H	5	0.14
(1,2265)	1:57:R:LEU:H	1:53:R:LEU:C	2	0.14
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG21	1	0.14
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG22	1	0.14
(1,2254)	1:127:R:VAL:HG11	1:177:R:VAL:HG23	1	0.14
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG21	1	0.14
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG22	1	0.14
(1,2254)	1:127:R:VAL:HG12	1:177:R:VAL:HG23	1	0.14
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG21	1	0.14
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG22	1	0.14
(1,2254)	1:127:R:VAL:HG13	1:177:R:VAL:HG23	1	0.14
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG21	1	0.14
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG22	1	0.14
(1,2254)	1:127:R:VAL:HG21	1:177:R:VAL:HG23	1	0.14
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG21	1	0.14
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG22	1	0.14
(1,2254)	1:127:R:VAL:HG22	1:177:R:VAL:HG23	1	0.14
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG21	1	0.14
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG22	1	0.14
(1,2254)	1:127:R:VAL:HG23	1:177:R:VAL:HG23	1	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2222)	1:158:R:GLY:HA2	1:159:R:TRP:HB3	4	0.14
(1,2221)	1:156:R:SER:H	1:155:R:THR:HA	4	0.14
(1,2205)	1:153:R:CYS:HB3	1:153:R:CYS:HA	2	0.14
(1,2174)	1:125:R:CYS:H	1:125:R:CYS:HB3	3	0.14
(1,2116)	1:87:R:GLU:H	1:87:R:GLU:HA	3	0.14
(1,2116)	1:87:R:GLU:H	1:87:R:GLU:HA	4	0.14
(1,2078)	1:52:R:TRP:H	1:52:R:TRP:HA	1	0.14
(1,2078)	1:52:R:TRP:H	1:52:R:TRP:HA	4	0.14
(1,2060)	1:177:R:VAL:H	1:177:R:VAL:HG11	5	0.14
(1,2060)	1:177:R:VAL:H	1:177:R:VAL:HG12	5	0.14
(1,2060)	1:177:R:VAL:H	1:177:R:VAL:HG13	5	0.14
(1,2019)	1:178:R:LEU:HD11	1:127:R:VAL:HG21	4	0.14
(1,2019)	1:178:R:LEU:HD11	1:127:R:VAL:HG22	4	0.14
(1,2019)	1:178:R:LEU:HD11	1:127:R:VAL:HG23	4	0.14
(1,2019)	1:178:R:LEU:HD12	1:127:R:VAL:HG21	4	0.14
(1,2019)	1:178:R:LEU:HD12	1:127:R:VAL:HG22	4	0.14
(1,2019)	1:178:R:LEU:HD12	1:127:R:VAL:HG23	4	0.14
(1,2019)	1:178:R:LEU:HD13	1:127:R:VAL:HG21	4	0.14
(1,2019)	1:178:R:LEU:HD13	1:127:R:VAL:HG22	4	0.14
(1,2019)	1:178:R:LEU:HD13	1:127:R:VAL:HG23	4	0.14
(1,2019)	1:178:R:LEU:HD21	1:127:R:VAL:HG21	4	0.14
(1,2019)	1:178:R:LEU:HD21	1:127:R:VAL:HG22	4	0.14
(1,2019)	1:178:R:LEU:HD21	1:127:R:VAL:HG23	4	0.14
(1,2019)	1:178:R:LEU:HD22	1:127:R:VAL:HG21	4	0.14
(1,2019)	1:178:R:LEU:HD22	1:127:R:VAL:HG22	4	0.14
(1,2019)	1:178:R:LEU:HD22	1:127:R:VAL:HG23	4	0.14
(1,2019)	1:178:R:LEU:HD23	1:127:R:VAL:HG21	4	0.14
(1,2019)	1:178:R:LEU:HD23	1:127:R:VAL:HG22	4	0.14
(1,2019)	1:178:R:LEU:HD23	1:127:R:VAL:HG23	4	0.14
(1,2005)	1:115:R:ILE:HD11	1:113:R:THR:HG22	5	0.14
(1,1995)	1:103:R:VAL:HA	1:103:R:VAL:HG21	1	0.14
(1,1995)	1:103:R:VAL:HA	1:103:R:VAL:HG22	1	0.14
(1,1995)	1:103:R:VAL:HA	1:103:R:VAL:HG23	1	0.14
(1,1990)	1:103:R:VAL:HG21	1:103:R:VAL:HA	1	0.14
(1,1990)	1:103:R:VAL:HG22	1:103:R:VAL:HA	1	0.14
(1,1990)	1:103:R:VAL:HG23	1:103:R:VAL:HA	1	0.14
(1,1913)	1:161:R:ALA:HB1	1:170:R:TRP:HB2	5	0.14
(1,1913)	1:161:R:ALA:HB2	1:170:R:TRP:HB2	5	0.14
(1,1913)	1:161:R:ALA:HB3	1:170:R:TRP:HB2	5	0.14
(1,1894)	1:170:R:TRP:HB2	1:161:R:ALA:HB1	5	0.14
(1,1894)	1:170:R:TRP:HB2	1:161:R:ALA:HB2	5	0.14
(1,1894)	1:170:R:TRP:HB2	1:161:R:ALA:HB3	5	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1837)	1:126:R:VAL:H	1:126:R:VAL:HG21	3	0.14
(1,1837)	1:126:R:VAL:H	1:126:R:VAL:HG22	3	0.14
(1,1837)	1:126:R:VAL:H	1:126:R:VAL:HG23	3	0.14
(1,1719)	1:56:R:ILE:H	1:56:R:ILE:HD11	4	0.14
(1,1719)	1:56:R:ILE:H	1:56:R:ILE:HD12	4	0.14
(1,1719)	1:56:R:ILE:H	1:56:R:ILE:HD13	4	0.14
(1,1712)	1:53:R:LEU:HA	1:53:R:LEU:HD21	3	0.14
(1,1712)	1:53:R:LEU:HA	1:53:R:LEU:HD22	3	0.14
(1,1712)	1:53:R:LEU:HA	1:53:R:LEU:HD23	3	0.14
(1,1689)	1:194:R:ALA:H	1:193:R:LYS:HB3	2	0.14
(1,1641)	1:160:R:TYR:H	1:154:R:VAL:HG21	1	0.14
(1,1641)	1:160:R:TYR:H	1:154:R:VAL:HG22	1	0.14
(1,1641)	1:160:R:TYR:H	1:154:R:VAL:HG23	1	0.14
(1,1626)	1:153:R:CYS:H	1:139:R:ALA:H	4	0.14
(1,1626)	1:153:R:CYS:H	1:139:R:ALA:H	5	0.14
(1,1583)	1:127:R:VAL:H	1:180:R:PHE:H	2	0.14
(1,1488)	1:87:R:GLU:H	1:94:R:LEU:HD21	5	0.14
(1,1488)	1:87:R:GLU:H	1:94:R:LEU:HD22	5	0.14
(1,1488)	1:87:R:GLU:H	1:94:R:LEU:HD23	5	0.14
(1,1487)	1:87:R:GLU:H	1:85:R:GLN:H	3	0.14
(1,1484)	1:85:R:GLN:H	1:87:R:GLU:H	3	0.14
(1,1482)	1:85:R:GLN:H	1:83:R:ILE:HA	3	0.14
(1,1414)	1:60:R:PHE:H	1:57:R:LEU:HD11	3	0.14
(1,1414)	1:60:R:PHE:H	1:57:R:LEU:HD12	3	0.14
(1,1414)	1:60:R:PHE:H	1:57:R:LEU:HD13	3	0.14
(1,1414)	1:60:R:PHE:H	1:57:R:LEU:HD21	3	0.14
(1,1414)	1:60:R:PHE:H	1:57:R:LEU:HD22	3	0.14
(1,1414)	1:60:R:PHE:H	1:57:R:LEU:HD23	3	0.14
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD11	5	0.14
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD12	5	0.14
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD13	5	0.14
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD21	5	0.14
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD22	5	0.14
(1,1404)	1:54:R:ASN:H	1:57:R:LEU:HD23	5	0.14
(1,1401)	1:54:R:ASN:H	1:52:R:TRP:H	4	0.14
(1,1382)	1:43:R:SER:H	1:42:R:TYR:HD1	2	0.14
(1,1382)	1:43:R:SER:H	1:42:R:TYR:HD2	2	0.14
(1,1346)	1:32:R:THR:H	1:38:R:LYS:HA	4	0.14
(1,1059)	1:107:R:ILE:H	1:105:R:TRP:HB2	5	0.14
(1,1025)	1:95:R:HIS:H	1:94:R:LEU:HD11	5	0.14
(1,1025)	1:95:R:HIS:H	1:94:R:LEU:HD12	5	0.14
(1,1025)	1:95:R:HIS:H	1:94:R:LEU:HD13	5	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	1:90:R:THR:H	1:89:R:LEU:HB2	3	0.14
(1,982)	1:83:R:ILE:H	1:53:R:LEU:HD11	1	0.14
(1,982)	1:83:R:ILE:H	1:53:R:LEU:HD12	1	0.14
(1,982)	1:83:R:ILE:H	1:53:R:LEU:HD13	1	0.14
(1,849)	1:46:R:ASN:H	1:44:R:ARG:H	2	0.14
(1,773)	1:181:R:VAL:H	1:180:R:PHE:HE1	3	0.14
(1,773)	1:181:R:VAL:H	1:180:R:PHE:HE2	3	0.14
(1,695)	1:160:R:TYR:H	1:158:R:GLY:HA2	1	0.14
(1,695)	1:160:R:TYR:H	1:158:R:GLY:HA3	1	0.14
(1,689)	1:159:R:TRP:H	1:155:R:THR:H	2	0.14
(1,443)	1:97:R:GLY:H	1:52:R:TRP:HE1	4	0.14
(1,216)	1:42:R:TYR:H	1:42:R:TYR:HE1	4	0.14
(1,216)	1:42:R:TYR:H	1:42:R:TYR:HE2	4	0.14
(2,109)	1:140:R:GLY:H	1:152:R:ALA:O	1	0.13
(2,97)	1:104:R:ILE:H	1:100:R:PRO:O	1	0.13
(2,75)	1:163:R:ASP:N	1:166:R:ASP:O	3	0.13
(2,63)	1:140:R:GLY:H	1:152:R:ALA:O	1	0.13
(2,60)	1:141:R:ILE:N	1:179:R:VAL:O	2	0.13
(2,60)	1:141:R:ILE:N	1:179:R:VAL:O	4	0.13
(2,55)	1:180:R:PHE:O	1:125:R:CYS:N	2	0.13
(2,33)	1:88:R:ASP:H	1:84:R:LYS:O	4	0.13
(2,20)	1:69:R:ASP:O	1:73:R:SER:N	5	0.13
(2,12)	1:61:R:ARG:N	1:57:R:LEU:O	2	0.13
(2,11)	1:61:R:ARG:H	1:57:R:LEU:O	4	0.13
(2,7)	1:59:R:LEU:H	1:55:R:ALA:O	2	0.13
(2,3)	1:57:R:LEU:H	1:53:R:LEU:O	1	0.13
(2,3)	1:57:R:LEU:H	1:53:R:LEU:O	5	0.13
(1,2317)	1:140:R:GLY:H	1:152:R:ALA:C	4	0.13
(1,2307)	1:50:R:ASN:C	1:54:R:ASN:H	4	0.13
(1,2294)	1:140:R:GLY:H	1:152:R:ALA:C	4	0.13
(1,2292)	1:141:R:ILE:H	1:179:R:VAL:C	4	0.13
(1,2289)	1:116:R:GLY:H	1:124:R:VAL:C	5	0.13
(1,2287)	1:31:R:LEU:C	1:39:R:LYS:H	5	0.13
(1,2280)	1:85:R:GLN:C	1:89:R:LEU:H	3	0.13
(1,2268)	1:61:R:ARG:H	1:57:R:LEU:C	4	0.13
(1,2264)	1:51:R:ALA:C	1:55:R:ALA:H	3	0.13
(1,2228)	1:162:R:ILE:H	1:162:R:ILE:HA	5	0.13
(1,2181)	1:134:R:LEU:H	1:134:R:LEU:HA	4	0.13
(1,2156)	1:111:R:LEU:HB2	1:112:R:HIS:HB3	3	0.13
(1,2133)	1:94:R:LEU:HB2	1:94:R:LEU:HG	5	0.13
(1,2078)	1:52:R:TRP:H	1:52:R:TRP:HA	3	0.13
(1,2078)	1:52:R:TRP:H	1:52:R:TRP:HA	5	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2072)	1:41:R:PHE:HD1	1:31:R:LEU:HG	5	0.13
(1,2072)	1:41:R:PHE:HD2	1:31:R:LEU:HG	5	0.13
(1,2060)	1:177:R:VAL:H	1:177:R:VAL:HG11	4	0.13
(1,2060)	1:177:R:VAL:H	1:177:R:VAL:HG12	4	0.13
(1,2060)	1:177:R:VAL:H	1:177:R:VAL:HG13	4	0.13
(1,2044)	1:155:R:THR:HG23	1:155:R:THR:HA	3	0.13
(1,2041)	1:34:R:TYR:HB2	1:154:R:VAL:HG11	1	0.13
(1,2041)	1:34:R:TYR:HB2	1:154:R:VAL:HG12	1	0.13
(1,2041)	1:34:R:TYR:HB2	1:154:R:VAL:HG13	1	0.13
(1,2041)	1:34:R:TYR:HB3	1:154:R:VAL:HG11	1	0.13
(1,2041)	1:34:R:TYR:HB3	1:154:R:VAL:HG12	1	0.13
(1,2041)	1:34:R:TYR:HB3	1:154:R:VAL:HG13	1	0.13
(1,2041)	1:34:R:TYR:HB2	1:154:R:VAL:HG11	2	0.13
(1,2041)	1:34:R:TYR:HB2	1:154:R:VAL:HG12	2	0.13
(1,2041)	1:34:R:TYR:HB2	1:154:R:VAL:HG13	2	0.13
(1,2041)	1:34:R:TYR:HB3	1:154:R:VAL:HG11	2	0.13
(1,2041)	1:34:R:TYR:HB3	1:154:R:VAL:HG12	2	0.13
(1,2041)	1:34:R:TYR:HB3	1:154:R:VAL:HG13	2	0.13
(1,1997)	1:110:R:LEU:HD11	1:110:R:LEU:HA	2	0.13
(1,1997)	1:110:R:LEU:HD12	1:110:R:LEU:HA	2	0.13
(1,1997)	1:110:R:LEU:HD13	1:110:R:LEU:HA	2	0.13
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG21	1	0.13
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG22	1	0.13
(1,1953)	1:56:R:ILE:HD11	1:56:R:ILE:HG23	1	0.13
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG21	1	0.13
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG22	1	0.13
(1,1953)	1:56:R:ILE:HD12	1:56:R:ILE:HG23	1	0.13
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG21	1	0.13
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG22	1	0.13
(1,1953)	1:56:R:ILE:HD13	1:56:R:ILE:HG23	1	0.13
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG21	4	0.13
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG22	4	0.13
(1,1928)	1:177:R:VAL:H	1:177:R:VAL:HG23	4	0.13
(1,1907)	1:162:R:ILE:HG13	1:162:R:ILE:HG21	1	0.13
(1,1907)	1:162:R:ILE:HG13	1:162:R:ILE:HG22	1	0.13
(1,1907)	1:162:R:ILE:HG13	1:162:R:ILE:HG23	1	0.13
(1,1848)	1:134:R:LEU:HD21	1:134:R:LEU:HA	1	0.13
(1,1848)	1:134:R:LEU:HD22	1:134:R:LEU:HA	1	0.13
(1,1848)	1:134:R:LEU:HD23	1:134:R:LEU:HA	1	0.13
(1,1827)	1:124:R:VAL:HG21	1:124:R:VAL:HA	2	0.13
(1,1827)	1:124:R:VAL:HG22	1:124:R:VAL:HA	2	0.13
(1,1827)	1:124:R:VAL:HG23	1:124:R:VAL:HA	2	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1794)	1:107:R:ILE:HD11	1:103:R:VAL:HG11	2	0.13
(1,1794)	1:107:R:ILE:HD11	1:103:R:VAL:HG12	2	0.13
(1,1794)	1:107:R:ILE:HD11	1:103:R:VAL:HG13	2	0.13
(1,1794)	1:107:R:ILE:HD12	1:103:R:VAL:HG11	2	0.13
(1,1794)	1:107:R:ILE:HD12	1:103:R:VAL:HG12	2	0.13
(1,1794)	1:107:R:ILE:HD12	1:103:R:VAL:HG13	2	0.13
(1,1794)	1:107:R:ILE:HD13	1:103:R:VAL:HG11	2	0.13
(1,1794)	1:107:R:ILE:HD13	1:103:R:VAL:HG12	2	0.13
(1,1794)	1:107:R:ILE:HD13	1:103:R:VAL:HG13	2	0.13
(1,1759)	1:83:R:ILE:HG21	1:83:R:ILE:HA	2	0.13
(1,1759)	1:83:R:ILE:HG22	1:83:R:ILE:HA	2	0.13
(1,1759)	1:83:R:ILE:HG23	1:83:R:ILE:HA	2	0.13
(1,1729)	1:59:R:LEU:HA	1:59:R:LEU:HD11	2	0.13
(1,1729)	1:59:R:LEU:HA	1:59:R:LEU:HD12	2	0.13
(1,1729)	1:59:R:LEU:HA	1:59:R:LEU:HD13	2	0.13
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD11	3	0.13
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD12	3	0.13
(1,1710)	1:83:R:ILE:HD11	1:53:R:LEU:HD13	3	0.13
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD11	3	0.13
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD12	3	0.13
(1,1710)	1:83:R:ILE:HD12	1:53:R:LEU:HD13	3	0.13
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD11	3	0.13
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD12	3	0.13
(1,1710)	1:83:R:ILE:HD13	1:53:R:LEU:HD13	3	0.13
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB1	2	0.13
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB2	2	0.13
(1,1700)	1:50:R:ASN:H	1:51:R:ALA:HB3	2	0.13
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD11	2	0.13
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD12	2	0.13
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD13	2	0.13
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD21	2	0.13
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD22	2	0.13
(1,1692)	1:41:R:PHE:HD1	1:31:R:LEU:HD23	2	0.13
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD11	2	0.13
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD12	2	0.13
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD13	2	0.13
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD21	2	0.13
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD22	2	0.13
(1,1692)	1:41:R:PHE:HD2	1:31:R:LEU:HD23	2	0.13
(1,1499)	1:95:R:HIS:H	1:97:R:GLY:H	3	0.13
(1,1487)	1:87:R:GLU:H	1:85:R:GLN:H	5	0.13
(1,1484)	1:85:R:GLN:H	1:87:R:GLU:H	5	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1472)	1:82:R:ALA:H	1:71:R:VAL:HG21	5	0.13
(1,1472)	1:82:R:ALA:H	1:71:R:VAL:HG22	5	0.13
(1,1472)	1:82:R:ALA:H	1:71:R:VAL:HG23	5	0.13
(1,1368)	1:37:R:GLU:H	1:34:R:TYR:H	1	0.13
(1,1365)	1:36:R:GLY:H	1:33:R:LEU:H	1	0.13
(1,1363)	1:35:R:ASN:H	1:155:R:THR:HA	3	0.13
(1,1352)	1:33:R:LEU:H	1:37:R:GLU:H	1	0.13
(1,1351)	1:33:R:LEU:H	1:36:R:GLY:H	1	0.13
(1,1346)	1:32:R:THR:H	1:38:R:LYS:HA	5	0.13
(1,1189)	1:144:R:LYS:H	1:149:R:ALA:H	4	0.13
(1,1128)	1:124:R:VAL:H	1:181:R:VAL:HA	3	0.13
(1,1001)	1:87:R:GLU:H	1:94:R:LEU:H	3	0.13
(1,742)	1:177:R:VAL:H	1:175:R:SER:HA	4	0.13
(1,594)	1:131:R:ASP:H	1:132:R:MET:H	2	0.13
(1,424)	1:92:R:LEU:H	1:90:R:THR:HA	1	0.13
(1,192)	1:37:R:GLU:H	1:35:R:ASN:H	4	0.13
(1,192)	1:37:R:GLU:H	1:35:R:ASN:H	5	0.13
(2,98)	1:104:R:ILE:N	1:100:R:PRO:O	4	0.12
(2,95)	1:91:R:GLY:H	1:87:R:GLU:O	2	0.12
(2,54)	1:116:R:GLY:N	1:124:R:VAL:O	1	0.12
(2,39)	1:87:R:GLU:O	1:91:R:GLY:H	2	0.12
(2,38)	1:86:R:LEU:O	1:90:R:THR:N	2	0.12
(2,12)	1:61:R:ARG:N	1:57:R:LEU:O	5	0.12
(1,2319)	1:142:R:PHE:C	1:150:R:VAL:H	4	0.12
(1,2317)	1:140:R:GLY:H	1:152:R:ALA:C	2	0.12
(1,2294)	1:140:R:GLY:H	1:152:R:ALA:C	2	0.12
(1,2285)	1:29:R:MET:C	1:41:R:PHE:H	3	0.12
(1,2268)	1:61:R:ARG:H	1:57:R:LEU:C	5	0.12
(1,2265)	1:57:R:LEU:H	1:53:R:LEU:C	1	0.12
(1,2265)	1:57:R:LEU:H	1:53:R:LEU:C	5	0.12
(1,2250)	1:177:R:VAL:HG11	1:177:R:VAL:HA	4	0.12
(1,2250)	1:177:R:VAL:HG12	1:177:R:VAL:HA	4	0.12
(1,2250)	1:177:R:VAL:HG13	1:177:R:VAL:HA	4	0.12
(1,2233)	1:162:R:ILE:HA	1:162:R:ILE:HG13	1	0.12
(1,2226)	1:162:R:ILE:HG13	1:162:R:ILE:HA	1	0.12
(1,2221)	1:156:R:SER:H	1:155:R:THR:HA	3	0.12
(1,2137)	1:95:R:HIS:H	1:95:R:HIS:HB3	2	0.12
(1,2116)	1:87:R:GLU:H	1:87:R:GLU:HA	1	0.12
(1,2058)	1:142:R:PHE:HD1	1:177:R:VAL:HG11	5	0.12
(1,2058)	1:142:R:PHE:HD1	1:177:R:VAL:HG12	5	0.12
(1,2058)	1:142:R:PHE:HD1	1:177:R:VAL:HG13	5	0.12
(1,2058)	1:142:R:PHE:HD2	1:177:R:VAL:HG11	5	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2058)	1:142:R:PHE:HD2	1:177:R:VAL:HG12	5	0.12
(1,2058)	1:142:R:PHE:HD2	1:177:R:VAL:HG13	5	0.12
(1,1995)	1:103:R:VAL:HA	1:103:R:VAL:HG21	2	0.12
(1,1995)	1:103:R:VAL:HA	1:103:R:VAL:HG22	2	0.12
(1,1995)	1:103:R:VAL:HA	1:103:R:VAL:HG23	2	0.12
(1,1990)	1:103:R:VAL:HG21	1:103:R:VAL:HA	2	0.12
(1,1990)	1:103:R:VAL:HG22	1:103:R:VAL:HA	2	0.12
(1,1990)	1:103:R:VAL:HG23	1:103:R:VAL:HA	2	0.12
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB1	4	0.12
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB2	4	0.12
(1,1973)	1:71:R:VAL:HG21	1:82:R:ALA:HB3	4	0.12
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB1	4	0.12
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB2	4	0.12
(1,1973)	1:71:R:VAL:HG22	1:82:R:ALA:HB3	4	0.12
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB1	4	0.12
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB2	4	0.12
(1,1973)	1:71:R:VAL:HG23	1:82:R:ALA:HB3	4	0.12
(1,1954)	1:56:R:ILE:HG13	1:56:R:ILE:HG21	2	0.12
(1,1954)	1:56:R:ILE:HG13	1:56:R:ILE:HG22	2	0.12
(1,1954)	1:56:R:ILE:HG13	1:56:R:ILE:HG23	2	0.12
(1,1944)	1:82:R:ALA:HB1	1:53:R:LEU:HD11	1	0.12
(1,1944)	1:82:R:ALA:HB1	1:53:R:LEU:HD12	1	0.12
(1,1944)	1:82:R:ALA:HB1	1:53:R:LEU:HD13	1	0.12
(1,1944)	1:82:R:ALA:HB2	1:53:R:LEU:HD11	1	0.12
(1,1944)	1:82:R:ALA:HB2	1:53:R:LEU:HD12	1	0.12
(1,1944)	1:82:R:ALA:HB2	1:53:R:LEU:HD13	1	0.12
(1,1944)	1:82:R:ALA:HB3	1:53:R:LEU:HD11	1	0.12
(1,1944)	1:82:R:ALA:HB3	1:53:R:LEU:HD12	1	0.12
(1,1944)	1:82:R:ALA:HB3	1:53:R:LEU:HD13	1	0.12
(1,1884)	1:154:R:VAL:H	1:154:R:VAL:HG21	4	0.12
(1,1884)	1:154:R:VAL:H	1:154:R:VAL:HG22	4	0.12
(1,1884)	1:154:R:VAL:H	1:154:R:VAL:HG23	4	0.12
(1,1852)	1:134:R:LEU:HD11	1:134:R:LEU:HG	3	0.12
(1,1852)	1:134:R:LEU:HD12	1:134:R:LEU:HG	3	0.12
(1,1852)	1:134:R:LEU:HD13	1:134:R:LEU:HG	3	0.12
(1,1852)	1:134:R:LEU:HD21	1:134:R:LEU:HG	3	0.12
(1,1852)	1:134:R:LEU:HD22	1:134:R:LEU:HG	3	0.12
(1,1852)	1:134:R:LEU:HD23	1:134:R:LEU:HG	3	0.12
(1,1852)	1:134:R:LEU:HD11	1:134:R:LEU:HG	4	0.12
(1,1852)	1:134:R:LEU:HD12	1:134:R:LEU:HG	4	0.12
(1,1852)	1:134:R:LEU:HD13	1:134:R:LEU:HG	4	0.12
(1,1852)	1:134:R:LEU:HD21	1:134:R:LEU:HG	4	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1852)	1:134:R:LEU:HD22	1:134:R:LEU:HG	4	0.12
(1,1852)	1:134:R:LEU:HD23	1:134:R:LEU:HG	4	0.12
(1,1848)	1:134:R:LEU:HD21	1:134:R:LEU:HA	4	0.12
(1,1848)	1:134:R:LEU:HD22	1:134:R:LEU:HA	4	0.12
(1,1848)	1:134:R:LEU:HD23	1:134:R:LEU:HA	4	0.12
(1,1842)	1:127:R:VAL:HA	1:127:R:VAL:HG21	5	0.12
(1,1842)	1:127:R:VAL:HA	1:127:R:VAL:HG22	5	0.12
(1,1842)	1:127:R:VAL:HA	1:127:R:VAL:HG23	5	0.12
(1,1792)	1:103:R:VAL:HA	1:103:R:VAL:HG11	4	0.12
(1,1792)	1:103:R:VAL:HA	1:103:R:VAL:HG12	4	0.12
(1,1792)	1:103:R:VAL:HA	1:103:R:VAL:HG13	4	0.12
(1,1788)	1:103:R:VAL:HG11	1:103:R:VAL:HA	4	0.12
(1,1788)	1:103:R:VAL:HG12	1:103:R:VAL:HA	4	0.12
(1,1788)	1:103:R:VAL:HG13	1:103:R:VAL:HA	4	0.12
(1,1763)	1:83:R:ILE:HG21	1:83:R:ILE:HG12	2	0.12
(1,1763)	1:83:R:ILE:HG22	1:83:R:ILE:HG12	2	0.12
(1,1763)	1:83:R:ILE:HG23	1:83:R:ILE:HG12	2	0.12
(1,1713)	1:53:R:LEU:HB2	1:53:R:LEU:HD21	2	0.12
(1,1713)	1:53:R:LEU:HB2	1:53:R:LEU:HD22	2	0.12
(1,1713)	1:53:R:LEU:HB2	1:53:R:LEU:HD23	2	0.12
(1,1713)	1:53:R:LEU:HB2	1:53:R:LEU:HD21	5	0.12
(1,1713)	1:53:R:LEU:HB2	1:53:R:LEU:HD22	5	0.12
(1,1713)	1:53:R:LEU:HB2	1:53:R:LEU:HD23	5	0.12
(1,1691)	1:31:R:LEU:HB3	1:31:R:LEU:HD11	1	0.12
(1,1691)	1:31:R:LEU:HB3	1:31:R:LEU:HD12	1	0.12
(1,1691)	1:31:R:LEU:HB3	1:31:R:LEU:HD13	1	0.12
(1,1691)	1:31:R:LEU:HB3	1:31:R:LEU:HD21	1	0.12
(1,1691)	1:31:R:LEU:HB3	1:31:R:LEU:HD22	1	0.12
(1,1691)	1:31:R:LEU:HB3	1:31:R:LEU:HD23	1	0.12
(1,1681)	1:179:R:VAL:H	1:180:R:PHE:H	1	0.12
(1,1668)	1:170:R:TRP:H	1:160:R:TYR:H	4	0.12
(1,1643)	1:160:R:TYR:H	1:170:R:TRP:H	4	0.12
(1,1535)	1:111:R:LEU:H	1:109:R:HIS:H	2	0.12
(1,1529)	1:110:R:LEU:H	1:109:R:HIS:HB3	4	0.12
(1,1527)	1:109:R:HIS:H	1:111:R:LEU:H	2	0.12
(1,1487)	1:87:R:GLU:H	1:85:R:GLN:H	2	0.12
(1,1486)	1:87:R:GLU:H	1:83:R:ILE:HA	5	0.12
(1,1484)	1:85:R:GLN:H	1:87:R:GLU:H	2	0.12
(1,1401)	1:54:R:ASN:H	1:52:R:TRP:H	1	0.12
(1,1387)	1:46:R:ASN:H	1:44:R:ARG:H	3	0.12
(1,1150)	1:130:R:THR:H	1:128:R:ASP:HB2	3	0.12
(1,982)	1:83:R:ILE:H	1:53:R:LEU:HD11	4	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,982)	1:83:R:ILE:H	1:53:R:LEU:HD12	4	0.12
(1,982)	1:83:R:ILE:H	1:53:R:LEU:HD13	4	0.12
(1,958)	1:78:R:LEU:H	1:78:R:LEU:HA	3	0.12
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD11	4	0.12
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD12	4	0.12
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD13	4	0.12
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD21	4	0.12
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD22	4	0.12
(1,939)	1:72:R:TYR:H	1:57:R:LEU:HD23	4	0.12
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD11	3	0.12
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD12	3	0.12
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD13	3	0.12
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD21	3	0.12
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD22	3	0.12
(1,833)	1:41:R:PHE:H	1:31:R:LEU:HD23	3	0.12
(1,818)	1:36:R:GLY:H	1:34:R:TYR:H	4	0.12
(1,778)	1:183:R:TYR:H	1:137:R:PHE:HA	2	0.12
(1,689)	1:159:R:TRP:H	1:155:R:THR:H	4	0.12
(1,656)	1:152:R:ALA:H	1:153:R:CYS:H	2	0.12
(1,608)	1:139:R:ALA:H	1:181:R:VAL:HG11	3	0.12
(1,608)	1:139:R:ALA:H	1:181:R:VAL:HG12	3	0.12
(1,608)	1:139:R:ALA:H	1:181:R:VAL:HG13	3	0.12
(1,512)	1:113:R:THR:H	1:112:R:HIS:HB2	3	0.12
(1,52)	1:95:R:HIS:H	1:94:R:LEU:H	1	0.12
(2,100)	1:103:R:VAL:H	1:99:R:PRO:O	2	0.11
(2,92)	1:66:R:PRO:O	1:69:R:ASP:N	2	0.11
(2,87)	1:60:R:PHE:O	1:65:R:GLU:H	3	0.11
(2,77)	1:163:R:ASP:O	1:166:R:ASP:N	4	0.11
(2,35)	1:85:R:GLN:O	1:89:R:LEU:H	5	0.11
(2,30)	1:82:R:ALA:O	1:86:R:LEU:N	5	0.11
(2,19)	1:69:R:ASP:O	1:73:R:SER:H	2	0.11
(2,17)	1:68:R:PHE:O	1:72:R:TYR:H	5	0.11
(2,6)	1:54:R:ASN:O	1:58:R:GLN:N	4	0.11
(2,4)	1:57:R:LEU:N	1:53:R:LEU:O	3	0.11
(1,2316)	1:139:R:ALA:C	1:181:R:VAL:H	3	0.11
(1,2301)	1:163:R:ASP:C	1:166:R:ASP:H	1	0.11
(1,2299)	1:162:R:ILE:H	1:151:R:PHE:C	4	0.11
(1,2287)	1:31:R:LEU:C	1:39:R:LYS:H	4	0.11
(1,2247)	1:134:R:LEU:HD11	1:171:R:THR:HA	5	0.11
(1,2247)	1:134:R:LEU:HD12	1:171:R:THR:HA	5	0.11
(1,2247)	1:134:R:LEU:HD13	1:171:R:THR:HA	5	0.11
(1,2247)	1:134:R:LEU:HD21	1:171:R:THR:HA	5	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2247)	1:134:R:LEU:HD22	1:171:R:THR:HA	5	0.11
(1,2247)	1:134:R:LEU:HD23	1:171:R:THR:HA	5	0.11
(1,2244)	1:170:R:TRP:HA	1:170:R:TRP:HB2	2	0.11
(1,2243)	1:170:R:TRP:HA	1:170:R:TRP:HB3	2	0.11
(1,2235)	1:162:R:ILE:H	1:162:R:ILE:HG12	4	0.11
(1,2198)	1:141:R:ILE:HA	1:151:R:PHE:HA	5	0.11
(1,2164)	1:117:R:THR:H	1:117:R:THR:HA	5	0.11
(1,2060)	1:177:R:VAL:H	1:177:R:VAL:HG11	1	0.11
(1,2060)	1:177:R:VAL:H	1:177:R:VAL:HG12	1	0.11
(1,2060)	1:177:R:VAL:H	1:177:R:VAL:HG13	1	0.11
(1,2004)	1:113:R:THR:HG1	1:113:R:THR:HA	2	0.11
(1,1994)	1:94:R:LEU:HD21	1:103:R:VAL:HG21	4	0.11
(1,1994)	1:94:R:LEU:HD21	1:103:R:VAL:HG22	4	0.11
(1,1994)	1:94:R:LEU:HD21	1:103:R:VAL:HG23	4	0.11
(1,1994)	1:94:R:LEU:HD22	1:103:R:VAL:HG21	4	0.11
(1,1994)	1:94:R:LEU:HD22	1:103:R:VAL:HG22	4	0.11
(1,1994)	1:94:R:LEU:HD22	1:103:R:VAL:HG23	4	0.11
(1,1994)	1:94:R:LEU:HD23	1:103:R:VAL:HG21	4	0.11
(1,1994)	1:94:R:LEU:HD23	1:103:R:VAL:HG22	4	0.11
(1,1994)	1:94:R:LEU:HD23	1:103:R:VAL:HG23	4	0.11
(1,1985)	1:95:R:HIS:HB2	1:95:R:HIS:HA	3	0.11
(1,1985)	1:95:R:HIS:HB3	1:95:R:HIS:HA	3	0.11
(1,1899)	1:162:R:ILE:HB	1:162:R:ILE:HD11	3	0.11
(1,1899)	1:162:R:ILE:HB	1:162:R:ILE:HD12	3	0.11
(1,1899)	1:162:R:ILE:HB	1:162:R:ILE:HD13	3	0.11
(1,1868)	1:150:R:VAL:H	1:150:R:VAL:HG21	5	0.11
(1,1868)	1:150:R:VAL:H	1:150:R:VAL:HG22	5	0.11
(1,1868)	1:150:R:VAL:H	1:150:R:VAL:HG23	5	0.11
(1,1852)	1:134:R:LEU:HD11	1:134:R:LEU:HG	1	0.11
(1,1852)	1:134:R:LEU:HD12	1:134:R:LEU:HG	1	0.11
(1,1852)	1:134:R:LEU:HD13	1:134:R:LEU:HG	1	0.11
(1,1852)	1:134:R:LEU:HD21	1:134:R:LEU:HG	1	0.11
(1,1852)	1:134:R:LEU:HD22	1:134:R:LEU:HG	1	0.11
(1,1852)	1:134:R:LEU:HD23	1:134:R:LEU:HG	1	0.11
(1,1852)	1:134:R:LEU:HD11	1:134:R:LEU:HG	2	0.11
(1,1852)	1:134:R:LEU:HD12	1:134:R:LEU:HG	2	0.11
(1,1852)	1:134:R:LEU:HD13	1:134:R:LEU:HG	2	0.11
(1,1852)	1:134:R:LEU:HD21	1:134:R:LEU:HG	2	0.11
(1,1852)	1:134:R:LEU:HD22	1:134:R:LEU:HG	2	0.11
(1,1852)	1:134:R:LEU:HD23	1:134:R:LEU:HG	2	0.11
(1,1794)	1:107:R:ILE:HD11	1:103:R:VAL:HG11	4	0.11
(1,1794)	1:107:R:ILE:HD11	1:103:R:VAL:HG12	4	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1794)	1:107:R:ILE:HD11	1:103:R:VAL:HG13	4	0.11
(1,1794)	1:107:R:ILE:HD12	1:103:R:VAL:HG11	4	0.11
(1,1794)	1:107:R:ILE:HD12	1:103:R:VAL:HG12	4	0.11
(1,1794)	1:107:R:ILE:HD12	1:103:R:VAL:HG13	4	0.11
(1,1794)	1:107:R:ILE:HD13	1:103:R:VAL:HG11	4	0.11
(1,1794)	1:107:R:ILE:HD13	1:103:R:VAL:HG12	4	0.11
(1,1794)	1:107:R:ILE:HD13	1:103:R:VAL:HG13	4	0.11
(1,1783)	1:100:R:PRO:CB	1:100:R:PRO:HG2	1	0.11
(1,1783)	1:100:R:PRO:CB	1:100:R:PRO:HG3	1	0.11
(1,1783)	1:100:R:PRO:CB	1:100:R:PRO:HG2	2	0.11
(1,1783)	1:100:R:PRO:CB	1:100:R:PRO:HG3	2	0.11
(1,1783)	1:100:R:PRO:CB	1:100:R:PRO:HG2	3	0.11
(1,1783)	1:100:R:PRO:CB	1:100:R:PRO:HG3	3	0.11
(1,1783)	1:100:R:PRO:CB	1:100:R:PRO:HG2	4	0.11
(1,1783)	1:100:R:PRO:CB	1:100:R:PRO:HG3	4	0.11
(1,1783)	1:100:R:PRO:CB	1:100:R:PRO:HG2	5	0.11
(1,1783)	1:100:R:PRO:CB	1:100:R:PRO:HG3	5	0.11
(1,1770)	1:89:R:LEU:HD11	1:89:R:LEU:HG	3	0.11
(1,1770)	1:89:R:LEU:HD12	1:89:R:LEU:HG	3	0.11
(1,1770)	1:89:R:LEU:HD13	1:89:R:LEU:HG	3	0.11
(1,1770)	1:89:R:LEU:HD21	1:89:R:LEU:HG	3	0.11
(1,1770)	1:89:R:LEU:HD22	1:89:R:LEU:HG	3	0.11
(1,1770)	1:89:R:LEU:HD23	1:89:R:LEU:HG	3	0.11
(1,1770)	1:89:R:LEU:HD11	1:89:R:LEU:HG	4	0.11
(1,1770)	1:89:R:LEU:HD12	1:89:R:LEU:HG	4	0.11
(1,1770)	1:89:R:LEU:HD13	1:89:R:LEU:HG	4	0.11
(1,1770)	1:89:R:LEU:HD21	1:89:R:LEU:HG	4	0.11
(1,1770)	1:89:R:LEU:HD22	1:89:R:LEU:HG	4	0.11
(1,1770)	1:89:R:LEU:HD23	1:89:R:LEU:HG	4	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD11	3	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD12	3	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD13	3	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD21	3	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD22	3	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD23	3	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD11	4	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD12	4	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD13	4	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD21	4	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD22	4	0.11
(1,1769)	1:89:R:LEU:HG	1:89:R:LEU:HD23	4	0.11
(1,1757)	1:82:R:ALA:H	1:82:R:ALA:HB1	3	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1757)	1:82:R:ALA:H	1:82:R:ALA:HB2	3	0.11
(1,1757)	1:82:R:ALA:H	1:82:R:ALA:HB3	3	0.11
(1,1732)	1:63:R:VAL:HG11	1:63:R:VAL:HB	1	0.11
(1,1732)	1:63:R:VAL:HG12	1:63:R:VAL:HB	1	0.11
(1,1732)	1:63:R:VAL:HG13	1:63:R:VAL:HB	1	0.11
(1,1732)	1:63:R:VAL:HG21	1:63:R:VAL:HB	1	0.11
(1,1732)	1:63:R:VAL:HG22	1:63:R:VAL:HB	1	0.11
(1,1732)	1:63:R:VAL:HG23	1:63:R:VAL:HB	1	0.11
(1,1732)	1:63:R:VAL:HG11	1:63:R:VAL:HB	2	0.11
(1,1732)	1:63:R:VAL:HG12	1:63:R:VAL:HB	2	0.11
(1,1732)	1:63:R:VAL:HG13	1:63:R:VAL:HB	2	0.11
(1,1732)	1:63:R:VAL:HG21	1:63:R:VAL:HB	2	0.11
(1,1732)	1:63:R:VAL:HG22	1:63:R:VAL:HB	2	0.11
(1,1732)	1:63:R:VAL:HG23	1:63:R:VAL:HB	2	0.11
(1,1732)	1:63:R:VAL:HG11	1:63:R:VAL:HB	3	0.11
(1,1732)	1:63:R:VAL:HG12	1:63:R:VAL:HB	3	0.11
(1,1732)	1:63:R:VAL:HG13	1:63:R:VAL:HB	3	0.11
(1,1732)	1:63:R:VAL:HG21	1:63:R:VAL:HB	3	0.11
(1,1732)	1:63:R:VAL:HG22	1:63:R:VAL:HB	3	0.11
(1,1732)	1:63:R:VAL:HG23	1:63:R:VAL:HB	3	0.11
(1,1732)	1:63:R:VAL:HG11	1:63:R:VAL:HB	4	0.11
(1,1732)	1:63:R:VAL:HG12	1:63:R:VAL:HB	4	0.11
(1,1732)	1:63:R:VAL:HG13	1:63:R:VAL:HB	4	0.11
(1,1732)	1:63:R:VAL:HG21	1:63:R:VAL:HB	4	0.11
(1,1732)	1:63:R:VAL:HG22	1:63:R:VAL:HB	4	0.11
(1,1732)	1:63:R:VAL:HG23	1:63:R:VAL:HB	4	0.11
(1,1732)	1:63:R:VAL:HG11	1:63:R:VAL:HB	5	0.11
(1,1732)	1:63:R:VAL:HG12	1:63:R:VAL:HB	5	0.11
(1,1732)	1:63:R:VAL:HG13	1:63:R:VAL:HB	5	0.11
(1,1732)	1:63:R:VAL:HG21	1:63:R:VAL:HB	5	0.11
(1,1732)	1:63:R:VAL:HG22	1:63:R:VAL:HB	5	0.11
(1,1732)	1:63:R:VAL:HG23	1:63:R:VAL:HB	5	0.11
(1,1713)	1:53:R:LEU:HB2	1:53:R:LEU:HD21	3	0.11
(1,1713)	1:53:R:LEU:HB2	1:53:R:LEU:HD22	3	0.11
(1,1713)	1:53:R:LEU:HB2	1:53:R:LEU:HD23	3	0.11
(1,1642)	1:160:R:TYR:H	1:159:R:TRP:H	2	0.11
(1,1497)	1:94:R:LEU:H	1:93:R:GLU:H	4	0.11
(1,1491)	1:90:R:THR:H	1:89:R:LEU:HG	4	0.11
(1,1481)	1:85:R:GLN:H	1:81:R:GLU:HA	2	0.11
(1,1410)	1:59:R:LEU:H	1:57:R:LEU:H	4	0.11
(1,1259)	1:161:R:ALA:H	1:163:R:ASP:H	4	0.11
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD11	2	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD12	2	0.11
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD13	2	0.11
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD21	2	0.11
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD22	2	0.11
(1,1006)	1:90:R:THR:H	1:89:R:LEU:HD23	2	0.11
(1,1004)	1:90:R:THR:H	1:89:R:LEU:HB3	4	0.11
(1,923)	1:68:R:PHE:H	1:68:R:PHE:HB2	5	0.11
(1,773)	1:181:R:VAL:H	1:180:R:PHE:HE1	1	0.11
(1,773)	1:181:R:VAL:H	1:180:R:PHE:HE2	1	0.11
(1,695)	1:160:R:TYR:H	1:158:R:GLY:HA2	5	0.11
(1,695)	1:160:R:TYR:H	1:158:R:GLY:HA3	5	0.11
(1,583)	1:129:R:GLY:H	1:128:R:ASP:HB2	5	0.11
(1,218)	1:43:R:SER:H	1:42:R:TYR:H	2	0.11
(1,196)	1:38:R:LYS:H	1:37:R:GLU:H	4	0.11
(1,194)	1:37:R:GLU:H	1:38:R:LYS:H	4	0.11
(1,156)	1:179:R:VAL:H	1:141:R:ILE:HB	2	0.11
(2,85)	1:52:R:TRP:O	1:56:R:ILE:H	5	0.1
(2,36)	1:85:R:GLN:O	1:89:R:LEU:N	2	0.1
(2,11)	1:61:R:ARG:H	1:57:R:LEU:O	5	0.1
(1,2307)	1:50:R:ASN:C	1:54:R:ASN:H	2	0.1
(1,2270)	1:63:R:VAL:H	1:59:R:LEU:C	4	0.1
(1,2089)	1:56:R:ILE:HG21	1:56:R:ILE:HG12	5	0.1
(1,2089)	1:56:R:ILE:HG22	1:56:R:ILE:HG12	5	0.1
(1,2089)	1:56:R:ILE:HG23	1:56:R:ILE:HG12	5	0.1
(1,2031)	1:181:R:VAL:HB	1:139:R:ALA:HB1	1	0.1
(1,2031)	1:181:R:VAL:HB	1:139:R:ALA:HB2	1	0.1
(1,2031)	1:181:R:VAL:HB	1:139:R:ALA:HB3	1	0.1
(1,2031)	1:181:R:VAL:HB	1:139:R:ALA:HB1	4	0.1
(1,2031)	1:181:R:VAL:HB	1:139:R:ALA:HB2	4	0.1
(1,2031)	1:181:R:VAL:HB	1:139:R:ALA:HB3	4	0.1
(1,1948)	1:57:R:LEU:HD11	1:53:R:LEU:HD21	3	0.1
(1,1948)	1:57:R:LEU:HD11	1:53:R:LEU:HD22	3	0.1
(1,1948)	1:57:R:LEU:HD11	1:53:R:LEU:HD23	3	0.1
(1,1948)	1:57:R:LEU:HD12	1:53:R:LEU:HD21	3	0.1
(1,1948)	1:57:R:LEU:HD12	1:53:R:LEU:HD22	3	0.1
(1,1948)	1:57:R:LEU:HD12	1:53:R:LEU:HD23	3	0.1
(1,1948)	1:57:R:LEU:HD13	1:53:R:LEU:HD21	3	0.1
(1,1948)	1:57:R:LEU:HD13	1:53:R:LEU:HD22	3	0.1
(1,1948)	1:57:R:LEU:HD13	1:53:R:LEU:HD23	3	0.1
(1,1948)	1:57:R:LEU:HD21	1:53:R:LEU:HD21	3	0.1
(1,1948)	1:57:R:LEU:HD21	1:53:R:LEU:HD22	3	0.1
(1,1948)	1:57:R:LEU:HD21	1:53:R:LEU:HD23	3	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1948)	1:57:R:LEU:HD22	1:53:R:LEU:HD21	3	0.1
(1,1948)	1:57:R:LEU:HD22	1:53:R:LEU:HD22	3	0.1
(1,1948)	1:57:R:LEU:HD22	1:53:R:LEU:HD23	3	0.1
(1,1948)	1:57:R:LEU:HD23	1:53:R:LEU:HD21	3	0.1
(1,1948)	1:57:R:LEU:HD23	1:53:R:LEU:HD22	3	0.1
(1,1948)	1:57:R:LEU:HD23	1:53:R:LEU:HD23	3	0.1
(1,1944)	1:82:R:ALA:HB1	1:53:R:LEU:HD11	3	0.1
(1,1944)	1:82:R:ALA:HB1	1:53:R:LEU:HD12	3	0.1
(1,1944)	1:82:R:ALA:HB1	1:53:R:LEU:HD13	3	0.1
(1,1944)	1:82:R:ALA:HB2	1:53:R:LEU:HD11	3	0.1
(1,1944)	1:82:R:ALA:HB2	1:53:R:LEU:HD12	3	0.1
(1,1944)	1:82:R:ALA:HB2	1:53:R:LEU:HD13	3	0.1
(1,1944)	1:82:R:ALA:HB3	1:53:R:LEU:HD11	3	0.1
(1,1944)	1:82:R:ALA:HB3	1:53:R:LEU:HD12	3	0.1
(1,1944)	1:82:R:ALA:HB3	1:53:R:LEU:HD13	3	0.1
(1,1922)	1:177:R:VAL:HA	1:177:R:VAL:HG11	3	0.1
(1,1922)	1:177:R:VAL:HA	1:177:R:VAL:HG12	3	0.1
(1,1922)	1:177:R:VAL:HA	1:177:R:VAL:HG13	3	0.1
(1,1913)	1:161:R:ALA:HB1	1:170:R:TRP:HB2	4	0.1
(1,1913)	1:161:R:ALA:HB2	1:170:R:TRP:HB2	4	0.1
(1,1913)	1:161:R:ALA:HB3	1:170:R:TRP:HB2	4	0.1
(1,1908)	1:162:R:ILE:HG12	1:162:R:ILE:HG21	3	0.1
(1,1908)	1:162:R:ILE:HG12	1:162:R:ILE:HG22	3	0.1
(1,1908)	1:162:R:ILE:HG12	1:162:R:ILE:HG23	3	0.1
(1,1894)	1:170:R:TRP:HB2	1:161:R:ALA:HB1	4	0.1
(1,1894)	1:170:R:TRP:HB2	1:161:R:ALA:HB2	4	0.1
(1,1894)	1:170:R:TRP:HB2	1:161:R:ALA:HB3	4	0.1
(1,1827)	1:124:R:VAL:HG21	1:124:R:VAL:HA	1	0.1
(1,1827)	1:124:R:VAL:HG22	1:124:R:VAL:HA	1	0.1
(1,1827)	1:124:R:VAL:HG23	1:124:R:VAL:HA	1	0.1
(1,1827)	1:124:R:VAL:HG21	1:124:R:VAL:HA	5	0.1
(1,1827)	1:124:R:VAL:HG22	1:124:R:VAL:HA	5	0.1
(1,1827)	1:124:R:VAL:HG23	1:124:R:VAL:HA	5	0.1
(1,1713)	1:53:R:LEU:HB2	1:53:R:LEU:HD21	4	0.1
(1,1713)	1:53:R:LEU:HB2	1:53:R:LEU:HD22	4	0.1
(1,1713)	1:53:R:LEU:HB2	1:53:R:LEU:HD23	4	0.1
(1,1669)	1:170:R:TRP:H	1:168:R:TYR:HD1	3	0.1
(1,1669)	1:170:R:TRP:H	1:168:R:TYR:HD2	3	0.1
(1,1667)	1:170:R:TRP:H	1:152:R:ALA:HB1	5	0.1
(1,1667)	1:170:R:TRP:H	1:152:R:ALA:HB2	5	0.1
(1,1667)	1:170:R:TRP:H	1:152:R:ALA:HB3	5	0.1
(1,1653)	1:163:R:ASP:H	1:168:R:TYR:H	2	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1455)	1:73:R:SER:H	1:71:R:VAL:H	5	0.1
(1,1446)	1:71:R:VAL:H	1:73:R:SER:H	5	0.1
(1,1420)	1:61:R:ARG:H	1:59:R:LEU:H	5	0.1
(1,1412)	1:59:R:LEU:H	1:61:R:ARG:H	5	0.1
(1,1369)	1:37:R:GLU:H	1:35:R:ASN:HB3	2	0.1
(1,1353)	1:33:R:LEU:H	1:38:R:LYS:H	2	0.1
(1,1297)	1:173:R:ASP:H	1:176:R:ASP:H	3	0.1
(1,1084)	1:112:R:HIS:H	1:113:R:THR:HB	2	0.1
(1,886)	1:58:R:GLN:H	1:54:R:ASN:HA	2	0.1
(1,660)	1:153:R:CYS:H	1:155:R:THR:H	4	0.1
(1,424)	1:92:R:LEU:H	1:90:R:THR:HA	3	0.1
(1,424)	1:92:R:LEU:H	1:90:R:THR:HA	5	0.1
(1,196)	1:38:R:LYS:H	1:37:R:GLU:H	5	0.1
(1,194)	1:37:R:GLU:H	1:38:R:LYS:H	5	0.1

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

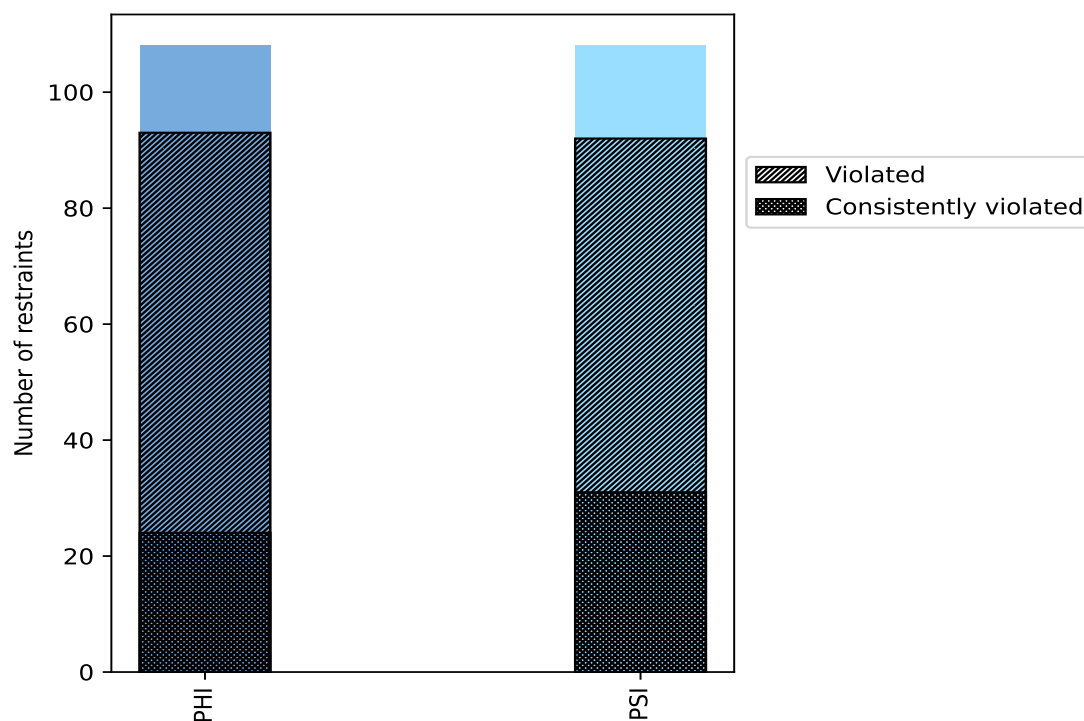
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	108	50.0	93	86.1	43.1	24	22.2	11.1
PSI	108	50.0	92	85.2	42.6	31	28.7	14.4
Total	216	100.0	185	85.6	85.6	55	25.5	25.5

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

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



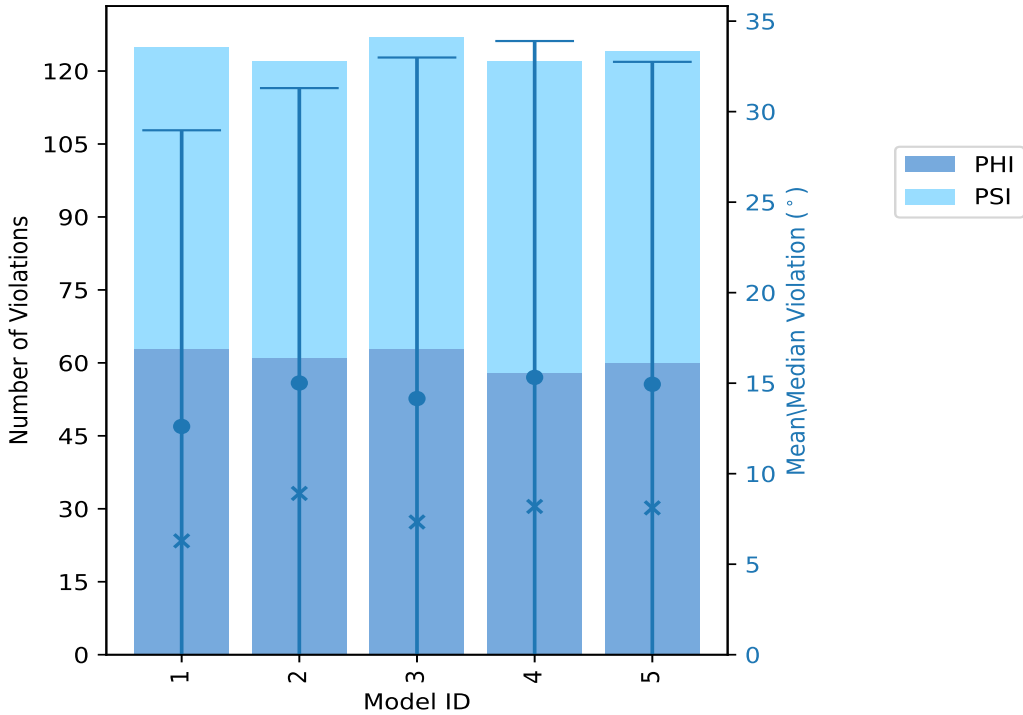
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	63	62	125	12.61	93.38	16.36	6.29
2	61	61	122	15.01	97.72	16.29	8.91
3	63	64	127	14.15	98.76	18.84	7.33
4	58	64	122	15.32	110.88	18.58	8.19
5	60	64	124	14.94	114.55	17.81	8.11

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



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

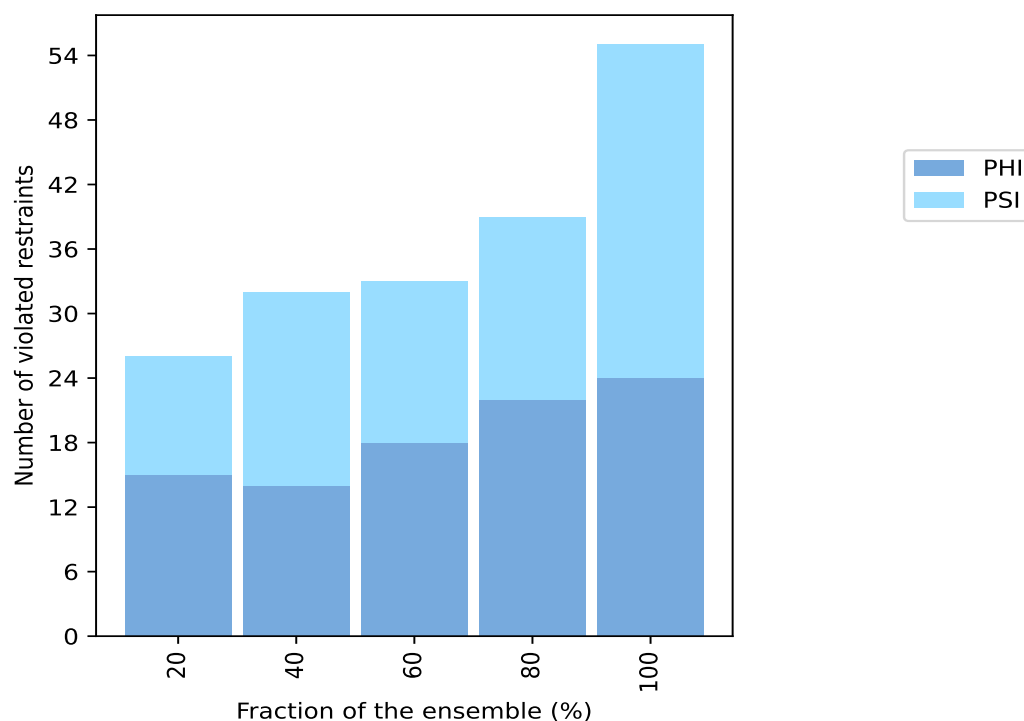
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
15	11	26	1	20.0
14	18	32	2	40.0
18	15	33	3	60.0
22	17	39	4	80.0
24	31	55	5	100.0

¹ Number of models with violations

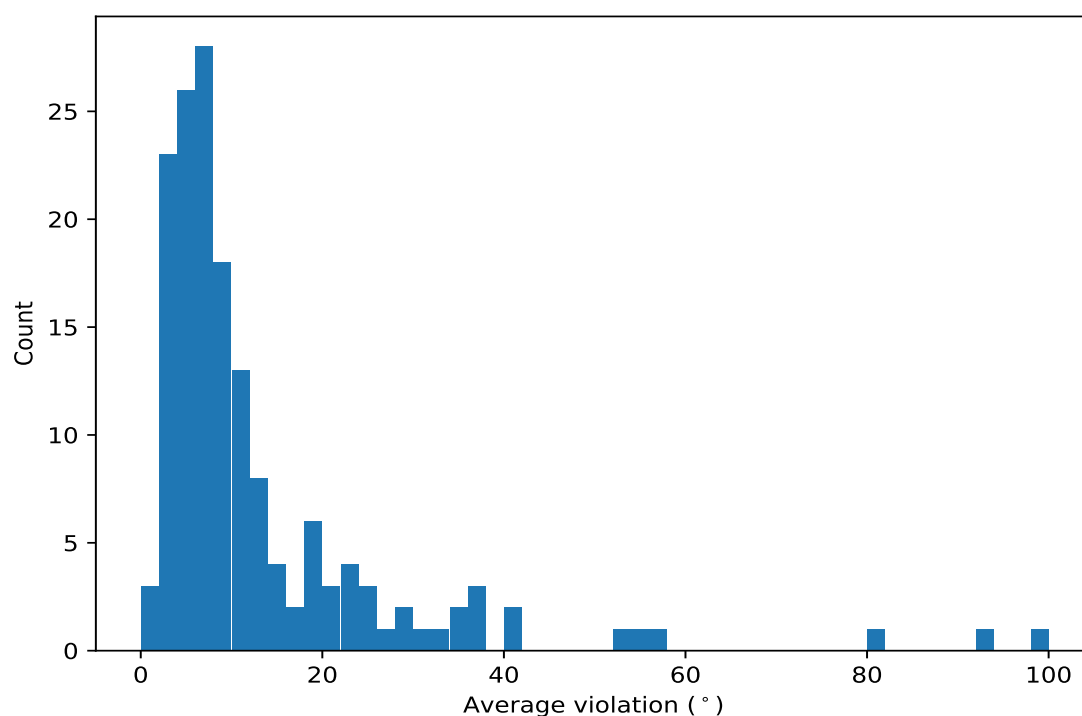
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



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 [i](#)

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,208)	1:178:R:LEU:N	1:178:R:LEU:CA	1:178:R:LEU:C	1:179:R:VAL:N	5	99.25	11.45	95.66
(1,156)	1:138:R:HIS:N	1:138:R:HIS:CA	1:138:R:HIS:C	1:139:R:ALA:N	5	56.0	6.94	55.34
(1,196)	1:170:R:TRP:N	1:170:R:TRP:CA	1:170:R:TRP:C	1:171:R:THR:N	5	54.84	36.04	37.73
(1,126)	1:112:R:HIS:N	1:112:R:HIS:CA	1:112:R:HIS:C	1:113:R:THR:N	5	52.77	7.06	51.58
(1,60)	1:66:R:PRO:N	1:66:R:PRO:CA	1:66:R:PRO:C	1:67:R:PHE:N	5	40.3	4.55	41.77
(1,209)	1:178:R:LEU:C	1:179:R:VAL:N	1:179:R:VAL:CA	1:179:R:VAL:C	5	35.91	7.77	34.61
(1,212)	1:180:R:PHE:N	1:180:R:PHE:CA	1:180:R:PHE:C	1:181:R:VAL:N	5	34.09	4.58	35.53
(1,10)	1:35:R:ASN:N	1:35:R:ASN:CA	1:35:R:ASN:C	1:36:R:GLY:N	5	32.42	23.47	49.41
(1,197)	1:170:R:TRP:C	1:171:R:THR:N	1:171:R:THR:CA	1:171:R:THR:C	5	31.98	28.69	13.74
(1,182)	1:159:R:TRP:N	1:159:R:TRP:CA	1:159:R:TRP:C	1:160:R:TYR:N	5	28.82	6.87	28.36
(1,108)	1:102:R:LEU:N	1:102:R:LEU:CA	1:102:R:LEU:C	1:103:R:VAL:N	5	28.82	12.62	32.58
(1,125)	1:111:R:LEU:C	1:112:R:HIS:N	1:112:R:HIS:CA	1:112:R:HIS:C	5	27.06	18.18	35.9
(1,25)	1:43:R:SER:C	1:44:R:ARG:N	1:44:R:ARG:CA	1:44:R:ARG:C	5	25.93	16.03	16.72
(1,28)	1:45:R:PRO:N	1:45:R:PRO:CA	1:45:R:PRO:C	1:46:R:ASN:N	5	24.52	12.49	31.26
(1,177)	1:152:R:ALA:C	1:153:R:CYS:N	1:153:R:CYS:CA	1:153:R:CYS:C	5	24.03	4.2	23.56
(1,105)	1:100:R:PRO:C	1:101:R:ALA:N	1:101:R:ALA:CA	1:101:R:ALA:C	5	22.92	10.79	27.78
(1,11)	1:35:R:ASN:C	1:36:R:GLY:N	1:36:R:GLY:CA	1:36:R:GLY:C	5	22.89	15.95	30.33
(1,186)	1:162:R:ILE:N	1:162:R:ILE:CA	1:162:R:ILE:C	1:163:R:ASP:N	5	22.76	3.1	21.59
(1,7)	1:33:R:LEU:C	1:34:R:TYR:N	1:34:R:TYR:CA	1:34:R:TYR:C	5	21.01	9.52	19.44
(1,119)	1:107:R:ILE:C	1:108:R:LYS:N	1:108:R:LYS:CA	1:108:R:LYS:C	5	20.63	1.95	19.53
(1,83)	1:82:R:ALA:C	1:83:R:ILE:N	1:83:R:ILE:CA	1:83:R:ILE:C	5	19.84	0.84	20.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,57)	1:64:R:GLU:C	1:65:R:GLU:N	1:65:R:GLU:CA	1:65:R:GLU:C	5	19.55	12.75	14.28
(1,40)	1:55:R:ALA:N	1:55:R:ALA:CA	1:55:R:ALA:C	1:56:R:ILE:N	5	19.17	4.9	18.72
(1,34)	1:52:R:TRP:N	1:52:R:TRP:CA	1:52:R:TRP:C	1:53:R:LEU:N	5	16.42	1.08	16.9
(1,179)	1:153:R:CYS:C	1:154:R:VAL:N	1:154:R:VAL:CA	1:154:R:VAL:C	5	15.01	4.26	15.45
(1,176)	1:152:R:ALA:N	1:152:R:ALA:CA	1:152:R:ALA:C	1:153:R:CYS:N	5	14.36	2.54	14.0
(1,44)	1:57:R:LEU:N	1:57:R:LEU:CA	1:57:R:LEU:C	1:58:R:GLN:N	5	14.28	6.03	12.87
(1,146)	1:130:R:THR:N	1:130:R:THR:CA	1:130:R:THR:C	1:131:R:ASP:N	5	13.62	6.85	11.62
(1,68)	1:71:R:VAL:N	1:71:R:VAL:CA	1:71:R:VAL:C	1:72:R:TYR:N	5	13.29	5.91	14.22
(1,128)	1:114:R:GLY:N	1:114:R:GLY:CA	1:114:R:GLY:C	1:115:R:ILE:N	5	13.29	8.39	12.6
(1,131)	1:116:R:GLY:C	1:117:R:THR:N	1:117:R:THR:CA	1:117:R:THR:C	5	13.18	18.02	4.63
(1,194)	1:169:R:PRO:N	1:169:R:PRO:CA	1:169:R:PRO:C	1:170:R:TRP:N	5	12.45	2.86	10.62
(1,97)	1:89:R:LEU:C	1:90:R:THR:N	1:90:R:THR:CA	1:90:R:THR:C	5	11.81	3.26	11.42
(1,203)	1:175:R:SER:C	1:176:R:ASP:N	1:176:R:ASP:CA	1:176:R:ASP:C	5	11.42	2.91	10.6
(1,161)	1:141:R:ILE:C	1:142:R:PHE:N	1:142:R:PHE:CA	1:142:R:PHE:C	5	11.19	2.18	11.52
(1,8)	1:34:R:TYR:N	1:34:R:TYR:CA	1:34:R:TYR:C	1:35:R:ASN:N	5	11.04	7.33	10.27
(1,59)	1:65:R:GLU:C	1:66:R:PRO:N	1:66:R:PRO:CA	1:66:R:PRO:C	5	10.01	4.33	8.27
(1,37)	1:53:R:LEU:C	1:54:R:ASN:N	1:54:R:ASN:CA	1:54:R:ASN:C	5	9.88	3.88	10.08
(1,58)	1:65:R:GLU:N	1:65:R:GLU:CA	1:65:R:GLU:C	1:66:R:PRO:N	5	9.74	5.22	13.26
(1,100)	1:91:R:GLY:N	1:91:R:GLY:CA	1:91:R:GLY:C	1:92:R:LEU:N	5	9.61	2.77	10.15
(1,78)	1:80:R:LEU:N	1:80:R:LEU:CA	1:80:R:LEU:C	1:81:R:GLU:N	5	9.45	3.06	8.26
(1,120)	1:108:R:LYS:N	1:108:R:LYS:CA	1:108:R:LYS:C	1:109:R:HIS:N	5	9.4	3.11	10.93
(1,16)	1:38:R:LYS:N	1:38:R:LYS:CA	1:38:R:LYS:C	1:39:R:LYS:N	5	9.04	7.8	6.04
(1,61)	1:66:R:PRO:C	1:67:R:PHE:N	1:67:R:PHE:CA	1:67:R:PHE:C	5	8.83	5.74	8.78
(1,130)	1:115:R:ILE:N	1:115:R:ILE:CA	1:115:R:ILE:C	1:116:R:GLY:N	5	8.68	7.3	5.75
(1,29)	1:46:R:ASN:C	1:47:R:ASN:N	1:47:R:ASN:CA	1:47:R:ASN:C	5	8.35	4.23	6.61
(1,210)	1:179:R:VAL:N	1:179:R:VAL:CA	1:179:R:VAL:C	1:180:R:PHE:N	5	8.04	4.39	7.87
(1,77)	1:79:R:THR:C	1:80:R:LEU:N	1:80:R:LEU:CA	1:80:R:LEU:C	5	7.91	0.51	8.14
(1,127)	1:113:R:THR:C	1:114:R:GLY:N	1:114:R:GLY:CA	1:114:R:GLY:C	5	7.35	5.27	8.34
(1,138)	1:123:R:GLU:N	1:123:R:GLU:CA	1:123:R:GLU:C	1:124:R:VAL:N	5	6.37	2.12	7.16
(1,85)	1:83:R:ILE:C	1:84:R:LYS:N	1:84:R:LYS:CA	1:84:R:LYS:C	5	6.19	0.41	6.19
(1,38)	1:54:R:ASN:N	1:54:R:ASN:CA	1:54:R:ASN:C	1:55:R:ALA:N	5	6.17	1.81	6.89
(1,96)	1:89:R:LEU:N	1:89:R:LEU:CA	1:89:R:LEU:C	1:90:R:THR:N	5	6.07	1.86	6.25
(1,33)	1:51:R:ALA:C	1:52:R:TRP:N	1:52:R:TRP:CA	1:52:R:TRP:C	5	5.95	1.17	5.87
(1,80)	1:81:R:GLU:N	1:81:R:GLU:CA	1:81:R:GLU:C	1:82:R:ALA:N	5	5.95	1.73	6.78
(1,107)	1:101:R:ALA:C	1:102:R:LEU:N	1:102:R:LEU:CA	1:102:R:LEU:C	4	92.07	2.22	91.92
(1,106)	1:101:R:ALA:N	1:101:R:ALA:CA	1:101:R:ALA:C	1:102:R:LEU:N	4	81.61	1.09	81.85
(1,13)	1:36:R:GLY:C	1:37:R:GLU:N	1:37:R:GLU:CA	1:37:R:GLU:C	4	41.49	21.19	53.25
(1,157)	1:138:R:HIS:C	1:139:R:ALA:N	1:139:R:ALA:CA	1:139:R:ALA:C	4	36.46	3.93	35.66
(1,12)	1:36:R:GLY:N	1:36:R:GLY:CA	1:36:R:GLY:C	1:37:R:GLU:N	4	21.26	9.56	26.26
(1,144)	1:126:R:VAL:N	1:126:R:VAL:CA	1:126:R:VAL:C	1:127:R:VAL:N	4	19.5	5.7	18.94
(1,154)	1:137:R:PHE:N	1:137:R:PHE:CA	1:137:R:PHE:C	1:138:R:HIS:N	4	18.76	16.25	14.02
(1,30)	1:47:R:ASN:N	1:47:R:ASN:CA	1:47:R:ASN:C	1:48:R:HIS:N	4	18.14	4.57	18.55
(1,140)	1:124:R:VAL:N	1:124:R:VAL:CA	1:124:R:VAL:C	1:125:R:CYS:N	4	17.26	13.71	13.43
(1,143)	1:125:R:CYS:C	1:126:R:VAL:N	1:126:R:VAL:CA	1:126:R:VAL:C	4	13.55	4.36	12.42
(1,123)	1:109:R:HIS:C	1:110:R:LEU:N	1:110:R:LEU:CA	1:110:R:LEU:C	4	11.14	3.79	11.52
(1,23)	1:41:R:PHE:C	1:42:R:TYR:N	1:42:R:TYR:CA	1:42:R:TYR:C	4	10.32	8.52	6.83
(1,155)	1:137:R:PHE:C	1:138:R:HIS:N	1:138:R:HIS:CA	1:138:R:HIS:C	4	9.94	8.12	6.64
(1,189)	1:165:R:GLU:C	1:166:R:ASP:N	1:166:R:ASP:CA	1:166:R:ASP:C	4	9.8	2.38	9.22
(1,9)	1:34:R:TYR:C	1:35:R:ASN:N	1:35:R:ASN:CA	1:35:R:ASN:C	4	9.17	10.83	3.75
(1,55)	1:62:R:TYR:C	1:63:R:VAL:N	1:63:R:VAL:CA	1:63:R:VAL:C	4	9.16	2.87	8.52
(1,56)	1:63:R:VAL:N	1:63:R:VAL:CA	1:63:R:VAL:C	1:64:R:GLU:N	4	8.35	4.51	8.78

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,6)	1:32:R:THR:N	1:32:R:THR:CA	1:32:R:THR:C	1:33:R:LEU:N	4	7.53	6.07	5.82
(1,188)	1:163:R:ASP:N	1:163:R:ASP:CA	1:163:R:ASP:C	1:164:R:ASP:N	4	7.36	3.25	8.36
(1,178)	1:153:R:CYS:N	1:153:R:CYS:CA	1:153:R:CYS:C	1:154:R:VAL:N	4	7.19	4.85	5.21
(1,63)	1:68:R:PHE:C	1:69:R:ASP:N	1:69:R:ASP:CA	1:69:R:ASP:C	4	7.19	4.07	6.04
(1,150)	1:133:R:CYS:N	1:133:R:CYS:CA	1:133:R:CYS:C	1:134:R:LEU:N	4	6.99	4.36	5.9
(1,82)	1:82:R:ALA:N	1:82:R:ALA:CA	1:82:R:ALA:C	1:83:R:ILE:N	4	6.89	3.64	6.4
(1,21)	1:40:R:THR:C	1:41:R:PHE:N	1:41:R:PHE:CA	1:41:R:PHE:C	4	6.69	3.33	7.36
(1,95)	1:88:R:ASP:C	1:89:R:LEU:N	1:89:R:LEU:CA	1:89:R:LEU:C	4	6.54	3.56	5.99
(1,62)	1:67:R:PHE:N	1:67:R:PHE:CA	1:67:R:PHE:C	1:68:R:PHE:N	4	6.46	3.03	7.77
(1,167)	1:147:R:GLU:C	1:148:R:HIS:N	1:148:R:HIS:CA	1:148:R:HIS:C	4	5.86	1.91	5.78
(1,129)	1:114:R:GLY:C	1:115:R:ILE:N	1:115:R:ILE:CA	1:115:R:ILE:C	4	5.8	5.58	3.06
(1,159)	1:140:R:GLY:C	1:141:R:ILE:N	1:141:R:ILE:CA	1:141:R:ILE:C	4	5.45	3.63	4.48
(1,46)	1:58:R:GLN:N	1:58:R:GLN:CA	1:58:R:GLN:C	1:59:R:LEU:N	4	5.39	1.41	5.53
(1,99)	1:90:R:THR:C	1:91:R:GLY:N	1:91:R:GLY:CA	1:91:R:GLY:C	4	5.29	2.69	4.96
(1,101)	1:94:R:LEU:C	1:95:R:HIS:N	1:95:R:HIS:CA	1:95:R:HIS:C	4	4.35	1.35	3.6
(1,71)	1:72:R:TYR:C	1:73:R:SER:N	1:73:R:SER:CA	1:73:R:SER:C	4	4.15	1.2	3.71
(1,185)	1:161:R:ALA:C	1:162:R:ILE:N	1:162:R:ILE:CA	1:162:R:ILE:C	4	3.96	2.39	3.54
(1,112)	1:104:R:ILE:N	1:104:R:ILE:CA	1:104:R:ILE:C	1:105:R:TRP:N	4	3.85	1.06	3.68
(1,43)	1:56:R:ILE:C	1:57:R:LEU:N	1:57:R:LEU:CA	1:57:R:LEU:C	4	3.37	1.86	3.39
(1,32)	1:51:R:ALA:N	1:51:R:ALA:CA	1:51:R:ALA:C	1:52:R:TRP:N	4	3.14	1.25	3.08
(1,142)	1:125:R:CYS:N	1:125:R:CYS:CA	1:125:R:CYS:C	1:126:R:VAL:N	4	3.14	1.03	2.9
(1,47)	1:58:R:GLN:C	1:59:R:LEU:N	1:59:R:LEU:CA	1:59:R:LEU:C	4	2.87	1.09	3.22
(1,14)	1:37:R:GLU:N	1:37:R:GLU:CA	1:37:R:GLU:C	1:38:R:LYS:N	3	37.07	6.85	36.86
(1,15)	1:37:R:GLU:C	1:38:R:LYS:N	1:38:R:LYS:CA	1:38:R:LYS:C	3	22.13	9.3	24.71
(1,118)	1:107:R:ILE:N	1:107:R:ILE:CA	1:107:R:ILE:C	1:108:R:LYS:N	3	15.6	6.44	16.69
(1,199)	1:172:R:PRO:C	1:173:R:ASP:N	1:173:R:ASP:CA	1:173:R:ASP:C	3	11.29	7.27	14.48
(1,190)	1:166:R:ASP:N	1:166:R:ASP:CA	1:166:R:ASP:C	1:167:R:PHE:N	3	10.65	7.03	12.92
(1,145)	1:129:R:GLY:C	1:130:R:THR:N	1:130:R:THR:CA	1:130:R:THR:C	3	10.27	6.26	7.53
(1,24)	1:42:R:TYR:N	1:42:R:TYR:CA	1:42:R:TYR:C	1:43:R:SER:N	3	9.09	6.32	6.22
(1,132)	1:117:R:THR:N	1:117:R:THR:CA	1:117:R:THR:C	1:118:R:ALA:N	3	9.05	4.76	5.8
(1,148)	1:132:R:MET:N	1:132:R:MET:CA	1:132:R:MET:C	1:133:R:CYS:N	3	7.9	4.38	9.19
(1,53)	1:61:R:ARG:C	1:62:R:TYR:N	1:62:R:TYR:CA	1:62:R:TYR:C	3	7.89	2.6	8.69
(1,26)	1:44:R:ARG:N	1:44:R:ARG:CA	1:44:R:ARG:C	1:45:R:PRO:N	3	7.47	4.84	6.71
(1,180)	1:154:R:VAL:N	1:154:R:VAL:CA	1:154:R:VAL:C	1:155:R:THR:N	3	6.94	2.87	8.75
(1,42)	1:56:R:ILE:N	1:56:R:ILE:CA	1:56:R:ILE:C	1:57:R:LEU:N	3	6.61	3.04	5.36
(1,139)	1:123:R:GLU:C	1:124:R:VAL:N	1:124:R:VAL:CA	1:124:R:VAL:C	3	6.05	6.3	2.17
(1,115)	1:105:R:TRP:C	1:106:R:ASN:N	1:106:R:ASN:CA	1:106:R:ASN:C	3	6.0	1.23	6.87
(1,195)	1:169:R:PRO:C	1:170:R:TRP:N	1:170:R:TRP:CA	1:170:R:TRP:C	3	5.89	2.93	5.9
(1,19)	1:39:R:LYS:C	1:40:R:THR:N	1:40:R:THR:CA	1:40:R:THR:C	3	5.81	0.69	5.6
(1,45)	1:57:R:LEU:C	1:58:R:GLN:N	1:58:R:GLN:CA	1:58:R:GLN:C	3	5.42	1.98	5.15
(1,91)	1:86:R:LEU:C	1:87:R:GLU:N	1:87:R:GLU:CA	1:87:R:GLU:C	3	5.29	3.17	4.87
(1,160)	1:141:R:ILE:N	1:141:R:ILE:CA	1:141:R:ILE:C	1:142:R:PHE:N	3	4.97	1.66	3.82
(1,50)	1:60:R:PHE:N	1:60:R:PHE:CA	1:60:R:PHE:C	1:61:R:ARG:N	3	4.74	3.07	3.28
(1,116)	1:106:R:ASN:N	1:106:R:ASN:CA	1:106:R:ASN:C	1:107:R:ILE:N	3	4.73	2.01	5.81
(1,122)	1:109:R:HIS:N	1:109:R:HIS:CA	1:109:R:HIS:C	1:110:R:LEU:N	3	4.69	2.46	5.32
(1,54)	1:62:R:TYR:N	1:62:R:TYR:CA	1:62:R:TYR:C	1:63:R:VAL:N	3	4.61	3.12	2.7
(1,109)	1:102:R:LEU:C	1:103:R:VAL:N	1:103:R:VAL:CA	1:103:R:VAL:C	3	4.11	1.76	3.98
(1,207)	1:177:R:VAL:C	1:178:R:LEU:N	1:178:R:LEU:CA	1:178:R:LEU:C	3	3.52	1.54	4.1
(1,147)	1:131:R:ASP:C	1:132:R:MET:N	1:132:R:MET:CA	1:132:R:MET:C	3	3.29	1.84	2.17
(1,31)	1:50:R:ASN:C	1:51:R:ALA:N	1:51:R:ALA:CA	1:51:R:ALA:C	3	3.04	1.04	2.32
(1,75)	1:78:R:LEU:C	1:79:R:THR:N	1:79:R:THR:CA	1:79:R:THR:C	3	2.64	1.47	1.99

Continued on next page...

Continued from previous page...

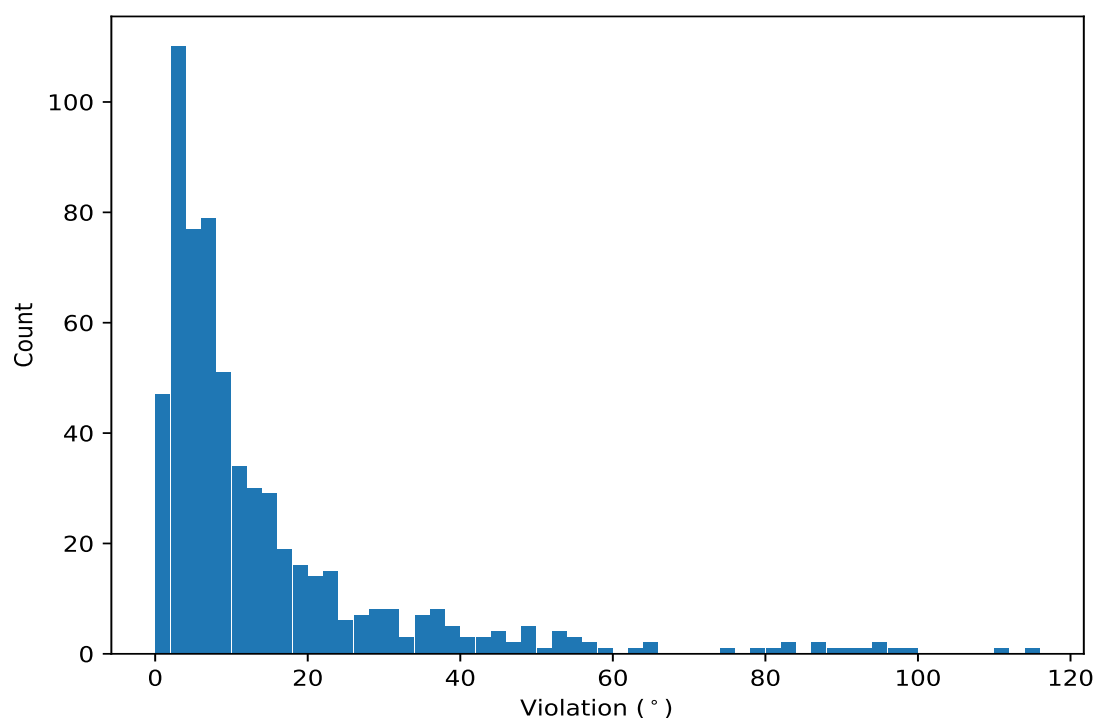
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,173)	1:150:R:VAL:C	1:151:R:PHE:N	1:151:R:PHE:CA	1:151:R:PHE:C	3	2.45	0.97	2.89
(1,39)	1:54:R:ASN:C	1:55:R:ALA:N	1:55:R:ALA:CA	1:55:R:ALA:C	3	2.44	0.23	2.52
(1,70)	1:72:R:TYR:N	1:72:R:TYR:CA	1:72:R:TYR:C	1:73:R:SER:N	3	2.16	0.43	2.25
(1,165)	1:143:R:LEU:C	1:144:R:LYS:N	1:144:R:LYS:CA	1:144:R:LYS:C	3	1.92	0.14	1.85
(1,141)	1:124:R:VAL:C	1:125:R:CYS:N	1:125:R:CYS:CA	1:125:R:CYS:C	2	36.07	22.19	36.07
(1,153)	1:136:R:ASP:C	1:137:R:PHE:N	1:137:R:PHE:CA	1:137:R:PHE:C	2	13.45	5.08	13.45
(1,184)	1:161:R:ALA:N	1:161:R:ALA:CA	1:161:R:ALA:C	1:162:R:ILE:N	2	12.76	9.0	12.76
(1,111)	1:103:R:VAL:C	1:104:R:ILE:N	1:104:R:ILE:CA	1:104:R:ILE:C	2	11.85	4.29	11.85
(1,124)	1:110:R:LEU:N	1:110:R:LEU:CA	1:110:R:LEU:C	1:111:R:LEU:N	2	10.19	0.7	10.19
(1,200)	1:173:R:ASP:N	1:173:R:ASP:CA	1:173:R:ASP:C	1:174:R:PRO:N	2	10.07	1.83	10.07
(1,41)	1:55:R:ALA:C	1:56:R:ILE:N	1:56:R:ILE:CA	1:56:R:ILE:C	2	9.53	6.66	9.53
(1,76)	1:79:R:THR:N	1:79:R:THR:CA	1:79:R:THR:C	1:80:R:LEU:N	2	7.24	0.01	7.24
(1,198)	1:171:R:THR:N	1:171:R:THR:CA	1:171:R:THR:C	1:172:R:PRO:N	2	7.22	1.04	7.22
(1,4)	1:31:R:LEU:N	1:31:R:LEU:CA	1:31:R:LEU:C	1:32:R:THR:N	2	7.1	1.7	7.1
(1,201)	1:174:R:PRO:C	1:175:R:SER:N	1:175:R:SER:CA	1:175:R:SER:C	2	6.74	0.41	6.74
(1,49)	1:59:R:LEU:C	1:60:R:PHE:N	1:60:R:PHE:CA	1:60:R:PHE:C	2	6.59	1.73	6.59
(1,22)	1:41:R:PHE:N	1:41:R:PHE:CA	1:41:R:PHE:C	1:42:R:TYR:N	2	6.28	1.54	6.28
(1,117)	1:106:R:ASN:C	1:107:R:ILE:N	1:107:R:ILE:CA	1:107:R:ILE:C	2	5.96	1.56	5.96
(1,202)	1:175:R:SER:N	1:175:R:SER:CA	1:175:R:SER:C	1:176:R:ASP:N	2	5.74	1.45	5.74
(1,20)	1:40:R:THR:N	1:40:R:THR:CA	1:40:R:THR:C	1:41:R:PHE:N	2	5.1	3.82	5.1
(1,152)	1:135:R:ALA:N	1:135:R:ALA:CA	1:135:R:ALA:C	1:136:R:ASP:N	2	4.96	1.44	4.96
(1,104)	1:100:R:PRO:N	1:100:R:PRO:CA	1:100:R:PRO:C	1:101:R:ALA:N	2	4.58	0.46	4.58
(1,18)	1:39:R:LYS:N	1:39:R:LYS:CA	1:39:R:LYS:C	1:40:R:THR:N	2	4.18	1.05	4.18
(1,149)	1:132:R:MET:C	1:133:R:CYS:N	1:133:R:CYS:CA	1:133:R:CYS:C	2	4.04	1.26	4.04
(1,187)	1:162:R:ILE:C	1:163:R:ASP:N	1:163:R:ASP:CA	1:163:R:ASP:C	2	3.5	1.5	3.5
(1,81)	1:81:R:GLU:C	1:82:R:ALA:N	1:82:R:ALA:CA	1:82:R:ALA:C	2	3.4	1.3	3.4
(1,73)	1:73:R:SER:C	1:74:R:SER:N	1:74:R:SER:CA	1:74:R:SER:C	2	3.09	0.29	3.09
(1,206)	1:177:R:VAL:N	1:177:R:VAL:CA	1:177:R:VAL:C	1:178:R:LEU:N	2	2.84	0.53	2.84
(1,3)	1:30:R:GLU:C	1:31:R:LEU:N	1:31:R:LEU:CA	1:31:R:LEU:C	2	2.58	0.38	2.58
(1,84)	1:83:R:ILE:N	1:83:R:ILE:CA	1:83:R:ILE:C	1:84:R:LYS:N	2	2.38	1.0	2.38
(1,121)	1:108:R:LYS:C	1:109:R:HIS:N	1:109:R:HIS:CA	1:109:R:HIS:C	2	2.24	0.25	2.24
(1,94)	1:88:R:ASP:N	1:88:R:ASP:CA	1:88:R:ASP:C	1:89:R:LEU:N	2	2.14	0.5	2.14
(1,192)	1:167:R:PHE:N	1:167:R:PHE:CA	1:167:R:PHE:C	1:168:R:TYR:N	2	2.13	0.2	2.13
(1,114)	1:105:R:TRP:N	1:105:R:TRP:CA	1:105:R:TRP:C	1:106:R:ASN:N	2	2.08	0.82	2.08
(1,51)	1:60:R:PHE:C	1:61:R:ARG:N	1:61:R:ARG:CA	1:61:R:ARG:C	2	1.82	0.31	1.82
(1,110)	1:103:R:VAL:N	1:103:R:VAL:CA	1:103:R:VAL:C	1:104:R:ILE:N	2	1.62	0.23	1.62

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,208)	1:178:R:LEU:N	1:178:R:LEU:CA	1:178:R:LEU:C	1:179:R:VAL:N	5	114.55
(1,208)	1:178:R:LEU:N	1:178:R:LEU:CA	1:178:R:LEU:C	1:179:R:VAL:N	4	110.88
(1,196)	1:170:R:TRP:N	1:170:R:TRP:CA	1:170:R:TRP:C	1:171:R:THR:N	3	98.76
(1,196)	1:170:R:TRP:N	1:170:R:TRP:CA	1:170:R:TRP:C	1:171:R:THR:N	2	97.72
(1,208)	1:178:R:LEU:N	1:178:R:LEU:CA	1:178:R:LEU:C	1:179:R:VAL:N	2	95.66
(1,107)	1:101:R:ALA:C	1:102:R:LEU:N	1:102:R:LEU:CA	1:102:R:LEU:C	4	95.0
(1,107)	1:101:R:ALA:C	1:102:R:LEU:N	1:102:R:LEU:CA	1:102:R:LEU:C	1	93.38
(1,107)	1:101:R:ALA:C	1:102:R:LEU:N	1:102:R:LEU:CA	1:102:R:LEU:C	5	90.46
(1,107)	1:101:R:ALA:C	1:102:R:LEU:N	1:102:R:LEU:CA	1:102:R:LEU:C	3	89.45
(1,208)	1:178:R:LEU:N	1:178:R:LEU:CA	1:178:R:LEU:C	1:179:R:VAL:N	3	87.74
(1,208)	1:178:R:LEU:N	1:178:R:LEU:CA	1:178:R:LEU:C	1:179:R:VAL:N	1	87.4
(1,106)	1:101:R:ALA:N	1:101:R:ALA:CA	1:101:R:ALA:C	1:102:R:LEU:N	1	82.82
(1,106)	1:101:R:ALA:N	1:101:R:ALA:CA	1:101:R:ALA:C	1:102:R:LEU:N	4	82.27
(1,106)	1:101:R:ALA:N	1:101:R:ALA:CA	1:101:R:ALA:C	1:102:R:LEU:N	3	81.44
(1,106)	1:101:R:ALA:N	1:101:R:ALA:CA	1:101:R:ALA:C	1:102:R:LEU:N	5	79.92
(1,197)	1:170:R:TRP:C	1:171:R:THR:N	1:171:R:THR:CA	1:171:R:THR:C	3	75.78
(1,126)	1:112:R:HIS:N	1:112:R:HIS:CA	1:112:R:HIS:C	1:113:R:THR:N	3	65.87
(1,156)	1:138:R:HIS:N	1:138:R:HIS:CA	1:138:R:HIS:C	1:139:R:ALA:N	1	64.42
(1,156)	1:138:R:HIS:N	1:138:R:HIS:CA	1:138:R:HIS:C	1:139:R:ALA:N	3	63.37
(1,141)	1:124:R:VAL:C	1:125:R:CYS:N	1:125:R:CYS:CA	1:125:R:CYS:C	4	58.26
(1,197)	1:170:R:TRP:C	1:171:R:THR:N	1:171:R:THR:CA	1:171:R:THR:C	2	56.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,25)	1:43:R:SER:C	1:44:R:ARG:N	1:44:R:ARG:CA	1:44:R:ARG:C	3	56.13
(1,156)	1:138:R:HIS:N	1:138:R:HIS:CA	1:138:R:HIS:C	1:139:R:ALA:N	4	55.34
(1,13)	1:36:R:GLY:C	1:37:R:GLU:N	1:37:R:GLU:CA	1:37:R:GLU:C	5	54.63
(1,13)	1:36:R:GLY:C	1:37:R:GLU:N	1:37:R:GLU:CA	1:37:R:GLU:C	2	54.32
(1,10)	1:35:R:ASN:N	1:35:R:ASN:CA	1:35:R:ASN:C	1:36:R:GLY:N	5	53.1
(1,126)	1:112:R:HIS:N	1:112:R:HIS:CA	1:112:R:HIS:C	1:113:R:THR:N	5	52.44
(1,13)	1:36:R:GLY:C	1:37:R:GLU:N	1:37:R:GLU:CA	1:37:R:GLU:C	4	52.18
(1,10)	1:35:R:ASN:N	1:35:R:ASN:CA	1:35:R:ASN:C	1:36:R:GLY:N	4	52.13
(1,126)	1:112:R:HIS:N	1:112:R:HIS:CA	1:112:R:HIS:C	1:113:R:THR:N	1	51.58
(1,10)	1:35:R:ASN:N	1:35:R:ASN:CA	1:35:R:ASN:C	1:36:R:GLY:N	2	49.41
(1,126)	1:112:R:HIS:N	1:112:R:HIS:CA	1:112:R:HIS:C	1:113:R:THR:N	4	49.09
(1,131)	1:116:R:GLY:C	1:117:R:THR:N	1:117:R:THR:CA	1:117:R:THR:C	4	48.95
(1,156)	1:138:R:HIS:N	1:138:R:HIS:CA	1:138:R:HIS:C	1:139:R:ALA:N	5	48.82
(1,156)	1:138:R:HIS:N	1:138:R:HIS:CA	1:138:R:HIS:C	1:139:R:ALA:N	2	48.04
(1,209)	1:178:R:LEU:C	1:179:R:VAL:N	1:179:R:VAL:CA	1:179:R:VAL:C	5	47.57
(1,125)	1:111:R:LEU:C	1:112:R:HIS:N	1:112:R:HIS:CA	1:112:R:HIS:C	1	47.38
(1,14)	1:37:R:GLU:N	1:37:R:GLU:CA	1:37:R:GLU:C	1:38:R:LYS:N	4	45.57
(1,154)	1:137:R:PHE:N	1:137:R:PHE:CA	1:137:R:PHE:C	1:138:R:HIS:N	3	45.3
(1,60)	1:66:R:PRO:N	1:66:R:PRO:CA	1:66:R:PRO:C	1:67:R:PHE:N	1	44.88
(1,126)	1:112:R:HIS:N	1:112:R:HIS:CA	1:112:R:HIS:C	1:113:R:THR:N	2	44.86
(1,11)	1:35:R:ASN:C	1:36:R:GLY:N	1:36:R:GLY:CA	1:36:R:GLY:C	2	43.75
(1,60)	1:66:R:PRO:N	1:66:R:PRO:CA	1:66:R:PRO:C	1:67:R:PHE:N	2	43.45
(1,157)	1:138:R:HIS:C	1:139:R:ALA:N	1:139:R:ALA:CA	1:139:R:ALA:C	1	42.48
(1,60)	1:66:R:PRO:N	1:66:R:PRO:CA	1:66:R:PRO:C	1:67:R:PHE:N	3	41.77
(1,125)	1:111:R:LEU:C	1:112:R:HIS:N	1:112:R:HIS:CA	1:112:R:HIS:C	2	41.53
(1,182)	1:159:R:TRP:N	1:159:R:TRP:CA	1:159:R:TRP:C	1:160:R:TYR:N	2	40.83
(1,60)	1:66:R:PRO:N	1:66:R:PRO:CA	1:66:R:PRO:C	1:67:R:PHE:N	4	39.44
(1,209)	1:178:R:LEU:C	1:179:R:VAL:N	1:179:R:VAL:CA	1:179:R:VAL:C	4	39.31
(1,108)	1:102:R:LEU:N	1:102:R:LEU:CA	1:102:R:LEU:C	1:103:R:VAL:N	5	39.27
(1,140)	1:124:R:VAL:N	1:124:R:VAL:CA	1:124:R:VAL:C	1:125:R:CYS:N	5	38.52
(1,212)	1:180:R:PHE:N	1:180:R:PHE:CA	1:180:R:PHE:C	1:181:R:VAL:N	4	38.19
(1,196)	1:170:R:TRP:N	1:170:R:TRP:CA	1:170:R:TRP:C	1:171:R:THR:N	4	37.73
(1,57)	1:64:R:GLU:C	1:65:R:GLU:N	1:65:R:GLU:CA	1:65:R:GLU:C	1	37.72
(1,7)	1:33:R:LEU:C	1:34:R:TYR:N	1:34:R:TYR:CA	1:34:R:TYR:C	2	37.42
(1,157)	1:138:R:HIS:C	1:139:R:ALA:N	1:139:R:ALA:CA	1:139:R:ALA:C	4	37.19
(1,28)	1:45:R:PRO:N	1:45:R:PRO:CA	1:45:R:PRO:C	1:46:R:ASN:N	5	37.12
(1,14)	1:37:R:GLU:N	1:37:R:GLU:CA	1:37:R:GLU:C	1:38:R:LYS:N	5	36.86
(1,108)	1:102:R:LEU:N	1:102:R:LEU:CA	1:102:R:LEU:C	1:103:R:VAL:N	1	36.74
(1,212)	1:180:R:PHE:N	1:180:R:PHE:CA	1:180:R:PHE:C	1:181:R:VAL:N	2	36.44
(1,125)	1:111:R:LEU:C	1:112:R:HIS:N	1:112:R:HIS:CA	1:112:R:HIS:C	5	35.9
(1,212)	1:180:R:PHE:N	1:180:R:PHE:CA	1:180:R:PHE:C	1:181:R:VAL:N	3	35.53
(1,28)	1:45:R:PRO:N	1:45:R:PRO:CA	1:45:R:PRO:C	1:46:R:ASN:N	4	35.41
(1,212)	1:180:R:PHE:N	1:180:R:PHE:CA	1:180:R:PHE:C	1:181:R:VAL:N	5	35.14
(1,209)	1:178:R:LEU:C	1:179:R:VAL:N	1:179:R:VAL:CA	1:179:R:VAL:C	1	34.61
(1,209)	1:178:R:LEU:C	1:179:R:VAL:N	1:179:R:VAL:CA	1:179:R:VAL:C	3	34.43
(1,157)	1:138:R:HIS:C	1:139:R:ALA:N	1:139:R:ALA:CA	1:139:R:ALA:C	5	34.12
(1,108)	1:102:R:LEU:N	1:102:R:LEU:CA	1:102:R:LEU:C	1:103:R:VAL:N	4	32.58
(1,157)	1:138:R:HIS:C	1:139:R:ALA:N	1:139:R:ALA:CA	1:139:R:ALA:C	2	32.04
(1,15)	1:37:R:GLU:C	1:38:R:LYS:N	1:38:R:LYS:CA	1:38:R:LYS:C	5	32.02
(1,60)	1:66:R:PRO:N	1:66:R:PRO:CA	1:66:R:PRO:C	1:67:R:PHE:N	5	31.94
(1,11)	1:35:R:ASN:C	1:36:R:GLY:N	1:36:R:GLY:CA	1:36:R:GLY:C	5	31.63

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,57)	1:64:R:GLU:C	1:65:R:GLU:N	1:65:R:GLU:CA	1:65:R:GLU:C	3	31.56
(1,177)	1:152:R:ALA:C	1:153:R:CYS:N	1:153:R:CYS:CA	1:153:R:CYS:C	4	31.29
(1,108)	1:102:R:LEU:N	1:102:R:LEU:CA	1:102:R:LEU:C	1:103:R:VAL:N	3	31.26
(1,28)	1:45:R:PRO:N	1:45:R:PRO:CA	1:45:R:PRO:C	1:46:R:ASN:N	3	31.26
(1,182)	1:159:R:TRP:N	1:159:R:TRP:CA	1:159:R:TRP:C	1:160:R:TYR:N	4	30.5
(1,11)	1:35:R:ASN:C	1:36:R:GLY:N	1:36:R:GLY:CA	1:36:R:GLY:C	4	30.33
(1,105)	1:100:R:PRO:C	1:101:R:ALA:N	1:101:R:ALA:CA	1:101:R:ALA:C	3	29.65
(1,128)	1:114:R:GLY:N	1:114:R:GLY:CA	1:114:R:GLY:C	1:115:R:ILE:N	5	28.85
(1,14)	1:37:R:GLU:N	1:37:R:GLU:CA	1:37:R:GLU:C	1:38:R:LYS:N	2	28.79
(1,25)	1:43:R:SER:C	1:44:R:ARG:N	1:44:R:ARG:CA	1:44:R:ARG:C	2	28.64
(1,182)	1:159:R:TRP:N	1:159:R:TRP:CA	1:159:R:TRP:C	1:160:R:TYR:N	3	28.36
(1,186)	1:162:R:ILE:N	1:162:R:ILE:CA	1:162:R:ILE:C	1:163:R:ASP:N	2	28.31
(1,105)	1:100:R:PRO:C	1:101:R:ALA:N	1:101:R:ALA:CA	1:101:R:ALA:C	1	28.13
(1,144)	1:126:R:VAL:N	1:126:R:VAL:CA	1:126:R:VAL:C	1:127:R:VAL:N	1	28.06
(1,9)	1:34:R:TYR:C	1:35:R:ASN:N	1:35:R:ASN:CA	1:35:R:ASN:C	2	27.84
(1,12)	1:36:R:GLY:N	1:36:R:GLY:CA	1:36:R:GLY:C	1:37:R:GLU:N	2	27.8
(1,105)	1:100:R:PRO:C	1:101:R:ALA:N	1:101:R:ALA:CA	1:101:R:ALA:C	4	27.78
(1,105)	1:100:R:PRO:C	1:101:R:ALA:N	1:101:R:ALA:CA	1:101:R:ALA:C	5	27.66
(1,146)	1:130:R:THR:N	1:130:R:THR:CA	1:130:R:THR:C	1:131:R:ASP:N	1	26.33
(1,12)	1:36:R:GLY:N	1:36:R:GLY:CA	1:36:R:GLY:C	1:37:R:GLU:N	4	26.27
(1,12)	1:36:R:GLY:N	1:36:R:GLY:CA	1:36:R:GLY:C	1:37:R:GLU:N	5	26.25
(1,40)	1:55:R:ALA:N	1:55:R:ALA:CA	1:55:R:ALA:C	1:56:R:ILE:N	5	25.8
(1,212)	1:180:R:PHE:N	1:180:R:PHE:CA	1:180:R:PHE:C	1:181:R:VAL:N	1	25.17
(1,15)	1:37:R:GLU:C	1:38:R:LYS:N	1:38:R:LYS:CA	1:38:R:LYS:C	4	24.71
(1,23)	1:41:R:PHE:C	1:42:R:TYR:N	1:42:R:TYR:CA	1:42:R:TYR:C	3	24.65
(1,177)	1:152:R:ALA:C	1:153:R:CYS:N	1:153:R:CYS:CA	1:153:R:CYS:C	5	24.63
(1,16)	1:38:R:LYS:N	1:38:R:LYS:CA	1:38:R:LYS:C	1:39:R:LYS:N	2	24.27
(1,30)	1:47:R:ASN:N	1:47:R:ASN:CA	1:47:R:ASN:C	1:48:R:HIS:N	1	23.77
(1,186)	1:162:R:ILE:N	1:162:R:ILE:CA	1:162:R:ILE:C	1:163:R:ASP:N	5	23.72
(1,209)	1:178:R:LEU:C	1:179:R:VAL:N	1:179:R:VAL:CA	1:179:R:VAL:C	2	23.63
(1,177)	1:152:R:ALA:C	1:153:R:CYS:N	1:153:R:CYS:CA	1:153:R:CYS:C	2	23.56
(1,44)	1:57:R:LEU:N	1:57:R:LEU:CA	1:57:R:LEU:C	1:58:R:GLN:N	1	23.52
(1,7)	1:33:R:LEU:C	1:34:R:TYR:N	1:34:R:TYR:CA	1:34:R:TYR:C	4	23.52
(1,119)	1:107:R:ILE:C	1:108:R:LYS:N	1:108:R:LYS:CA	1:108:R:LYS:C	2	23.42
(1,155)	1:137:R:PHE:C	1:138:R:HIS:N	1:138:R:HIS:CA	1:138:R:HIS:C	3	23.32
(1,130)	1:115:R:ILE:N	1:115:R:ILE:CA	1:115:R:ILE:C	1:116:R:GLY:N	5	23.14
(1,182)	1:159:R:TRP:N	1:159:R:TRP:CA	1:159:R:TRP:C	1:160:R:TYR:N	5	23.01
(1,68)	1:71:R:VAL:N	1:71:R:VAL:CA	1:71:R:VAL:C	1:72:R:TYR:N	2	22.97
(1,118)	1:107:R:ILE:N	1:107:R:ILE:CA	1:107:R:ILE:C	1:108:R:LYS:N	2	22.88
(1,119)	1:107:R:ILE:C	1:108:R:LYS:N	1:108:R:LYS:CA	1:108:R:LYS:C	1	22.51
(1,177)	1:152:R:ALA:C	1:153:R:CYS:N	1:153:R:CYS:CA	1:153:R:CYS:C	1	22.3
(1,8)	1:34:R:TYR:N	1:34:R:TYR:CA	1:34:R:TYR:C	1:35:R:ASN:N	2	22.28
(1,40)	1:55:R:ALA:N	1:55:R:ALA:CA	1:55:R:ALA:C	1:56:R:ILE:N	2	21.99
(1,196)	1:170:R:TRP:N	1:170:R:TRP:CA	1:170:R:TRP:C	1:171:R:THR:N	1	21.81
(1,137)	1:122:R:SER:C	1:123:R:GLU:N	1:123:R:GLU:CA	1:123:R:GLU:C	5	21.8
(1,184)	1:161:R:ALA:N	1:161:R:ALA:CA	1:161:R:ALA:C	1:162:R:ILE:N	2	21.77
(1,186)	1:162:R:ILE:N	1:162:R:ILE:CA	1:162:R:ILE:C	1:163:R:ASP:N	1	21.59
(1,182)	1:159:R:TRP:N	1:159:R:TRP:CA	1:159:R:TRP:C	1:160:R:TYR:N	1	21.42
(1,83)	1:82:R:ALA:C	1:83:R:ILE:N	1:83:R:ILE:CA	1:83:R:ILE:C	4	20.76
(1,30)	1:47:R:ASN:N	1:47:R:ASN:CA	1:47:R:ASN:C	1:48:R:HIS:N	2	20.76
(1,186)	1:162:R:ILE:N	1:162:R:ILE:CA	1:162:R:ILE:C	1:163:R:ASP:N	3	20.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,143)	1:125:R:CYS:C	1:126:R:VAL:N	1:126:R:VAL:CA	1:126:R:VAL:C	4	20.55
(1,83)	1:82:R:ALA:C	1:83:R:ILE:N	1:83:R:ILE:CA	1:83:R:ILE:C	3	20.36
(1,83)	1:82:R:ALA:C	1:83:R:ILE:N	1:83:R:ILE:CA	1:83:R:ILE:C	5	20.26
(1,179)	1:153:R:CYS:C	1:154:R:VAL:N	1:154:R:VAL:CA	1:154:R:VAL:C	3	20.09
(1,140)	1:124:R:VAL:N	1:124:R:VAL:CA	1:124:R:VAL:C	1:125:R:CYS:N	4	20.0
(1,144)	1:126:R:VAL:N	1:126:R:VAL:CA	1:126:R:VAL:C	1:127:R:VAL:N	4	19.6
(1,186)	1:162:R:ILE:N	1:162:R:ILE:CA	1:162:R:ILE:C	1:163:R:ASP:N	4	19.54
(1,119)	1:107:R:ILE:C	1:108:R:LYS:N	1:108:R:LYS:CA	1:108:R:LYS:C	4	19.53
(1,7)	1:33:R:LEU:C	1:34:R:TYR:N	1:34:R:TYR:CA	1:34:R:TYR:C	5	19.44
(1,83)	1:82:R:ALA:C	1:83:R:ILE:N	1:83:R:ILE:CA	1:83:R:ILE:C	2	19.4
(1,119)	1:107:R:ILE:C	1:108:R:LYS:N	1:108:R:LYS:CA	1:108:R:LYS:C	3	19.04
(1,145)	1:129:R:GLY:C	1:130:R:THR:N	1:130:R:THR:CA	1:130:R:THR:C	1	18.93
(1,40)	1:55:R:ALA:N	1:55:R:ALA:CA	1:55:R:ALA:C	1:56:R:ILE:N	1	18.72
(1,119)	1:107:R:ILE:C	1:108:R:LYS:N	1:108:R:LYS:CA	1:108:R:LYS:C	5	18.63
(1,153)	1:136:R:ASP:C	1:137:R:PHE:N	1:137:R:PHE:CA	1:137:R:PHE:C	2	18.53
(1,83)	1:82:R:ALA:C	1:83:R:ILE:N	1:83:R:ILE:CA	1:83:R:ILE:C	1	18.41
(1,177)	1:152:R:ALA:C	1:153:R:CYS:N	1:153:R:CYS:CA	1:153:R:CYS:C	3	18.37
(1,40)	1:55:R:ALA:N	1:55:R:ALA:CA	1:55:R:ALA:C	1:56:R:ILE:N	3	18.37
(1,144)	1:126:R:VAL:N	1:126:R:VAL:CA	1:126:R:VAL:C	1:127:R:VAL:N	2	18.27
(1,196)	1:170:R:TRP:N	1:170:R:TRP:CA	1:170:R:TRP:C	1:171:R:THR:N	5	18.18
(1,199)	1:172:R:PRO:C	1:173:R:ASP:N	1:173:R:ASP:CA	1:173:R:ASP:C	3	18.15
(1,176)	1:152:R:ALA:N	1:152:R:ALA:CA	1:152:R:ALA:C	1:153:R:CYS:N	1	17.93
(1,190)	1:166:R:ASP:N	1:166:R:ASP:CA	1:166:R:ASP:C	1:167:R:PHE:N	3	17.9
(1,24)	1:42:R:TYR:N	1:42:R:TYR:CA	1:42:R:TYR:C	1:43:R:SER:N	3	17.86
(1,44)	1:57:R:LEU:N	1:57:R:LEU:CA	1:57:R:LEU:C	1:58:R:GLN:N	5	17.72
(1,34)	1:52:R:TRP:N	1:52:R:TRP:CA	1:52:R:TRP:C	1:53:R:LEU:N	4	17.63
(1,179)	1:153:R:CYS:C	1:154:R:VAL:N	1:154:R:VAL:CA	1:154:R:VAL:C	5	17.62
(1,97)	1:89:R:LEU:C	1:90:R:THR:N	1:90:R:THR:CA	1:90:R:THR:C	2	17.28
(1,6)	1:32:R:THR:N	1:32:R:THR:CA	1:32:R:THR:C	1:33:R:LEU:N	3	17.24
(1,34)	1:52:R:TRP:N	1:52:R:TRP:CA	1:52:R:TRP:C	1:53:R:LEU:N	2	17.17
(1,34)	1:52:R:TRP:N	1:52:R:TRP:CA	1:52:R:TRP:C	1:53:R:LEU:N	5	16.9
(1,203)	1:175:R:SER:C	1:176:R:ASP:N	1:176:R:ASP:CA	1:176:R:ASP:C	4	16.86
(1,154)	1:137:R:PHE:N	1:137:R:PHE:CA	1:137:R:PHE:C	1:138:R:HIS:N	2	16.81
(1,25)	1:43:R:SER:C	1:44:R:ARG:N	1:44:R:ARG:CA	1:44:R:ARG:C	4	16.72
(1,118)	1:107:R:ILE:N	1:107:R:ILE:CA	1:107:R:ILE:C	1:108:R:LYS:N	1	16.69
(1,30)	1:47:R:ASN:N	1:47:R:ASN:CA	1:47:R:ASN:C	1:48:R:HIS:N	4	16.33
(1,194)	1:169:R:PRO:N	1:169:R:PRO:CA	1:169:R:PRO:C	1:170:R:TRP:N	2	16.3
(1,41)	1:55:R:ALA:C	1:56:R:ILE:N	1:56:R:ILE:CA	1:56:R:ILE:C	2	16.19
(1,111)	1:103:R:VAL:C	1:104:R:ILE:N	1:104:R:ILE:CA	1:104:R:ILE:C	3	16.14
(1,123)	1:109:R:HIS:C	1:110:R:LEU:N	1:110:R:LEU:CA	1:110:R:LEU:C	2	16.11
(1,127)	1:113:R:THR:C	1:114:R:GLY:N	1:114:R:GLY:CA	1:114:R:GLY:C	5	15.92
(1,176)	1:152:R:ALA:N	1:152:R:ALA:CA	1:152:R:ALA:C	1:153:R:CYS:N	3	15.91
(1,7)	1:33:R:LEU:C	1:34:R:TYR:N	1:34:R:TYR:CA	1:34:R:TYR:C	1	15.81
(1,8)	1:34:R:TYR:N	1:34:R:TYR:CA	1:34:R:TYR:C	1:35:R:ASN:N	3	15.8
(1,132)	1:117:R:THR:N	1:117:R:THR:CA	1:117:R:THR:C	1:118:R:ALA:N	5	15.79
(1,34)	1:52:R:TRP:N	1:52:R:TRP:CA	1:52:R:TRP:C	1:53:R:LEU:N	1	15.78
(1,37)	1:53:R:LEU:C	1:54:R:ASN:N	1:54:R:ASN:CA	1:54:R:ASN:C	2	15.72
(1,59)	1:65:R:GLU:C	1:66:R:PRO:N	1:66:R:PRO:CA	1:66:R:PRO:C	3	15.69
(1,194)	1:169:R:PRO:N	1:169:R:PRO:CA	1:169:R:PRO:C	1:170:R:TRP:N	1	15.48
(1,179)	1:153:R:CYS:C	1:154:R:VAL:N	1:154:R:VAL:CA	1:154:R:VAL:C	2	15.45
(1,178)	1:153:R:CYS:N	1:153:R:CYS:CA	1:153:R:CYS:C	1:154:R:VAL:N	4	15.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,78)	1:80:R:LEU:N	1:80:R:LEU:CA	1:80:R:LEU:C	1:81:R:GLU:N	1	15.39
(1,61)	1:66:R:PRO:C	1:67:R:PHE:N	1:67:R:PHE:CA	1:67:R:PHE:C	2	15.35
(1,129)	1:114:R:GLY:C	1:115:R:ILE:N	1:115:R:ILE:CA	1:115:R:ILE:C	5	15.33
(1,61)	1:66:R:PRO:C	1:67:R:PHE:N	1:67:R:PHE:CA	1:67:R:PHE:C	4	14.98
(1,139)	1:123:R:GLU:C	1:124:R:VAL:N	1:124:R:VAL:CA	1:124:R:VAL:C	5	14.93
(1,58)	1:65:R:GLU:N	1:65:R:GLU:CA	1:65:R:GLU:C	1:66:R:PRO:N	4	14.82
(1,158)	1:139:R:ALA:N	1:139:R:ALA:CA	1:139:R:ALA:C	1:140:R:GLY:N	3	14.69
(1,34)	1:52:R:TRP:N	1:52:R:TRP:CA	1:52:R:TRP:C	1:53:R:LEU:N	3	14.64
(1,68)	1:71:R:VAL:N	1:71:R:VAL:CA	1:71:R:VAL:C	1:72:R:TYR:N	1	14.63
(1,25)	1:43:R:SER:C	1:44:R:ARG:N	1:44:R:ARG:CA	1:44:R:ARG:C	5	14.51
(1,179)	1:153:R:CYS:C	1:154:R:VAL:N	1:154:R:VAL:CA	1:154:R:VAL:C	1	14.5
(1,199)	1:172:R:PRO:C	1:173:R:ASP:N	1:173:R:ASP:CA	1:173:R:ASP:C	2	14.48
(1,5)	1:31:R:LEU:C	1:32:R:THR:N	1:32:R:THR:CA	1:32:R:THR:C	2	14.47
(1,59)	1:65:R:GLU:C	1:66:R:PRO:N	1:66:R:PRO:CA	1:66:R:PRO:C	1	14.45
(1,57)	1:64:R:GLU:C	1:65:R:GLU:N	1:65:R:GLU:CA	1:65:R:GLU:C	5	14.28
(1,68)	1:71:R:VAL:N	1:71:R:VAL:CA	1:71:R:VAL:C	1:72:R:TYR:N	4	14.22
(1,100)	1:91:R:GLY:N	1:91:R:GLY:CA	1:91:R:GLY:C	1:92:R:LEU:N	5	14.04
(1,176)	1:152:R:ALA:N	1:152:R:ALA:CA	1:152:R:ALA:C	1:153:R:CYS:N	2	14.0
(1,141)	1:124:R:VAL:C	1:125:R:CYS:N	1:125:R:CYS:CA	1:125:R:CYS:C	5	13.88
(1,58)	1:65:R:GLU:N	1:65:R:GLU:CA	1:65:R:GLU:C	1:66:R:PRO:N	2	13.85
(1,63)	1:68:R:PHE:C	1:69:R:ASP:N	1:69:R:ASP:CA	1:69:R:ASP:C	4	13.8
(1,29)	1:46:R:ASN:C	1:47:R:ASN:N	1:47:R:ASN:CA	1:47:R:ASN:C	4	13.78
(1,197)	1:170:R:TRP:C	1:171:R:THR:N	1:171:R:THR:CA	1:171:R:THR:C	5	13.74
(1,26)	1:44:R:ARG:N	1:44:R:ARG:CA	1:44:R:ARG:C	1:45:R:PRO:N	4	13.74
(1,161)	1:141:R:ILE:C	1:142:R:PHE:N	1:142:R:PHE:CA	1:142:R:PHE:C	1	13.72
(1,25)	1:43:R:SER:C	1:44:R:ARG:N	1:44:R:ARG:CA	1:44:R:ARG:C	1	13.67
(1,176)	1:152:R:ALA:N	1:152:R:ALA:CA	1:152:R:ALA:C	1:153:R:CYS:N	5	13.65
(1,189)	1:165:R:GLU:C	1:166:R:ASP:N	1:166:R:ASP:CA	1:166:R:ASP:C	3	13.5
(1,55)	1:62:R:TYR:C	1:63:R:VAL:N	1:63:R:VAL:CA	1:63:R:VAL:C	5	13.37
(1,150)	1:133:R:CYS:N	1:133:R:CYS:CA	1:133:R:CYS:C	1:134:R:LEU:N	4	13.36
(1,143)	1:125:R:CYS:C	1:126:R:VAL:N	1:126:R:VAL:CA	1:126:R:VAL:C	2	13.36
(1,146)	1:130:R:THR:N	1:130:R:THR:CA	1:130:R:THR:C	1:131:R:ASP:N	4	13.32
(1,161)	1:141:R:ILE:C	1:142:R:PHE:N	1:142:R:PHE:CA	1:142:R:PHE:C	2	13.28
(1,58)	1:65:R:GLU:N	1:65:R:GLU:CA	1:65:R:GLU:C	1:66:R:PRO:N	5	13.26
(1,128)	1:114:R:GLY:N	1:114:R:GLY:CA	1:114:R:GLY:C	1:115:R:ILE:N	2	13.16
(1,97)	1:89:R:LEU:C	1:90:R:THR:N	1:90:R:THR:CA	1:90:R:THR:C	1	13.11
(1,190)	1:166:R:ASP:N	1:166:R:ASP:CA	1:166:R:ASP:C	1:167:R:PHE:N	1	12.92
(1,44)	1:57:R:LEU:N	1:57:R:LEU:CA	1:57:R:LEU:C	1:58:R:GLN:N	2	12.87
(1,56)	1:63:R:VAL:N	1:63:R:VAL:CA	1:63:R:VAL:C	1:64:R:GLU:N	3	12.85
(1,210)	1:179:R:VAL:N	1:179:R:VAL:CA	1:179:R:VAL:C	1:180:R:PHE:N	5	12.84
(1,210)	1:179:R:VAL:N	1:179:R:VAL:CA	1:179:R:VAL:C	1:180:R:PHE:N	1	12.83
(1,56)	1:63:R:VAL:N	1:63:R:VAL:CA	1:63:R:VAL:C	1:64:R:GLU:N	1	12.79
(1,120)	1:108:R:LYS:N	1:108:R:LYS:CA	1:108:R:LYS:C	1:109:R:HIS:N	3	12.73
(1,128)	1:114:R:GLY:N	1:114:R:GLY:CA	1:114:R:GLY:C	1:115:R:ILE:N	3	12.6
(1,29)	1:46:R:ASN:C	1:47:R:ASN:N	1:47:R:ASN:CA	1:47:R:ASN:C	3	12.55
(1,148)	1:132:R:MET:N	1:132:R:MET:CA	1:132:R:MET:C	1:133:R:CYS:N	2	12.5
(1,82)	1:82:R:ALA:N	1:82:R:ALA:CA	1:82:R:ALA:C	1:83:R:ILE:N	5	12.31
(1,144)	1:126:R:VAL:N	1:126:R:VAL:CA	1:126:R:VAL:C	1:127:R:VAL:N	3	12.08
(1,120)	1:108:R:LYS:N	1:108:R:LYS:CA	1:108:R:LYS:C	1:109:R:HIS:N	2	11.99
(1,200)	1:173:R:ASP:N	1:173:R:ASP:CA	1:173:R:ASP:C	1:174:R:PRO:N	2	11.9
(1,44)	1:57:R:LEU:N	1:57:R:LEU:CA	1:57:R:LEU:C	1:58:R:GLN:N	4	11.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,30)	1:47:R:ASN:N	1:47:R:ASN:CA	1:47:R:ASN:C	1:48:R:HIS:N	5	11.69
(1,146)	1:130:R:THR:N	1:130:R:THR:CA	1:130:R:THR:C	1:131:R:ASP:N	2	11.62
(1,95)	1:88:R:ASP:C	1:89:R:LEU:N	1:89:R:LEU:CA	1:89:R:LEU:C	3	11.61
(1,123)	1:109:R:HIS:C	1:110:R:LEU:N	1:110:R:LEU:CA	1:110:R:LEU:C	4	11.54
(1,161)	1:141:R:ILE:C	1:142:R:PHE:N	1:142:R:PHE:CA	1:142:R:PHE:C	4	11.52
(1,123)	1:109:R:HIS:C	1:110:R:LEU:N	1:110:R:LEU:CA	1:110:R:LEU:C	5	11.49
(1,143)	1:125:R:CYS:C	1:126:R:VAL:N	1:126:R:VAL:CA	1:126:R:VAL:C	3	11.47
(1,97)	1:89:R:LEU:C	1:90:R:THR:N	1:90:R:THR:CA	1:90:R:THR:C	4	11.42
(1,37)	1:53:R:LEU:C	1:54:R:ASN:N	1:54:R:ASN:CA	1:54:R:ASN:C	4	11.4
(1,154)	1:137:R:PHE:N	1:137:R:PHE:CA	1:137:R:PHE:C	1:138:R:HIS:N	4	11.23
(1,159)	1:140:R:GLY:C	1:141:R:ILE:N	1:141:R:ILE:CA	1:141:R:ILE:C	4	11.2
(1,203)	1:175:R:SER:C	1:176:R:ASP:N	1:176:R:ASP:CA	1:176:R:ASP:C	5	11.16
(1,146)	1:130:R:THR:N	1:130:R:THR:CA	1:130:R:THR:C	1:131:R:ASP:N	5	11.11
(1,40)	1:55:R:ALA:N	1:55:R:ALA:CA	1:55:R:ALA:C	1:56:R:ILE:N	4	10.98
(1,120)	1:108:R:LYS:N	1:108:R:LYS:CA	1:108:R:LYS:C	1:109:R:HIS:N	4	10.93
(1,124)	1:110:R:LEU:N	1:110:R:LEU:CA	1:110:R:LEU:C	1:111:R:LEU:N	5	10.89
(1,42)	1:56:R:ILE:N	1:56:R:ILE:CA	1:56:R:ILE:C	1:57:R:LEU:N	3	10.8
(1,188)	1:163:R:ASP:N	1:163:R:ASP:CA	1:163:R:ASP:C	1:164:R:ASP:N	3	10.74
(1,194)	1:169:R:PRO:N	1:169:R:PRO:CA	1:169:R:PRO:C	1:170:R:TRP:N	3	10.62
(1,203)	1:175:R:SER:C	1:176:R:ASP:N	1:176:R:ASP:CA	1:176:R:ASP:C	1	10.6
(1,53)	1:61:R:ARG:C	1:62:R:TYR:N	1:62:R:TYR:CA	1:62:R:TYR:C	3	10.6
(1,21)	1:40:R:THR:C	1:41:R:PHE:N	1:41:R:PHE:CA	1:41:R:PHE:C	2	10.58
(1,194)	1:169:R:PRO:N	1:169:R:PRO:CA	1:169:R:PRO:C	1:170:R:TRP:N	4	10.55
(1,203)	1:175:R:SER:C	1:176:R:ASP:N	1:176:R:ASP:CA	1:176:R:ASP:C	3	10.41
(1,100)	1:91:R:GLY:N	1:91:R:GLY:CA	1:91:R:GLY:C	1:92:R:LEU:N	1	10.35
(1,176)	1:152:R:ALA:N	1:152:R:ALA:CA	1:152:R:ALA:C	1:153:R:CYS:N	4	10.29
(1,8)	1:34:R:TYR:N	1:34:R:TYR:CA	1:34:R:TYR:C	1:35:R:ASN:N	1	10.27
(1,55)	1:62:R:TYR:C	1:63:R:VAL:N	1:63:R:VAL:CA	1:63:R:VAL:C	2	10.23
(1,189)	1:165:R:GLU:C	1:166:R:ASP:N	1:166:R:ASP:CA	1:166:R:ASP:C	4	10.19
(1,100)	1:91:R:GLY:N	1:91:R:GLY:CA	1:91:R:GLY:C	1:92:R:LEU:N	4	10.15
(1,37)	1:53:R:LEU:C	1:54:R:ASN:N	1:54:R:ASN:CA	1:54:R:ASN:C	1	10.08
(1,15)	1:37:R:GLU:C	1:38:R:LYS:N	1:38:R:LYS:CA	1:38:R:LYS:C	2	9.67
(1,28)	1:45:R:PRO:N	1:45:R:PRO:CA	1:45:R:PRO:C	1:46:R:ASN:N	2	9.65
(1,155)	1:137:R:PHE:C	1:138:R:HIS:N	1:138:R:HIS:CA	1:138:R:HIS:C	2	9.53
(1,124)	1:110:R:LEU:N	1:110:R:LEU:CA	1:110:R:LEU:C	1:111:R:LEU:N	1	9.49
(1,195)	1:169:R:PRO:C	1:170:R:TRP:N	1:170:R:TRP:CA	1:170:R:TRP:C	4	9.47
(1,97)	1:89:R:LEU:C	1:90:R:THR:N	1:90:R:THR:CA	1:90:R:THR:C	3	9.4
(1,91)	1:86:R:LEU:C	1:87:R:GLU:N	1:87:R:GLU:CA	1:87:R:GLU:C	2	9.37
(1,194)	1:169:R:PRO:N	1:169:R:PRO:CA	1:169:R:PRO:C	1:170:R:TRP:N	5	9.29
(1,161)	1:141:R:ILE:C	1:142:R:PHE:N	1:142:R:PHE:CA	1:142:R:PHE:C	5	9.24
(1,68)	1:71:R:VAL:N	1:71:R:VAL:CA	1:71:R:VAL:C	1:72:R:TYR:N	3	9.2
(1,180)	1:154:R:VAL:N	1:154:R:VAL:CA	1:154:R:VAL:C	1:155:R:THR:N	5	9.19
(1,148)	1:132:R:MET:N	1:132:R:MET:CA	1:132:R:MET:C	1:133:R:CYS:N	5	9.19
(1,99)	1:90:R:THR:C	1:91:R:GLY:N	1:91:R:GLY:CA	1:91:R:GLY:C	2	9.17
(1,28)	1:45:R:PRO:N	1:45:R:PRO:CA	1:45:R:PRO:C	1:46:R:ASN:N	1	9.17
(1,78)	1:80:R:LEU:N	1:80:R:LEU:CA	1:80:R:LEU:C	1:81:R:GLU:N	3	9.12
(1,62)	1:67:R:PHE:N	1:67:R:PHE:CA	1:67:R:PHE:C	1:68:R:PHE:N	1	9.02
(1,50)	1:60:R:PHE:N	1:60:R:PHE:CA	1:60:R:PHE:C	1:61:R:ARG:N	1	9.02
(1,54)	1:62:R:TYR:N	1:62:R:TYR:CA	1:62:R:TYR:C	1:63:R:VAL:N	4	9.01
(1,20)	1:40:R:THR:N	1:40:R:THR:CA	1:40:R:THR:C	1:41:R:PHE:N	2	8.92
(1,127)	1:113:R:THR:C	1:114:R:GLY:N	1:114:R:GLY:CA	1:114:R:GLY:C	2	8.9

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,7)	1:33:R:LEU:C	1:34:R:TYR:N	1:34:R:TYR:CA	1:34:R:TYR:C	3	8.86
(1,4)	1:31:R:LEU:N	1:31:R:LEU:CA	1:31:R:LEU:C	1:32:R:THR:N	2	8.81
(1,143)	1:125:R:CYS:C	1:126:R:VAL:N	1:126:R:VAL:CA	1:126:R:VAL:C	1	8.8
(1,61)	1:66:R:PRO:C	1:67:R:PHE:N	1:67:R:PHE:CA	1:67:R:PHE:C	5	8.78
(1,180)	1:154:R:VAL:N	1:154:R:VAL:CA	1:154:R:VAL:C	1:155:R:THR:N	4	8.75
(1,138)	1:123:R:GLU:N	1:123:R:GLU:CA	1:123:R:GLU:C	1:124:R:VAL:N	2	8.74
(1,53)	1:61:R:ARG:C	1:62:R:TYR:N	1:62:R:TYR:CA	1:62:R:TYR:C	1	8.69
(1,150)	1:133:R:CYS:N	1:133:R:CYS:CA	1:133:R:CYS:C	1:134:R:LEU:N	3	8.68
(1,96)	1:89:R:LEU:N	1:89:R:LEU:CA	1:89:R:LEU:C	1:90:R:THR:N	5	8.68
(1,23)	1:41:R:PHE:C	1:42:R:TYR:N	1:42:R:TYR:CA	1:42:R:TYR:C	2	8.6
(1,188)	1:163:R:ASP:N	1:163:R:ASP:CA	1:163:R:ASP:C	1:164:R:ASP:N	1	8.54
(1,167)	1:147:R:GLU:C	1:148:R:HIS:N	1:148:R:HIS:CA	1:148:R:HIS:C	3	8.47
(1,77)	1:79:R:THR:C	1:80:R:LEU:N	1:80:R:LEU:CA	1:80:R:LEU:C	5	8.44
(1,153)	1:136:R:ASP:C	1:137:R:PHE:N	1:137:R:PHE:CA	1:137:R:PHE:C	3	8.37
(1,37)	1:53:R:LEU:C	1:54:R:ASN:N	1:54:R:ASN:CA	1:54:R:ASN:C	5	8.35
(1,127)	1:113:R:THR:C	1:114:R:GLY:N	1:114:R:GLY:CA	1:114:R:GLY:C	1	8.34
(1,49)	1:59:R:LEU:C	1:60:R:PHE:N	1:60:R:PHE:CA	1:60:R:PHE:C	1	8.32
(1,59)	1:65:R:GLU:C	1:66:R:PRO:N	1:66:R:PRO:CA	1:66:R:PRO:C	4	8.27
(1,198)	1:171:R:THR:N	1:171:R:THR:CA	1:171:R:THR:C	1:172:R:PRO:N	3	8.26
(1,189)	1:165:R:GLU:C	1:166:R:ASP:N	1:166:R:ASP:CA	1:166:R:ASP:C	1	8.26
(1,78)	1:80:R:LEU:N	1:80:R:LEU:CA	1:80:R:LEU:C	1:81:R:GLU:N	2	8.26
(1,200)	1:173:R:ASP:N	1:173:R:ASP:CA	1:173:R:ASP:C	1:174:R:PRO:N	4	8.24
(1,161)	1:141:R:ILE:C	1:142:R:PHE:N	1:142:R:PHE:CA	1:142:R:PHE:C	3	8.18
(1,188)	1:163:R:ASP:N	1:163:R:ASP:CA	1:163:R:ASP:C	1:164:R:ASP:N	5	8.17
(1,77)	1:79:R:THR:C	1:80:R:LEU:N	1:80:R:LEU:CA	1:80:R:LEU:C	3	8.15
(1,77)	1:79:R:THR:C	1:80:R:LEU:N	1:80:R:LEU:CA	1:80:R:LEU:C	4	8.14
(1,203)	1:175:R:SER:C	1:176:R:ASP:N	1:176:R:ASP:CA	1:176:R:ASP:C	2	8.09
(1,95)	1:88:R:ASP:C	1:89:R:LEU:N	1:89:R:LEU:CA	1:89:R:LEU:C	2	8.07
(1,131)	1:116:R:GLY:C	1:117:R:THR:N	1:117:R:THR:CA	1:117:R:THR:C	2	8.05
(1,21)	1:40:R:THR:C	1:41:R:PHE:N	1:41:R:PHE:CA	1:41:R:PHE:C	5	8.05
(1,38)	1:54:R:ASN:N	1:54:R:ASN:CA	1:54:R:ASN:C	1:55:R:ALA:N	4	8.02
(1,33)	1:51:R:ALA:C	1:52:R:TRP:N	1:52:R:TRP:CA	1:52:R:TRP:C	2	7.99
(1,45)	1:57:R:LEU:C	1:58:R:GLN:N	1:58:R:GLN:CA	1:58:R:GLN:C	3	7.97
(1,138)	1:123:R:GLU:N	1:123:R:GLU:CA	1:123:R:GLU:C	1:124:R:VAL:N	3	7.9
(1,16)	1:38:R:LYS:N	1:38:R:LYS:CA	1:38:R:LYS:C	1:39:R:LYS:N	4	7.9
(1,62)	1:67:R:PHE:N	1:67:R:PHE:CA	1:67:R:PHE:C	1:68:R:PHE:N	2	7.89
(1,57)	1:64:R:GLU:C	1:65:R:GLU:N	1:65:R:GLU:CA	1:65:R:GLU:C	4	7.88
(1,210)	1:179:R:VAL:N	1:179:R:VAL:CA	1:179:R:VAL:C	1:180:R:PHE:N	2	7.87
(1,77)	1:79:R:THR:C	1:80:R:LEU:N	1:80:R:LEU:CA	1:80:R:LEU:C	2	7.87
(1,97)	1:89:R:LEU:C	1:90:R:THR:N	1:90:R:THR:CA	1:90:R:THR:C	5	7.86
(1,22)	1:41:R:PHE:N	1:41:R:PHE:CA	1:41:R:PHE:C	1:42:R:TYR:N	5	7.82
(1,6)	1:32:R:THR:N	1:32:R:THR:CA	1:32:R:THR:C	1:33:R:LEU:N	1	7.76
(1,197)	1:170:R:TRP:C	1:171:R:THR:N	1:171:R:THR:CA	1:171:R:THR:C	4	7.73
(1,82)	1:82:R:ALA:N	1:82:R:ALA:CA	1:82:R:ALA:C	1:83:R:ILE:N	2	7.7
(1,78)	1:80:R:LEU:N	1:80:R:LEU:CA	1:80:R:LEU:C	1:81:R:GLU:N	5	7.65
(1,62)	1:67:R:PHE:N	1:67:R:PHE:CA	1:67:R:PHE:C	1:68:R:PHE:N	3	7.65
(1,100)	1:91:R:GLY:N	1:91:R:GLY:CA	1:91:R:GLY:C	1:92:R:LEU:N	3	7.61
(1,111)	1:103:R:VAL:C	1:104:R:ILE:N	1:104:R:ILE:CA	1:104:R:ILE:C	1	7.56
(1,185)	1:161:R:ALA:C	1:162:R:ILE:N	1:162:R:ILE:CA	1:162:R:ILE:C	4	7.53
(1,145)	1:129:R:GLY:C	1:130:R:THR:N	1:130:R:THR:CA	1:130:R:THR:C	4	7.53
(1,117)	1:106:R:ASN:C	1:107:R:ILE:N	1:107:R:ILE:CA	1:107:R:ILE:C	3	7.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,96)	1:89:R:LEU:N	1:89:R:LEU:CA	1:89:R:LEU:C	1:90:R:THR:N	2	7.45
(1,179)	1:153:R:CYS:C	1:154:R:VAL:N	1:154:R:VAL:CA	1:154:R:VAL:C	4	7.41
(1,11)	1:35:R:ASN:C	1:36:R:GLY:N	1:36:R:GLY:CA	1:36:R:GLY:C	1	7.41
(1,122)	1:109:R:HIS:N	1:109:R:HIS:CA	1:109:R:HIS:C	1:110:R:LEU:N	3	7.33
(1,160)	1:141:R:ILE:N	1:141:R:ILE:CA	1:141:R:ILE:C	1:142:R:PHE:N	3	7.31
(1,189)	1:165:R:GLU:C	1:166:R:ASP:N	1:166:R:ASP:CA	1:166:R:ASP:C	5	7.26
(1,76)	1:79:R:THR:N	1:79:R:THR:CA	1:79:R:THR:C	1:80:R:LEU:N	5	7.25
(1,76)	1:79:R:THR:N	1:79:R:THR:CA	1:79:R:THR:C	1:80:R:LEU:N	2	7.23
(1,46)	1:58:R:GLN:N	1:58:R:GLN:CA	1:58:R:GLN:C	1:59:R:LEU:N	2	7.23
(1,118)	1:107:R:ILE:N	1:107:R:ILE:CA	1:107:R:ILE:C	1:108:R:LYS:N	5	7.22
(1,202)	1:175:R:SER:N	1:175:R:SER:CA	1:175:R:SER:C	1:176:R:ASP:N	4	7.19
(1,138)	1:123:R:GLU:N	1:123:R:GLU:CA	1:123:R:GLU:C	1:124:R:VAL:N	4	7.16
(1,201)	1:174:R:PRO:C	1:175:R:SER:N	1:175:R:SER:CA	1:175:R:SER:C	3	7.15
(1,59)	1:65:R:GLU:C	1:66:R:PRO:N	1:66:R:PRO:CA	1:66:R:PRO:C	2	7.09
(1,80)	1:81:R:GLU:N	1:81:R:GLU:CA	1:81:R:GLU:C	1:82:R:ALA:N	2	7.08
(1,80)	1:81:R:GLU:N	1:81:R:GLU:CA	1:81:R:GLU:C	1:82:R:ALA:N	1	7.0
(1,38)	1:54:R:ASN:N	1:54:R:ASN:CA	1:54:R:ASN:C	1:55:R:ALA:N	5	7.0
(1,77)	1:79:R:THR:C	1:80:R:LEU:N	1:80:R:LEU:CA	1:80:R:LEU:C	1	6.96
(1,38)	1:54:R:ASN:N	1:54:R:ASN:CA	1:54:R:ASN:C	1:55:R:ALA:N	1	6.89
(1,115)	1:105:R:TRP:C	1:106:R:ASN:N	1:106:R:ASN:CA	1:106:R:ASN:C	3	6.88
(1,115)	1:105:R:TRP:C	1:106:R:ASN:N	1:106:R:ASN:CA	1:106:R:ASN:C	4	6.87
(1,63)	1:68:R:PHE:C	1:69:R:ASP:N	1:69:R:ASP:CA	1:69:R:ASP:C	5	6.87
(1,140)	1:124:R:VAL:N	1:124:R:VAL:CA	1:124:R:VAL:C	1:125:R:CYS:N	3	6.86
(1,78)	1:80:R:LEU:N	1:80:R:LEU:CA	1:80:R:LEU:C	1:81:R:GLU:N	4	6.84
(1,55)	1:62:R:TYR:C	1:63:R:VAL:N	1:63:R:VAL:CA	1:63:R:VAL:C	3	6.82
(1,85)	1:83:R:ILE:C	1:84:R:LYS:N	1:84:R:LYS:CA	1:84:R:LYS:C	5	6.8
(1,80)	1:81:R:GLU:N	1:81:R:GLU:CA	1:81:R:GLU:C	1:82:R:ALA:N	3	6.78
(1,19)	1:39:R:LYS:C	1:40:R:THR:N	1:40:R:THR:CA	1:40:R:THR:C	5	6.74
(1,26)	1:44:R:ARG:N	1:44:R:ARG:CA	1:44:R:ARG:C	1:45:R:PRO:N	5	6.71
(1,167)	1:147:R:GLU:C	1:148:R:HIS:N	1:148:R:HIS:CA	1:148:R:HIS:C	5	6.7
(1,101)	1:94:R:LEU:C	1:95:R:HIS:N	1:95:R:HIS:CA	1:95:R:HIS:C	2	6.69
(1,21)	1:40:R:THR:C	1:41:R:PHE:N	1:41:R:PHE:CA	1:41:R:PHE:C	3	6.67
(1,128)	1:114:R:GLY:N	1:114:R:GLY:CA	1:114:R:GLY:C	1:115:R:ILE:N	4	6.64
(1,29)	1:46:R:ASN:C	1:47:R:ASN:N	1:47:R:ASN:CA	1:47:R:ASN:C	1	6.61
(1,116)	1:106:R:ASN:N	1:106:R:ASN:CA	1:106:R:ASN:C	1:107:R:ILE:N	3	6.47
(1,130)	1:115:R:ILE:N	1:115:R:ILE:CA	1:115:R:ILE:C	1:116:R:GLY:N	2	6.44
(1,29)	1:46:R:ASN:C	1:47:R:ASN:N	1:47:R:ASN:CA	1:47:R:ASN:C	5	6.43
(1,152)	1:135:R:ALA:N	1:135:R:ALA:CA	1:135:R:ALA:C	1:136:R:ASP:N	2	6.41
(1,135)	1:118:R:ALA:C	1:119:R:SER:N	1:119:R:SER:CA	1:119:R:SER:C	5	6.38
(1,80)	1:81:R:GLU:N	1:81:R:GLU:CA	1:81:R:GLU:C	1:82:R:ALA:N	4	6.37
(1,201)	1:174:R:PRO:C	1:175:R:SER:N	1:175:R:SER:CA	1:175:R:SER:C	5	6.34
(1,57)	1:64:R:GLU:C	1:65:R:GLU:N	1:65:R:GLU:CA	1:65:R:GLU:C	2	6.33
(1,109)	1:102:R:LEU:C	1:103:R:VAL:N	1:103:R:VAL:CA	1:103:R:VAL:C	1	6.32
(1,33)	1:51:R:ALA:C	1:52:R:TRP:N	1:52:R:TRP:CA	1:52:R:TRP:C	1	6.29
(1,85)	1:83:R:ILE:C	1:84:R:LYS:N	1:84:R:LYS:CA	1:84:R:LYS:C	3	6.26
(1,96)	1:89:R:LEU:N	1:89:R:LEU:CA	1:89:R:LEU:C	1:90:R:THR:N	4	6.25
(1,55)	1:62:R:TYR:C	1:63:R:VAL:N	1:63:R:VAL:CA	1:63:R:VAL:C	1	6.24
(1,151)	1:134:R:LEU:C	1:135:R:ALA:N	1:135:R:ALA:CA	1:135:R:ALA:C	3	6.23
(1,99)	1:90:R:THR:C	1:91:R:GLY:N	1:91:R:GLY:CA	1:91:R:GLY:C	5	6.22
(1,24)	1:42:R:TYR:N	1:42:R:TYR:CA	1:42:R:TYR:C	1:43:R:SER:N	4	6.22
(1,38)	1:54:R:ASN:N	1:54:R:ASN:CA	1:54:R:ASN:C	1:55:R:ALA:N	3	6.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,85)	1:83:R:ILE:C	1:84:R:LYS:N	1:84:R:LYS:CA	1:84:R:LYS:C	2	6.19
(1,85)	1:83:R:ILE:C	1:84:R:LYS:N	1:84:R:LYS:CA	1:84:R:LYS:C	1	6.18
(1,198)	1:171:R:THR:N	1:171:R:THR:CA	1:171:R:THR:C	1:172:R:PRO:N	4	6.17
(1,71)	1:72:R:TYR:C	1:73:R:SER:N	1:73:R:SER:CA	1:73:R:SER:C	1	6.17
(1,125)	1:111:R:LEU:C	1:112:R:HIS:N	1:112:R:HIS:CA	1:112:R:HIS:C	3	6.14
(1,120)	1:108:R:LYS:N	1:108:R:LYS:CA	1:108:R:LYS:C	1:109:R:HIS:N	5	6.14
(1,197)	1:170:R:TRP:C	1:171:R:THR:N	1:171:R:THR:CA	1:171:R:THR:C	1	6.07
(1,16)	1:38:R:LYS:N	1:38:R:LYS:CA	1:38:R:LYS:C	1:39:R:LYS:N	5	6.04
(1,178)	1:153:R:CYS:N	1:153:R:CYS:CA	1:153:R:CYS:C	1:154:R:VAL:N	3	5.91
(1,195)	1:169:R:PRO:C	1:170:R:TRP:N	1:170:R:TRP:CA	1:170:R:TRP:C	1	5.9
(1,100)	1:91:R:GLY:N	1:91:R:GLY:CA	1:91:R:GLY:C	1:92:R:LEU:N	2	5.89
(1,147)	1:131:R:ASP:C	1:132:R:MET:N	1:132:R:MET:CA	1:132:R:MET:C	1	5.88
(1,33)	1:51:R:ALA:C	1:52:R:TRP:N	1:52:R:TRP:CA	1:52:R:TRP:C	3	5.87
(1,116)	1:106:R:ASN:N	1:106:R:ASN:CA	1:106:R:ASN:C	1:107:R:ILE:N	4	5.81
(1,132)	1:117:R:THR:N	1:117:R:THR:CA	1:117:R:THR:C	1:118:R:ALA:N	4	5.8
(1,159)	1:140:R:GLY:C	1:141:R:ILE:N	1:141:R:ILE:CA	1:141:R:ILE:C	5	5.77
(1,130)	1:115:R:ILE:N	1:115:R:ILE:CA	1:115:R:ILE:C	1:116:R:GLY:N	4	5.75
(1,46)	1:58:R:GLN:N	1:58:R:GLN:CA	1:58:R:GLN:C	1:59:R:LEU:N	5	5.74
(1,146)	1:130:R:THR:N	1:130:R:THR:CA	1:130:R:THR:C	1:131:R:ASP:N	3	5.71
(1,69)	1:71:R:VAL:C	1:72:R:TYR:N	1:72:R:TYR:CA	1:72:R:TYR:C	2	5.65
(1,43)	1:56:R:ILE:C	1:57:R:LEU:N	1:57:R:LEU:CA	1:57:R:LEU:C	1	5.61
(1,19)	1:39:R:LYS:C	1:40:R:THR:N	1:40:R:THR:CA	1:40:R:THR:C	4	5.6
(1,132)	1:117:R:THR:N	1:117:R:THR:CA	1:117:R:THR:C	1:118:R:ALA:N	3	5.57
(1,44)	1:57:R:LEU:N	1:57:R:LEU:CA	1:57:R:LEU:C	1:58:R:GLN:N	3	5.57
(1,85)	1:83:R:ILE:C	1:84:R:LYS:N	1:84:R:LYS:CA	1:84:R:LYS:C	4	5.51
(1,112)	1:104:R:ILE:N	1:104:R:ILE:CA	1:104:R:ILE:C	1:105:R:TRP:N	2	5.47
(1,68)	1:71:R:VAL:N	1:71:R:VAL:CA	1:71:R:VAL:C	1:72:R:TYR:N	5	5.44
(1,123)	1:109:R:HIS:C	1:110:R:LEU:N	1:110:R:LEU:CA	1:110:R:LEU:C	1	5.43
(1,4)	1:31:R:LEU:N	1:31:R:LEU:CA	1:31:R:LEU:C	1:32:R:THR:N	4	5.4
(1,172)	1:150:R:VAL:N	1:150:R:VAL:CA	1:150:R:VAL:C	1:151:R:PHE:N	3	5.37
(1,42)	1:56:R:ILE:N	1:56:R:ILE:CA	1:56:R:ILE:C	1:57:R:LEU:N	5	5.36
(1,122)	1:109:R:HIS:N	1:109:R:HIS:CA	1:109:R:HIS:C	1:110:R:LEU:N	4	5.32
(1,52)	1:61:R:ARG:N	1:61:R:ARG:CA	1:61:R:ARG:C	1:62:R:TYR:N	3	5.32
(1,46)	1:58:R:GLN:N	1:58:R:GLN:CA	1:58:R:GLN:C	1:59:R:LEU:N	1	5.32
(1,149)	1:132:R:MET:C	1:133:R:CYS:N	1:133:R:CYS:CA	1:133:R:CYS:C	3	5.31
(1,138)	1:123:R:GLU:N	1:123:R:GLU:CA	1:123:R:GLU:C	1:124:R:VAL:N	1	5.24
(1,18)	1:39:R:LYS:N	1:39:R:LYS:CA	1:39:R:LYS:C	1:40:R:THR:N	3	5.23
(1,120)	1:108:R:LYS:N	1:108:R:LYS:CA	1:108:R:LYS:C	1:109:R:HIS:N	1	5.22
(1,128)	1:114:R:GLY:N	1:114:R:GLY:CA	1:114:R:GLY:C	1:115:R:ILE:N	1	5.2
(1,63)	1:68:R:PHE:C	1:69:R:ASP:N	1:69:R:ASP:CA	1:69:R:ASP:C	2	5.2
(1,45)	1:57:R:LEU:C	1:58:R:GLN:N	1:58:R:GLN:CA	1:58:R:GLN:C	1	5.15
(1,82)	1:82:R:ALA:N	1:82:R:ALA:CA	1:82:R:ALA:C	1:83:R:ILE:N	1	5.1
(1,19)	1:39:R:LYS:C	1:40:R:THR:N	1:40:R:THR:CA	1:40:R:THR:C	1	5.1
(1,210)	1:179:R:VAL:N	1:179:R:VAL:CA	1:179:R:VAL:C	1:180:R:PHE:N	3	5.08
(1,23)	1:41:R:PHE:C	1:42:R:TYR:N	1:42:R:TYR:CA	1:42:R:TYR:C	1	5.06
(1,207)	1:177:R:VAL:C	1:178:R:LEU:N	1:178:R:LEU:CA	1:178:R:LEU:C	3	5.05
(1,104)	1:100:R:PRO:N	1:100:R:PRO:CA	1:100:R:PRO:C	1:101:R:ALA:N	1	5.03
(1,187)	1:162:R:ILE:C	1:163:R:ASP:N	1:163:R:ASP:CA	1:163:R:ASP:C	2	4.99
(1,10)	1:35:R:ASN:N	1:35:R:ASN:CA	1:35:R:ASN:C	1:36:R:GLY:N	3	4.99
(1,33)	1:51:R:ALA:C	1:52:R:TRP:N	1:52:R:TRP:CA	1:52:R:TRP:C	4	4.9
(1,91)	1:86:R:LEU:C	1:87:R:GLU:N	1:87:R:GLU:CA	1:87:R:GLU:C	5	4.87

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,167)	1:147:R:GLU:C	1:148:R:HIS:N	1:148:R:HIS:CA	1:148:R:HIS:C	4	4.86
(1,49)	1:59:R:LEU:C	1:60:R:PHE:N	1:60:R:PHE:CA	1:60:R:PHE:C	3	4.86
(1,13)	1:36:R:GLY:C	1:37:R:GLU:N	1:37:R:GLU:CA	1:37:R:GLU:C	3	4.82
(1,142)	1:125:R:CYS:N	1:125:R:CYS:CA	1:125:R:CYS:C	1:126:R:VAL:N	2	4.78
(1,56)	1:63:R:VAL:N	1:63:R:VAL:CA	1:63:R:VAL:C	1:64:R:GLU:N	5	4.77
(1,43)	1:56:R:ILE:C	1:57:R:LEU:N	1:57:R:LEU:CA	1:57:R:LEU:C	2	4.75
(1,12)	1:36:R:GLY:N	1:36:R:GLY:CA	1:36:R:GLY:C	1:37:R:GLU:N	3	4.74
(1,22)	1:41:R:PHE:N	1:41:R:PHE:CA	1:41:R:PHE:C	1:42:R:TYR:N	3	4.73
(1,33)	1:51:R:ALA:C	1:52:R:TRP:N	1:52:R:TRP:CA	1:52:R:TRP:C	5	4.72
(1,81)	1:81:R:GLU:C	1:82:R:ALA:N	1:82:R:ALA:CA	1:82:R:ALA:C	1	4.71
(1,8)	1:34:R:TYR:N	1:34:R:TYR:CA	1:34:R:TYR:C	1:35:R:ASN:N	5	4.69
(1,75)	1:78:R:LEU:C	1:79:R:THR:N	1:79:R:THR:CA	1:79:R:THR:C	2	4.67
(1,131)	1:116:R:GLY:C	1:117:R:THR:N	1:117:R:THR:CA	1:117:R:THR:C	3	4.63
(1,185)	1:161:R:ALA:C	1:162:R:ILE:N	1:162:R:ILE:CA	1:162:R:ILE:C	2	4.57
(1,130)	1:115:R:ILE:N	1:115:R:ILE:CA	1:115:R:ILE:C	1:116:R:GLY:N	1	4.55
(1,32)	1:51:R:ALA:N	1:51:R:ALA:CA	1:51:R:ALA:C	1:52:R:TRP:N	4	4.54
(1,59)	1:65:R:GLU:C	1:66:R:PRO:N	1:66:R:PRO:CA	1:66:R:PRO:C	5	4.53
(1,178)	1:153:R:CYS:N	1:153:R:CYS:CA	1:153:R:CYS:C	1:154:R:VAL:N	5	4.51
(1,31)	1:50:R:ASN:C	1:51:R:ALA:N	1:51:R:ALA:CA	1:51:R:ALA:C	3	4.51
(1,175)	1:151:R:PHE:C	1:152:R:ALA:N	1:152:R:ALA:CA	1:152:R:ALA:C	5	4.44
(1,117)	1:106:R:ASN:C	1:107:R:ILE:N	1:107:R:ILE:CA	1:107:R:ILE:C	4	4.4
(1,53)	1:61:R:ARG:C	1:62:R:TYR:N	1:62:R:TYR:CA	1:62:R:TYR:C	5	4.39
(1,125)	1:111:R:LEU:C	1:112:R:HIS:N	1:112:R:HIS:CA	1:112:R:HIS:C	4	4.37
(1,145)	1:129:R:GLY:C	1:130:R:THR:N	1:130:R:THR:CA	1:130:R:THR:C	2	4.34
(1,202)	1:175:R:SER:N	1:175:R:SER:CA	1:175:R:SER:C	1:176:R:ASP:N	1	4.3
(1,115)	1:105:R:TRP:C	1:106:R:ASN:N	1:106:R:ASN:CA	1:106:R:ASN:C	2	4.26
(1,108)	1:102:R:LEU:N	1:102:R:LEU:CA	1:102:R:LEU:C	1:103:R:VAL:N	2	4.25
(1,32)	1:51:R:ALA:N	1:51:R:ALA:CA	1:51:R:ALA:C	1:52:R:TRP:N	2	4.24
(1,104)	1:100:R:PRO:N	1:100:R:PRO:CA	1:100:R:PRO:C	1:101:R:ALA:N	4	4.12
(1,207)	1:177:R:VAL:C	1:178:R:LEU:N	1:178:R:LEU:CA	1:178:R:LEU:C	2	4.1
(1,129)	1:114:R:GLY:C	1:115:R:ILE:N	1:115:R:ILE:CA	1:115:R:ILE:C	4	4.1
(1,96)	1:89:R:LEU:N	1:89:R:LEU:CA	1:89:R:LEU:C	1:90:R:THR:N	3	4.1
(1,9)	1:34:R:TYR:C	1:35:R:ASN:N	1:35:R:ASN:CA	1:35:R:ASN:C	1	4.07
(1,61)	1:66:R:PRO:C	1:67:R:PHE:N	1:67:R:PHE:CA	1:67:R:PHE:C	3	4.05
(1,109)	1:102:R:LEU:C	1:103:R:VAL:N	1:103:R:VAL:CA	1:103:R:VAL:C	5	3.98
(1,47)	1:58:R:GLN:C	1:59:R:LEU:N	1:59:R:LEU:CA	1:59:R:LEU:C	4	3.97
(1,16)	1:38:R:LYS:N	1:38:R:LYS:CA	1:38:R:LYS:C	1:39:R:LYS:N	3	3.97
(1,112)	1:104:R:ILE:N	1:104:R:ILE:CA	1:104:R:ILE:C	1:105:R:TRP:N	3	3.91
(1,95)	1:88:R:ASP:C	1:89:R:LEU:N	1:89:R:LEU:CA	1:89:R:LEU:C	4	3.91
(1,96)	1:89:R:LEU:N	1:89:R:LEU:CA	1:89:R:LEU:C	1:90:R:THR:N	1	3.89
(1,6)	1:32:R:THR:N	1:32:R:THR:CA	1:32:R:THR:C	1:33:R:LEU:N	5	3.88
(1,37)	1:53:R:LEU:C	1:54:R:ASN:N	1:54:R:ASN:CA	1:54:R:ASN:C	3	3.85
(1,160)	1:141:R:ILE:N	1:141:R:ILE:CA	1:141:R:ILE:C	1:142:R:PHE:N	2	3.82
(1,160)	1:141:R:ILE:N	1:141:R:ILE:CA	1:141:R:ILE:C	1:142:R:PHE:N	1	3.77
(1,71)	1:72:R:TYR:C	1:73:R:SER:N	1:73:R:SER:CA	1:73:R:SER:C	5	3.77
(1,184)	1:161:R:ALA:N	1:161:R:ALA:CA	1:161:R:ALA:C	1:162:R:ILE:N	4	3.76
(1,155)	1:137:R:PHE:C	1:138:R:HIS:N	1:138:R:HIS:CA	1:138:R:HIS:C	5	3.76
(1,183)	1:160:R:TYR:C	1:161:R:ALA:N	1:161:R:ALA:CA	1:161:R:ALA:C	1	3.73
(1,99)	1:90:R:THR:C	1:91:R:GLY:N	1:91:R:GLY:CA	1:91:R:GLY:C	4	3.71
(1,58)	1:65:R:GLU:N	1:65:R:GLU:CA	1:65:R:GLU:C	1:66:R:PRO:N	1	3.68
(1,42)	1:56:R:ILE:N	1:56:R:ILE:CA	1:56:R:ILE:C	1:57:R:LEU:N	1	3.68

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,140)	1:124:R:VAL:N	1:124:R:VAL:CA	1:124:R:VAL:C	1:125:R:CYS:N	2	3.67
(1,71)	1:72:R:TYR:C	1:73:R:SER:N	1:73:R:SER:CA	1:73:R:SER:C	4	3.65
(1,101)	1:94:R:LEU:C	1:95:R:HIS:N	1:95:R:HIS:CA	1:95:R:HIS:C	1	3.61
(1,101)	1:94:R:LEU:C	1:95:R:HIS:N	1:95:R:HIS:CA	1:95:R:HIS:C	4	3.58
(1,98)	1:90:R:THR:N	1:90:R:THR:CA	1:90:R:THR:C	1:91:R:GLY:N	5	3.58
(1,152)	1:135:R:ALA:N	1:135:R:ALA:CA	1:135:R:ALA:C	1:136:R:ASP:N	4	3.52
(1,130)	1:115:R:ILE:N	1:115:R:ILE:CA	1:115:R:ILE:C	1:116:R:GLY:N	3	3.5
(1,101)	1:94:R:LEU:C	1:95:R:HIS:N	1:95:R:HIS:CA	1:95:R:HIS:C	5	3.5
(1,112)	1:104:R:ILE:N	1:104:R:ILE:CA	1:104:R:ILE:C	1:105:R:TRP:N	1	3.46
(1,47)	1:58:R:GLN:C	1:59:R:LEU:N	1:59:R:LEU:CA	1:59:R:LEU:C	1	3.43
(1,9)	1:34:R:TYR:C	1:35:R:ASN:N	1:35:R:ASN:CA	1:35:R:ASN:C	3	3.43
(1,167)	1:147:R:GLU:C	1:148:R:HIS:N	1:148:R:HIS:CA	1:148:R:HIS:C	1	3.41
(1,84)	1:83:R:ILE:N	1:83:R:ILE:CA	1:83:R:ILE:C	1:84:R:LYS:N	2	3.38
(1,73)	1:73:R:SER:C	1:74:R:SER:N	1:74:R:SER:CA	1:74:R:SER:C	3	3.38
(1,206)	1:177:R:VAL:N	1:177:R:VAL:CA	1:177:R:VAL:C	1:178:R:LEU:N	5	3.37
(1,173)	1:150:R:VAL:C	1:151:R:PHE:N	1:151:R:PHE:CA	1:151:R:PHE:C	2	3.35
(1,174)	1:151:R:PHE:N	1:151:R:PHE:CA	1:151:R:PHE:C	1:152:R:ALA:N	2	3.32
(1,50)	1:60:R:PHE:N	1:60:R:PHE:CA	1:60:R:PHE:C	1:61:R:ARG:N	3	3.28
(1,46)	1:58:R:GLN:N	1:58:R:GLN:CA	1:58:R:GLN:C	1:59:R:LEU:N	3	3.27
(1,159)	1:140:R:GLY:C	1:141:R:ILE:N	1:141:R:ILE:CA	1:141:R:ILE:C	2	3.2
(1,24)	1:42:R:TYR:N	1:42:R:TYR:CA	1:42:R:TYR:C	1:43:R:SER:N	5	3.2
(1,87)	1:84:R:LYS:C	1:85:R:GLN:N	1:85:R:GLN:CA	1:85:R:GLN:C	1	3.15
(1,45)	1:57:R:LEU:C	1:58:R:GLN:N	1:58:R:GLN:CA	1:58:R:GLN:C	5	3.15
(1,155)	1:137:R:PHE:C	1:138:R:HIS:N	1:138:R:HIS:CA	1:138:R:HIS:C	4	3.14
(1,150)	1:133:R:CYS:N	1:133:R:CYS:CA	1:133:R:CYS:C	1:134:R:LEU:N	1	3.13
(1,18)	1:39:R:LYS:N	1:39:R:LYS:CA	1:39:R:LYS:C	1:40:R:THR:N	2	3.13
(1,142)	1:125:R:CYS:N	1:125:R:CYS:CA	1:125:R:CYS:C	1:126:R:VAL:N	3	3.1
(1,58)	1:65:R:GLU:N	1:65:R:GLU:CA	1:65:R:GLU:C	1:66:R:PRO:N	3	3.08
(1,162)	1:142:R:PHE:N	1:142:R:PHE:CA	1:142:R:PHE:C	1:143:R:LEU:N	1	3.06
(1,16)	1:38:R:LYS:N	1:38:R:LYS:CA	1:38:R:LYS:C	1:39:R:LYS:N	1	3.04
(1,131)	1:116:R:GLY:C	1:117:R:THR:N	1:117:R:THR:CA	1:117:R:THR:C	1	3.03
(1,47)	1:58:R:GLN:C	1:59:R:LEU:N	1:59:R:LEU:CA	1:59:R:LEU:C	5	3.02
(1,71)	1:72:R:TYR:C	1:73:R:SER:N	1:73:R:SER:CA	1:73:R:SER:C	3	3.01
(1,56)	1:63:R:VAL:N	1:63:R:VAL:CA	1:63:R:VAL:C	1:64:R:GLU:N	2	2.99
(1,23)	1:41:R:PHE:C	1:42:R:TYR:N	1:42:R:TYR:CA	1:42:R:TYR:C	5	2.96
(1,3)	1:30:R:GLU:C	1:31:R:LEU:N	1:31:R:LEU:CA	1:31:R:LEU:C	1	2.96
(1,178)	1:153:R:CYS:N	1:153:R:CYS:CA	1:153:R:CYS:C	1:154:R:VAL:N	1	2.95
(1,74)	1:74:R:SER:N	1:74:R:SER:CA	1:74:R:SER:C	1:75:R:PRO:N	3	2.93
(1,114)	1:105:R:TRP:N	1:105:R:TRP:CA	1:105:R:TRP:C	1:106:R:ASN:N	5	2.9
(1,180)	1:154:R:VAL:N	1:154:R:VAL:CA	1:154:R:VAL:C	1:155:R:THR:N	1	2.89
(1,173)	1:150:R:VAL:C	1:151:R:PHE:N	1:151:R:PHE:CA	1:151:R:PHE:C	5	2.89
(1,63)	1:68:R:PHE:C	1:69:R:ASP:N	1:69:R:ASP:CA	1:69:R:ASP:C	1	2.88
(1,41)	1:55:R:ALA:C	1:56:R:ILE:N	1:56:R:ILE:CA	1:56:R:ILE:C	1	2.87
(1,138)	1:123:R:GLU:N	1:123:R:GLU:CA	1:123:R:GLU:C	1:124:R:VAL:N	5	2.82
(1,73)	1:73:R:SER:C	1:74:R:SER:N	1:74:R:SER:CA	1:74:R:SER:C	1	2.8
(1,133)	1:117:R:THR:C	1:118:R:ALA:N	1:118:R:ALA:CA	1:118:R:ALA:C	1	2.79
(1,150)	1:133:R:CYS:N	1:133:R:CYS:CA	1:133:R:CYS:C	1:134:R:LEU:N	2	2.78
(1,149)	1:132:R:MET:C	1:133:R:CYS:N	1:133:R:CYS:CA	1:133:R:CYS:C	2	2.78
(1,164)	1:143:R:LEU:N	1:143:R:LEU:CA	1:143:R:LEU:C	1:144:R:LYS:N	1	2.77
(1,38)	1:54:R:ASN:N	1:54:R:ASN:CA	1:54:R:ASN:C	1:55:R:ALA:N	2	2.74
(1,36)	1:53:R:LEU:N	1:53:R:LEU:CA	1:53:R:LEU:C	1:54:R:ASN:N	2	2.73

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,103)	1:99:R:PRO:C	1:100:R:PRO:N	1:100:R:PRO:CA	1:100:R:PRO:C	2	2.71
(1,54)	1:62:R:TYR:N	1:62:R:TYR:CA	1:62:R:TYR:C	1:63:R:VAL:N	1	2.7
(1,142)	1:125:R:CYS:N	1:125:R:CYS:CA	1:125:R:CYS:C	1:126:R:VAL:N	5	2.69
(1,39)	1:54:R:ASN:C	1:55:R:ALA:N	1:55:R:ALA:CA	1:55:R:ALA:C	5	2.67
(1,94)	1:88:R:ASP:N	1:88:R:ASP:CA	1:88:R:ASP:C	1:89:R:LEU:N	5	2.64
(1,70)	1:72:R:TYR:N	1:72:R:TYR:CA	1:72:R:TYR:C	1:73:R:SER:N	1	2.64
(1,134)	1:118:R:ALA:N	1:118:R:ALA:CA	1:118:R:ALA:C	1:119:R:SER:N	4	2.62
(1,95)	1:88:R:ASP:C	1:89:R:LEU:N	1:89:R:LEU:CA	1:89:R:LEU:C	1	2.59
(1,112)	1:104:R:ILE:N	1:104:R:ILE:CA	1:104:R:ILE:C	1:105:R:TRP:N	5	2.55
(1,80)	1:81:R:GLU:N	1:81:R:GLU:CA	1:81:R:GLU:C	1:82:R:ALA:N	5	2.52
(1,39)	1:54:R:ASN:C	1:55:R:ALA:N	1:55:R:ALA:CA	1:55:R:ALA:C	4	2.52
(1,185)	1:161:R:ALA:C	1:162:R:ILE:N	1:162:R:ILE:CA	1:162:R:ILE:C	3	2.51
(1,121)	1:108:R:LYS:C	1:109:R:HIS:N	1:109:R:HIS:CA	1:109:R:HIS:C	1	2.49
(1,10)	1:35:R:ASN:N	1:35:R:ASN:CA	1:35:R:ASN:C	1:36:R:GLY:N	1	2.47
(1,166)	1:144:R:LYS:N	1:144:R:LYS:CA	1:144:R:LYS:C	1:145:R:GLY:N	5	2.46
(1,82)	1:82:R:ALA:N	1:82:R:ALA:CA	1:82:R:ALA:C	1:83:R:ILE:N	4	2.45
(1,181)	1:158:R:GLY:C	1:159:R:TRP:N	1:159:R:TRP:CA	1:159:R:TRP:C	5	2.42
(1,29)	1:46:R:ASN:C	1:47:R:ASN:N	1:47:R:ASN:CA	1:47:R:ASN:C	2	2.39
(1,192)	1:167:R:PHE:N	1:167:R:PHE:CA	1:167:R:PHE:C	1:168:R:TYR:N	5	2.34
(1,127)	1:113:R:THR:C	1:114:R:GLY:N	1:114:R:GLY:CA	1:114:R:GLY:C	3	2.33
(1,206)	1:177:R:VAL:N	1:177:R:VAL:CA	1:177:R:VAL:C	1:178:R:LEU:N	4	2.32
(1,31)	1:50:R:ASN:C	1:51:R:ALA:N	1:51:R:ALA:CA	1:51:R:ALA:C	1	2.32
(1,195)	1:169:R:PRO:C	1:170:R:TRP:N	1:170:R:TRP:CA	1:170:R:TRP:C	2	2.3
(1,31)	1:50:R:ASN:C	1:51:R:ALA:N	1:51:R:ALA:CA	1:51:R:ALA:C	4	2.3
(1,70)	1:72:R:TYR:N	1:72:R:TYR:CA	1:72:R:TYR:C	1:73:R:SER:N	3	2.25
(1,3)	1:30:R:GLU:C	1:31:R:LEU:N	1:31:R:LEU:CA	1:31:R:LEU:C	2	2.2
(1,8)	1:34:R:TYR:N	1:34:R:TYR:CA	1:34:R:TYR:C	1:35:R:ASN:N	4	2.18
(1,147)	1:131:R:ASP:C	1:132:R:MET:N	1:132:R:MET:CA	1:132:R:MET:C	2	2.17
(1,139)	1:123:R:GLU:C	1:124:R:VAL:N	1:124:R:VAL:CA	1:124:R:VAL:C	4	2.17
(1,51)	1:60:R:PHE:C	1:61:R:ARG:N	1:61:R:ARG:CA	1:61:R:ARG:C	1	2.13
(1,39)	1:54:R:ASN:C	1:55:R:ALA:N	1:55:R:ALA:CA	1:55:R:ALA:C	1	2.13
(1,165)	1:143:R:LEU:C	1:144:R:LYS:N	1:144:R:LYS:CA	1:144:R:LYS:C	3	2.12
(1,54)	1:62:R:TYR:N	1:62:R:TYR:CA	1:62:R:TYR:C	1:63:R:VAL:N	5	2.12
(1,81)	1:81:R:GLU:C	1:82:R:ALA:N	1:82:R:ALA:CA	1:82:R:ALA:C	2	2.1
(1,99)	1:90:R:THR:C	1:91:R:GLY:N	1:91:R:GLY:CA	1:91:R:GLY:C	1	2.05
(1,43)	1:56:R:ILE:C	1:57:R:LEU:N	1:57:R:LEU:CA	1:57:R:LEU:C	4	2.03
(1,109)	1:102:R:LEU:C	1:103:R:VAL:N	1:103:R:VAL:CA	1:103:R:VAL:C	4	2.02
(1,129)	1:114:R:GLY:C	1:115:R:ILE:N	1:115:R:ILE:CA	1:115:R:ILE:C	2	2.01
(1,188)	1:163:R:ASP:N	1:163:R:ASP:CA	1:163:R:ASP:C	1:164:R:ASP:N	4	2.0
(1,187)	1:162:R:ILE:C	1:163:R:ASP:N	1:163:R:ASP:CA	1:163:R:ASP:C	3	2.0
(1,148)	1:132:R:MET:N	1:132:R:MET:CA	1:132:R:MET:C	1:133:R:CYS:N	1	2.0
(1,121)	1:108:R:LYS:C	1:109:R:HIS:N	1:109:R:HIS:CA	1:109:R:HIS:C	3	2.0
(1,75)	1:78:R:LEU:C	1:79:R:THR:N	1:79:R:THR:CA	1:79:R:THR:C	1	1.99
(1,142)	1:125:R:CYS:N	1:125:R:CYS:CA	1:125:R:CYS:C	1:126:R:VAL:N	4	1.97
(1,26)	1:44:R:ARG:N	1:44:R:ARG:CA	1:44:R:ARG:C	1:45:R:PRO:N	3	1.97
(1,192)	1:167:R:PHE:N	1:167:R:PHE:CA	1:167:R:PHE:C	1:168:R:TYR:N	4	1.93
(1,50)	1:60:R:PHE:N	1:60:R:PHE:CA	1:60:R:PHE:C	1:61:R:ARG:N	4	1.93
(1,32)	1:51:R:ALA:N	1:51:R:ALA:CA	1:51:R:ALA:C	1:52:R:TRP:N	1	1.93
(1,116)	1:106:R:ASN:N	1:106:R:ASN:CA	1:106:R:ASN:C	1:107:R:ILE:N	1	1.92
(1,89)	1:85:R:GLN:C	1:86:R:LEU:N	1:86:R:LEU:CA	1:86:R:LEU:C	3	1.89
(1,32)	1:51:R:ALA:N	1:51:R:ALA:CA	1:51:R:ALA:C	1:52:R:TRP:N	3	1.86

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,165)	1:143:R:LEU:C	1:144:R:LYS:N	1:144:R:LYS:CA	1:144:R:LYS:C	5	1.85
(1,110)	1:103:R:VAL:N	1:103:R:VAL:CA	1:103:R:VAL:C	1:104:R:ILE:N	2	1.85
(1,147)	1:131:R:ASP:C	1:132:R:MET:N	1:132:R:MET:CA	1:132:R:MET:C	4	1.81
(1,163)	1:142:R:PHE:C	1:143:R:LEU:N	1:143:R:LEU:CA	1:143:R:LEU:C	3	1.8
(1,165)	1:143:R:LEU:C	1:144:R:LYS:N	1:144:R:LYS:CA	1:144:R:LYS:C	4	1.79
(1,129)	1:114:R:GLY:C	1:115:R:ILE:N	1:115:R:ILE:CA	1:115:R:ILE:C	3	1.76
(1,27)	1:44:R:ARG:C	1:45:R:PRO:N	1:45:R:PRO:CA	1:45:R:PRO:C	3	1.72
(1,154)	1:137:R:PHE:N	1:137:R:PHE:CA	1:137:R:PHE:C	1:138:R:HIS:N	1	1.69
(1,159)	1:140:R:GLY:C	1:141:R:ILE:N	1:141:R:ILE:CA	1:141:R:ILE:C	3	1.65
(1,94)	1:88:R:ASP:N	1:88:R:ASP:CA	1:88:R:ASP:C	1:89:R:LEU:N	1	1.64
(1,91)	1:86:R:LEU:C	1:87:R:GLU:N	1:87:R:GLU:CA	1:87:R:GLU:C	3	1.63
(1,70)	1:72:R:TYR:N	1:72:R:TYR:CA	1:72:R:TYR:C	1:73:R:SER:N	5	1.6
(1,210)	1:179:R:VAL:N	1:179:R:VAL:CA	1:179:R:VAL:C	1:180:R:PHE:N	4	1.58
(1,51)	1:60:R:PHE:C	1:61:R:ARG:N	1:61:R:ARG:CA	1:61:R:ARG:C	5	1.5
(1,191)	1:166:R:ASP:C	1:167:R:PHE:N	1:167:R:PHE:CA	1:167:R:PHE:C	3	1.48
(1,21)	1:40:R:THR:C	1:41:R:PHE:N	1:41:R:PHE:CA	1:41:R:PHE:C	1	1.46
(1,207)	1:177:R:VAL:C	1:178:R:LEU:N	1:178:R:LEU:CA	1:178:R:LEU:C	4	1.41
(1,122)	1:109:R:HIS:N	1:109:R:HIS:CA	1:109:R:HIS:C	1:110:R:LEU:N	2	1.41
(1,110)	1:103:R:VAL:N	1:103:R:VAL:CA	1:103:R:VAL:C	1:104:R:ILE:N	5	1.4
(1,105)	1:100:R:PRO:C	1:101:R:ALA:N	1:101:R:ALA:CA	1:101:R:ALA:C	2	1.4
(1,84)	1:83:R:ILE:N	1:83:R:ILE:CA	1:83:R:ILE:C	1:84:R:LYS:N	5	1.38
(1,9)	1:34:R:TYR:C	1:35:R:ASN:N	1:35:R:ASN:CA	1:35:R:ASN:C	4	1.34
(1,11)	1:35:R:ASN:C	1:36:R:GLY:N	1:36:R:GLY:CA	1:36:R:GLY:C	3	1.31
(1,62)	1:67:R:PHE:N	1:67:R:PHE:CA	1:67:R:PHE:C	1:68:R:PHE:N	4	1.29
(1,20)	1:40:R:THR:N	1:40:R:THR:CA	1:40:R:THR:C	1:41:R:PHE:N	1	1.28
(1,127)	1:113:R:THR:C	1:114:R:GLY:N	1:114:R:GLY:CA	1:114:R:GLY:C	4	1.27
(1,131)	1:116:R:GLY:C	1:117:R:THR:N	1:117:R:THR:CA	1:117:R:THR:C	5	1.26
(1,114)	1:105:R:TRP:N	1:105:R:TRP:CA	1:105:R:TRP:C	1:106:R:ASN:N	3	1.26
(1,75)	1:78:R:LEU:C	1:79:R:THR:N	1:79:R:THR:CA	1:79:R:THR:C	3	1.25
(1,199)	1:172:R:PRO:C	1:173:R:ASP:N	1:173:R:ASP:CA	1:173:R:ASP:C	1	1.23
(1,6)	1:32:R:THR:N	1:32:R:THR:CA	1:32:R:THR:C	1:33:R:LEU:N	2	1.23
(1,185)	1:161:R:ALA:C	1:162:R:ILE:N	1:162:R:ILE:CA	1:162:R:ILE:C	5	1.21
(1,190)	1:166:R:ASP:N	1:166:R:ASP:CA	1:166:R:ASP:C	1:167:R:PHE:N	4	1.14
(1,173)	1:150:R:VAL:C	1:151:R:PHE:N	1:151:R:PHE:CA	1:151:R:PHE:C	4	1.11
(1,43)	1:56:R:ILE:C	1:57:R:LEU:N	1:57:R:LEU:CA	1:57:R:LEU:C	5	1.1
(1,47)	1:58:R:GLN:C	1:59:R:LEU:N	1:59:R:LEU:CA	1:59:R:LEU:C	2	1.07
(1,139)	1:123:R:GLU:C	1:124:R:VAL:N	1:124:R:VAL:CA	1:124:R:VAL:C	3	1.05
(1,61)	1:66:R:PRO:C	1:67:R:PHE:N	1:67:R:PHE:CA	1:67:R:PHE:C	1	1.0