



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 12:16 AM UTC

PDB ID : 6L8V / pdb_00006l8v
BMRB ID : 36294
Title : membrane-bound Bax helix2-helix5 domain
Authors : OuYang, B.; Lv, F.
Deposited on : 2019-11-07

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

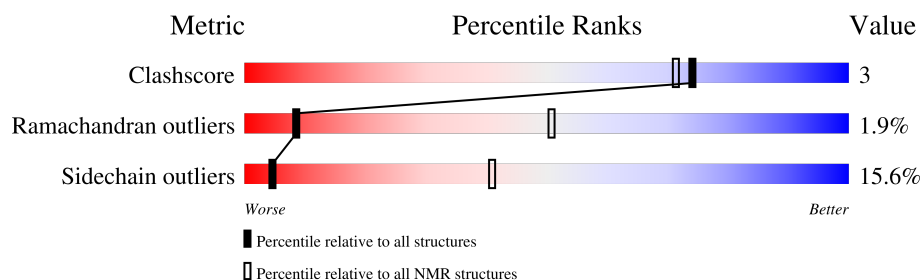
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 18%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	81	
1	B	81	

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:55-A:128, B:56-B:128 (147)	1.22	15

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2520 atoms, of which 1262 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apoptosis regulator BAX.

Mol	Chain	Residues	Atoms						Trace
1	A	81	Total	C	H	N	O	S	0
			1260	398	631	107	120	4	
1	B	81	Total	C	H	N	O	S	0
			1260	398	631	107	120	4	

There are 14 discrepancies between the modelled and reference sequences:

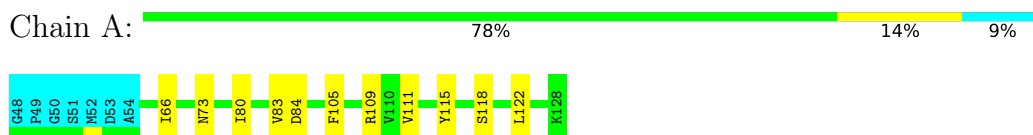
Chain	Residue	Modelled	Actual	Comment	Reference
A	48	GLY	-	expression tag	UNP Q07812
A	49	PRO	-	expression tag	UNP Q07812
A	50	GLY	-	expression tag	UNP Q07812
A	51	SER	-	expression tag	UNP Q07812
A	52	MET	-	expression tag	UNP Q07812
A	62	SER	CYS	engineered mutation	UNP Q07812
A	126	SER	CYS	engineered mutation	UNP Q07812
B	48	GLY	-	expression tag	UNP Q07812
B	49	PRO	-	expression tag	UNP Q07812
B	50	GLY	-	expression tag	UNP Q07812
B	51	SER	-	expression tag	UNP Q07812
B	52	MET	-	expression tag	UNP Q07812
B	62	SER	CYS	engineered mutation	UNP Q07812
B	126	SER	CYS	engineered mutation	UNP Q07812

4 Residue-property plots

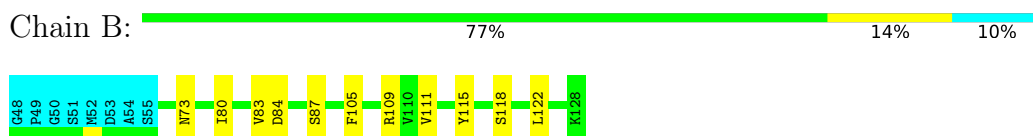
4.1 Average score per residue in the NMR ensemble

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: Apoptosis regulator BAX



- Molecule 1: Apoptosis regulator BAX

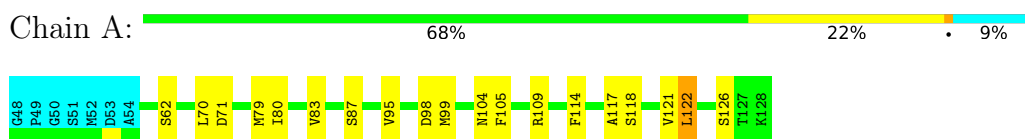


4.2 Scores per residue for each member of the ensemble

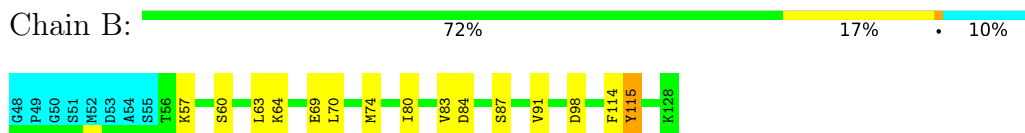
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Apoptosis regulator BAX



- Molecule 1: Apoptosis regulator BAX



4.2.2 Score per residue for model 2

- Molecule 1: Apoptosis regulator BAX

Chain A: 



- Molecule 1: Apoptosis regulator BAX

Chain B: 



4.2.3 Score per residue for model 3

- Molecule 1: Apoptosis regulator BAX

Chain A: 



- Molecule 1: Apoptosis regulator BAX

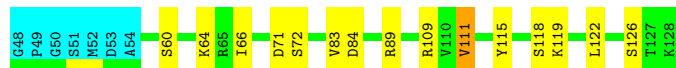
Chain B: 



4.2.4 Score per residue for model 4

- Molecule 1: Apoptosis regulator BAX

Chain A: 



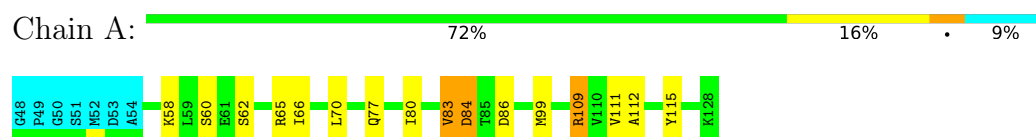
- Molecule 1: Apoptosis regulator BAX

Chain B: 

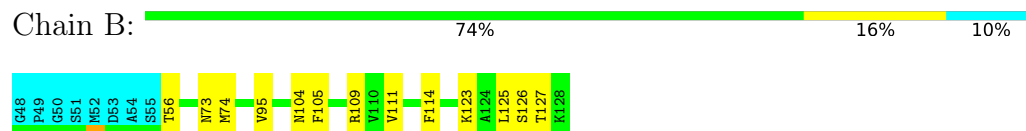


4.2.5 Score per residue for model 5

- Molecule 1: Apoptosis regulator BAX

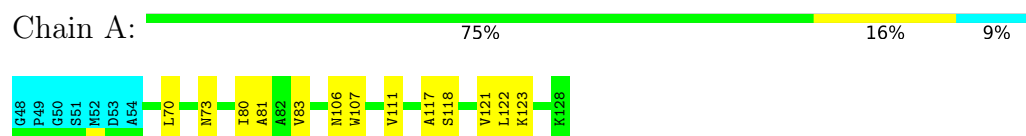


- Molecule 1: Apoptosis regulator BAX

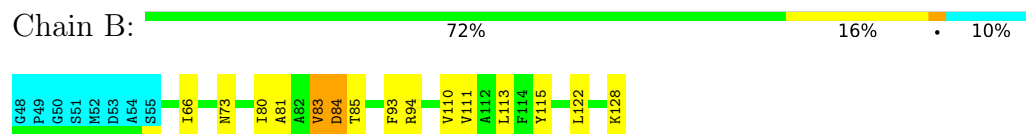


4.2.6 Score per residue for model 6

- Molecule 1: Apoptosis regulator BAX

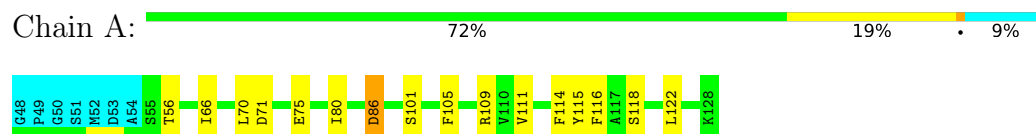


- Molecule 1: Apoptosis regulator BAX

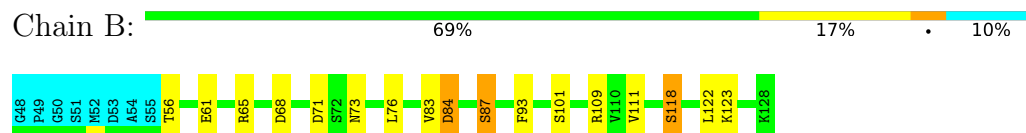


4.2.7 Score per residue for model 7

- Molecule 1: Apoptosis regulator BAX

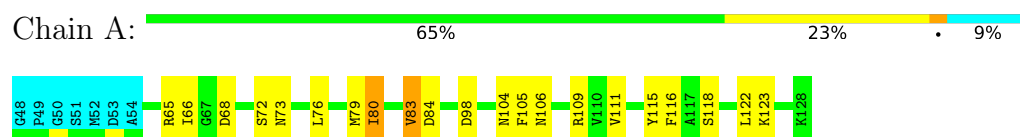


- Molecule 1: Apoptosis regulator BAX

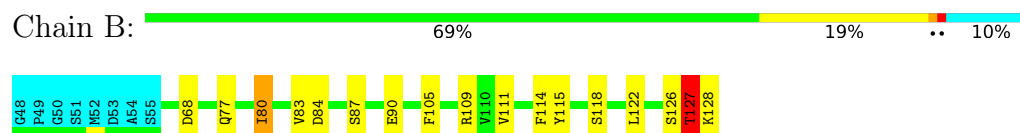


4.2.8 Score per residue for model 8

- Molecule 1: Apoptosis regulator BAX

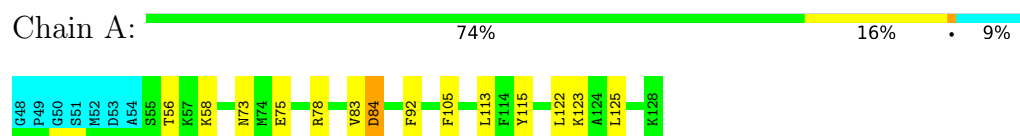


- Molecule 1: Apoptosis regulator BAX

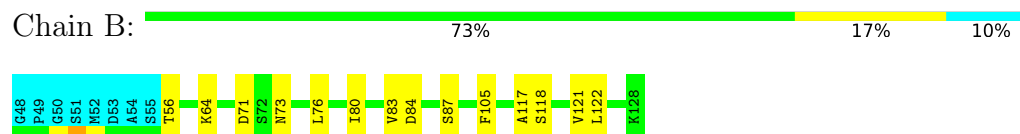


4.2.9 Score per residue for model 9

- Molecule 1: Apoptosis regulator BAX

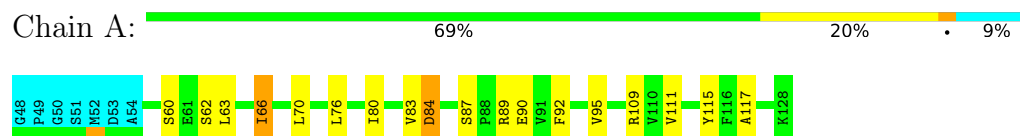


- Molecule 1: Apoptosis regulator BAX

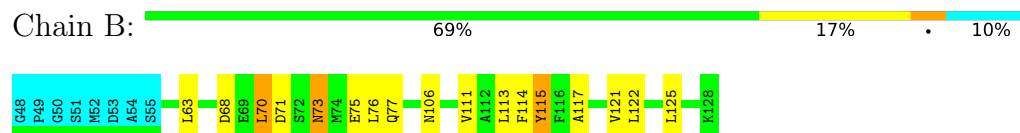


4.2.10 Score per residue for model 10

- Molecule 1: Apoptosis regulator BAX



- Molecule 1: Apoptosis regulator BAX



4.2.11 Score per residue for model 11

- Molecule 1: Apoptosis regulator BAX

Chain A:  77% 14% 9%



- Molecule 1: Apoptosis regulator BAX

Chain B:  79% 11% 10%



4.2.12 Score per residue for model 12

- Molecule 1: Apoptosis regulator BAX

Chain A:  73% 19% 9%



- Molecule 1: Apoptosis regulator BAX

Chain B:  70% 19% 10%



4.2.13 Score per residue for model 13

- Molecule 1: Apoptosis regulator BAX

Chain A:  68% 22% 9%



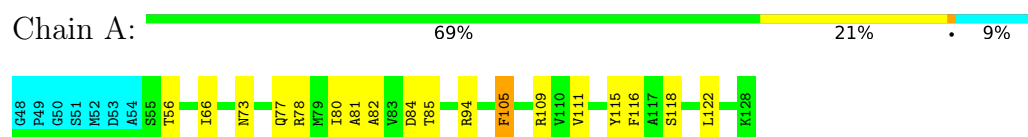
- Molecule 1: Apoptosis regulator BAX

Chain B:  73% 15% 10%

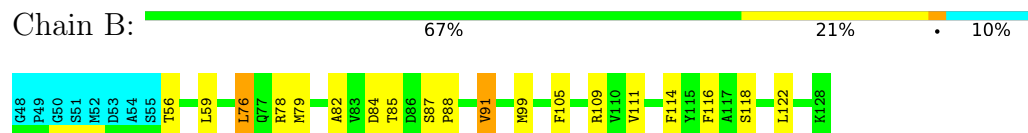


4.2.14 Score per residue for model 14

- Molecule 1: Apoptosis regulator BAX

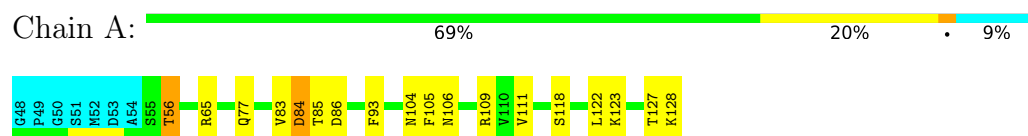


- Molecule 1: Apoptosis regulator BAX

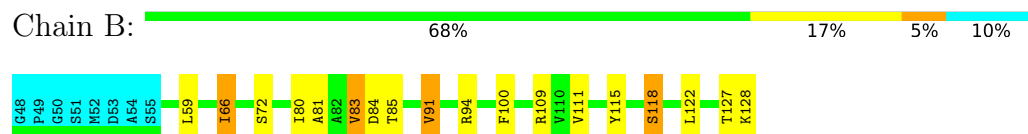


4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Apoptosis regulator BAX



- Molecule 1: Apoptosis regulator BAX



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	
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	387
Number of shifts mapped to atoms	387
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	18%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.38±0.01	0±0/596 (0.0± 0.0%)	1.02±0.01	0±0/799 (0.0± 0.1%)
1	B	1.37±0.01	0±0/590 (0.0± 0.0%)	1.03±0.02	0±0/791 (0.0± 0.0%)
All	All	1.38	1/17790 (0.0%)	1.02	4/23850 (0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	87	SER	N-CA	6.12	1.50	1.46	7	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	A	116	PHE	CA-CB-CG	-6.15	107.65	113.80	8	3
1	B	110	VAL	N-CA-C	-5.71	104.96	110.72	13	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	587	593	593	5±2
1	B	581	588	588	4±2
All	All	17520	17715	17715	111

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:VAL:HG12	1:B:111:VAL:HG13	0.72	1.61	10	2
1:A:111:VAL:CG1	1:B:111:VAL:HG13	0.67	2.20	10	2
1:A:80:ILE:O	1:A:83:VAL:HG13	0.63	1.93	13	3
1:A:125:LEU:O	1:A:125:LEU:HD13	0.60	1.94	3	1
1:A:62:SER:CB	1:B:79:MET:HE1	0.57	2.29	12	1
1:A:111:VAL:HG13	1:B:111:VAL:CG1	0.56	2.30	6	3
1:A:111:VAL:HG13	1:B:111:VAL:HG12	0.56	1.75	15	6
1:A:117:ALA:O	1:A:121:VAL:HG12	0.56	2.00	6	1
1:A:79:MET:HE3	1:B:59:LEU:HD11	0.56	1.78	11	1
1:B:76:LEU:HD23	1:B:79:MET:HE2	0.56	1.77	14	1
1:A:111:VAL:HG22	1:B:111:VAL:HG12	0.55	1.78	5	4
1:B:117:ALA:O	1:B:121:VAL:HG12	0.55	2.02	10	3
1:B:126:SER:O	1:B:127:THR:HG23	0.55	2.02	8	1
1:A:80:ILE:HD12	1:A:81:ALA:N	0.54	2.18	11	3
1:B:88:PRO:O	1:B:91:VAL:HG13	0.54	2.02	14	1
1:B:80:ILE:O	1:B:83:VAL:HG22	0.54	2.02	13	1
1:B:80:ILE:O	1:B:83:VAL:HG13	0.53	2.03	9	4
1:B:59:LEU:O	1:B:63:LEU:HD12	0.53	2.04	13	2
1:A:115:TYR:HB2	1:B:111:VAL:HG21	0.52	1.80	10	1
1:B:76:LEU:C	1:B:76:LEU:HD13	0.51	2.30	7	2
1:A:76:LEU:CD2	1:A:80:ILE:HD11	0.50	2.37	10	1
1:B:80:ILE:HD12	1:B:81:ALA:N	0.50	2.21	6	2
1:B:80:ILE:O	1:B:83:VAL:HG23	0.49	2.08	12	1
1:A:62:SER:O	1:A:66:ILE:HD13	0.49	2.08	10	1
1:B:83:VAL:HG12	1:B:91:VAL:HG21	0.49	1.85	15	1
1:A:78:ARG:O	1:A:82:ALA:HB2	0.48	2.07	14	2
1:B:115:TYR:CD2	1:B:115:TYR:C	0.48	2.91	1	1
1:B:70:LEU:O	1:B:70:LEU:HD13	0.47	2.09	10	1
1:A:127:THR:O	1:A:128:LYS:C	0.47	2.57	3	2
1:B:118:SER:O	1:B:122:LEU:HD13	0.47	2.10	9	6
1:A:76:LEU:O	1:A:80:ILE:HD13	0.47	2.09	3	1
1:A:111:VAL:CG1	1:B:111:VAL:HG12	0.47	2.39	13	1
1:B:88:PRO:HA	1:B:91:VAL:HG13	0.47	1.86	14	1
1:A:118:SER:O	1:A:122:LEU:HD13	0.47	2.10	15	7
1:A:111:VAL:HG21	1:B:115:TYR:HB2	0.46	1.87	15	1
1:A:70:LEU:HD23	1:A:70:LEU:O	0.46	2.10	6	5
1:A:80:ILE:O	1:A:83:VAL:HG23	0.45	2.12	10	2
1:A:92:PHE:CZ	1:A:117:ALA:HB2	0.45	2.47	13	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:83:VAL:O	1:B:83:VAL:HG23	0.45	2.12	13	1
1:B:127:THR:HG23	1:B:127:THR:O	0.44	2.13	5	1
1:B:83:VAL:CG1	1:B:91:VAL:HG21	0.44	2.42	15	1
1:A:127:THR:O	1:A:127:THR:HG22	0.44	2.13	3	1
1:A:83:VAL:O	1:A:84:ASP:C	0.43	2.60	10	2
1:B:115:TYR:CD1	1:B:115:TYR:C	0.43	2.95	10	1
1:B:70:LEU:HD23	1:B:70:LEU:O	0.43	2.14	3	1
1:B:121:VAL:HG13	1:B:122:LEU:HD12	0.43	1.91	9	1
1:A:76:LEU:HG	1:A:79:MET:HE2	0.42	1.90	8	1
1:A:118:SER:O	1:A:122:LEU:HD22	0.42	2.15	1	1
1:A:115:TYR:CD2	1:A:115:TYR:C	0.42	2.98	13	2
1:A:83:VAL:HG23	1:A:83:VAL:O	0.41	2.15	13	1
1:B:78:ARG:O	1:B:82:ALA:HB2	0.41	2.15	14	1
1:A:83:VAL:O	1:A:83:VAL:HG23	0.41	2.15	3	2
1:B:76:LEU:HD23	1:B:79:MET:CE	0.41	2.43	14	1
1:B:73:ASN:ND2	1:B:76:LEU:HD12	0.41	2.31	10	1
1:A:117:ALA:O	1:A:121:VAL:HG22	0.41	2.16	1	1
1:A:126:SER:O	1:A:127:THR:C	0.41	2.63	3	1
1:A:77:GLN:O	1:A:81:ALA:HB3	0.41	2.15	14	1
1:A:80:ILE:HD13	1:A:116:PHE:CE2	0.41	2.51	14	1
1:B:99:MET:HE3	1:B:105:PHE:CE1	0.41	2.50	14	1
1:B:66:ILE:O	1:B:66:ILE:HD13	0.41	2.16	15	1
1:B:83:VAL:O	1:B:84:ASP:C	0.41	2.62	1	1
1:B:76:LEU:HD13	1:B:76:LEU:O	0.40	2.16	9	1
1:A:109:ARG:NH1	1:A:112:ALA:HB3	0.40	2.32	5	1
1:B:117:ALA:O	1:B:121:VAL:HG22	0.40	2.15	13	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	73/81 (90%)	67±2 (92±2%)	4±2 (5±3%)	2±1 (2±1%)	7	45
1	B	72/81 (89%)	66±1 (92±2%)	4±1 (6±1%)	1±1 (1±1%)	11	57
All	All	2175/2430 (90%)	2007 (92%)	127 (6%)	41 (2%)	8	51

All 13 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	84	ASP	9
1	A	83	VAL	6
1	B	84	ASP	6
1	B	73	ASN	4
1	A	87	SER	3
1	B	86	ASP	2
1	B	83	VAL	2
1	A	86	ASP	2
1	A	105	PHE	2
1	A	73	ASN	2
1	A	127	THR	1
1	B	127	THR	1
1	B	87	SER	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	64/68 (94%)	54±3 (84±4%)	10±3 (16±4%)	4	41
1	B	63/68 (93%)	53±3 (84±4%)	10±3 (16±4%)	4	41
All	All	1905/2040 (93%)	1607 (84%)	298 (16%)	4	41

All 98 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	109	ARG	12
1	A	105	PHE	9
1	A	115	TYR	9
1	B	87	SER	8
1	B	109	ARG	8
1	B	115	TYR	7
1	A	66	ILE	7
1	B	105	PHE	7
1	B	114	PHE	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	56	THR	6
1	A	73	ASN	6
1	B	68	ASP	6
1	B	91	VAL	5
1	B	71	ASP	5
1	A	123	LYS	5
1	A	65	ARG	5
1	A	95	VAL	4
1	A	104	ASN	4
1	A	122	LEU	4
1	B	63	LEU	4
1	B	70	LEU	4
1	A	84	ASP	4
1	A	89	ARG	4
1	B	77	GLN	4
1	B	84	ASP	4
1	B	66	ILE	4
1	A	58	LYS	4
1	B	56	THR	4
1	A	106	ASN	4
1	A	71	ASP	3
1	B	60	SER	3
1	B	69	GLU	3
1	B	74	MET	3
1	A	68	ASP	3
1	A	72	SER	3
1	B	65	ARG	3
1	B	127	THR	3
1	A	80	ILE	3
1	A	93	PHE	3
1	B	106	ASN	3
1	A	60	SER	3
1	B	73	ASN	3
1	B	100	PHE	3
1	B	113	LEU	3
1	A	86	ASP	3
1	B	85	THR	3
1	B	93	PHE	3
1	B	128	LYS	3
1	A	62	SER	2
1	A	79	MET	2
1	A	98	ASP	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	99	MET	2
1	A	114	PHE	2
1	A	126	SER	2
1	B	57	LYS	2
1	B	64	LYS	2
1	A	70	LEU	2
1	A	119	LYS	2
1	B	80	ILE	2
1	A	59	LEU	2
1	A	125	LEU	2
1	A	64	LYS	2
1	B	61	GLU	2
1	B	72	SER	2
1	B	75	GLU	2
1	A	77	GLN	2
1	B	123	LYS	2
1	B	125	LEU	2
1	B	94	ARG	2
1	B	110	VAL	2
1	B	122	LEU	2
1	A	75	GLU	2
1	B	118	SER	2
1	A	94	ARG	2
1	A	85	THR	2
1	B	59	LEU	2
1	B	98	ASP	1
1	A	128	LYS	1
1	A	111	VAL	1
1	B	95	VAL	1
1	B	104	ASN	1
1	B	126	SER	1
1	A	107	TRP	1
1	A	101	SER	1
1	B	101	SER	1
1	B	90	GLU	1
1	A	78	ARG	1
1	A	92	PHE	1
1	A	113	LEU	1
1	A	63	LEU	1
1	A	87	SER	1
1	A	90	GLU	1
1	A	100	PHE	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	102	ASP	1
1	A	120	LEU	1
1	B	76	LEU	1
1	B	116	PHE	1
1	B	83	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 18% for the well-defined parts and 18% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *bax2-5CS_V3.str*

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	387
Number of shifts mapped to atoms	387
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	80	0.14 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	73	1.36 ± 0.10	Should be checked
$^{13}\text{C}'$	80	0.06 ± 0.11	None needed (< 0.5 ppm)
^{15}N	77	-0.10 ± 0.18	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 18%, i.e. 360 atoms were assigned a chemical shift out of a possible 2044. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	292/737 (40%)	72/298 (24%)	148/294 (50%)	72/145 (50%)
Sidechain	68/1145 (6%)	0/744 (0%)	68/351 (19%)	0/50 (0%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/162 (0%)	0/80 (0%)	0/80 (0%)	0/2 (0%)
Overall	360/2044 (18%)	72/1122 (6%)	216/725 (30%)	72/197 (37%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 18%, i.e. 387 atoms were assigned a chemical shift out of a possible 2182. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	314/812 (39%)	77/330 (23%)	160/324 (49%)	77/158 (49%)
Sidechain	73/1208 (6%)	0/786 (0%)	73/372 (20%)	0/50 (0%)
Aromatic	0/162 (0%)	0/80 (0%)	0/80 (0%)	0/2 (0%)
Overall	387/2182 (18%)	77/1196 (6%)	233/776 (30%)	77/210 (37%)

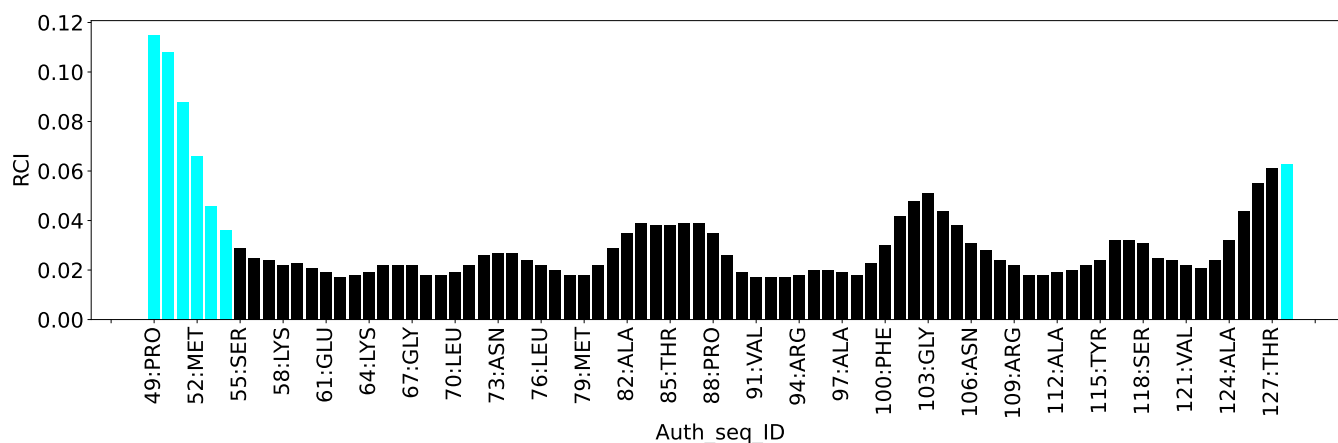
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1464
Intra-residue ($ i-j =0$)	110
Sequential ($ i-j =1$)	850
Medium range ($ i-j >1$ and $ i-j <5$)	362
Long range ($ i-j \geq 5$)	142
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	9.0
Number of long range restraints per residue ¹	0.9

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)	83.6	0.2
0.2-0.5 (Medium)	62.3	0.5
>0.5 (Large)	51.7	30.32

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

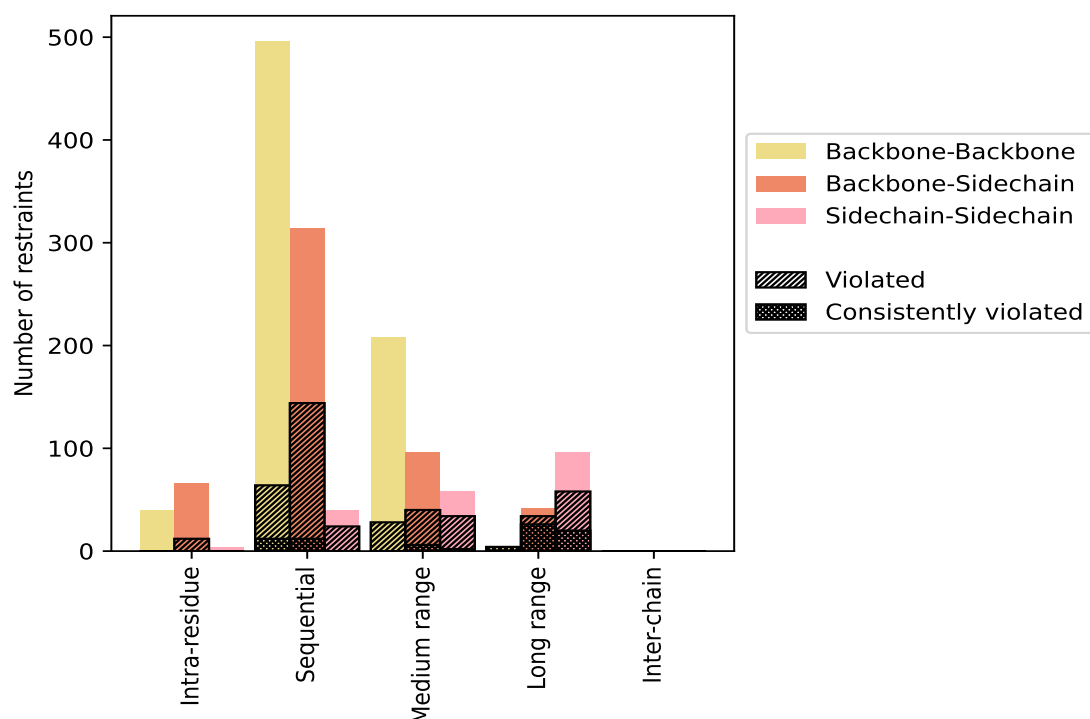
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	110	7.5	12	10.9	0.8	0	0.0	0.0
Backbone-Backbone	40	2.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	66	4.5	12	18.2	0.8	0	0.0	0.0
Sidechain-Sidechain	4	0.3	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	850	58.1	232	27.3	15.8	24	2.8	1.6
Backbone-Backbone	496	33.9	64	12.9	4.4	12	2.4	0.8
Backbone-Sidechain	314	21.4	144	45.9	9.8	12	3.8	0.8
Sidechain-Sidechain	40	2.7	24	60.0	1.6	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	362	24.7	102	28.2	7.0	8	2.2	0.5
Backbone-Backbone	208	14.2	28	13.5	1.9	0	0.0	0.0
Backbone-Sidechain	96	6.6	40	41.7	2.7	6	6.2	0.4
Sidechain-Sidechain	58	4.0	34	58.6	2.3	2	3.4	0.1
Long range ($i-j \geq 5$)	142	9.7	96	67.6	6.6	50	35.2	3.4
Backbone-Backbone	4	0.3	4	100.0	0.3	4	100.0	0.3
Backbone-Sidechain	42	2.9	34	81.0	2.3	26	61.9	1.8
Sidechain-Sidechain	96	6.6	58	60.4	4.0	20	20.8	1.4
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	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1464	100.0	442	30.2	30.2	82	5.6	5.6
Backbone-Backbone	748	51.1	96	12.8	6.6	16	2.1	1.1
Backbone-Sidechain	518	35.4	230	44.4	15.7	44	8.5	3.0
Sidechain-Sidechain	198	13.5	116	58.6	7.9	22	11.1	1.5

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	4	84	34	66	0	188	3.81	28.53	7.15	0.22
2	0	92	26	56	0	174	3.97	29.45	7.36	0.25
3	0	116	26	70	0	212	3.36	28.88	6.85	0.23
4	0	100	22	62	0	184	3.89	30.32	7.33	0.24
5	0	124	26	68	0	218	3.28	29.2	6.8	0.21
6	0	116	42	74	0	232	3.11	28.17	6.58	0.21
7	0	100	26	68	0	194	3.59	28.91	7.06	0.23
8	0	112	30	62	0	204	3.39	29.6	6.89	0.2
9	0	100	26	68	0	194	3.71	29.97	7.2	0.25
10	0	88	46	62	0	196	3.63	27.45	6.91	0.22

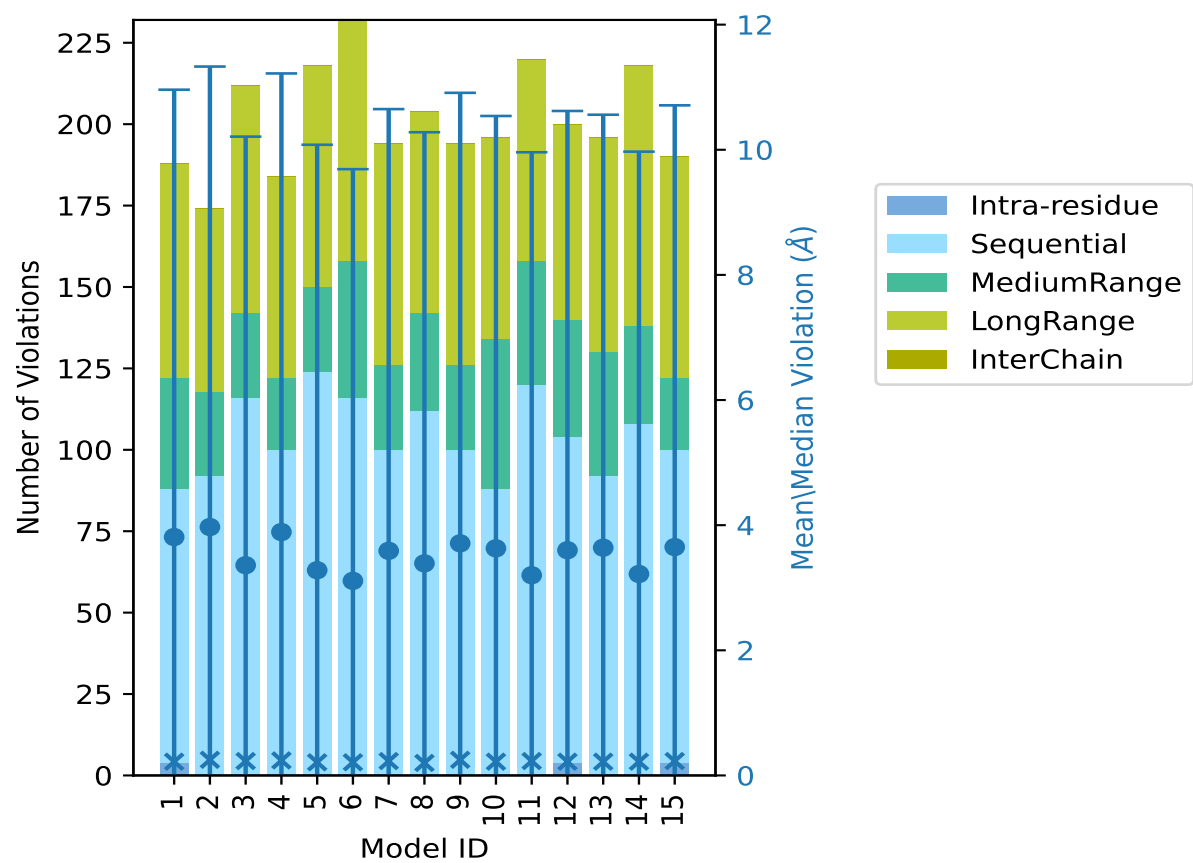
Continued on next page...

Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	120	38	62	0	220	3.2	29.63	6.76	0.23
12	4	100	36	60	0	200	3.6	28.16	7.02	0.22
13	0	92	38	66	0	196	3.64	27.66	6.92	0.22
14	0	108	30	80	0	218	3.22	29.54	6.75	0.22
15	4	96	22	68	0	190	3.65	29.56	7.06	0.23

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

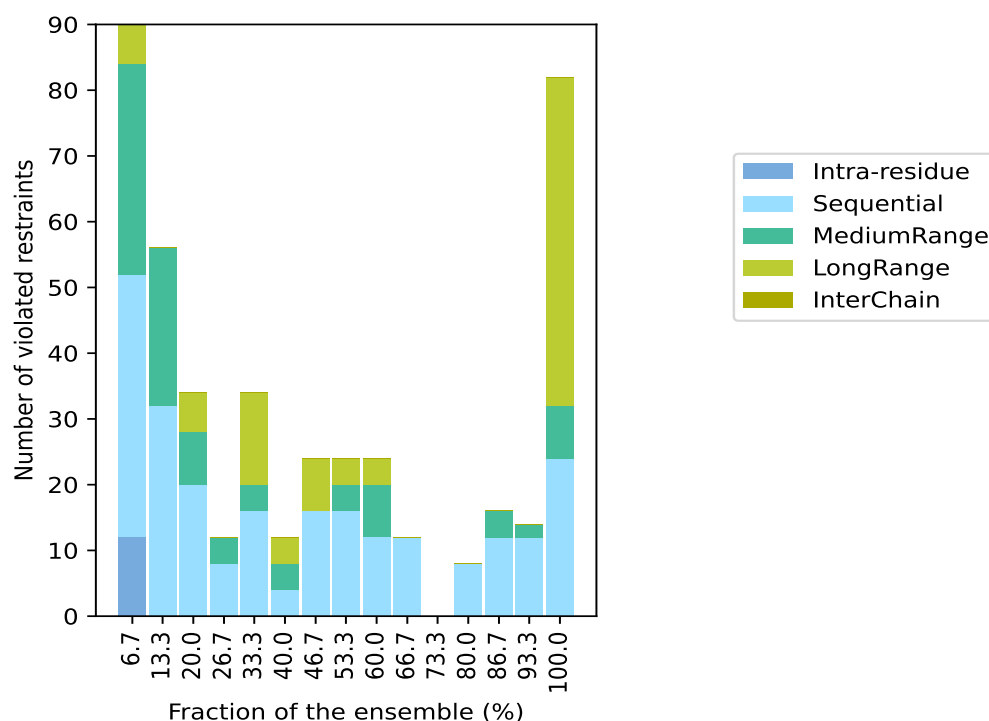
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1022(IR:98, SQ:618, MR:260, LR:46, IC:0) restraints are not 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	%
12	40	32	6	0	90	1	6.7
0	32	24	0	0	56	2	13.3
0	20	8	6	0	34	3	20.0
0	8	4	0	0	12	4	26.7
0	16	4	14	0	34	5	33.3
0	4	4	4	0	12	6	40.0
0	16	0	8	0	24	7	46.7
0	16	4	4	0	24	8	53.3
0	12	8	4	0	24	9	60.0
0	12	0	0	0	12	10	66.7
0	0	0	0	0	0	11	73.3
0	8	0	0	0	8	12	80.0
0	12	4	0	0	16	13	86.7
0	12	2	0	0	14	14	93.3
0	24	8	50	0	82	15	100.0

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

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

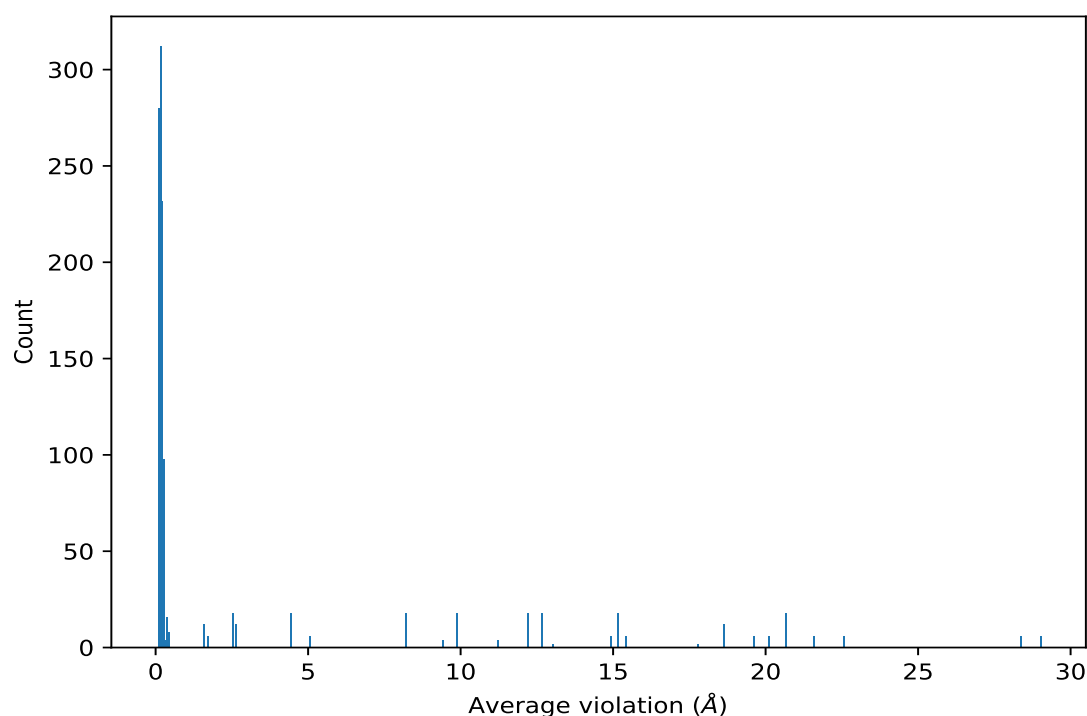
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG21	15	29.0	0.82	29.2
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG22	15	29.0	0.82	29.2
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG23	15	29.0	0.82	29.2
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG21	15	29.0	0.82	29.2
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG22	15	29.0	0.82	29.2
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG23	15	29.0	0.82	29.2
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG21	15	28.37	0.83	28.53
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG22	15	28.37	0.83	28.53
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG23	15	28.37	0.83	28.53
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG21	15	28.37	0.83	28.53
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG22	15	28.37	0.83	28.53
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG23	15	28.37	0.83	28.53
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG21	15	22.57	0.46	22.72
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG22	15	22.57	0.46	22.72
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG23	15	22.57	0.46	22.72
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG21	15	22.57	0.46	22.72

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG22	15	22.57	0.46	22.72
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG23	15	22.57	0.46	22.72
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG11	15	21.58	0.88	21.41
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG12	15	21.58	0.88	21.41
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG13	15	21.58	0.88	21.41
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG11	15	21.58	0.88	21.41
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG12	15	21.58	0.88	21.41
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG13	15	21.58	0.88	21.41
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG21	15	20.69	0.65	20.75
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG22	15	20.69	0.65	20.75
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG23	15	20.69	0.65	20.75
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG21	15	20.69	0.65	20.75
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG22	15	20.69	0.65	20.75
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG23	15	20.69	0.65	20.75
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG21	15	20.69	0.65	20.75
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG22	15	20.69	0.65	20.75
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG23	15	20.69	0.65	20.75
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG21	15	20.69	0.65	20.75
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG22	15	20.69	0.65	20.75
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG23	15	20.69	0.65	20.75
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG21	15	20.69	0.65	20.75
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG22	15	20.69	0.65	20.75
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG23	15	20.69	0.65	20.75
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG21	15	20.69	0.65	20.75
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG22	15	20.69	0.65	20.75
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG23	15	20.69	0.65	20.75
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD11	15	20.13	0.79	19.86
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD12	15	20.13	0.79	19.86
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD13	15	20.13	0.79	19.86
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD11	15	20.13	0.79	19.86
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD12	15	20.13	0.79	19.86
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD13	15	20.13	0.79	19.86
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD21	15	19.63	0.75	19.83
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD22	15	19.63	0.75	19.83
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD23	15	19.63	0.75	19.83
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD21	15	19.63	0.75	19.83
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD22	15	19.63	0.75	19.83
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD23	15	19.63	0.75	19.83
(1,35)	1:95:A:VAL:HG11	1:60:A:SER:H	15	18.63	0.53	18.53
(1,35)	1:95:A:VAL:HG12	1:60:A:SER:H	15	18.63	0.53	18.53
(1,35)	1:95:A:VAL:HG13	1:60:A:SER:H	15	18.63	0.53	18.53
(1,35)	1:95:A:VAL:HG21	1:60:A:SER:H	15	18.63	0.53	18.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,35)	1:95:A:VAL:HG22	1:60:A:SER:H	15	18.63	0.53	18.53
(1,35)	1:95:A:VAL:HG23	1:60:A:SER:H	15	18.63	0.53	18.53
(1,36)	1:95:A:VAL:HG11	1:60:A:SER:H	15	18.63	0.53	18.53
(1,36)	1:95:A:VAL:HG12	1:60:A:SER:H	15	18.63	0.53	18.53
(1,36)	1:95:A:VAL:HG13	1:60:A:SER:H	15	18.63	0.53	18.53
(1,36)	1:95:A:VAL:HG21	1:60:A:SER:H	15	18.63	0.53	18.53
(1,36)	1:95:A:VAL:HG22	1:60:A:SER:H	15	18.63	0.53	18.53
(1,36)	1:95:A:VAL:HG23	1:60:A:SER:H	15	18.63	0.53	18.53
(1,39)	1:107:A:TRP:HE1	1:119:A:LYS:HA	15	17.75	0.53	17.97
(1,40)	1:107:A:TRP:HE1	1:119:A:LYS:HA	15	17.75	0.53	17.97
(1,59)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	15	15.43	0.73	15.61
(1,59)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	15	15.43	0.73	15.61
(1,59)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	15	15.43	0.73	15.61
(1,60)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	15	15.43	0.73	15.61
(1,60)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	15	15.43	0.73	15.61
(1,60)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	15	15.43	0.73	15.61
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	15	15.18	0.67	15.43
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	15	15.18	0.67	15.43
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	15	15.18	0.67	15.43
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	15	15.18	0.67	15.43
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	15	15.18	0.67	15.43
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	15	15.18	0.67	15.43
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	15	15.18	0.67	15.43
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	15	15.18	0.67	15.43
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	15	15.18	0.67	15.43
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	15	15.18	0.67	15.43
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	15	15.18	0.67	15.43
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	15	15.18	0.67	15.43
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	15	15.18	0.67	15.43
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	15	15.18	0.67	15.43
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	15	15.18	0.67	15.43
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	15	15.18	0.67	15.43
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	15	15.18	0.67	15.43
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	15	15.18	0.67	15.43
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	15	14.92	0.47	14.99
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	15	14.92	0.47	14.99
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	15	14.92	0.47	14.99
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	15	14.92	0.47	14.99
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	15	14.92	0.47	14.99
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	15	14.92	0.47	14.99
(1,57)	1:118:A:SER:H	1:107:A:TRP:HE1	15	13.01	0.4	13.06
(1,58)	1:118:A:SER:H	1:107:A:TRP:HE1	15	13.01	0.4	13.06

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE1	15	12.67	1.15	12.22
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE2	15	12.67	1.15	12.22
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE3	15	12.67	1.15	12.22
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE1	15	12.67	1.15	12.22
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE2	15	12.67	1.15	12.22
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE3	15	12.67	1.15	12.22
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE1	15	12.67	1.15	12.22
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE2	15	12.67	1.15	12.22
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE3	15	12.67	1.15	12.22
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE1	15	12.67	1.15	12.22
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE2	15	12.67	1.15	12.22
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE3	15	12.67	1.15	12.22
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE1	15	12.67	1.15	12.22
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE2	15	12.67	1.15	12.22
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE3	15	12.67	1.15	12.22
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE1	15	12.67	1.15	12.22
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE2	15	12.67	1.15	12.22
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE3	15	12.67	1.15	12.22
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	15	12.23	0.43	12.18
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	15	12.23	0.43	12.18
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	15	12.23	0.43	12.18
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	15	12.23	0.43	12.18
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	15	12.23	0.43	12.18
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	15	12.23	0.43	12.18
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	15	12.23	0.43	12.18
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	15	12.23	0.43	12.18
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	15	12.23	0.43	12.18
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	15	12.23	0.43	12.18
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	15	12.23	0.43	12.18
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	15	12.23	0.43	12.18
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	15	12.23	0.43	12.18
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	15	12.23	0.43	12.18
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	15	12.23	0.43	12.18
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	15	12.23	0.43	12.18
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	15	12.23	0.43	12.18
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	15	12.23	0.43	12.18
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG2	15	11.24	0.85	10.78
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG3	15	11.24	0.85	10.78
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG2	15	11.24	0.85	10.78
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG3	15	11.24	0.85	10.78
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	15	9.89	0.4	9.93
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	15	9.89	0.4	9.93

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	15	9.89	0.4	9.93
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	15	9.89	0.4	9.93
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	15	9.89	0.4	9.93
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	15	9.89	0.4	9.93
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	15	9.89	0.4	9.93
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	15	9.89	0.4	9.93
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	15	9.89	0.4	9.93
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	15	9.89	0.4	9.93
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	15	9.89	0.4	9.93
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	15	9.89	0.4	9.93
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	15	9.89	0.4	9.93
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	15	9.89	0.4	9.93
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	15	9.89	0.4	9.93
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	15	9.89	0.4	9.93
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	15	9.89	0.4	9.93
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	15	9.89	0.4	9.93
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD2	15	9.4	1.39	9.13
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD3	15	9.4	1.39	9.13
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD2	15	9.4	1.39	9.13
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD3	15	9.4	1.39	9.13
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	15	8.22	0.57	8.24
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	15	8.22	0.57	8.24
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	15	8.22	0.57	8.24
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	15	8.22	0.57	8.24
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	15	8.22	0.57	8.24
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	15	8.22	0.57	8.24
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	15	8.22	0.57	8.24
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	15	8.22	0.57	8.24
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	15	8.22	0.57	8.24
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	15	8.22	0.57	8.24
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	15	8.22	0.57	8.24
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	15	8.22	0.57	8.24
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	15	8.22	0.57	8.24
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	15	8.22	0.57	8.24
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	15	8.22	0.57	8.24
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	15	8.22	0.57	8.24
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	15	8.22	0.57	8.24
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	15	8.22	0.57	8.24
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB1	15	5.1	1.06	4.7
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB2	15	5.1	1.06	4.7
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB3	15	5.1	1.06	4.7
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB1	15	5.1	1.06	4.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB2	15	5.1	1.06	4.7
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB3	15	5.1	1.06	4.7
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	15	4.4	0.64	4.33
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	15	4.4	0.64	4.33
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	15	4.4	0.64	4.33
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	15	4.4	0.64	4.33
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	15	4.4	0.64	4.33
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	15	4.4	0.64	4.33
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	15	4.4	0.64	4.33
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	15	4.4	0.64	4.33
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	15	4.4	0.64	4.33
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	15	4.4	0.64	4.33
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	15	4.4	0.64	4.33
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	15	4.4	0.64	4.33
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	15	4.4	0.64	4.33
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	15	4.4	0.64	4.33
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	15	4.4	0.64	4.33
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	15	4.4	0.64	4.33
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	15	4.4	0.64	4.33
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	15	4.4	0.64	4.33
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	15	2.61	1.08	2.13
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	15	2.61	1.08	2.13
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	15	2.61	1.08	2.13
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	15	2.61	1.08	2.13
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	15	2.61	1.08	2.13
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	15	2.61	1.08	2.13
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	15	2.61	1.08	2.13
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	15	2.61	1.08	2.13
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	15	2.61	1.08	2.13
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	15	2.61	1.08	2.13
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	15	2.61	1.08	2.13
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	15	2.61	1.08	2.13
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	15	2.51	0.58	2.6
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	15	2.51	0.58	2.6
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	15	2.51	0.58	2.6
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	15	2.51	0.58	2.6
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	15	2.51	0.58	2.6
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	15	2.51	0.58	2.6
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	15	2.51	0.58	2.6
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	15	2.51	0.58	2.6
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	15	2.51	0.58	2.6
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	15	2.51	0.58	2.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	15	2.51	0.58	2.6
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	15	2.51	0.58	2.6
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	15	2.51	0.58	2.6
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	15	2.51	0.58	2.6
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	15	2.51	0.58	2.6
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	15	2.51	0.58	2.6
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	15	2.51	0.58	2.6
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	15	2.51	0.58	2.6
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG21	15	1.72	0.2	1.72
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG22	15	1.72	0.2	1.72
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG23	15	1.72	0.2	1.72
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG21	15	1.72	0.2	1.72
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG22	15	1.72	0.2	1.72
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG23	15	1.72	0.2	1.72
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	15	1.57	0.32	1.5
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	15	1.57	0.32	1.5
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	15	1.57	0.32	1.5
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	15	1.57	0.32	1.5
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	15	1.57	0.32	1.5
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	15	1.57	0.32	1.5
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	15	1.57	0.32	1.5
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	15	1.57	0.32	1.5
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	15	1.57	0.32	1.5
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	15	1.57	0.32	1.5
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	15	1.57	0.32	1.5
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	15	1.57	0.32	1.5
(2,571)	1:118:A:SER:H	1:113:A:LEU:HA	15	0.37	0.07	0.35
(2,572)	1:118:A:SER:H	1:113:A:LEU:HA	15	0.37	0.07	0.35
(3,571)	1:118:A:SER:H	1:113:A:LEU:HA	15	0.37	0.07	0.35
(3,572)	1:118:A:SER:H	1:113:A:LEU:HA	15	0.37	0.07	0.35
(2,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	15	0.26	0.05	0.24
(2,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	15	0.26	0.05	0.24
(2,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	15	0.26	0.05	0.24
(2,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	15	0.26	0.05	0.24
(2,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	15	0.26	0.05	0.24
(2,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	15	0.26	0.05	0.24
(2,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	15	0.26	0.05	0.24
(2,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	15	0.26	0.05	0.24
(2,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	15	0.26	0.05	0.24
(2,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	15	0.26	0.05	0.24
(2,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	15	0.26	0.05	0.24
(2,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	15	0.26	0.05	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	15	0.26	0.05	0.24
(3,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	15	0.26	0.05	0.24
(3,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	15	0.26	0.05	0.24
(3,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	15	0.26	0.05	0.24
(3,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	15	0.26	0.05	0.24
(3,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	15	0.26	0.05	0.24
(3,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	15	0.26	0.05	0.24
(3,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	15	0.26	0.05	0.24
(3,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	15	0.26	0.05	0.24
(3,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	15	0.26	0.05	0.24
(3,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	15	0.26	0.05	0.24
(3,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	15	0.26	0.05	0.24
(2,245)	1:83:A:VAL:H	1:82:A:ALA:HA	15	0.25	0.07	0.25
(2,246)	1:83:A:VAL:H	1:82:A:ALA:HA	15	0.25	0.07	0.25
(3,245)	1:83:A:VAL:H	1:82:A:ALA:HA	15	0.25	0.07	0.25
(3,246)	1:83:A:VAL:H	1:82:A:ALA:HA	15	0.25	0.07	0.25
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	15	0.25	0.05	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	15	0.25	0.05	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	15	0.25	0.05	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	15	0.25	0.05	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	15	0.25	0.05	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	15	0.25	0.05	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	15	0.25	0.05	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	15	0.25	0.05	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	15	0.25	0.05	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	15	0.25	0.05	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	15	0.25	0.05	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	15	0.25	0.05	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	15	0.25	0.05	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	15	0.25	0.05	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	15	0.25	0.05	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	15	0.25	0.05	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	15	0.25	0.05	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	15	0.25	0.05	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	15	0.25	0.05	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	15	0.25	0.05	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	15	0.25	0.05	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	15	0.25	0.05	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	15	0.25	0.05	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	15	0.25	0.05	0.26
(2,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	15	0.23	0.05	0.24
(2,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	15	0.23	0.05	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	15	0.23	0.05	0.24
(2,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	15	0.23	0.05	0.24
(2,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	15	0.23	0.05	0.24
(2,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	15	0.23	0.05	0.24
(3,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	15	0.23	0.05	0.24
(3,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	15	0.23	0.05	0.24
(3,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	15	0.23	0.05	0.24
(3,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	15	0.23	0.05	0.24
(3,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	15	0.23	0.05	0.24
(3,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	15	0.23	0.05	0.24
(2,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	15	0.21	0.04	0.21
(2,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	15	0.21	0.04	0.21
(2,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	15	0.21	0.04	0.21
(2,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	15	0.21	0.04	0.21
(2,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	15	0.21	0.04	0.21
(2,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	15	0.21	0.04	0.21
(2,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	15	0.21	0.04	0.21
(2,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	15	0.21	0.04	0.21
(2,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	15	0.21	0.04	0.21
(2,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	15	0.21	0.04	0.21
(2,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	15	0.21	0.04	0.21
(2,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	15	0.21	0.04	0.21
(3,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	15	0.21	0.04	0.21
(3,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	15	0.21	0.04	0.21
(3,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	15	0.21	0.04	0.21
(3,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	15	0.21	0.04	0.21
(3,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	15	0.21	0.04	0.21
(3,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	15	0.21	0.04	0.21
(3,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	15	0.21	0.04	0.21
(3,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	15	0.21	0.04	0.21
(3,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	15	0.21	0.04	0.21
(3,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	15	0.21	0.04	0.21
(3,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	15	0.21	0.04	0.21
(3,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	15	0.21	0.04	0.21
(2,445)	1:101:A:SER:H	1:102:A:ASP:H	15	0.21	0.04	0.2
(2,446)	1:101:A:SER:H	1:102:A:ASP:H	15	0.21	0.04	0.2
(3,445)	1:101:A:SER:H	1:102:A:ASP:H	15	0.21	0.04	0.2
(3,446)	1:101:A:SER:H	1:102:A:ASP:H	15	0.21	0.04	0.2
(2,547)	1:116:A:PHE:H	1:115:A:TYR:H	15	0.2	0.04	0.21
(2,548)	1:116:A:PHE:H	1:115:A:TYR:H	15	0.2	0.04	0.21
(3,547)	1:116:A:PHE:H	1:115:A:TYR:H	15	0.2	0.04	0.21
(3,548)	1:116:A:PHE:H	1:115:A:TYR:H	15	0.2	0.04	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG21	14	0.3	0.14	0.29
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG22	14	0.3	0.14	0.29
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG23	14	0.3	0.14	0.29
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG21	14	0.3	0.14	0.29
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG22	14	0.3	0.14	0.29
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG23	14	0.3	0.14	0.29
(2,685)	1:126:A:SER:H	1:125:A:LEU:HG	14	0.22	0.2	0.16
(2,686)	1:126:A:SER:H	1:125:A:LEU:HG	14	0.22	0.2	0.16
(3,685)	1:126:A:SER:H	1:125:A:LEU:HG	14	0.22	0.2	0.16
(3,686)	1:126:A:SER:H	1:125:A:LEU:HG	14	0.22	0.2	0.16
(2,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	14	0.18	0.05	0.16
(2,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	14	0.18	0.05	0.16
(2,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	14	0.18	0.05	0.16
(2,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	14	0.18	0.05	0.16
(2,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	14	0.18	0.05	0.16
(2,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	14	0.18	0.05	0.16
(3,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	14	0.18	0.05	0.16
(3,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	14	0.18	0.05	0.16
(3,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	14	0.18	0.05	0.16
(3,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	14	0.18	0.05	0.16
(3,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	14	0.18	0.05	0.16
(3,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	14	0.18	0.05	0.16
(2,671)	1:125:A:LEU:H	1:126:A:SER:HA	14	0.16	0.03	0.15
(2,672)	1:125:A:LEU:H	1:126:A:SER:HA	14	0.16	0.03	0.15
(3,671)	1:125:A:LEU:H	1:126:A:SER:HA	14	0.16	0.03	0.15
(3,672)	1:125:A:LEU:H	1:126:A:SER:HA	14	0.16	0.03	0.15
(2,173)	1:71:A:ASP:H	1:70:A:LEU:HG	13	0.31	0.07	0.33
(2,174)	1:71:A:ASP:H	1:70:A:LEU:HG	13	0.31	0.07	0.33
(3,173)	1:71:A:ASP:H	1:70:A:LEU:HG	13	0.31	0.07	0.33
(3,174)	1:71:A:ASP:H	1:70:A:LEU:HG	13	0.31	0.07	0.33
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	13	0.18	0.05	0.18
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	13	0.18	0.05	0.18
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	13	0.18	0.05	0.18
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	13	0.18	0.05	0.18
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	13	0.18	0.05	0.18
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	13	0.18	0.05	0.18
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	13	0.18	0.05	0.18
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	13	0.18	0.05	0.18
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	13	0.18	0.05	0.18
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	13	0.18	0.05	0.18
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	13	0.18	0.05	0.18
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	13	0.18	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)
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	13	0.18	0.05	0.18
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	13	0.18	0.05	0.18
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	13	0.18	0.05	0.18
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	13	0.18	0.05	0.18
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	13	0.18	0.05	0.18
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	13	0.18	0.05	0.18
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	13	0.18	0.05	0.18
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	13	0.18	0.05	0.18
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	13	0.18	0.05	0.18
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	13	0.18	0.05	0.18
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	13	0.18	0.05	0.18
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	13	0.18	0.05	0.18
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB1	13	0.17	0.02	0.17
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB2	13	0.17	0.02	0.17
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB3	13	0.17	0.02	0.17
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB1	13	0.17	0.02	0.17
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB2	13	0.17	0.02	0.17
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB3	13	0.17	0.02	0.17
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB1	13	0.17	0.02	0.17
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB2	13	0.17	0.02	0.17
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB3	13	0.17	0.02	0.17
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB1	13	0.17	0.02	0.17
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB2	13	0.17	0.02	0.17
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB3	13	0.17	0.02	0.17
(2,185)	1:73:A:ASN:H	1:74:A:MET:H	13	0.17	0.04	0.15
(2,188)	1:73:A:ASN:H	1:74:A:MET:H	13	0.17	0.04	0.15
(3,185)	1:73:A:ASN:H	1:74:A:MET:H	13	0.17	0.04	0.15
(3,188)	1:73:A:ASN:H	1:74:A:MET:H	13	0.17	0.04	0.15
(2,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	12	0.19	0.06	0.17
(2,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	12	0.19	0.06	0.17
(2,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	12	0.19	0.06	0.17
(2,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	12	0.19	0.06	0.17
(2,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	12	0.19	0.06	0.17
(2,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	12	0.19	0.06	0.17
(3,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	12	0.19	0.06	0.17
(3,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	12	0.19	0.06	0.17
(3,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	12	0.19	0.06	0.17
(3,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	12	0.19	0.06	0.17
(3,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	12	0.19	0.06	0.17
(3,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	12	0.19	0.06	0.17
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	12	0.14	0.02	0.13
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	12	0.14	0.02	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	12	0.14	0.02	0.13
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	12	0.14	0.02	0.13
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	12	0.14	0.02	0.13
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	12	0.14	0.02	0.13
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	12	0.14	0.02	0.13
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	12	0.14	0.02	0.13
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	12	0.14	0.02	0.13
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	12	0.14	0.02	0.13
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	12	0.14	0.02	0.13
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	12	0.14	0.02	0.13
(2,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	10	0.36	0.03	0.36
(2,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	10	0.36	0.03	0.36
(2,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	10	0.36	0.03	0.36
(2,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	10	0.36	0.03	0.36
(2,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	10	0.36	0.03	0.36
(2,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	10	0.36	0.03	0.36
(3,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	10	0.36	0.03	0.36
(3,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	10	0.36	0.03	0.36
(3,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	10	0.36	0.03	0.36
(3,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	10	0.36	0.03	0.36
(3,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	10	0.36	0.03	0.36
(3,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	10	0.36	0.03	0.36
(2,271)	1:84:A:ASP:H	1:85:A:THR:HA	10	0.24	0.05	0.24
(2,272)	1:84:A:ASP:H	1:85:A:THR:HA	10	0.24	0.05	0.24
(3,271)	1:84:A:ASP:H	1:85:A:THR:HA	10	0.24	0.05	0.24
(3,272)	1:84:A:ASP:H	1:85:A:THR:HA	10	0.24	0.05	0.24
(2,291)	1:87:A:SER:H	1:86:A:ASP:HA	10	0.22	0.05	0.22
(2,292)	1:87:A:SER:H	1:86:A:ASP:HA	10	0.22	0.05	0.22
(3,291)	1:87:A:SER:H	1:86:A:ASP:HA	10	0.22	0.05	0.22
(3,292)	1:87:A:SER:H	1:86:A:ASP:HA	10	0.22	0.05	0.22
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	9	0.26	0.07	0.27
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	9	0.26	0.07	0.27
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	9	0.26	0.07	0.27
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	9	0.26	0.07	0.27
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	9	0.26	0.07	0.27
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	9	0.26	0.07	0.27
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	9	0.26	0.07	0.27
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	9	0.26	0.07	0.27
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	9	0.26	0.07	0.27
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	9	0.26	0.07	0.27
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	9	0.26	0.07	0.27
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	9	0.26	0.07	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	9	0.21	0.04	0.21
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	9	0.21	0.04	0.21
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	9	0.21	0.04	0.21
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	9	0.21	0.04	0.21
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	9	0.21	0.04	0.21
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	9	0.21	0.04	0.21
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	9	0.21	0.04	0.21
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	9	0.21	0.04	0.21
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	9	0.21	0.04	0.21
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	9	0.21	0.04	0.21
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	9	0.21	0.04	0.21
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	9	0.21	0.04	0.21
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	9	0.21	0.04	0.21
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	9	0.21	0.04	0.21
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	9	0.21	0.04	0.21
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	9	0.21	0.04	0.21
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	9	0.21	0.04	0.21
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	9	0.21	0.04	0.21
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	9	0.21	0.04	0.21
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	9	0.21	0.04	0.21
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	9	0.21	0.04	0.21
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	9	0.21	0.04	0.21
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	9	0.21	0.04	0.21
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	9	0.21	0.04	0.21
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	9	0.21	0.04	0.21
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	9	0.21	0.04	0.21
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	9	0.21	0.04	0.21
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	9	0.21	0.04	0.21
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	9	0.21	0.04	0.21
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	9	0.21	0.04	0.21
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	9	0.21	0.04	0.21
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	9	0.21	0.04	0.21
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	9	0.21	0.04	0.21
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	9	0.21	0.04	0.21
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	9	0.21	0.04	0.21
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	9	0.21	0.04	0.21
(2,33)	1:56:A:THR:H	1:55:A:SER:HB2	9	0.19	0.04	0.18
(2,33)	1:56:A:THR:H	1:55:A:SER:HB3	9	0.19	0.04	0.18
(2,34)	1:56:A:THR:H	1:55:A:SER:HB2	9	0.19	0.04	0.18
(2,34)	1:56:A:THR:H	1:55:A:SER:HB3	9	0.19	0.04	0.18
(3,33)	1:56:A:THR:H	1:55:A:SER:HB2	9	0.19	0.04	0.18
(3,33)	1:56:A:THR:H	1:55:A:SER:HB3	9	0.19	0.04	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,34)	1:56:A:THR:H	1:55:A:SER:HB2	9	0.19	0.04	0.18
(3,34)	1:56:A:THR:H	1:55:A:SER:HB3	9	0.19	0.04	0.18
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	9	0.16	0.05	0.13
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	9	0.16	0.05	0.13
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	9	0.16	0.05	0.13
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	9	0.16	0.05	0.13
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	9	0.16	0.05	0.13
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	9	0.16	0.05	0.13
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	9	0.16	0.05	0.13
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	9	0.16	0.05	0.13
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	9	0.15	0.03	0.14
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	9	0.15	0.03	0.14
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	9	0.15	0.03	0.14
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	9	0.15	0.03	0.14
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	9	0.15	0.03	0.14
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	9	0.15	0.03	0.14
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	9	0.15	0.03	0.14
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	9	0.15	0.03	0.14
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	9	0.15	0.03	0.14
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	9	0.15	0.03	0.14
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	9	0.15	0.03	0.14
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	9	0.15	0.03	0.14
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	9	0.15	0.03	0.14
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	9	0.15	0.03	0.14
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	9	0.15	0.03	0.14
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	9	0.15	0.03	0.14
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	9	0.15	0.03	0.14
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	9	0.15	0.03	0.14
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	9	0.15	0.03	0.14
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	9	0.15	0.03	0.14
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	9	0.15	0.03	0.14
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	9	0.15	0.03	0.14
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	9	0.15	0.03	0.14
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	9	0.15	0.03	0.14
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	9	0.12	0.02	0.12
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	9	0.12	0.02	0.12
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	9	0.12	0.02	0.12
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	9	0.12	0.02	0.12
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	9	0.12	0.02	0.12
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	9	0.12	0.02	0.12
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	9	0.12	0.02	0.12
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	9	0.12	0.02	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	9	0.12	0.02	0.12
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	9	0.12	0.02	0.12
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	9	0.12	0.02	0.12
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	9	0.12	0.02	0.12
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	9	0.12	0.02	0.12
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	9	0.12	0.02	0.12
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	9	0.12	0.02	0.12
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	9	0.12	0.02	0.12
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	9	0.12	0.02	0.12
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	9	0.12	0.02	0.12
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	9	0.12	0.02	0.12
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	9	0.12	0.02	0.12
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	9	0.12	0.02	0.12
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	9	0.12	0.02	0.12
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	9	0.12	0.02	0.12
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	9	0.12	0.02	0.12
(2,491)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	8	0.42	0.15	0.41
(2,491)	1:110:A:VAL:HG12	1:107:A:TRP:HZ3	8	0.42	0.15	0.41
(2,492)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	8	0.42	0.15	0.41
(2,492)	1:110:A:VAL:HG12	1:107:A:TRP:HZ3	8	0.42	0.15	0.41
(3,491)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	8	0.42	0.15	0.41
(3,491)	1:110:A:VAL:HG12	1:107:A:TRP:HZ3	8	0.42	0.15	0.41
(3,492)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	8	0.42	0.15	0.41
(3,492)	1:110:A:VAL:HG12	1:107:A:TRP:HZ3	8	0.42	0.15	0.41
(2,699)	1:127:A:THR:HG21	1:128:A:LYS:H	8	0.23	0.05	0.24
(2,699)	1:127:A:THR:HG22	1:128:A:LYS:H	8	0.23	0.05	0.24
(2,699)	1:127:A:THR:HG23	1:128:A:LYS:H	8	0.23	0.05	0.24
(2,700)	1:127:A:THR:HG21	1:128:A:LYS:H	8	0.23	0.05	0.24
(2,700)	1:127:A:THR:HG22	1:128:A:LYS:H	8	0.23	0.05	0.24
(2,700)	1:127:A:THR:HG23	1:128:A:LYS:H	8	0.23	0.05	0.24
(3,699)	1:127:A:THR:HG21	1:128:A:LYS:H	8	0.23	0.05	0.24
(3,699)	1:127:A:THR:HG22	1:128:A:LYS:H	8	0.23	0.05	0.24
(3,699)	1:127:A:THR:HG23	1:128:A:LYS:H	8	0.23	0.05	0.24
(3,700)	1:127:A:THR:HG21	1:128:A:LYS:H	8	0.23	0.05	0.24
(3,700)	1:127:A:THR:HG22	1:128:A:LYS:H	8	0.23	0.05	0.24
(3,700)	1:127:A:THR:HG23	1:128:A:LYS:H	8	0.23	0.05	0.24
(2,206)	1:77:A:GLN:H	1:76:A:LEU:HG	8	0.22	0.06	0.22
(2,209)	1:77:A:GLN:H	1:76:A:LEU:HG	8	0.22	0.06	0.22
(3,206)	1:77:A:GLN:H	1:76:A:LEU:HG	8	0.22	0.06	0.22
(3,209)	1:77:A:GLN:H	1:76:A:LEU:HG	8	0.22	0.06	0.22
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	8	0.16	0.05	0.15
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	8	0.16	0.05	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	8	0.16	0.05	0.15
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	8	0.16	0.05	0.15
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	8	0.16	0.05	0.15
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	8	0.16	0.05	0.15
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	8	0.16	0.05	0.15
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	8	0.16	0.05	0.15
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	8	0.16	0.05	0.15
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	8	0.16	0.05	0.15
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	8	0.16	0.05	0.15
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	8	0.16	0.05	0.15
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	8	0.16	0.05	0.15
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	8	0.16	0.05	0.15
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	8	0.16	0.05	0.15
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	8	0.16	0.05	0.15
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	8	0.16	0.05	0.15
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	8	0.16	0.05	0.15
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	8	0.16	0.05	0.15
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	8	0.16	0.05	0.15
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	8	0.16	0.05	0.15
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	8	0.16	0.05	0.15
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	8	0.16	0.05	0.15
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	8	0.16	0.05	0.15
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	8	0.16	0.03	0.15
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	8	0.16	0.03	0.15
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	8	0.16	0.03	0.15
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	8	0.16	0.03	0.15
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	8	0.16	0.03	0.15
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	8	0.16	0.03	0.15
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	8	0.16	0.03	0.15
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	8	0.16	0.03	0.15
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	8	0.16	0.03	0.15
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	8	0.16	0.03	0.15
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	8	0.16	0.03	0.15
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	8	0.16	0.03	0.15
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB2	8	0.15	0.03	0.15
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB3	8	0.15	0.03	0.15
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB2	8	0.15	0.03	0.15
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB3	8	0.15	0.03	0.15
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB2	8	0.15	0.03	0.15
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB3	8	0.15	0.03	0.15
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB2	8	0.15	0.03	0.15
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB3	8	0.15	0.03	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG21	7	0.23	0.03	0.23
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG22	7	0.23	0.03	0.23
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG23	7	0.23	0.03	0.23
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG21	7	0.23	0.03	0.23
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG22	7	0.23	0.03	0.23
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG23	7	0.23	0.03	0.23
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG21	7	0.23	0.03	0.23
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG22	7	0.23	0.03	0.23
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG23	7	0.23	0.03	0.23
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG21	7	0.23	0.03	0.23
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG22	7	0.23	0.03	0.23
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG23	7	0.23	0.03	0.23
(2,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	7	0.18	0.06	0.18
(2,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	7	0.18	0.06	0.18
(2,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	7	0.18	0.06	0.18
(2,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	7	0.18	0.06	0.18
(2,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	7	0.18	0.06	0.18
(2,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	7	0.18	0.06	0.18
(2,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	7	0.18	0.06	0.18
(2,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	7	0.18	0.06	0.18
(2,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	7	0.18	0.06	0.18
(2,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	7	0.18	0.06	0.18
(2,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	7	0.18	0.06	0.18
(2,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	7	0.18	0.06	0.18
(3,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	7	0.18	0.06	0.18
(3,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	7	0.18	0.06	0.18
(3,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	7	0.18	0.06	0.18
(3,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	7	0.18	0.06	0.18
(3,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	7	0.18	0.06	0.18
(3,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	7	0.18	0.06	0.18
(3,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	7	0.18	0.06	0.18
(3,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	7	0.18	0.06	0.18
(3,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	7	0.18	0.06	0.18
(3,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	7	0.18	0.06	0.18
(3,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	7	0.18	0.06	0.18
(3,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	7	0.18	0.06	0.18
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB1	7	0.16	0.06	0.12
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB2	7	0.16	0.06	0.12
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB3	7	0.16	0.06	0.12
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB1	7	0.16	0.06	0.12
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB2	7	0.16	0.06	0.12
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB3	7	0.16	0.06	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB1	7	0.16	0.06	0.12
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB2	7	0.16	0.06	0.12
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB3	7	0.16	0.06	0.12
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB1	7	0.16	0.06	0.12
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB2	7	0.16	0.06	0.12
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB3	7	0.16	0.06	0.12
(2,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	7	0.16	0.03	0.15
(2,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	7	0.16	0.03	0.15
(2,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	7	0.16	0.03	0.15
(2,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	7	0.16	0.03	0.15
(2,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	7	0.16	0.03	0.15
(2,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	7	0.16	0.03	0.15
(2,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	7	0.16	0.03	0.15
(2,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	7	0.16	0.03	0.15
(2,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	7	0.16	0.03	0.15
(2,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	7	0.16	0.03	0.15
(2,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	7	0.16	0.03	0.15
(2,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	7	0.16	0.03	0.15
(2,469)	1:102:A:ASP:H	1:101:A:SER:HB2	7	0.16	0.02	0.16
(2,469)	1:102:A:ASP:H	1:101:A:SER:HB3	7	0.16	0.02	0.16
(2,470)	1:102:A:ASP:H	1:101:A:SER:HB2	7	0.16	0.02	0.16
(2,470)	1:102:A:ASP:H	1:101:A:SER:HB3	7	0.16	0.02	0.16
(3,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	7	0.16	0.03	0.15
(3,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	7	0.16	0.03	0.15
(3,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	7	0.16	0.03	0.15
(3,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	7	0.16	0.03	0.15
(3,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	7	0.16	0.03	0.15
(3,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	7	0.16	0.03	0.15
(3,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	7	0.16	0.03	0.15
(3,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	7	0.16	0.03	0.15
(3,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	7	0.16	0.03	0.15
(3,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	7	0.16	0.03	0.15
(3,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	7	0.16	0.03	0.15
(3,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	7	0.16	0.03	0.15
(3,469)	1:102:A:ASP:H	1:101:A:SER:HB2	7	0.16	0.02	0.16
(3,469)	1:102:A:ASP:H	1:101:A:SER:HB3	7	0.16	0.02	0.16
(3,470)	1:102:A:ASP:H	1:101:A:SER:HB2	7	0.16	0.02	0.16
(3,470)	1:102:A:ASP:H	1:101:A:SER:HB3	7	0.16	0.02	0.16
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	7	0.15	0.03	0.15
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	7	0.15	0.03	0.15
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	7	0.15	0.03	0.15
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	7	0.15	0.03	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	7	0.15	0.03	0.15
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	7	0.15	0.03	0.15
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	7	0.15	0.03	0.15
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	7	0.15	0.03	0.15
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	7	0.15	0.03	0.15
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	7	0.15	0.03	0.15
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	7	0.15	0.03	0.15
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	7	0.15	0.03	0.15
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	7	0.15	0.03	0.15
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	7	0.15	0.03	0.15
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	7	0.15	0.03	0.15
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	7	0.15	0.03	0.15
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	7	0.15	0.03	0.15
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	7	0.15	0.03	0.15
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	7	0.15	0.03	0.15
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	7	0.15	0.03	0.15
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	7	0.15	0.03	0.15
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	7	0.15	0.03	0.15
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	7	0.15	0.03	0.15
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	7	0.15	0.03	0.15
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	7	0.15	0.03	0.15
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	7	0.15	0.03	0.15
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	7	0.15	0.03	0.15
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	7	0.15	0.03	0.15
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	7	0.15	0.03	0.15
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	7	0.15	0.03	0.15
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	7	0.15	0.03	0.15
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	7	0.15	0.03	0.15
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	7	0.15	0.03	0.15
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	7	0.15	0.03	0.15
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	7	0.15	0.03	0.15
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	7	0.15	0.03	0.15
(2,693)	1:127:A:THR:H	1:128:A:LYS:H	6	0.29	0.08	0.28
(2,694)	1:127:A:THR:H	1:128:A:LYS:H	6	0.29	0.08	0.28
(3,693)	1:127:A:THR:H	1:128:A:LYS:H	6	0.29	0.08	0.28
(3,694)	1:127:A:THR:H	1:128:A:LYS:H	6	0.29	0.08	0.28
(2,222)	1:81:A:ALA:H	1:83:A:VAL:H	6	0.18	0.01	0.18
(2,226)	1:81:A:ALA:H	1:83:A:VAL:H	6	0.18	0.01	0.18
(3,222)	1:81:A:ALA:H	1:83:A:VAL:H	6	0.18	0.01	0.18
(3,226)	1:81:A:ALA:H	1:83:A:VAL:H	6	0.18	0.01	0.18
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	6	0.16	0.06	0.12
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	6	0.16	0.06	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	6	0.16	0.06	0.12
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	6	0.16	0.06	0.12
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	6	0.16	0.06	0.12
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	6	0.16	0.06	0.12
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	6	0.16	0.06	0.12
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	6	0.16	0.06	0.12
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	6	0.16	0.06	0.12
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	6	0.16	0.06	0.12
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	6	0.16	0.06	0.12
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	6	0.16	0.06	0.12
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	6	0.16	0.06	0.12
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	6	0.16	0.06	0.12
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	6	0.16	0.06	0.12
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	6	0.16	0.06	0.12
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	6	0.16	0.06	0.12
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	6	0.16	0.06	0.12
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	6	0.16	0.06	0.12
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	6	0.16	0.06	0.12
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	6	0.16	0.06	0.12
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	6	0.16	0.06	0.12
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	6	0.16	0.06	0.12
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	6	0.16	0.06	0.12
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	6	0.16	0.06	0.12
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	6	0.16	0.06	0.12
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	6	0.16	0.06	0.12
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	6	0.16	0.06	0.12
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	6	0.16	0.06	0.12
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	6	0.16	0.06	0.12
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	6	0.16	0.06	0.12
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	6	0.16	0.06	0.12
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	6	0.16	0.06	0.12
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	6	0.16	0.06	0.12
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	6	0.16	0.06	0.12
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	6	0.16	0.06	0.12
(2,81)	1:60:A:SER:H	1:59:A:LEU:HG	5	0.21	0.04	0.2
(2,82)	1:60:A:SER:H	1:59:A:LEU:HG	5	0.21	0.04	0.2
(3,81)	1:60:A:SER:H	1:59:A:LEU:HG	5	0.21	0.04	0.2
(3,82)	1:60:A:SER:H	1:59:A:LEU:HG	5	0.21	0.04	0.2
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	5	0.2	0.04	0.21
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	5	0.2	0.04	0.21
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	5	0.2	0.04	0.21
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	5	0.2	0.04	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	5	0.2	0.04	0.21
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	5	0.2	0.04	0.21
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	5	0.2	0.04	0.21
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	5	0.2	0.04	0.21
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	5	0.2	0.04	0.21
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	5	0.2	0.04	0.21
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	5	0.2	0.04	0.21
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	5	0.2	0.04	0.21
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	5	0.2	0.04	0.21
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	5	0.2	0.04	0.21
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	5	0.2	0.04	0.21
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	5	0.2	0.04	0.21
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	5	0.2	0.04	0.21
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	5	0.2	0.04	0.21
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	5	0.2	0.04	0.21
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	5	0.2	0.04	0.21
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	5	0.2	0.04	0.21
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	5	0.2	0.04	0.21
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	5	0.2	0.04	0.21
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	5	0.2	0.04	0.21
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	5	0.2	0.04	0.21
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	5	0.2	0.04	0.21
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	5	0.2	0.04	0.21
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	5	0.2	0.04	0.21
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	5	0.2	0.04	0.21
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	5	0.2	0.04	0.21
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	5	0.2	0.04	0.21
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	5	0.2	0.04	0.21
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	5	0.2	0.04	0.21
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	5	0.2	0.04	0.21
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	5	0.2	0.04	0.21
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	5	0.2	0.04	0.21
(2,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	5	0.2	0.11	0.13
(2,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	5	0.2	0.11	0.13
(2,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	5	0.2	0.11	0.13
(2,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	5	0.2	0.11	0.13
(2,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	5	0.2	0.11	0.13
(2,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	5	0.2	0.11	0.13
(2,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	5	0.2	0.11	0.13
(2,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	5	0.2	0.11	0.13
(2,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	5	0.2	0.11	0.13
(2,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	5	0.2	0.11	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	5	0.2	0.11	0.13
(2,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	5	0.2	0.11	0.13
(3,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	5	0.2	0.11	0.13
(3,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	5	0.2	0.11	0.13
(3,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	5	0.2	0.11	0.13
(3,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	5	0.2	0.11	0.13
(3,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	5	0.2	0.11	0.13
(3,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	5	0.2	0.11	0.13
(3,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	5	0.2	0.11	0.13
(3,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	5	0.2	0.11	0.13
(3,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	5	0.2	0.11	0.13
(3,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	5	0.2	0.11	0.13
(3,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	5	0.2	0.11	0.13
(3,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	5	0.2	0.11	0.13
(2,483)	1:105:A:PHE:H	1:106:A:ASN:H	5	0.2	0.03	0.21
(2,484)	1:105:A:PHE:H	1:106:A:ASN:H	5	0.2	0.03	0.21
(2,485)	1:106:A:ASN:H	1:105:A:PHE:H	5	0.2	0.03	0.21
(2,486)	1:106:A:ASN:H	1:105:A:PHE:H	5	0.2	0.03	0.21
(3,483)	1:105:A:PHE:H	1:106:A:ASN:H	5	0.2	0.03	0.21
(3,484)	1:105:A:PHE:H	1:106:A:ASN:H	5	0.2	0.03	0.21
(3,485)	1:106:A:ASN:H	1:105:A:PHE:H	5	0.2	0.03	0.21
(3,486)	1:106:A:ASN:H	1:105:A:PHE:H	5	0.2	0.03	0.21
(2,135)	1:67:A:GLY:H	1:66:A:ILE:HB	5	0.16	0.05	0.15
(2,136)	1:67:A:GLY:H	1:66:A:ILE:HB	5	0.16	0.05	0.15
(3,135)	1:67:A:GLY:H	1:66:A:ILE:HB	5	0.16	0.05	0.15
(3,136)	1:67:A:GLY:H	1:66:A:ILE:HB	5	0.16	0.05	0.15
(2,527)	1:113:A:LEU:HD21	1:96:A:ALA:HA	5	0.15	0.03	0.14
(2,527)	1:113:A:LEU:HD22	1:96:A:ALA:HA	5	0.15	0.03	0.14
(2,527)	1:113:A:LEU:HD23	1:96:A:ALA:HA	5	0.15	0.03	0.14
(2,531)	1:113:A:LEU:HD21	1:96:A:ALA:HA	5	0.15	0.03	0.14
(2,531)	1:113:A:LEU:HD22	1:96:A:ALA:HA	5	0.15	0.03	0.14
(2,531)	1:113:A:LEU:HD23	1:96:A:ALA:HA	5	0.15	0.03	0.14
(3,527)	1:113:A:LEU:HD21	1:96:A:ALA:HA	5	0.15	0.03	0.14
(3,527)	1:113:A:LEU:HD22	1:96:A:ALA:HA	5	0.15	0.03	0.14
(3,527)	1:113:A:LEU:HD23	1:96:A:ALA:HA	5	0.15	0.03	0.14
(3,531)	1:113:A:LEU:HD21	1:96:A:ALA:HA	5	0.15	0.03	0.14
(3,531)	1:113:A:LEU:HD22	1:96:A:ALA:HA	5	0.15	0.03	0.14
(3,531)	1:113:A:LEU:HD23	1:96:A:ALA:HA	5	0.15	0.03	0.14
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD11	5	0.14	0.03	0.13
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD12	5	0.14	0.03	0.13
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD13	5	0.14	0.03	0.13
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD11	5	0.14	0.03	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD12	5	0.14	0.03	0.13
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD13	5	0.14	0.03	0.13
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD11	5	0.14	0.03	0.13
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD12	5	0.14	0.03	0.13
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD13	5	0.14	0.03	0.13
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD11	5	0.14	0.03	0.13
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD12	5	0.14	0.03	0.13
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD13	5	0.14	0.03	0.13
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD11	5	0.14	0.03	0.13
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD12	5	0.14	0.03	0.13
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD13	5	0.14	0.03	0.13
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD11	5	0.14	0.03	0.13
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD12	5	0.14	0.03	0.13
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD13	5	0.14	0.03	0.13
(2,315)	1:91:A:VAL:HG11	1:83:A:VAL:HA	5	0.14	0.02	0.14
(2,315)	1:91:A:VAL:HG12	1:83:A:VAL:HA	5	0.14	0.02	0.14
(2,315)	1:91:A:VAL:HG13	1:83:A:VAL:HA	5	0.14	0.02	0.14
(2,316)	1:91:A:VAL:HG11	1:83:A:VAL:HA	5	0.14	0.02	0.14
(2,316)	1:91:A:VAL:HG12	1:83:A:VAL:HA	5	0.14	0.02	0.14
(2,316)	1:91:A:VAL:HG13	1:83:A:VAL:HA	5	0.14	0.02	0.14
(3,315)	1:91:A:VAL:HG11	1:83:A:VAL:HA	5	0.14	0.02	0.14
(3,315)	1:91:A:VAL:HG12	1:83:A:VAL:HA	5	0.14	0.02	0.14
(3,315)	1:91:A:VAL:HG13	1:83:A:VAL:HA	5	0.14	0.02	0.14
(3,316)	1:91:A:VAL:HG11	1:83:A:VAL:HA	5	0.14	0.02	0.14
(3,316)	1:91:A:VAL:HG12	1:83:A:VAL:HA	5	0.14	0.02	0.14
(3,316)	1:91:A:VAL:HG13	1:83:A:VAL:HA	5	0.14	0.02	0.14
(2,299)	1:90:A:GLU:H	1:89:A:ARG:HB2	4	0.15	0.03	0.16
(2,299)	1:90:A:GLU:H	1:89:A:ARG:HB3	4	0.15	0.03	0.16
(2,300)	1:90:A:GLU:H	1:89:A:ARG:HB2	4	0.15	0.03	0.16
(2,300)	1:90:A:GLU:H	1:89:A:ARG:HB3	4	0.15	0.03	0.16
(3,299)	1:90:A:GLU:H	1:89:A:ARG:HB2	4	0.15	0.03	0.16
(3,299)	1:90:A:GLU:H	1:89:A:ARG:HB3	4	0.15	0.03	0.16
(3,300)	1:90:A:GLU:H	1:89:A:ARG:HB2	4	0.15	0.03	0.16
(3,300)	1:90:A:GLU:H	1:89:A:ARG:HB3	4	0.15	0.03	0.16
(2,385)	1:96:A:ALA:H	1:95:A:VAL:HG21	4	0.12	0.01	0.12
(2,385)	1:96:A:ALA:H	1:95:A:VAL:HG22	4	0.12	0.01	0.12
(2,385)	1:96:A:ALA:H	1:95:A:VAL:HG23	4	0.12	0.01	0.12
(2,386)	1:96:A:ALA:H	1:95:A:VAL:HG21	4	0.12	0.01	0.12
(2,386)	1:96:A:ALA:H	1:95:A:VAL:HG22	4	0.12	0.01	0.12
(2,386)	1:96:A:ALA:H	1:95:A:VAL:HG23	4	0.12	0.01	0.12
(2,653)	1:124:A:ALA:H	1:120:A:LEU:HA	4	0.12	0.01	0.12
(2,654)	1:124:A:ALA:H	1:120:A:LEU:HA	4	0.12	0.01	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,385)	1:96:A:ALA:H	1:95:A:VAL:HG21	4	0.12	0.01	0.12
(3,385)	1:96:A:ALA:H	1:95:A:VAL:HG22	4	0.12	0.01	0.12
(3,385)	1:96:A:ALA:H	1:95:A:VAL:HG23	4	0.12	0.01	0.12
(3,386)	1:96:A:ALA:H	1:95:A:VAL:HG21	4	0.12	0.01	0.12
(3,386)	1:96:A:ALA:H	1:95:A:VAL:HG22	4	0.12	0.01	0.12
(3,386)	1:96:A:ALA:H	1:95:A:VAL:HG23	4	0.12	0.01	0.12
(3,653)	1:124:A:ALA:H	1:120:A:LEU:HA	4	0.12	0.01	0.12
(3,654)	1:124:A:ALA:H	1:120:A:LEU:HA	4	0.12	0.01	0.12
(2,369)	1:95:A:VAL:HG21	1:92:A:PHE:HE2	3	0.2	0.06	0.22
(2,369)	1:95:A:VAL:HG22	1:92:A:PHE:HE2	3	0.2	0.06	0.22
(2,369)	1:95:A:VAL:HG23	1:92:A:PHE:HE2	3	0.2	0.06	0.22
(2,370)	1:95:A:VAL:HG21	1:92:A:PHE:HE2	3	0.2	0.06	0.22
(2,370)	1:95:A:VAL:HG22	1:92:A:PHE:HE2	3	0.2	0.06	0.22
(2,370)	1:95:A:VAL:HG23	1:92:A:PHE:HE2	3	0.2	0.06	0.22
(3,369)	1:95:A:VAL:HG21	1:92:A:PHE:HE2	3	0.2	0.06	0.22
(3,369)	1:95:A:VAL:HG22	1:92:A:PHE:HE2	3	0.2	0.06	0.22
(3,369)	1:95:A:VAL:HG23	1:92:A:PHE:HE2	3	0.2	0.06	0.22
(3,370)	1:95:A:VAL:HG21	1:92:A:PHE:HE2	3	0.2	0.06	0.22
(3,370)	1:95:A:VAL:HG22	1:92:A:PHE:HE2	3	0.2	0.06	0.22
(3,370)	1:95:A:VAL:HG23	1:92:A:PHE:HE2	3	0.2	0.06	0.22
(2,273)	1:85:A:THR:H	1:84:A:ASP:HB2	3	0.2	0.08	0.17
(2,273)	1:85:A:THR:H	1:84:A:ASP:HB3	3	0.2	0.08	0.17
(2,274)	1:85:A:THR:H	1:84:A:ASP:HB2	3	0.2	0.08	0.17
(2,274)	1:85:A:THR:H	1:84:A:ASP:HB3	3	0.2	0.08	0.17
(3,273)	1:85:A:THR:H	1:84:A:ASP:HB2	3	0.2	0.08	0.17
(3,273)	1:85:A:THR:H	1:84:A:ASP:HB3	3	0.2	0.08	0.17
(3,274)	1:85:A:THR:H	1:84:A:ASP:HB2	3	0.2	0.08	0.17
(3,274)	1:85:A:THR:H	1:84:A:ASP:HB3	3	0.2	0.08	0.17
(2,701)	1:128:A:LYS:H	1:127:A:THR:HB	3	0.19	0.04	0.19
(2,702)	1:128:A:LYS:H	1:127:A:THR:HB	3	0.19	0.04	0.19
(3,701)	1:128:A:LYS:H	1:127:A:THR:HB	3	0.19	0.04	0.19
(3,702)	1:128:A:LYS:H	1:127:A:THR:HB	3	0.19	0.04	0.19
(2,247)	1:83:A:VAL:H	1:84:A:ASP:H	3	0.17	0.04	0.17
(2,248)	1:83:A:VAL:H	1:84:A:ASP:H	3	0.17	0.04	0.17
(2,261)	1:84:A:ASP:H	1:83:A:VAL:H	3	0.17	0.04	0.17
(2,262)	1:84:A:ASP:H	1:83:A:VAL:H	3	0.17	0.04	0.17
(3,247)	1:83:A:VAL:H	1:84:A:ASP:H	3	0.17	0.04	0.17
(3,248)	1:83:A:VAL:H	1:84:A:ASP:H	3	0.17	0.04	0.17
(3,261)	1:84:A:ASP:H	1:83:A:VAL:H	3	0.17	0.04	0.17
(3,262)	1:84:A:ASP:H	1:83:A:VAL:H	3	0.17	0.04	0.17
(1,11)	1:66:A:ILE:HG21	1:70:A:LEU:HD11	3	0.16	0.01	0.17
(1,11)	1:66:A:ILE:HG21	1:70:A:LEU:HD12	3	0.16	0.01	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,11)	1:66:A:ILE:HG21	1:70:A:LEU:HD13	3	0.16	0.01	0.17
(1,11)	1:66:A:ILE:HG22	1:70:A:LEU:HD11	3	0.16	0.01	0.17
(1,11)	1:66:A:ILE:HG22	1:70:A:LEU:HD12	3	0.16	0.01	0.17
(1,11)	1:66:A:ILE:HG22	1:70:A:LEU:HD13	3	0.16	0.01	0.17
(1,11)	1:66:A:ILE:HG23	1:70:A:LEU:HD11	3	0.16	0.01	0.17
(1,11)	1:66:A:ILE:HG23	1:70:A:LEU:HD12	3	0.16	0.01	0.17
(1,11)	1:66:A:ILE:HG23	1:70:A:LEU:HD13	3	0.16	0.01	0.17
(1,12)	1:66:A:ILE:HG21	1:70:A:LEU:HD11	3	0.16	0.01	0.17
(1,12)	1:66:A:ILE:HG21	1:70:A:LEU:HD12	3	0.16	0.01	0.17
(1,12)	1:66:A:ILE:HG21	1:70:A:LEU:HD13	3	0.16	0.01	0.17
(1,12)	1:66:A:ILE:HG22	1:70:A:LEU:HD11	3	0.16	0.01	0.17
(1,12)	1:66:A:ILE:HG22	1:70:A:LEU:HD12	3	0.16	0.01	0.17
(1,12)	1:66:A:ILE:HG22	1:70:A:LEU:HD13	3	0.16	0.01	0.17
(1,12)	1:66:A:ILE:HG23	1:70:A:LEU:HD11	3	0.16	0.01	0.17
(1,12)	1:66:A:ILE:HG23	1:70:A:LEU:HD12	3	0.16	0.01	0.17
(1,12)	1:66:A:ILE:HG23	1:70:A:LEU:HD13	3	0.16	0.01	0.17
(1,19)	1:70:A:LEU:HD11	1:66:A:ILE:HG21	3	0.16	0.01	0.17
(1,19)	1:70:A:LEU:HD11	1:66:A:ILE:HG22	3	0.16	0.01	0.17
(1,19)	1:70:A:LEU:HD11	1:66:A:ILE:HG23	3	0.16	0.01	0.17
(1,19)	1:70:A:LEU:HD12	1:66:A:ILE:HG21	3	0.16	0.01	0.17
(1,19)	1:70:A:LEU:HD12	1:66:A:ILE:HG22	3	0.16	0.01	0.17
(1,19)	1:70:A:LEU:HD12	1:66:A:ILE:HG23	3	0.16	0.01	0.17
(1,19)	1:70:A:LEU:HD13	1:66:A:ILE:HG21	3	0.16	0.01	0.17
(1,19)	1:70:A:LEU:HD13	1:66:A:ILE:HG22	3	0.16	0.01	0.17
(1,19)	1:70:A:LEU:HD13	1:66:A:ILE:HG23	3	0.16	0.01	0.17
(1,20)	1:70:A:LEU:HD11	1:66:A:ILE:HG21	3	0.16	0.01	0.17
(1,20)	1:70:A:LEU:HD11	1:66:A:ILE:HG22	3	0.16	0.01	0.17
(1,20)	1:70:A:LEU:HD11	1:66:A:ILE:HG23	3	0.16	0.01	0.17
(1,20)	1:70:A:LEU:HD12	1:66:A:ILE:HG21	3	0.16	0.01	0.17
(1,20)	1:70:A:LEU:HD12	1:66:A:ILE:HG22	3	0.16	0.01	0.17
(1,20)	1:70:A:LEU:HD12	1:66:A:ILE:HG23	3	0.16	0.01	0.17
(1,20)	1:70:A:LEU:HD13	1:66:A:ILE:HG21	3	0.16	0.01	0.17
(1,20)	1:70:A:LEU:HD13	1:66:A:ILE:HG22	3	0.16	0.01	0.17
(1,20)	1:70:A:LEU:HD13	1:66:A:ILE:HG23	3	0.16	0.01	0.17
(2,243)	1:83:A:VAL:H	1:82:A:ALA:HB1	3	0.15	0.02	0.15
(2,243)	1:83:A:VAL:H	1:82:A:ALA:HB2	3	0.15	0.02	0.15
(2,243)	1:83:A:VAL:H	1:82:A:ALA:HB3	3	0.15	0.02	0.15
(2,244)	1:83:A:VAL:H	1:82:A:ALA:HB1	3	0.15	0.02	0.15
(2,244)	1:83:A:VAL:H	1:82:A:ALA:HB2	3	0.15	0.02	0.15
(2,244)	1:83:A:VAL:H	1:82:A:ALA:HB3	3	0.15	0.02	0.15
(3,243)	1:83:A:VAL:H	1:82:A:ALA:HB1	3	0.15	0.02	0.15
(3,243)	1:83:A:VAL:H	1:82:A:ALA:HB2	3	0.15	0.02	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,243)	1:83:A:VAL:H	1:82:A:ALA:HB3	3	0.15	0.02	0.15
(3,244)	1:83:A:VAL:H	1:82:A:ALA:HB1	3	0.15	0.02	0.15
(3,244)	1:83:A:VAL:H	1:82:A:ALA:HB2	3	0.15	0.02	0.15
(3,244)	1:83:A:VAL:H	1:82:A:ALA:HB3	3	0.15	0.02	0.15
(2,217)	1:80:A:ILE:HD11	1:116:A:PHE:HE1	3	0.14	0.04	0.11
(2,217)	1:80:A:ILE:HD11	1:116:A:PHE:HE2	3	0.14	0.04	0.11
(2,217)	1:80:A:ILE:HD12	1:116:A:PHE:HE1	3	0.14	0.04	0.11
(2,217)	1:80:A:ILE:HD12	1:116:A:PHE:HE2	3	0.14	0.04	0.11
(2,217)	1:80:A:ILE:HD13	1:116:A:PHE:HE1	3	0.14	0.04	0.11
(2,217)	1:80:A:ILE:HD13	1:116:A:PHE:HE2	3	0.14	0.04	0.11
(2,218)	1:80:A:ILE:HD11	1:116:A:PHE:HE1	3	0.14	0.04	0.11
(2,218)	1:80:A:ILE:HD11	1:116:A:PHE:HE2	3	0.14	0.04	0.11
(2,218)	1:80:A:ILE:HD12	1:116:A:PHE:HE1	3	0.14	0.04	0.11
(2,218)	1:80:A:ILE:HD12	1:116:A:PHE:HE2	3	0.14	0.04	0.11
(2,218)	1:80:A:ILE:HD13	1:116:A:PHE:HE1	3	0.14	0.04	0.11
(2,218)	1:80:A:ILE:HD13	1:116:A:PHE:HE2	3	0.14	0.04	0.11
(3,217)	1:80:A:ILE:HD11	1:116:A:PHE:HE1	3	0.14	0.04	0.11
(3,217)	1:80:A:ILE:HD11	1:116:A:PHE:HE2	3	0.14	0.04	0.11
(3,217)	1:80:A:ILE:HD12	1:116:A:PHE:HE1	3	0.14	0.04	0.11
(3,217)	1:80:A:ILE:HD12	1:116:A:PHE:HE2	3	0.14	0.04	0.11
(3,217)	1:80:A:ILE:HD13	1:116:A:PHE:HE1	3	0.14	0.04	0.11
(3,217)	1:80:A:ILE:HD13	1:116:A:PHE:HE2	3	0.14	0.04	0.11
(3,218)	1:80:A:ILE:HD11	1:116:A:PHE:HE1	3	0.14	0.04	0.11
(3,218)	1:80:A:ILE:HD11	1:116:A:PHE:HE2	3	0.14	0.04	0.11
(3,218)	1:80:A:ILE:HD12	1:116:A:PHE:HE1	3	0.14	0.04	0.11
(3,218)	1:80:A:ILE:HD12	1:116:A:PHE:HE2	3	0.14	0.04	0.11
(3,218)	1:80:A:ILE:HD13	1:116:A:PHE:HE1	3	0.14	0.04	0.11
(3,218)	1:80:A:ILE:HD13	1:116:A:PHE:HE2	3	0.14	0.04	0.11
(2,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD21	3	0.13	0.01	0.13
(2,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD22	3	0.13	0.01	0.13
(2,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD23	3	0.13	0.01	0.13
(2,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD21	3	0.13	0.01	0.13
(2,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD22	3	0.13	0.01	0.13
(2,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD23	3	0.13	0.01	0.13
(2,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD21	3	0.13	0.01	0.13
(2,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD22	3	0.13	0.01	0.13
(2,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD23	3	0.13	0.01	0.13
(3,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD21	3	0.13	0.01	0.13
(3,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD22	3	0.13	0.01	0.13
(3,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD23	3	0.13	0.01	0.13
(3,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD21	3	0.13	0.01	0.13
(3,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD22	3	0.13	0.01	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD23	3	0.13	0.01	0.13
(3,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD21	3	0.13	0.01	0.13
(3,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD22	3	0.13	0.01	0.13
(3,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD23	3	0.13	0.01	0.13
(2,259)	1:83:A:VAL:HG11	1:84:A:ASP:H	2	0.26	0.01	0.26
(2,259)	1:83:A:VAL:HG12	1:84:A:ASP:H	2	0.26	0.01	0.26
(2,259)	1:83:A:VAL:HG13	1:84:A:ASP:H	2	0.26	0.01	0.26
(2,259)	1:83:A:VAL:HG21	1:84:A:ASP:H	2	0.26	0.01	0.26
(2,259)	1:83:A:VAL:HG22	1:84:A:ASP:H	2	0.26	0.01	0.26
(2,259)	1:83:A:VAL:HG23	1:84:A:ASP:H	2	0.26	0.01	0.26
(2,260)	1:83:A:VAL:HG11	1:84:A:ASP:H	2	0.26	0.01	0.26
(2,260)	1:83:A:VAL:HG12	1:84:A:ASP:H	2	0.26	0.01	0.26
(2,260)	1:83:A:VAL:HG13	1:84:A:ASP:H	2	0.26	0.01	0.26
(2,260)	1:83:A:VAL:HG21	1:84:A:ASP:H	2	0.26	0.01	0.26
(2,260)	1:83:A:VAL:HG22	1:84:A:ASP:H	2	0.26	0.01	0.26
(2,260)	1:83:A:VAL:HG23	1:84:A:ASP:H	2	0.26	0.01	0.26
(3,259)	1:83:A:VAL:HG11	1:84:A:ASP:H	2	0.26	0.01	0.26
(3,259)	1:83:A:VAL:HG12	1:84:A:ASP:H	2	0.26	0.01	0.26
(3,259)	1:83:A:VAL:HG13	1:84:A:ASP:H	2	0.26	0.01	0.26
(3,259)	1:83:A:VAL:HG21	1:84:A:ASP:H	2	0.26	0.01	0.26
(3,259)	1:83:A:VAL:HG22	1:84:A:ASP:H	2	0.26	0.01	0.26
(3,259)	1:83:A:VAL:HG23	1:84:A:ASP:H	2	0.26	0.01	0.26
(3,260)	1:83:A:VAL:HG11	1:84:A:ASP:H	2	0.26	0.01	0.26
(3,260)	1:83:A:VAL:HG12	1:84:A:ASP:H	2	0.26	0.01	0.26
(3,260)	1:83:A:VAL:HG13	1:84:A:ASP:H	2	0.26	0.01	0.26
(3,260)	1:83:A:VAL:HG21	1:84:A:ASP:H	2	0.26	0.01	0.26
(3,260)	1:83:A:VAL:HG22	1:84:A:ASP:H	2	0.26	0.01	0.26
(3,260)	1:83:A:VAL:HG23	1:84:A:ASP:H	2	0.26	0.01	0.26
(2,301)	1:90:A:GLU:H	1:89:A:ARG:HD2	2	0.24	0.09	0.24
(2,301)	1:90:A:GLU:H	1:89:A:ARG:HD3	2	0.24	0.09	0.24
(2,302)	1:90:A:GLU:H	1:89:A:ARG:HD2	2	0.24	0.09	0.24
(2,302)	1:90:A:GLU:H	1:89:A:ARG:HD3	2	0.24	0.09	0.24
(3,301)	1:90:A:GLU:H	1:89:A:ARG:HD2	2	0.24	0.09	0.24
(3,301)	1:90:A:GLU:H	1:89:A:ARG:HD3	2	0.24	0.09	0.24
(3,302)	1:90:A:GLU:H	1:89:A:ARG:HD2	2	0.24	0.09	0.24
(3,302)	1:90:A:GLU:H	1:89:A:ARG:HD3	2	0.24	0.09	0.24
(2,637)	1:122:A:LEU:HD11	1:118:A:SER:HA	2	0.2	0.08	0.2
(2,637)	1:122:A:LEU:HD12	1:118:A:SER:HA	2	0.2	0.08	0.2
(2,637)	1:122:A:LEU:HD13	1:118:A:SER:HA	2	0.2	0.08	0.2
(2,638)	1:122:A:LEU:HD11	1:118:A:SER:HA	2	0.2	0.08	0.2
(2,638)	1:122:A:LEU:HD12	1:118:A:SER:HA	2	0.2	0.08	0.2
(2,638)	1:122:A:LEU:HD13	1:118:A:SER:HA	2	0.2	0.08	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,637)	1:122:A:LEU:HD11	1:118:A:SER:HA	2	0.2	0.08	0.2
(3,637)	1:122:A:LEU:HD12	1:118:A:SER:HA	2	0.2	0.08	0.2
(3,637)	1:122:A:LEU:HD13	1:118:A:SER:HA	2	0.2	0.08	0.2
(3,638)	1:122:A:LEU:HD11	1:118:A:SER:HA	2	0.2	0.08	0.2
(3,638)	1:122:A:LEU:HD12	1:118:A:SER:HA	2	0.2	0.08	0.2
(3,638)	1:122:A:LEU:HD13	1:118:A:SER:HA	2	0.2	0.08	0.2
(2,183)	1:73:A:ASN:H	1:72:A:SER:HB2	2	0.19	0.01	0.19
(2,183)	1:73:A:ASN:H	1:72:A:SER:HB3	2	0.19	0.01	0.19
(2,186)	1:73:A:ASN:H	1:72:A:SER:HB2	2	0.19	0.01	0.19
(2,186)	1:73:A:ASN:H	1:72:A:SER:HB3	2	0.19	0.01	0.19
(3,183)	1:73:A:ASN:H	1:72:A:SER:HB2	2	0.19	0.01	0.19
(3,183)	1:73:A:ASN:H	1:72:A:SER:HB3	2	0.19	0.01	0.19
(3,186)	1:73:A:ASN:H	1:72:A:SER:HB2	2	0.19	0.01	0.19
(3,186)	1:73:A:ASN:H	1:72:A:SER:HB3	2	0.19	0.01	0.19
(2,517)	1:112:A:ALA:HB1	1:115:A:TYR:HD1	2	0.16	0.05	0.16
(2,517)	1:112:A:ALA:HB1	1:115:A:TYR:HD2	2	0.16	0.05	0.16
(2,517)	1:112:A:ALA:HB2	1:115:A:TYR:HD1	2	0.16	0.05	0.16
(2,517)	1:112:A:ALA:HB2	1:115:A:TYR:HD2	2	0.16	0.05	0.16
(2,517)	1:112:A:ALA:HB3	1:115:A:TYR:HD1	2	0.16	0.05	0.16
(2,517)	1:112:A:ALA:HB3	1:115:A:TYR:HD2	2	0.16	0.05	0.16
(2,518)	1:112:A:ALA:HB1	1:115:A:TYR:HD1	2	0.16	0.05	0.16
(2,518)	1:112:A:ALA:HB1	1:115:A:TYR:HD2	2	0.16	0.05	0.16
(2,518)	1:112:A:ALA:HB2	1:115:A:TYR:HD1	2	0.16	0.05	0.16
(2,518)	1:112:A:ALA:HB2	1:115:A:TYR:HD2	2	0.16	0.05	0.16
(2,518)	1:112:A:ALA:HB3	1:115:A:TYR:HD1	2	0.16	0.05	0.16
(2,518)	1:112:A:ALA:HB3	1:115:A:TYR:HD2	2	0.16	0.05	0.16
(3,517)	1:112:A:ALA:HB1	1:115:A:TYR:HD1	2	0.16	0.05	0.16
(3,517)	1:112:A:ALA:HB1	1:115:A:TYR:HD2	2	0.16	0.05	0.16
(3,517)	1:112:A:ALA:HB2	1:115:A:TYR:HD1	2	0.16	0.05	0.16
(3,517)	1:112:A:ALA:HB2	1:115:A:TYR:HD2	2	0.16	0.05	0.16
(3,517)	1:112:A:ALA:HB3	1:115:A:TYR:HD1	2	0.16	0.05	0.16
(3,517)	1:112:A:ALA:HB3	1:115:A:TYR:HD2	2	0.16	0.05	0.16
(3,518)	1:112:A:ALA:HB1	1:115:A:TYR:HD1	2	0.16	0.05	0.16
(3,518)	1:112:A:ALA:HB1	1:115:A:TYR:HD2	2	0.16	0.05	0.16
(3,518)	1:112:A:ALA:HB2	1:115:A:TYR:HD1	2	0.16	0.05	0.16
(3,518)	1:112:A:ALA:HB2	1:115:A:TYR:HD2	2	0.16	0.05	0.16
(3,518)	1:112:A:ALA:HB3	1:115:A:TYR:HD1	2	0.16	0.05	0.16
(3,518)	1:112:A:ALA:HB3	1:115:A:TYR:HD2	2	0.16	0.05	0.16
(2,263)	1:84:A:ASP:H	1:83:A:VAL:HG11	2	0.14	0.02	0.14
(2,263)	1:84:A:ASP:H	1:83:A:VAL:HG12	2	0.14	0.02	0.14
(2,263)	1:84:A:ASP:H	1:83:A:VAL:HG13	2	0.14	0.02	0.14
(2,264)	1:84:A:ASP:H	1:83:A:VAL:HG11	2	0.14	0.02	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,264)	1:84:A:ASP:H	1:83:A:VAL:HG12	2	0.14	0.02	0.14
(2,264)	1:84:A:ASP:H	1:83:A:VAL:HG13	2	0.14	0.02	0.14
(2,277)	1:85:A:THR:H	1:86:A:ASP:HB2	2	0.14	0.01	0.14
(2,277)	1:85:A:THR:H	1:86:A:ASP:HB3	2	0.14	0.01	0.14
(2,278)	1:85:A:THR:H	1:86:A:ASP:HB2	2	0.14	0.01	0.14
(2,278)	1:85:A:THR:H	1:86:A:ASP:HB3	2	0.14	0.01	0.14
(2,435)	1:99:A:MET:H	1:97:A:ALA:HA	2	0.14	0.02	0.14
(2,436)	1:99:A:MET:H	1:97:A:ALA:HA	2	0.14	0.02	0.14
(3,263)	1:84:A:ASP:H	1:83:A:VAL:HG11	2	0.14	0.02	0.14
(3,263)	1:84:A:ASP:H	1:83:A:VAL:HG12	2	0.14	0.02	0.14
(3,263)	1:84:A:ASP:H	1:83:A:VAL:HG13	2	0.14	0.02	0.14
(3,264)	1:84:A:ASP:H	1:83:A:VAL:HG11	2	0.14	0.02	0.14
(3,264)	1:84:A:ASP:H	1:83:A:VAL:HG12	2	0.14	0.02	0.14
(3,264)	1:84:A:ASP:H	1:83:A:VAL:HG13	2	0.14	0.02	0.14
(3,277)	1:85:A:THR:H	1:86:A:ASP:HB2	2	0.14	0.01	0.14
(3,277)	1:85:A:THR:H	1:86:A:ASP:HB3	2	0.14	0.01	0.14
(3,278)	1:85:A:THR:H	1:86:A:ASP:HB2	2	0.14	0.01	0.14
(3,278)	1:85:A:THR:H	1:86:A:ASP:HB3	2	0.14	0.01	0.14
(3,435)	1:99:A:MET:H	1:97:A:ALA:HA	2	0.14	0.02	0.14
(3,436)	1:99:A:MET:H	1:97:A:ALA:HA	2	0.14	0.02	0.14
(2,585)	1:120:A:LEU:H	1:117:A:ALA:HA	2	0.13	0.02	0.13
(2,586)	1:120:A:LEU:H	1:117:A:ALA:HA	2	0.13	0.02	0.13
(3,585)	1:120:A:LEU:H	1:117:A:ALA:HA	2	0.13	0.02	0.13
(3,586)	1:120:A:LEU:H	1:117:A:ALA:HA	2	0.13	0.02	0.13
(2,237)	1:82:A:ALA:H	1:80:A:ILE:HB	2	0.12	0.01	0.12
(2,238)	1:82:A:ALA:H	1:80:A:ILE:HB	2	0.12	0.01	0.12
(3,237)	1:82:A:ALA:H	1:80:A:ILE:HB	2	0.12	0.01	0.12
(3,238)	1:82:A:ALA:H	1:80:A:ILE:HB	2	0.12	0.01	0.12
(2,275)	1:85:A:THR:H	1:86:A:ASP:H	2	0.12	0.02	0.12
(2,276)	1:85:A:THR:H	1:86:A:ASP:H	2	0.12	0.02	0.12
(2,283)	1:86:A:ASP:H	1:85:A:THR:H	2	0.12	0.02	0.12
(2,284)	1:86:A:ASP:H	1:85:A:THR:H	2	0.12	0.02	0.12
(3,275)	1:85:A:THR:H	1:86:A:ASP:H	2	0.12	0.02	0.12
(3,276)	1:85:A:THR:H	1:86:A:ASP:H	2	0.12	0.02	0.12
(3,283)	1:86:A:ASP:H	1:85:A:THR:H	2	0.12	0.02	0.12
(3,284)	1:86:A:ASP:H	1:85:A:THR:H	2	0.12	0.02	0.12
(2,675)	1:125:A:LEU:HD11	1:122:A:LEU:HA	2	0.12	0.0	0.12
(2,675)	1:125:A:LEU:HD12	1:122:A:LEU:HA	2	0.12	0.0	0.12
(2,675)	1:125:A:LEU:HD13	1:122:A:LEU:HA	2	0.12	0.0	0.12
(2,676)	1:125:A:LEU:HD11	1:122:A:LEU:HA	2	0.12	0.0	0.12
(2,676)	1:125:A:LEU:HD12	1:122:A:LEU:HA	2	0.12	0.0	0.12
(2,676)	1:125:A:LEU:HD13	1:122:A:LEU:HA	2	0.12	0.0	0.12

Continued on next page...

Continued from previous page...

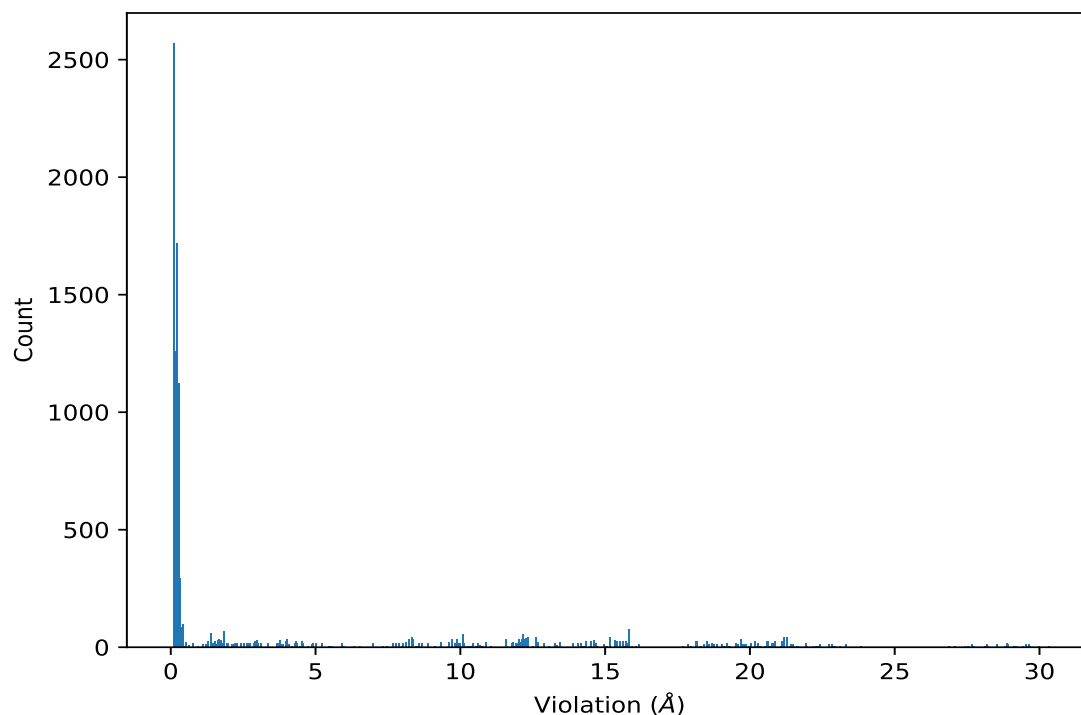
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,675)	1:125:A:LEU:HD11	1:122:A:LEU:HA	2	0.12	0.0	0.12
(3,675)	1:125:A:LEU:HD12	1:122:A:LEU:HA	2	0.12	0.0	0.12
(3,675)	1:125:A:LEU:HD13	1:122:A:LEU:HA	2	0.12	0.0	0.12
(3,676)	1:125:A:LEU:HD11	1:122:A:LEU:HA	2	0.12	0.0	0.12
(3,676)	1:125:A:LEU:HD12	1:122:A:LEU:HA	2	0.12	0.0	0.12
(3,676)	1:125:A:LEU:HD13	1:122:A:LEU:HA	2	0.12	0.0	0.12
(2,269)	1:84:A:ASP:H	1:83:A:VAL:HB	2	0.1	0.0	0.1
(2,270)	1:84:A:ASP:H	1:83:A:VAL:HB	2	0.1	0.0	0.1
(3,269)	1:84:A:ASP:H	1:83:A:VAL:HB	2	0.1	0.0	0.1
(3,270)	1:84:A:ASP:H	1:83:A:VAL:HB	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG21	4	30.32
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG22	4	30.32
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG23	4	30.32
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG21	4	30.32
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG22	4	30.32
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG23	4	30.32
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG21	9	29.97
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG22	9	29.97
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG23	9	29.97
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG21	9	29.97
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG22	9	29.97
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG23	9	29.97
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG21	4	29.67
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG22	4	29.67
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG23	4	29.67
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG21	4	29.67
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG22	4	29.67
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG23	4	29.67
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG21	11	29.63
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG22	11	29.63
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG23	11	29.63
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG21	11	29.63
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG22	11	29.63
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG23	11	29.63
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG21	8	29.6
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG22	8	29.6
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG23	8	29.6
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG21	8	29.6
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG22	8	29.6
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG23	8	29.6
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG21	15	29.56
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG22	15	29.56
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG23	15	29.56
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG21	15	29.56
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG22	15	29.56
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG23	15	29.56
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG21	14	29.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG22	14	29.54
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG23	14	29.54
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG21	14	29.54
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG22	14	29.54
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG23	14	29.54
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG21	9	29.53
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG22	9	29.53
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG23	9	29.53
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG21	9	29.53
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG22	9	29.53
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG23	9	29.53
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG21	2	29.45
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG22	2	29.45
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG23	2	29.45
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG21	2	29.45
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG22	2	29.45
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG23	2	29.45
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG21	5	29.2
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG22	5	29.2
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG23	5	29.2
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG21	5	29.2
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG22	5	29.2
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG23	5	29.2
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG21	2	29.14
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG22	2	29.14
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG23	2	29.14
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG21	2	29.14
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG22	2	29.14
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG23	2	29.14
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG21	15	28.93
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG22	15	28.93
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG23	15	28.93
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG21	15	28.93
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG22	15	28.93
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG23	15	28.93
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG21	7	28.91
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG22	7	28.91
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG23	7	28.91
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG21	7	28.91
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG22	7	28.91
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG23	7	28.91
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG21	8	28.88

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG22	8	28.88
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG23	8	28.88
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG21	8	28.88
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG22	8	28.88
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG23	8	28.88
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG21	3	28.88
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG22	3	28.88
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG23	3	28.88
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG21	3	28.88
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG22	3	28.88
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG23	3	28.88
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG21	11	28.86
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG22	11	28.86
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG23	11	28.86
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG21	11	28.86
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG22	11	28.86
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG23	11	28.86
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG21	14	28.81
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG22	14	28.81
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG23	14	28.81
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG21	14	28.81
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG22	14	28.81
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG23	14	28.81
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG21	5	28.53
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG22	5	28.53
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG23	5	28.53
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG21	5	28.53
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG22	5	28.53
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG23	5	28.53
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG21	1	28.53
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG22	1	28.53
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG23	1	28.53
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG21	1	28.53
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG22	1	28.53
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG23	1	28.53
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG21	7	28.23
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG22	7	28.23
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG23	7	28.23
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG21	7	28.23
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG22	7	28.23
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG23	7	28.23
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG21	6	28.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG22	6	28.17
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG23	6	28.17
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG21	6	28.17
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG22	6	28.17
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG23	6	28.17
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG21	12	28.16
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG22	12	28.16
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG23	12	28.16
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG21	12	28.16
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG22	12	28.16
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG23	12	28.16
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG21	3	28.12
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG22	3	28.12
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG23	3	28.12
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG21	3	28.12
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG22	3	28.12
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG23	3	28.12
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG21	12	27.72
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG22	12	27.72
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG23	12	27.72
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG21	12	27.72
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG22	12	27.72
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG23	12	27.72
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG21	1	27.7
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG22	1	27.7
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG23	1	27.7
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG21	1	27.7
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG22	1	27.7
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG23	1	27.7
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG21	13	27.66
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG22	13	27.66
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG23	13	27.66
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG21	13	27.66
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG22	13	27.66
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG23	13	27.66
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG21	6	27.53
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG22	6	27.53
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG23	6	27.53
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG21	6	27.53
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG22	6	27.53
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG23	6	27.53
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG21	10	27.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG22	10	27.45
(1,34)	1:94:A:ARG:H	1:56:A:THR:HG23	10	27.45
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG21	10	27.45
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG22	10	27.45
(1,33)	1:94:A:ARG:H	1:56:A:THR:HG23	10	27.45
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG21	13	27.07
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG22	13	27.07
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG23	13	27.07
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG21	13	27.07
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG22	13	27.07
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG23	13	27.07
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG21	10	26.86
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG22	10	26.86
(1,38)	1:95:A:VAL:H	1:56:A:THR:HG23	10	26.86
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG21	10	26.86
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG22	10	26.86
(1,37)	1:95:A:VAL:H	1:56:A:THR:HG23	10	26.86
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG11	9	23.8
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG12	9	23.8
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG13	9	23.8
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG11	9	23.8
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG12	9	23.8
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG13	9	23.8
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG11	12	23.34
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG12	12	23.34
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG13	12	23.34
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG11	12	23.34
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG12	12	23.34
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG13	12	23.34
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG21	12	23.32
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG22	12	23.32
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG23	12	23.32
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG21	12	23.32
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG22	12	23.32
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG23	12	23.32
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG21	4	23.13
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG22	4	23.13
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG23	4	23.13
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG21	4	23.13
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG22	4	23.13
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG23	4	23.13
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG21	5	22.94

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG22	5	22.94
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG23	5	22.94
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG21	5	22.94
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG22	5	22.94
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG23	5	22.94
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG21	6	22.86
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG22	6	22.86
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG23	6	22.86
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG21	6	22.86
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG22	6	22.86
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG23	6	22.86
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG21	3	22.84
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG22	3	22.84
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG23	3	22.84
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG21	3	22.84
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG22	3	22.84
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG23	3	22.84
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG21	15	22.81
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG22	15	22.81
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG23	15	22.81
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG21	15	22.81
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG22	15	22.81
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG23	15	22.81
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG21	1	22.72
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG22	1	22.72
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG23	1	22.72
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG21	9	22.72
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG22	9	22.72
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG23	9	22.72
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG21	1	22.72
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG22	1	22.72
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG23	1	22.72
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG21	9	22.72
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG22	9	22.72
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG23	9	22.72
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG21	13	22.44
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG22	13	22.44
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG23	13	22.44
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG21	13	22.44
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG22	13	22.44
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG23	13	22.44
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG21	14	22.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG22	14	22.42
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG23	14	22.42
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG21	14	22.42
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG22	14	22.42
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG23	14	22.42
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG21	7	22.37
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG22	7	22.37
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG23	7	22.37
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG21	7	22.37
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG22	7	22.37
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG23	7	22.37
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG21	11	22.31
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG22	11	22.31
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG23	11	22.31
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG21	11	22.31
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG22	11	22.31
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG23	11	22.31
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG21	10	22.28
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG22	10	22.28
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG23	10	22.28
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG21	10	22.28
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG22	10	22.28
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG23	10	22.28
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG11	1	22.19
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG12	1	22.19
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG13	1	22.19
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG11	1	22.19
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG12	1	22.19
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG13	1	22.19
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG21	8	21.97
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG22	8	21.97
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG23	8	21.97
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG21	8	21.97
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG22	8	21.97
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG23	8	21.97
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG21	4	21.91
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG22	4	21.91
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG23	4	21.91
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG21	4	21.91
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG22	4	21.91
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG23	4	21.91
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG21	4	21.91

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG22	4	21.91
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG23	4	21.91
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG21	4	21.91
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG22	4	21.91
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG23	4	21.91
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG21	4	21.91
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG22	4	21.91
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG23	4	21.91
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG21	4	21.91
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG22	4	21.91
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG23	4	21.91
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD11	6	21.67
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD12	6	21.67
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD13	6	21.67
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD11	6	21.67
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD12	6	21.67
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD13	6	21.67
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG11	4	21.62
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG12	4	21.62
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG13	4	21.62
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG11	4	21.62
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG12	4	21.62
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG13	4	21.62
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG11	5	21.53
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG12	5	21.53
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG13	5	21.53
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG11	5	21.53
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG12	5	21.53
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG13	5	21.53
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG11	2	21.47
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG12	2	21.47
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG13	2	21.47
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG11	15	21.47
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG12	15	21.47
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG13	15	21.47
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG11	2	21.47
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG12	2	21.47
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG13	2	21.47
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG11	15	21.47
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG12	15	21.47
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG13	15	21.47
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG21	2	21.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG22	2	21.42
(1,6)	1:60:A:SER:H	1:95:A:VAL:HG23	2	21.42
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG21	2	21.42
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG22	2	21.42
(1,5)	1:60:A:SER:H	1:95:A:VAL:HG23	2	21.42
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG11	13	21.41
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG12	13	21.41
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG13	13	21.41
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG11	13	21.41
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG12	13	21.41
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG13	13	21.41
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG11	10	21.4
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG12	10	21.4
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG13	10	21.4
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG11	10	21.4
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG12	10	21.4
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG13	10	21.4
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG21	15	21.28
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG22	15	21.28
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG23	15	21.28
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG21	15	21.28
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG22	15	21.28
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG23	15	21.28
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG21	15	21.28
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG22	15	21.28
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG23	15	21.28
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG21	15	21.28
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG22	15	21.28
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG23	15	21.28
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG21	15	21.28
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG22	15	21.28
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG23	15	21.28
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG21	15	21.28
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG22	15	21.28
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG23	15	21.28
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG11	3	21.27
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG12	3	21.27
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG13	3	21.27
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG11	3	21.27
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG12	3	21.27
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG13	3	21.27
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG21	8	21.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG22	8	21.25
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG23	8	21.25
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG21	8	21.25
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG22	8	21.25
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG23	8	21.25
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG21	8	21.25
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG22	8	21.25
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG23	8	21.25
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG21	8	21.25
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG22	8	21.25
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG23	8	21.25
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG21	8	21.25
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG22	8	21.25
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG23	8	21.25
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG21	8	21.25
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG22	8	21.25
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG23	8	21.25
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG21	11	21.2
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG22	11	21.2
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG23	11	21.2
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG21	11	21.2
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG22	11	21.2
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG23	11	21.2
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG21	11	21.2
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG22	11	21.2
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG23	11	21.2
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG21	11	21.2
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG22	11	21.2
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG23	11	21.2
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG21	11	21.2
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG22	11	21.2
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG23	11	21.2
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG21	11	21.2
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG22	11	21.2
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG23	11	21.2
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG21	9	21.18
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG22	9	21.18
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG23	9	21.18
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG21	9	21.18
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG22	9	21.18
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG23	9	21.18
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG21	9	21.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG22	9	21.18
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG23	9	21.18
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG21	9	21.18
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG22	9	21.18
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG23	9	21.18
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG21	9	21.18
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG22	9	21.18
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG23	9	21.18
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG21	9	21.18
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG22	9	21.18
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG23	9	21.18
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG11	6	21.16
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG12	6	21.16
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG13	6	21.16
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG11	6	21.16
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG12	6	21.16
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG13	6	21.16
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD11	4	21.12
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD12	4	21.12
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD13	4	21.12
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD11	4	21.12
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD12	4	21.12
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD13	4	21.12
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG21	14	21.11
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG22	14	21.11
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG23	14	21.11
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG21	14	21.11
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG22	14	21.11
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG23	14	21.11
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG21	14	21.11
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG22	14	21.11
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG23	14	21.11
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG21	14	21.11
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG22	14	21.11
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG23	14	21.11
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG21	14	21.11
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG22	14	21.11
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG23	14	21.11
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG21	14	21.11
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG22	14	21.11
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG23	14	21.11
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD11	1	21.08

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD12	1	21.08
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD13	1	21.08
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD11	1	21.08
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD12	1	21.08
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD13	1	21.08
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG21	5	20.9
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG22	5	20.9
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG23	5	20.9
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG21	5	20.9
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG22	5	20.9
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG23	5	20.9
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG21	5	20.9
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG22	5	20.9
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG23	5	20.9
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG21	5	20.9
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG22	5	20.9
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG23	5	20.9
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG21	5	20.9
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG22	5	20.9
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG23	5	20.9
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG21	5	20.9
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG22	5	20.9
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG23	5	20.9
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD11	9	20.85
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD12	9	20.85
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD13	9	20.85
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD11	9	20.85
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD12	9	20.85
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD13	9	20.85
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG11	7	20.81
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG12	7	20.81
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG13	7	20.81
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG11	11	20.81
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG12	11	20.81
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG13	11	20.81
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG11	7	20.81
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG12	7	20.81
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG13	7	20.81
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG11	11	20.81
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG12	11	20.81
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG13	11	20.81
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG11	14	20.8

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG12	14	20.8
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG13	14	20.8
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG11	14	20.8
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG12	14	20.8
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG13	14	20.8
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG21	7	20.75
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG22	7	20.75
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG23	7	20.75
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG21	7	20.75
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG22	7	20.75
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG23	7	20.75
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG21	7	20.75
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG22	7	20.75
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG23	7	20.75
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG21	7	20.75
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG22	7	20.75
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG23	7	20.75
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG21	7	20.75
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG22	7	20.75
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG23	7	20.75
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG21	7	20.75
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG22	7	20.75
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG23	7	20.75
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD11	11	20.72
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD12	11	20.72
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD13	11	20.72
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD11	11	20.72
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD12	11	20.72
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD13	11	20.72
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD21	2	20.7
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD22	2	20.7
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD23	2	20.7
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD21	2	20.7
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD22	2	20.7
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD23	2	20.7
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG21	3	20.63
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG22	3	20.63
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG23	3	20.63
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG21	3	20.63
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG22	3	20.63
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG23	3	20.63
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG21	3	20.63

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG22	3	20.63
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG23	3	20.63
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG21	3	20.63
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG22	3	20.63
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG23	3	20.63
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG21	3	20.63
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG22	3	20.63
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG23	3	20.63
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG21	3	20.63
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG22	3	20.63
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG23	3	20.63
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD21	12	20.6
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD22	12	20.6
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD23	12	20.6
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD21	12	20.6
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD22	12	20.6
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD23	12	20.6
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG11	8	20.56
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG12	8	20.56
(1,4)	1:60:A:SER:H	1:95:A:VAL:HG13	8	20.56
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG11	8	20.56
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG12	8	20.56
(1,3)	1:60:A:SER:H	1:95:A:VAL:HG13	8	20.56
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG21	2	20.55
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG22	2	20.55
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG23	2	20.55
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG21	2	20.55
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG22	2	20.55
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG23	2	20.55
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG21	2	20.55
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG22	2	20.55
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG23	2	20.55
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG21	2	20.55
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG22	2	20.55
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG23	2	20.55
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG21	2	20.55
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG22	2	20.55
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG23	2	20.55
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG21	2	20.55
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG22	2	20.55
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG23	2	20.55
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD11	15	20.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD12	15	20.52
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD13	15	20.52
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD11	15	20.52
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD12	15	20.52
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD13	15	20.52
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD21	7	20.36
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD22	7	20.36
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD23	7	20.36
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD21	7	20.36
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD22	7	20.36
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD23	7	20.36
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD11	3	20.34
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD12	3	20.34
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD13	3	20.34
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD11	3	20.34
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD12	3	20.34
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD13	3	20.34
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG21	6	20.28
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG22	6	20.28
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG23	6	20.28
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG21	6	20.28
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG22	6	20.28
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG23	6	20.28
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG21	6	20.28
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG22	6	20.28
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG23	6	20.28
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG21	6	20.28
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG22	6	20.28
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG23	6	20.28
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG21	6	20.28
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG22	6	20.28
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG23	6	20.28
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG21	6	20.28
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG22	6	20.28
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG23	6	20.28
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD21	14	20.22
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD22	14	20.22
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD23	14	20.22
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD21	14	20.22
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD22	14	20.22
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD23	14	20.22
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG21	12	20.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG22	12	20.17
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG23	12	20.17
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG21	12	20.17
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG22	12	20.17
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG23	12	20.17
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG21	12	20.17
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG22	12	20.17
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG23	12	20.17
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG21	12	20.17
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG22	12	20.17
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG23	12	20.17
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG21	12	20.17
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG22	12	20.17
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG23	12	20.17
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG21	12	20.17
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG22	12	20.17
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG23	12	20.17
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD21	5	20.16
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD22	5	20.16
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD23	5	20.16
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD21	5	20.16
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD22	5	20.16
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD23	5	20.16
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG21	1	20.01
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG22	1	20.01
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG23	1	20.01
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG21	1	20.01
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG22	1	20.01
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG23	1	20.01
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG21	1	20.01
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG22	1	20.01
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG23	1	20.01
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG21	1	20.01
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG22	1	20.01
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG23	1	20.01
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG21	1	20.01
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG22	1	20.01
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG23	1	20.01
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG21	1	20.01
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG22	1	20.01
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG23	1	20.01
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD21	8	19.97

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD22	8	19.97
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD23	8	19.97
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD21	8	19.97
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD22	8	19.97
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD23	8	19.97
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD21	3	19.89
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD22	3	19.89
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD23	3	19.89
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD21	3	19.89
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD22	3	19.89
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD23	3	19.89
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD11	7	19.86
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD12	7	19.86
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD13	7	19.86
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD11	7	19.86
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD12	7	19.86
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD13	7	19.86
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD21	11	19.83
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD22	11	19.83
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD23	11	19.83
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD21	11	19.83
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD22	11	19.83
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD23	11	19.83
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD11	8	19.83
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD12	8	19.83
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD13	8	19.83
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD11	8	19.83
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD12	8	19.83
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD13	8	19.83
(1,36)	1:95:A:VAL:HG11	1:60:A:SER:H	12	19.79
(1,36)	1:95:A:VAL:HG12	1:60:A:SER:H	12	19.79
(1,36)	1:95:A:VAL:HG13	1:60:A:SER:H	12	19.79
(1,36)	1:95:A:VAL:HG21	1:60:A:SER:H	12	19.79
(1,36)	1:95:A:VAL:HG22	1:60:A:SER:H	12	19.79
(1,36)	1:95:A:VAL:HG23	1:60:A:SER:H	12	19.79
(1,35)	1:95:A:VAL:HG11	1:60:A:SER:H	12	19.79
(1,35)	1:95:A:VAL:HG12	1:60:A:SER:H	12	19.79
(1,35)	1:95:A:VAL:HG13	1:60:A:SER:H	12	19.79
(1,35)	1:95:A:VAL:HG21	1:60:A:SER:H	12	19.79
(1,35)	1:95:A:VAL:HG22	1:60:A:SER:H	12	19.79
(1,35)	1:95:A:VAL:HG23	1:60:A:SER:H	12	19.79
(1,36)	1:95:A:VAL:HG11	1:60:A:SER:H	9	19.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:95:A:VAL:HG12	1:60:A:SER:H	9	19.7
(1,36)	1:95:A:VAL:HG13	1:60:A:SER:H	9	19.7
(1,36)	1:95:A:VAL:HG21	1:60:A:SER:H	9	19.7
(1,36)	1:95:A:VAL:HG22	1:60:A:SER:H	9	19.7
(1,36)	1:95:A:VAL:HG23	1:60:A:SER:H	9	19.7
(1,35)	1:95:A:VAL:HG11	1:60:A:SER:H	9	19.7
(1,35)	1:95:A:VAL:HG12	1:60:A:SER:H	9	19.7
(1,35)	1:95:A:VAL:HG13	1:60:A:SER:H	9	19.7
(1,35)	1:95:A:VAL:HG21	1:60:A:SER:H	9	19.7
(1,35)	1:95:A:VAL:HG22	1:60:A:SER:H	9	19.7
(1,35)	1:95:A:VAL:HG23	1:60:A:SER:H	9	19.7
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD21	13	19.69
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD22	13	19.69
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD23	13	19.69
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD21	13	19.69
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD22	13	19.69
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD23	13	19.69
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG21	13	19.67
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG22	13	19.67
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG23	13	19.67
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG21	13	19.67
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG22	13	19.67
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG23	13	19.67
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG21	13	19.67
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG22	13	19.67
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG23	13	19.67
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG21	13	19.67
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG22	13	19.67
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG23	13	19.67
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG21	13	19.67
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG22	13	19.67
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG23	13	19.67
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG21	13	19.67
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG22	13	19.67
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG23	13	19.67
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD11	2	19.58
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD12	2	19.58
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD13	2	19.58
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD11	12	19.58
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD12	12	19.58
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD13	12	19.58
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD11	2	19.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD12	2	19.58
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD13	2	19.58
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD11	12	19.58
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD12	12	19.58
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD13	12	19.58
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG21	10	19.5
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG22	10	19.5
(1,2)	1:56:A:THR:HG21	1:95:A:VAL:HG23	10	19.5
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG21	10	19.5
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG22	10	19.5
(1,2)	1:56:A:THR:HG22	1:95:A:VAL:HG23	10	19.5
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG21	10	19.5
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG22	10	19.5
(1,2)	1:56:A:THR:HG23	1:95:A:VAL:HG23	10	19.5
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG21	10	19.5
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG22	10	19.5
(1,1)	1:56:A:THR:HG21	1:95:A:VAL:HG23	10	19.5
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG21	10	19.5
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG22	10	19.5
(1,1)	1:56:A:THR:HG22	1:95:A:VAL:HG23	10	19.5
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG21	10	19.5
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG22	10	19.5
(1,1)	1:56:A:THR:HG23	1:95:A:VAL:HG23	10	19.5
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD21	10	19.34
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD22	10	19.34
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD23	10	19.34
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD21	10	19.34
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD22	10	19.34
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD23	10	19.34
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD21	6	19.27
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD22	6	19.27
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD23	6	19.27
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD21	6	19.27
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD22	6	19.27
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD23	6	19.27
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD11	10	19.24
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD12	10	19.24
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD13	10	19.24
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD11	10	19.24
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD12	10	19.24
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD13	10	19.24
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD11	5	19.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD12	5	19.23
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD13	5	19.23
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD11	14	19.23
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD12	14	19.23
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD13	14	19.23
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD11	5	19.23
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD12	5	19.23
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD13	5	19.23
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD11	14	19.23
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD12	14	19.23
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD13	14	19.23
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD11	13	19.15
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD12	13	19.15
(1,26)	1:80:A:ILE:H	1:59:A:LEU:HD13	13	19.15
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD11	13	19.15
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD12	13	19.15
(1,25)	1:80:A:ILE:H	1:59:A:LEU:HD13	13	19.15
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD21	1	19.08
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD22	1	19.08
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD23	1	19.08
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD21	1	19.08
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD22	1	19.08
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD23	1	19.08
(1,36)	1:95:A:VAL:HG11	1:60:A:SER:H	1	19.0
(1,36)	1:95:A:VAL:HG12	1:60:A:SER:H	1	19.0
(1,36)	1:95:A:VAL:HG13	1:60:A:SER:H	1	19.0
(1,36)	1:95:A:VAL:HG21	1:60:A:SER:H	1	19.0
(1,36)	1:95:A:VAL:HG22	1:60:A:SER:H	1	19.0
(1,36)	1:95:A:VAL:HG23	1:60:A:SER:H	1	19.0
(1,35)	1:95:A:VAL:HG11	1:60:A:SER:H	1	19.0
(1,35)	1:95:A:VAL:HG12	1:60:A:SER:H	1	19.0
(1,35)	1:95:A:VAL:HG13	1:60:A:SER:H	1	19.0
(1,35)	1:95:A:VAL:HG21	1:60:A:SER:H	1	19.0
(1,35)	1:95:A:VAL:HG22	1:60:A:SER:H	1	19.0
(1,35)	1:95:A:VAL:HG23	1:60:A:SER:H	1	19.0
(1,36)	1:95:A:VAL:HG11	1:60:A:SER:H	4	18.87
(1,36)	1:95:A:VAL:HG12	1:60:A:SER:H	4	18.87
(1,36)	1:95:A:VAL:HG13	1:60:A:SER:H	4	18.87
(1,36)	1:95:A:VAL:HG21	1:60:A:SER:H	4	18.87
(1,36)	1:95:A:VAL:HG22	1:60:A:SER:H	4	18.87
(1,36)	1:95:A:VAL:HG23	1:60:A:SER:H	4	18.87
(1,35)	1:95:A:VAL:HG11	1:60:A:SER:H	4	18.87

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:95:A:VAL:HG12	1:60:A:SER:H	4	18.87
(1,35)	1:95:A:VAL:HG13	1:60:A:SER:H	4	18.87
(1,35)	1:95:A:VAL:HG21	1:60:A:SER:H	4	18.87
(1,35)	1:95:A:VAL:HG22	1:60:A:SER:H	4	18.87
(1,35)	1:95:A:VAL:HG23	1:60:A:SER:H	4	18.87
(1,36)	1:95:A:VAL:HG11	1:60:A:SER:H	5	18.76
(1,36)	1:95:A:VAL:HG12	1:60:A:SER:H	5	18.76
(1,36)	1:95:A:VAL:HG13	1:60:A:SER:H	5	18.76
(1,36)	1:95:A:VAL:HG21	1:60:A:SER:H	5	18.76
(1,36)	1:95:A:VAL:HG22	1:60:A:SER:H	5	18.76
(1,36)	1:95:A:VAL:HG23	1:60:A:SER:H	5	18.76
(1,35)	1:95:A:VAL:HG11	1:60:A:SER:H	5	18.76
(1,35)	1:95:A:VAL:HG12	1:60:A:SER:H	5	18.76
(1,35)	1:95:A:VAL:HG13	1:60:A:SER:H	5	18.76
(1,35)	1:95:A:VAL:HG21	1:60:A:SER:H	5	18.76
(1,35)	1:95:A:VAL:HG22	1:60:A:SER:H	5	18.76
(1,35)	1:95:A:VAL:HG23	1:60:A:SER:H	5	18.76
(1,36)	1:95:A:VAL:HG11	1:60:A:SER:H	15	18.68
(1,36)	1:95:A:VAL:HG12	1:60:A:SER:H	15	18.68
(1,36)	1:95:A:VAL:HG13	1:60:A:SER:H	15	18.68
(1,36)	1:95:A:VAL:HG21	1:60:A:SER:H	15	18.68
(1,36)	1:95:A:VAL:HG22	1:60:A:SER:H	15	18.68
(1,36)	1:95:A:VAL:HG23	1:60:A:SER:H	15	18.68
(1,35)	1:95:A:VAL:HG11	1:60:A:SER:H	15	18.68
(1,35)	1:95:A:VAL:HG12	1:60:A:SER:H	15	18.68
(1,35)	1:95:A:VAL:HG13	1:60:A:SER:H	15	18.68
(1,35)	1:95:A:VAL:HG21	1:60:A:SER:H	15	18.68
(1,35)	1:95:A:VAL:HG22	1:60:A:SER:H	15	18.68
(1,35)	1:95:A:VAL:HG23	1:60:A:SER:H	15	18.68
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD21	4	18.67
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD22	4	18.67
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD23	4	18.67
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD21	4	18.67
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD22	4	18.67
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD23	4	18.67
(1,40)	1:107:A:TRP:HE1	1:119:A:LYS:HA	3	18.63
(1,39)	1:107:A:TRP:HE1	1:119:A:LYS:HA	3	18.63
(1,36)	1:95:A:VAL:HG11	1:60:A:SER:H	3	18.59
(1,36)	1:95:A:VAL:HG12	1:60:A:SER:H	3	18.59
(1,36)	1:95:A:VAL:HG13	1:60:A:SER:H	3	18.59
(1,36)	1:95:A:VAL:HG21	1:60:A:SER:H	3	18.59
(1,36)	1:95:A:VAL:HG22	1:60:A:SER:H	3	18.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:95:A:VAL:HG23	1:60:A:SER:H	3	18.59
(1,35)	1:95:A:VAL:HG11	1:60:A:SER:H	3	18.59
(1,35)	1:95:A:VAL:HG12	1:60:A:SER:H	3	18.59
(1,35)	1:95:A:VAL:HG13	1:60:A:SER:H	3	18.59
(1,35)	1:95:A:VAL:HG21	1:60:A:SER:H	3	18.59
(1,35)	1:95:A:VAL:HG22	1:60:A:SER:H	3	18.59
(1,35)	1:95:A:VAL:HG23	1:60:A:SER:H	3	18.59
(1,36)	1:95:A:VAL:HG11	1:60:A:SER:H	6	18.53
(1,36)	1:95:A:VAL:HG12	1:60:A:SER:H	6	18.53
(1,36)	1:95:A:VAL:HG13	1:60:A:SER:H	6	18.53
(1,36)	1:95:A:VAL:HG21	1:60:A:SER:H	6	18.53
(1,36)	1:95:A:VAL:HG22	1:60:A:SER:H	6	18.53
(1,36)	1:95:A:VAL:HG23	1:60:A:SER:H	6	18.53
(1,35)	1:95:A:VAL:HG11	1:60:A:SER:H	6	18.53
(1,35)	1:95:A:VAL:HG12	1:60:A:SER:H	6	18.53
(1,35)	1:95:A:VAL:HG13	1:60:A:SER:H	6	18.53
(1,35)	1:95:A:VAL:HG21	1:60:A:SER:H	6	18.53
(1,35)	1:95:A:VAL:HG22	1:60:A:SER:H	6	18.53
(1,35)	1:95:A:VAL:HG23	1:60:A:SER:H	6	18.53
(1,36)	1:95:A:VAL:HG11	1:60:A:SER:H	13	18.51
(1,36)	1:95:A:VAL:HG12	1:60:A:SER:H	13	18.51
(1,36)	1:95:A:VAL:HG13	1:60:A:SER:H	13	18.51
(1,36)	1:95:A:VAL:HG21	1:60:A:SER:H	13	18.51
(1,36)	1:95:A:VAL:HG22	1:60:A:SER:H	13	18.51
(1,36)	1:95:A:VAL:HG23	1:60:A:SER:H	13	18.51
(1,35)	1:95:A:VAL:HG11	1:60:A:SER:H	13	18.51
(1,35)	1:95:A:VAL:HG12	1:60:A:SER:H	13	18.51
(1,35)	1:95:A:VAL:HG13	1:60:A:SER:H	13	18.51
(1,35)	1:95:A:VAL:HG21	1:60:A:SER:H	13	18.51
(1,35)	1:95:A:VAL:HG22	1:60:A:SER:H	13	18.51
(1,35)	1:95:A:VAL:HG23	1:60:A:SER:H	13	18.51
(1,36)	1:95:A:VAL:HG11	1:60:A:SER:H	10	18.44
(1,36)	1:95:A:VAL:HG12	1:60:A:SER:H	10	18.44
(1,36)	1:95:A:VAL:HG13	1:60:A:SER:H	10	18.44
(1,36)	1:95:A:VAL:HG21	1:60:A:SER:H	10	18.44
(1,36)	1:95:A:VAL:HG22	1:60:A:SER:H	10	18.44
(1,36)	1:95:A:VAL:HG23	1:60:A:SER:H	10	18.44
(1,35)	1:95:A:VAL:HG11	1:60:A:SER:H	10	18.44
(1,35)	1:95:A:VAL:HG12	1:60:A:SER:H	10	18.44
(1,35)	1:95:A:VAL:HG13	1:60:A:SER:H	10	18.44
(1,35)	1:95:A:VAL:HG21	1:60:A:SER:H	10	18.44
(1,35)	1:95:A:VAL:HG22	1:60:A:SER:H	10	18.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:95:A:VAL:HG23	1:60:A:SER:H	10	18.44
(1,40)	1:107:A:TRP:HE1	1:119:A:LYS:HA	5	18.39
(1,39)	1:107:A:TRP:HE1	1:119:A:LYS:HA	5	18.39
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD21	9	18.33
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD22	9	18.33
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD23	9	18.33
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD21	9	18.33
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD22	9	18.33
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD23	9	18.33
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD21	15	18.28
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD22	15	18.28
(1,28)	1:80:A:ILE:H	1:59:A:LEU:HD23	15	18.28
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD21	15	18.28
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD22	15	18.28
(1,27)	1:80:A:ILE:H	1:59:A:LEU:HD23	15	18.28
(1,40)	1:107:A:TRP:HE1	1:119:A:LYS:HA	14	18.21
(1,39)	1:107:A:TRP:HE1	1:119:A:LYS:HA	14	18.21
(1,36)	1:95:A:VAL:HG11	1:60:A:SER:H	14	18.19
(1,36)	1:95:A:VAL:HG12	1:60:A:SER:H	14	18.19
(1,36)	1:95:A:VAL:HG13	1:60:A:SER:H	14	18.19
(1,36)	1:95:A:VAL:HG21	1:60:A:SER:H	14	18.19
(1,36)	1:95:A:VAL:HG22	1:60:A:SER:H	14	18.19
(1,36)	1:95:A:VAL:HG23	1:60:A:SER:H	14	18.19
(1,35)	1:95:A:VAL:HG11	1:60:A:SER:H	14	18.19
(1,35)	1:95:A:VAL:HG12	1:60:A:SER:H	14	18.19
(1,35)	1:95:A:VAL:HG13	1:60:A:SER:H	14	18.19
(1,35)	1:95:A:VAL:HG21	1:60:A:SER:H	14	18.19
(1,35)	1:95:A:VAL:HG22	1:60:A:SER:H	14	18.19
(1,35)	1:95:A:VAL:HG23	1:60:A:SER:H	14	18.19
(1,36)	1:95:A:VAL:HG11	1:60:A:SER:H	7	18.17
(1,36)	1:95:A:VAL:HG12	1:60:A:SER:H	7	18.17
(1,36)	1:95:A:VAL:HG13	1:60:A:SER:H	7	18.17
(1,36)	1:95:A:VAL:HG21	1:60:A:SER:H	7	18.17
(1,36)	1:95:A:VAL:HG22	1:60:A:SER:H	7	18.17
(1,36)	1:95:A:VAL:HG23	1:60:A:SER:H	7	18.17
(1,35)	1:95:A:VAL:HG11	1:60:A:SER:H	7	18.17
(1,35)	1:95:A:VAL:HG12	1:60:A:SER:H	7	18.17
(1,35)	1:95:A:VAL:HG13	1:60:A:SER:H	7	18.17
(1,35)	1:95:A:VAL:HG21	1:60:A:SER:H	7	18.17
(1,35)	1:95:A:VAL:HG22	1:60:A:SER:H	7	18.17
(1,35)	1:95:A:VAL:HG23	1:60:A:SER:H	7	18.17
(1,40)	1:107:A:TRP:HE1	1:119:A:LYS:HA	6	18.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:107:A:TRP:HE1	1:119:A:LYS:HA	6	18.15
(1,36)	1:95:A:VAL:HG11	1:60:A:SER:H	11	18.15
(1,36)	1:95:A:VAL:HG12	1:60:A:SER:H	11	18.15
(1,36)	1:95:A:VAL:HG13	1:60:A:SER:H	11	18.15
(1,36)	1:95:A:VAL:HG21	1:60:A:SER:H	11	18.15
(1,36)	1:95:A:VAL:HG22	1:60:A:SER:H	11	18.15
(1,36)	1:95:A:VAL:HG23	1:60:A:SER:H	11	18.15
(1,35)	1:95:A:VAL:HG11	1:60:A:SER:H	11	18.15
(1,35)	1:95:A:VAL:HG12	1:60:A:SER:H	11	18.15
(1,35)	1:95:A:VAL:HG13	1:60:A:SER:H	11	18.15
(1,35)	1:95:A:VAL:HG21	1:60:A:SER:H	11	18.15
(1,35)	1:95:A:VAL:HG22	1:60:A:SER:H	11	18.15
(1,35)	1:95:A:VAL:HG23	1:60:A:SER:H	11	18.15
(1,36)	1:95:A:VAL:HG11	1:60:A:SER:H	2	18.11
(1,36)	1:95:A:VAL:HG12	1:60:A:SER:H	2	18.11
(1,36)	1:95:A:VAL:HG13	1:60:A:SER:H	2	18.11
(1,36)	1:95:A:VAL:HG21	1:60:A:SER:H	2	18.11
(1,36)	1:95:A:VAL:HG22	1:60:A:SER:H	2	18.11
(1,36)	1:95:A:VAL:HG23	1:60:A:SER:H	2	18.11
(1,35)	1:95:A:VAL:HG11	1:60:A:SER:H	2	18.11
(1,35)	1:95:A:VAL:HG12	1:60:A:SER:H	2	18.11
(1,35)	1:95:A:VAL:HG13	1:60:A:SER:H	2	18.11
(1,35)	1:95:A:VAL:HG21	1:60:A:SER:H	2	18.11
(1,35)	1:95:A:VAL:HG22	1:60:A:SER:H	2	18.11
(1,35)	1:95:A:VAL:HG23	1:60:A:SER:H	2	18.11
(1,40)	1:107:A:TRP:HE1	1:119:A:LYS:HA	11	18.06
(1,39)	1:107:A:TRP:HE1	1:119:A:LYS:HA	11	18.06
(1,40)	1:107:A:TRP:HE1	1:119:A:LYS:HA	2	18.0
(1,39)	1:107:A:TRP:HE1	1:119:A:LYS:HA	2	18.0
(1,40)	1:107:A:TRP:HE1	1:119:A:LYS:HA	7	17.99
(1,39)	1:107:A:TRP:HE1	1:119:A:LYS:HA	7	17.99
(1,40)	1:107:A:TRP:HE1	1:119:A:LYS:HA	8	17.97
(1,39)	1:107:A:TRP:HE1	1:119:A:LYS:HA	8	17.97
(1,36)	1:95:A:VAL:HG11	1:60:A:SER:H	8	17.9
(1,36)	1:95:A:VAL:HG12	1:60:A:SER:H	8	17.9
(1,36)	1:95:A:VAL:HG13	1:60:A:SER:H	8	17.9
(1,36)	1:95:A:VAL:HG21	1:60:A:SER:H	8	17.9
(1,36)	1:95:A:VAL:HG22	1:60:A:SER:H	8	17.9
(1,36)	1:95:A:VAL:HG23	1:60:A:SER:H	8	17.9
(1,35)	1:95:A:VAL:HG11	1:60:A:SER:H	8	17.9
(1,35)	1:95:A:VAL:HG12	1:60:A:SER:H	8	17.9
(1,35)	1:95:A:VAL:HG13	1:60:A:SER:H	8	17.9

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:95:A:VAL:HG21	1:60:A:SER:H	8	17.9
(1,35)	1:95:A:VAL:HG22	1:60:A:SER:H	8	17.9
(1,35)	1:95:A:VAL:HG23	1:60:A:SER:H	8	17.9
(1,40)	1:107:A:TRP:HE1	1:119:A:LYS:HA	4	17.67
(1,39)	1:107:A:TRP:HE1	1:119:A:LYS:HA	4	17.67
(1,40)	1:107:A:TRP:HE1	1:119:A:LYS:HA	9	17.66
(1,39)	1:107:A:TRP:HE1	1:119:A:LYS:HA	9	17.66
(1,40)	1:107:A:TRP:HE1	1:119:A:LYS:HA	13	17.47
(1,39)	1:107:A:TRP:HE1	1:119:A:LYS:HA	13	17.47
(1,40)	1:107:A:TRP:HE1	1:119:A:LYS:HA	12	17.26
(1,39)	1:107:A:TRP:HE1	1:119:A:LYS:HA	12	17.26
(1,40)	1:107:A:TRP:HE1	1:119:A:LYS:HA	15	17.15
(1,39)	1:107:A:TRP:HE1	1:119:A:LYS:HA	15	17.15
(1,40)	1:107:A:TRP:HE1	1:119:A:LYS:HA	10	16.94
(1,39)	1:107:A:TRP:HE1	1:119:A:LYS:HA	10	16.94
(1,40)	1:107:A:TRP:HE1	1:119:A:LYS:HA	1	16.75
(1,39)	1:107:A:TRP:HE1	1:119:A:LYS:HA	1	16.75
(1,60)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	3	16.19
(1,60)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	3	16.19
(1,60)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	3	16.19
(1,59)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	3	16.19
(1,59)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	3	16.19
(1,59)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	3	16.19
(1,60)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	13	16.18
(1,60)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	13	16.18
(1,60)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	13	16.18
(1,59)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	13	16.18
(1,59)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	13	16.18
(1,59)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	13	16.18
(1,60)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	5	16.06
(1,60)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	5	16.06
(1,60)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	5	16.06
(1,59)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	5	16.06
(1,59)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	5	16.06
(1,59)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	5	16.06
(1,60)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	11	15.9
(1,60)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	11	15.9
(1,60)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	11	15.9
(1,59)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	11	15.9
(1,59)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	11	15.9
(1,59)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	11	15.9
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	2	15.83

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	2	15.83
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	2	15.83
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	2	15.83
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	2	15.83
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	2	15.83
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	2	15.83
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	2	15.83
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	2	15.83
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	3	15.83
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	3	15.83
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	3	15.83
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	3	15.83
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	3	15.83
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	3	15.83
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	3	15.83
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	3	15.83
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	3	15.83
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	10	15.83
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	10	15.83
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	10	15.83
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	10	15.83
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	10	15.83
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	10	15.83
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	10	15.83
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	10	15.83
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	10	15.83
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	2	15.83
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	2	15.83
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	2	15.83
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	2	15.83
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	2	15.83
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	2	15.83
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	2	15.83
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	2	15.83
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	2	15.83
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	3	15.83
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	3	15.83
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	3	15.83
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	3	15.83
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	3	15.83
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	3	15.83
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	3	15.83

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	3	15.83
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	3	15.83
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	10	15.83
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	10	15.83
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	10	15.83
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	10	15.83
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	10	15.83
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	10	15.83
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	10	15.83
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	10	15.83
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	10	15.83
(1,60)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	6	15.81
(1,60)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	6	15.81
(1,60)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	6	15.81
(1,59)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	6	15.81
(1,59)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	6	15.81
(1,59)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	6	15.81
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	12	15.81
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	12	15.81
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	12	15.81
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	12	15.81
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	12	15.81
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	12	15.81
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	12	15.81
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	12	15.81
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	12	15.81
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	12	15.81
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	12	15.81
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	12	15.81
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	12	15.81
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	12	15.81
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	12	15.81
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	12	15.81
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	12	15.81
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	12	15.81
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	7	15.79
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	7	15.79
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	7	15.79
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	7	15.79
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	7	15.79
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	7	15.79
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	7	15.79

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	7	15.79
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	7	15.79
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	7	15.79
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	7	15.79
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	7	15.79
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	7	15.79
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	7	15.79
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	7	15.79
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	7	15.79
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	7	15.79
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	7	15.79
(1,60)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	14	15.73
(1,60)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	14	15.73
(1,60)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	14	15.73
(1,59)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	14	15.73
(1,59)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	14	15.73
(1,59)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	14	15.73
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	5	15.71
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	5	15.71
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	5	15.71
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	5	15.71
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	5	15.71
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	5	15.71
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	5	15.71
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	5	15.71
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	5	15.71
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	5	15.71
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	5	15.71
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	5	15.71
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	5	15.71
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	5	15.71
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	5	15.71
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	5	15.71
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	5	15.71
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	5	15.71
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	5	15.66
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	5	15.66
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	5	15.66
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	5	15.66
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	5	15.66
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	5	15.66
(1,60)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	9	15.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	9	15.64
(1,60)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	9	15.64
(1,59)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	9	15.64
(1,59)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	9	15.64
(1,59)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	9	15.64
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	1	15.62
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	1	15.62
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	1	15.62
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	1	15.62
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	1	15.62
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	1	15.62
(1,60)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	7	15.61
(1,60)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	7	15.61
(1,60)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	7	15.61
(1,60)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	8	15.61
(1,60)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	8	15.61
(1,60)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	8	15.61
(1,59)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	7	15.61
(1,59)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	7	15.61
(1,59)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	7	15.61
(1,59)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	8	15.61
(1,59)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	8	15.61
(1,59)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	8	15.61
(1,60)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	2	15.53
(1,60)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	2	15.53
(1,60)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	2	15.53
(1,59)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	2	15.53
(1,59)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	2	15.53
(1,59)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	2	15.53
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	8	15.51
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	8	15.51
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	8	15.51
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	8	15.51
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	8	15.51
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	8	15.51
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	8	15.51
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	8	15.51
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	8	15.51
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	8	15.51
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	8	15.51
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	8	15.51
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	8	15.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	8	15.51
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	8	15.51
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	8	15.51
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	8	15.51
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	8	15.51
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	11	15.44
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	11	15.44
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	11	15.44
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	11	15.44
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	11	15.44
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	11	15.44
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	14	15.43
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	14	15.43
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	14	15.43
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	14	15.43
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	14	15.43
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	14	15.43
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	14	15.43
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	14	15.43
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	14	15.43
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	14	15.43
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	14	15.43
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	14	15.43
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	14	15.43
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	14	15.43
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	14	15.43
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	14	15.43
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	14	15.43
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	14	15.43
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	3	15.36
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	3	15.36
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	3	15.36
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	3	15.36
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	3	15.36
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	3	15.36
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE1	10	15.35
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE2	10	15.35
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE3	10	15.35
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE1	10	15.35
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE2	10	15.35
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE3	10	15.35
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE1	10	15.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE2	10	15.35
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE3	10	15.35
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE1	10	15.35
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE2	10	15.35
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE3	10	15.35
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE1	10	15.35
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE2	10	15.35
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE3	10	15.35
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE1	10	15.35
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE2	10	15.35
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE3	10	15.35
(1,60)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	4	15.31
(1,60)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	4	15.31
(1,60)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	4	15.31
(1,60)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	12	15.31
(1,60)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	12	15.31
(1,60)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	12	15.31
(1,59)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	4	15.31
(1,59)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	4	15.31
(1,59)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	4	15.31
(1,59)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	12	15.31
(1,59)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	12	15.31
(1,59)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	12	15.31
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	13	15.18
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	13	15.18
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	13	15.18
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	13	15.18
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	13	15.18
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	13	15.18
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	13	15.18
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	13	15.18
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	13	15.18
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	13	15.18
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	13	15.18
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	13	15.18
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	13	15.18
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	13	15.18
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	13	15.18
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	13	15.18
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	13	15.18
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	13	15.18
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	11	15.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	11	15.17
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	11	15.17
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	11	15.17
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	11	15.17
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	11	15.17
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	11	15.17
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	11	15.17
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	11	15.17
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	11	15.17
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	11	15.17
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	11	15.17
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	11	15.17
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	11	15.17
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	11	15.17
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	11	15.17
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	11	15.17
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	11	15.17
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	7	15.16
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	7	15.16
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	7	15.16
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	7	15.16
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	7	15.16
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	7	15.16
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	14	15.06
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	14	15.06
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	14	15.06
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	14	15.06
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	14	15.06
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	14	15.06
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	2	15.04
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	2	15.04
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	2	15.04
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	2	15.04
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	2	15.04
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	2	15.04
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	6	14.99
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	6	14.99
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	6	14.99
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	6	14.99
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	6	14.99
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	6	14.99
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	8	14.97

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	8	14.97
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	8	14.97
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	8	14.97
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	8	14.97
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	8	14.97
(1,60)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	15	14.73
(1,60)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	15	14.73
(1,60)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	15	14.73
(1,59)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	15	14.73
(1,59)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	15	14.73
(1,59)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	15	14.73
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	6	14.65
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	6	14.65
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	6	14.65
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	6	14.65
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	6	14.65
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	6	14.65
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	6	14.65
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	6	14.65
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	6	14.65
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	6	14.65
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	6	14.65
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	6	14.65
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	6	14.65
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	6	14.65
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	6	14.65
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	6	14.65
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	6	14.65
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	6	14.65
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	4	14.62
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	4	14.62
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	4	14.62
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	4	14.62
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	4	14.62
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	4	14.62
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	1	14.62
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	1	14.62
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	1	14.62
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	1	14.62
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	1	14.62
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	1	14.62
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	1	14.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	1	14.62
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	1	14.62
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	1	14.62
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	1	14.62
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	1	14.62
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	1	14.62
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	1	14.62
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	1	14.62
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	1	14.62
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	1	14.62
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	1	14.62
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	9	14.61
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	9	14.61
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	9	14.61
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	9	14.61
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	9	14.61
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	9	14.61
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE1	13	14.53
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE2	13	14.53
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE3	13	14.53
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE1	13	14.53
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE2	13	14.53
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE3	13	14.53
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE1	13	14.53
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE2	13	14.53
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE3	13	14.53
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE1	13	14.53
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE2	13	14.53
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE3	13	14.53
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE1	13	14.53
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE2	13	14.53
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE3	13	14.53
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE1	13	14.53
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE2	13	14.53
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE3	13	14.53
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	13	14.52
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	13	14.52
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	13	14.52
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	13	14.52
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	13	14.52
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	13	14.52
(1,60)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	10	14.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	10	14.48
(1,60)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	10	14.48
(1,59)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	10	14.48
(1,59)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	10	14.48
(1,59)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	10	14.48
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	10	14.31
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	10	14.31
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	10	14.31
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	10	14.31
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	10	14.31
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	10	14.31
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	4	14.3
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	4	14.3
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	4	14.3
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	4	14.3
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	4	14.3
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	4	14.3
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	4	14.3
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	4	14.3
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	4	14.3
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	4	14.3
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	4	14.3
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	4	14.3
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	4	14.3
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	4	14.3
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	4	14.3
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	4	14.3
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	4	14.3
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	4	14.3
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	12	14.25
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	12	14.25
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	12	14.25
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	12	14.25
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	12	14.25
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	12	14.25
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	15	14.21
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	15	14.21
(1,42)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	15	14.21
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD11	15	14.21
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD12	15	14.21
(1,41)	1:107:A:TRP:HE1	1:122:A:LEU:HD13	15	14.21
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE1	1	14.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE2	1	14.15
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE3	1	14.15
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE1	1	14.15
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE2	1	14.15
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE3	1	14.15
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE1	1	14.15
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE2	1	14.15
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE3	1	14.15
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE1	1	14.15
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE2	1	14.15
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE3	1	14.15
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE1	1	14.15
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE2	1	14.15
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE3	1	14.15
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE1	1	14.15
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE2	1	14.15
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE3	1	14.15
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	9	14.1
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	9	14.1
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	9	14.1
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	9	14.1
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	9	14.1
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	9	14.1
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	9	14.1
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	9	14.1
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	9	14.1
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	9	14.1
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	9	14.1
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	9	14.1
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	9	14.1
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	9	14.1
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	9	14.1
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	9	14.1
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	9	14.1
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	9	14.1
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	15	13.87
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	15	13.87
(1,30)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	15	13.87
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	15	13.87
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	15	13.87
(1,30)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	15	13.87
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	15	13.87

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	15	13.87
(1,30)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	15	13.87
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD21	15	13.87
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD22	15	13.87
(1,29)	1:80:A:ILE:HG21	1:59:A:LEU:HD23	15	13.87
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD21	15	13.87
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD22	15	13.87
(1,29)	1:80:A:ILE:HG22	1:59:A:LEU:HD23	15	13.87
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD21	15	13.87
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD22	15	13.87
(1,29)	1:80:A:ILE:HG23	1:59:A:LEU:HD23	15	13.87
(1,58)	1:118:A:SER:H	1:107:A:TRP:HE1	5	13.63
(1,57)	1:118:A:SER:H	1:107:A:TRP:HE1	5	13.63
(1,58)	1:118:A:SER:H	1:107:A:TRP:HE1	3	13.51
(1,57)	1:118:A:SER:H	1:107:A:TRP:HE1	3	13.51
(1,58)	1:118:A:SER:H	1:107:A:TRP:HE1	6	13.42
(1,57)	1:118:A:SER:H	1:107:A:TRP:HE1	6	13.42
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE1	7	13.4
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE2	7	13.4
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE3	7	13.4
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE1	7	13.4
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE2	7	13.4
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE3	7	13.4
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE1	7	13.4
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE2	7	13.4
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE3	7	13.4
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE1	7	13.4
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE2	7	13.4
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE3	7	13.4
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE1	7	13.4
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE2	7	13.4
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE3	7	13.4
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE1	7	13.4
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE2	7	13.4
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE3	7	13.4
(1,58)	1:118:A:SER:H	1:107:A:TRP:HE1	11	13.37
(1,57)	1:118:A:SER:H	1:107:A:TRP:HE1	11	13.37
(1,58)	1:118:A:SER:H	1:107:A:TRP:HE1	14	13.33
(1,57)	1:118:A:SER:H	1:107:A:TRP:HE1	14	13.33
(1,60)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	1	13.32
(1,60)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	1	13.32
(1,60)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	1	13.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:122:A:LEU:HD21	1:107:A:TRP:HE1	1	13.32
(1,59)	1:122:A:LEU:HD22	1:107:A:TRP:HE1	1	13.32
(1,59)	1:122:A:LEU:HD23	1:107:A:TRP:HE1	1	13.32
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	10	13.28
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	10	13.28
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	10	13.28
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	10	13.28
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	10	13.28
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	10	13.28
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	10	13.28
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	10	13.28
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	10	13.28
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	10	13.28
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	10	13.28
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	10	13.28
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	10	13.28
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	10	13.28
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	10	13.28
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	10	13.28
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	10	13.28
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	10	13.28
(1,58)	1:118:A:SER:H	1:107:A:TRP:HE1	7	13.13
(1,57)	1:118:A:SER:H	1:107:A:TRP:HE1	7	13.13
(1,58)	1:118:A:SER:H	1:107:A:TRP:HE1	2	13.1
(1,57)	1:118:A:SER:H	1:107:A:TRP:HE1	2	13.1
(1,58)	1:118:A:SER:H	1:107:A:TRP:HE1	8	13.06
(1,57)	1:118:A:SER:H	1:107:A:TRP:HE1	8	13.06
(1,58)	1:118:A:SER:H	1:107:A:TRP:HE1	9	13.04
(1,57)	1:118:A:SER:H	1:107:A:TRP:HE1	9	13.04
(1,58)	1:118:A:SER:H	1:107:A:TRP:HE1	4	12.92
(1,57)	1:118:A:SER:H	1:107:A:TRP:HE1	4	12.92
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE1	6	12.86
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE2	6	12.86
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE3	6	12.86
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE1	6	12.86
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE2	6	12.86
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE3	6	12.86
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE1	6	12.86
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE2	6	12.86
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE3	6	12.86
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE1	6	12.86
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE2	6	12.86

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE3	6	12.86
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE1	6	12.86
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE2	6	12.86
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE3	6	12.86
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE1	6	12.86
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE2	6	12.86
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE3	6	12.86
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	1	12.68
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	1	12.68
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	1	12.68
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	1	12.68
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	1	12.68
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	1	12.68
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	1	12.68
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	1	12.68
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	1	12.68
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	1	12.68
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	1	12.68
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	1	12.68
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	1	12.68
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	1	12.68
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	1	12.68
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	1	12.68
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	1	12.68
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	1	12.68
(1,58)	1:118:A:SER:H	1:107:A:TRP:HE1	10	12.67
(1,57)	1:118:A:SER:H	1:107:A:TRP:HE1	10	12.67
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	6	12.64
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	6	12.64
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	6	12.64
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	6	12.64
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	6	12.64
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	6	12.64
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	6	12.64
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	6	12.64
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	6	12.64
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	12	12.64
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	12	12.64
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	12	12.64
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	12	12.64
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	12	12.64
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	12	12.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	12	12.64
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	12	12.64
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	12	12.64
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	6	12.64
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	6	12.64
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	6	12.64
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	6	12.64
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	6	12.64
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	6	12.64
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	6	12.64
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	6	12.64
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	6	12.64
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	12	12.64
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	12	12.64
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	12	12.64
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	12	12.64
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	12	12.64
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	12	12.64
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	12	12.64
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	12	12.64
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	12	12.64
(1,58)	1:118:A:SER:H	1:107:A:TRP:HE1	1	12.63
(1,57)	1:118:A:SER:H	1:107:A:TRP:HE1	1	12.63
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG2	1	12.62
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG3	1	12.62
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG2	1	12.62
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG3	1	12.62
(1,58)	1:118:A:SER:H	1:107:A:TRP:HE1	12	12.57
(1,57)	1:118:A:SER:H	1:107:A:TRP:HE1	12	12.57
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG2	12	12.54
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG3	12	12.54
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG2	12	12.54
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG3	12	12.54
(1,58)	1:118:A:SER:H	1:107:A:TRP:HE1	13	12.35
(1,58)	1:118:A:SER:H	1:107:A:TRP:HE1	15	12.35
(1,57)	1:118:A:SER:H	1:107:A:TRP:HE1	13	12.35
(1,57)	1:118:A:SER:H	1:107:A:TRP:HE1	15	12.35
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	3	12.35
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	3	12.35
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	3	12.35
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	3	12.35
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	3	12.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	3	12.35
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	3	12.35
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	3	12.35
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	3	12.35
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	3	12.35
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	3	12.35
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	3	12.35
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	3	12.35
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	3	12.35
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	3	12.35
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	3	12.35
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	3	12.35
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	3	12.35
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG2	13	12.35
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG3	13	12.35
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG2	13	12.35
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG3	13	12.35
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE1	2	12.33
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE2	2	12.33
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE3	2	12.33
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE1	2	12.33
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE2	2	12.33
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE3	2	12.33
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE1	2	12.33
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE2	2	12.33
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE3	2	12.33
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE1	2	12.33
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE2	2	12.33
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE3	2	12.33
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE1	2	12.33
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE2	2	12.33
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE3	2	12.33
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE1	2	12.33
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE2	2	12.33
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE3	2	12.33
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG2	10	12.28
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG3	10	12.28
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG2	10	12.28
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG3	10	12.28
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE1	11	12.27
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE2	11	12.27
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE3	11	12.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE1	11	12.27
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE2	11	12.27
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE3	11	12.27
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE1	11	12.27
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE2	11	12.27
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE3	11	12.27
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE1	11	12.27
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE2	11	12.27
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE3	11	12.27
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE1	11	12.27
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE2	11	12.27
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE3	11	12.27
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE1	11	12.27
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE2	11	12.27
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE3	11	12.27
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	7	12.25
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	7	12.25
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	7	12.25
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	7	12.25
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	7	12.25
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	7	12.25
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	7	12.25
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	7	12.25
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	7	12.25
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	7	12.25
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	7	12.25
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	7	12.25
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	7	12.25
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	7	12.25
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	7	12.25
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	7	12.25
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	7	12.25
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	7	12.25
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	4	12.24
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	4	12.24
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	4	12.24
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	4	12.24
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	4	12.24
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	4	12.24
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	4	12.24
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	4	12.24
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	4	12.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	4	12.24
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	4	12.24
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	4	12.24
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	4	12.24
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	4	12.24
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	4	12.24
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	4	12.24
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	4	12.24
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	4	12.24
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE1	14	12.22
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE2	14	12.22
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE3	14	12.22
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE1	14	12.22
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE2	14	12.22
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE3	14	12.22
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE1	14	12.22
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE2	14	12.22
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE3	14	12.22
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE1	14	12.22
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE2	14	12.22
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE3	14	12.22
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE1	14	12.22
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE2	14	12.22
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE3	14	12.22
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE1	14	12.22
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE2	14	12.22
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE3	14	12.22
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE1	3	12.2
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE2	3	12.2
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE3	3	12.2
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE1	3	12.2
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE2	3	12.2
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE3	3	12.2
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE1	3	12.2
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE2	3	12.2
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE3	3	12.2
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE1	3	12.2
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE2	3	12.2
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE3	3	12.2
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE1	3	12.2
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE2	3	12.2
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE3	3	12.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE1	3	12.2
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE2	3	12.2
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE3	3	12.2
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE1	12	12.19
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE2	12	12.19
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE3	12	12.19
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE1	12	12.19
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE2	12	12.19
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE3	12	12.19
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE1	12	12.19
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE2	12	12.19
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE3	12	12.19
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE1	12	12.19
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE2	12	12.19
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE3	12	12.19
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE1	12	12.19
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE2	12	12.19
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE3	12	12.19
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE1	12	12.19
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE2	12	12.19
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE3	12	12.19
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	2	12.18
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	2	12.18
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	2	12.18
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	2	12.18
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	2	12.18
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	2	12.18
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	2	12.18
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	2	12.18
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	2	12.18
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	2	12.18
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	2	12.18
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	2	12.18
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	2	12.18
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	2	12.18
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	2	12.18
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	2	12.18
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	2	12.18
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	2	12.18
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	5	12.11
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	5	12.11
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	5	12.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	5	12.11
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	5	12.11
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	5	12.11
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	5	12.11
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	5	12.11
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	5	12.11
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	9	12.11
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	9	12.11
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	9	12.11
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	9	12.11
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	9	12.11
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	9	12.11
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	9	12.11
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	9	12.11
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	9	12.11
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	5	12.11
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	5	12.11
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	5	12.11
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	5	12.11
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	5	12.11
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	5	12.11
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	5	12.11
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	5	12.11
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	5	12.11
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	9	12.11
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	9	12.11
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	9	12.11
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	9	12.11
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	9	12.11
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	9	12.11
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	9	12.11
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	9	12.11
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	9	12.11
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	11	12.08
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	11	12.08
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	11	12.08
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	11	12.08
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	11	12.08
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	11	12.08
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	11	12.08
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	11	12.08
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	11	12.08

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	11	12.08
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	11	12.08
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	11	12.08
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	11	12.08
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	11	12.08
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	11	12.08
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	11	12.08
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	11	12.08
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	11	12.08
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD2	10	12.05
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD3	10	12.05
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD2	10	12.05
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD3	10	12.05
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE1	4	12.03
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE2	4	12.03
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE3	4	12.03
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE1	4	12.03
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE2	4	12.03
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE3	4	12.03
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE1	4	12.03
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE2	4	12.03
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE3	4	12.03
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE1	15	12.03
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE2	15	12.03
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE3	15	12.03
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE1	15	12.03
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE2	15	12.03
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE3	15	12.03
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE1	15	12.03
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE2	15	12.03
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE3	15	12.03
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE1	4	12.03
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE2	4	12.03
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE3	4	12.03
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE1	4	12.03
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE2	4	12.03
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE3	4	12.03
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE1	4	12.03
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE2	4	12.03
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE3	4	12.03
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE1	15	12.03
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE2	15	12.03

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE3	15	12.03
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE1	15	12.03
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE2	15	12.03
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE3	15	12.03
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE1	15	12.03
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE2	15	12.03
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE3	15	12.03
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	8	11.99
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	8	11.99
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	8	11.99
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	8	11.99
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	8	11.99
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	8	11.99
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	8	11.99
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	8	11.99
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	8	11.99
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	8	11.99
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	8	11.99
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	8	11.99
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	8	11.99
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	8	11.99
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	8	11.99
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	8	11.99
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	8	11.99
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	8	11.99
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE1	9	11.92
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE2	9	11.92
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE3	9	11.92
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE1	9	11.92
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE2	9	11.92
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE3	9	11.92
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE1	9	11.92
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE2	9	11.92
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE3	9	11.92
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE1	9	11.92
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE2	9	11.92
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE3	9	11.92
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE1	9	11.92
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE2	9	11.92
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE3	9	11.92
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE1	9	11.92
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE2	9	11.92

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE3	9	11.92
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD2	13	11.89
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD3	13	11.89
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD2	13	11.89
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD3	13	11.89
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	13	11.81
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	13	11.81
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	13	11.81
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	13	11.81
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	13	11.81
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	13	11.81
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	13	11.81
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	13	11.81
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	13	11.81
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	13	11.81
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	13	11.81
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	13	11.81
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	13	11.81
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	13	11.81
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	13	11.81
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	13	11.81
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	13	11.81
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	13	11.81
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG2	4	11.8
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG3	4	11.8
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG2	4	11.8
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG3	4	11.8
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE1	5	11.77
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE2	5	11.77
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE3	5	11.77
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE1	5	11.77
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE2	5	11.77
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE3	5	11.77
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE1	5	11.77
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE2	5	11.77
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE3	5	11.77
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE1	5	11.77
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE2	5	11.77
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE3	5	11.77
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE1	5	11.77
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE2	5	11.77
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE3	5	11.77

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE1	5	11.77
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE2	5	11.77
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE3	5	11.77
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG2	9	11.64
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG3	9	11.64
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG2	9	11.64
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG3	9	11.64
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	15	11.58
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	15	11.58
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	15	11.58
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	15	11.58
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	15	11.58
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	15	11.58
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	15	11.58
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	15	11.58
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	15	11.58
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	15	11.58
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	15	11.58
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	15	11.58
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	15	11.58
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	15	11.58
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	15	11.58
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	15	11.58
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	15	11.58
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	15	11.58
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	14	11.55
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	14	11.55
(1,32)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	14	11.55
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	14	11.55
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	14	11.55
(1,32)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	14	11.55
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	14	11.55
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	14	11.55
(1,32)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	14	11.55
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD11	14	11.55
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD12	14	11.55
(1,31)	1:80:A:ILE:HG21	1:63:A:LEU:HD13	14	11.55
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD11	14	11.55
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD12	14	11.55
(1,31)	1:80:A:ILE:HG22	1:63:A:LEU:HD13	14	11.55
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD11	14	11.55
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD12	14	11.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:80:A:ILE:HG23	1:63:A:LEU:HD13	14	11.55
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG2	5	11.06
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG3	5	11.06
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG2	5	11.06
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG3	5	11.06
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE1	8	10.87
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE2	8	10.87
(1,8)	1:63:A:LEU:HD11	1:79:A:MET:HE3	8	10.87
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE1	8	10.87
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE2	8	10.87
(1,8)	1:63:A:LEU:HD12	1:79:A:MET:HE3	8	10.87
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE1	8	10.87
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE2	8	10.87
(1,8)	1:63:A:LEU:HD13	1:79:A:MET:HE3	8	10.87
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE1	8	10.87
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE2	8	10.87
(1,7)	1:63:A:LEU:HD11	1:79:A:MET:HE3	8	10.87
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE1	8	10.87
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE2	8	10.87
(1,7)	1:63:A:LEU:HD12	1:79:A:MET:HE3	8	10.87
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE1	8	10.87
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE2	8	10.87
(1,7)	1:63:A:LEU:HD13	1:79:A:MET:HE3	8	10.87
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD2	6	10.86
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD3	6	10.86
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD2	6	10.86
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD3	6	10.86
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG2	6	10.78
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG3	6	10.78
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG2	6	10.78
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG3	6	10.78
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG2	15	10.73
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG3	15	10.73
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG2	15	10.73
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG3	15	10.73
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG2	3	10.66
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG3	3	10.66
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG2	7	10.66
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG3	7	10.66
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG2	3	10.66
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG3	3	10.66
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG2	7	10.66

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG3	7	10.66
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	6	10.61
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	6	10.61
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	6	10.61
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	6	10.61
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	6	10.61
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	6	10.61
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	6	10.61
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	6	10.61
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	6	10.61
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	6	10.61
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	6	10.61
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	6	10.61
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	6	10.61
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	6	10.61
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	6	10.61
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	6	10.61
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	6	10.61
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	6	10.61
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG2	14	10.57
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG3	14	10.57
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG2	14	10.57
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG3	14	10.57
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD2	1	10.54
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD3	1	10.54
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD2	1	10.54
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD3	1	10.54
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	2	10.4
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	2	10.4
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	2	10.4
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	2	10.4
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	2	10.4
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	2	10.4
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	2	10.4
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	2	10.4
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	2	10.4
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	2	10.4
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	2	10.4
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	2	10.4
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	2	10.4
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	2	10.4
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	2	10.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	2	10.4
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	2	10.4
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	2	10.4
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG2	11	10.39
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG3	11	10.39
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG2	11	10.39
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG3	11	10.39
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD2	12	10.34
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD3	12	10.34
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD2	12	10.34
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD3	12	10.34
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG2	8	10.29
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG3	8	10.29
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG2	8	10.29
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG3	8	10.29
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG2	2	10.19
(1,18)	1:68:A:ASP:H	1:109:A:ARG:HG3	2	10.19
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG2	2	10.19
(1,17)	1:68:A:ASP:H	1:109:A:ARG:HG3	2	10.19
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	7	10.12
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	7	10.12
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	7	10.12
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	7	10.12
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	7	10.12
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	7	10.12
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	7	10.12
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	7	10.12
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	7	10.12
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	7	10.12
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	7	10.12
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	7	10.12
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	7	10.12
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	7	10.12
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	7	10.12
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	7	10.12
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	7	10.12
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	7	10.12
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	1	10.08
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	1	10.08
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	1	10.08
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	1	10.08
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	1	10.08

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	1	10.08
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	1	10.08
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	1	10.08
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	1	10.08
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	1	10.08
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	1	10.08
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	1	10.08
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	1	10.08
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	1	10.08
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	1	10.08
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	1	10.08
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	1	10.08
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	1	10.08
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	9	10.07
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	9	10.07
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	9	10.07
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	9	10.07
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	9	10.07
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	9	10.07
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	9	10.07
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	9	10.07
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	9	10.07
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	15	10.07
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	15	10.07
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	15	10.07
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	15	10.07
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	15	10.07
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	15	10.07
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	15	10.07
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	15	10.07
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	15	10.07
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	9	10.07
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	9	10.07
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	9	10.07
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	9	10.07
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	9	10.07
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	9	10.07
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	9	10.07
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	9	10.07
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	9	10.07
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	15	10.07
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	15	10.07

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	15	10.07
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	15	10.07
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	15	10.07
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	15	10.07
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	15	10.07
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	15	10.07
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	15	10.07
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	4	9.98
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	4	9.98
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	4	9.98
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	4	9.98
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	4	9.98
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	4	9.98
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	4	9.98
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	4	9.98
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	4	9.98
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	4	9.98
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	4	9.98
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	4	9.98
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	4	9.98
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	4	9.98
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	4	9.98
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	4	9.98
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	4	9.98
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	4	9.98
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	5	9.93
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	5	9.93
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	5	9.93
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	5	9.93
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	5	9.93
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	5	9.93
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	5	9.93
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	5	9.93
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	5	9.93
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	5	9.93
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	5	9.93
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	5	9.93
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	5	9.93
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	5	9.93
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	5	9.93
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	5	9.93
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	5	9.93

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	5	9.93
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	10	9.87
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	10	9.87
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	10	9.87
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	10	9.87
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	10	9.87
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	10	9.87
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	10	9.87
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	10	9.87
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	10	9.87
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	10	9.87
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	10	9.87
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	10	9.87
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	10	9.87
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	10	9.87
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	10	9.87
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	10	9.87
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	10	9.87
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	10	9.87
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	3	9.86
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	3	9.86
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	3	9.86
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	3	9.86
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	3	9.86
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	3	9.86
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	3	9.86
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	3	9.86
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	3	9.86
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	3	9.86
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	3	9.86
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	3	9.86
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	3	9.86
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	3	9.86
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	3	9.86
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	3	9.86
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	3	9.86
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	3	9.86
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	11	9.84
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	11	9.84
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	11	9.84
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	11	9.84
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	11	9.84

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	11	9.84
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	11	9.84
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	11	9.84
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	11	9.84
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	11	9.84
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	11	9.84
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	11	9.84
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	11	9.84
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	11	9.84
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	11	9.84
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	11	9.84
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	11	9.84
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	11	9.84
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	14	9.74
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	14	9.74
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	14	9.74
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	14	9.74
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	14	9.74
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	14	9.74
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	14	9.74
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	14	9.74
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	14	9.74
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	14	9.74
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	14	9.74
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	14	9.74
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	14	9.74
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	14	9.74
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	14	9.74
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	14	9.74
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	14	9.74
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	14	9.74
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	1	9.71
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	1	9.71
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	1	9.71
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	1	9.71
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	1	9.71
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	1	9.71
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	1	9.71
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	1	9.71
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	1	9.71
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	1	9.71
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	1	9.71

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	1	9.71
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	1	9.71
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	1	9.71
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	1	9.71
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	1	9.71
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	1	9.71
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	1	9.71
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	13	9.63
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	13	9.63
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	13	9.63
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	13	9.63
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	13	9.63
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	13	9.63
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	13	9.63
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	13	9.63
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	13	9.63
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	13	9.63
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	13	9.63
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	13	9.63
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	13	9.63
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	13	9.63
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	13	9.63
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	13	9.63
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	13	9.63
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	13	9.63
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD2	5	9.63
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD3	5	9.63
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD2	5	9.63
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD3	5	9.63
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	8	9.33
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	8	9.33
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	8	9.33
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	8	9.33
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	8	9.33
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	8	9.33
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	8	9.33
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	8	9.33
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	8	9.33
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	8	9.33
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	8	9.33
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	8	9.33
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	8	9.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	8	9.33
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	8	9.33
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	8	9.33
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	8	9.33
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	8	9.33
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD2	4	9.32
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD3	4	9.32
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD2	4	9.32
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD3	4	9.32
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD2	9	9.13
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD3	9	9.13
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD2	9	9.13
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD3	9	9.13
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	12	8.88
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	12	8.88
(1,22)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	12	8.88
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	12	8.88
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	12	8.88
(1,22)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	12	8.88
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	12	8.88
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	12	8.88
(1,22)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	12	8.88
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD11	12	8.88
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD12	12	8.88
(1,21)	1:76:A:LEU:HD21	1:63:A:LEU:HD13	12	8.88
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD11	12	8.88
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD12	12	8.88
(1,21)	1:76:A:LEU:HD22	1:63:A:LEU:HD13	12	8.88
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD11	12	8.88
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD12	12	8.88
(1,21)	1:76:A:LEU:HD23	1:63:A:LEU:HD13	12	8.88
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	6	8.7
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	6	8.7
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	6	8.7
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	6	8.7
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	6	8.7
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	6	8.7
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	6	8.7
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	6	8.7
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	6	8.7
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	6	8.7
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	6	8.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	6	8.7
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	6	8.7
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	6	8.7
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	6	8.7
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	6	8.7
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	6	8.7
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	6	8.7
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	2	8.57
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	2	8.57
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	2	8.57
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	2	8.57
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	2	8.57
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	2	8.57
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	2	8.57
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	2	8.57
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	2	8.57
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	2	8.57
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	2	8.57
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	2	8.57
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	2	8.57
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	2	8.57
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	2	8.57
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	2	8.57
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	2	8.57
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	2	8.57
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD2	15	8.52
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD3	15	8.52
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD2	15	8.52
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD3	15	8.52
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD2	3	8.48
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD3	3	8.48
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD2	3	8.48
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD3	3	8.48
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	4	8.36
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	4	8.36
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	4	8.36
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	4	8.36
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	4	8.36
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	4	8.36
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	4	8.36
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	4	8.36
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	4	8.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	4	8.36
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	4	8.36
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	4	8.36
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	4	8.36
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	4	8.36
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	4	8.36
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	4	8.36
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	4	8.36
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	4	8.36
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	7	8.35
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	7	8.35
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	7	8.35
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	7	8.35
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	7	8.35
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	7	8.35
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	7	8.35
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	7	8.35
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	7	8.35
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	7	8.35
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	7	8.35
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	7	8.35
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	7	8.35
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	7	8.35
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	7	8.35
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	7	8.35
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	7	8.35
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	7	8.35
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	15	8.34
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	15	8.34
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	15	8.34
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	15	8.34
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	15	8.34
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	15	8.34
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	15	8.34
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	15	8.34
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	15	8.34
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	15	8.34
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	15	8.34
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	15	8.34
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	15	8.34
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	15	8.34
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	15	8.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	15	8.34
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	15	8.34
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	15	8.34
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD2	7	8.32
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD3	7	8.32
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD2	7	8.32
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD3	7	8.32
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	11	8.31
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	11	8.31
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	11	8.31
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	11	8.31
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	11	8.31
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	11	8.31
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	11	8.31
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	11	8.31
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	11	8.31
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	11	8.31
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	11	8.31
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	11	8.31
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	11	8.31
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	11	8.31
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	11	8.31
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	11	8.31
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	11	8.31
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	11	8.31
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD2	14	8.3
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD3	14	8.3
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD2	14	8.3
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD3	14	8.3
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	9	8.24
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	9	8.24
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	9	8.24
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	9	8.24
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	9	8.24
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	9	8.24
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	9	8.24
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	9	8.24
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	9	8.24
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	10	8.24
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	10	8.24
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	10	8.24
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	10	8.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	10	8.24
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	10	8.24
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	10	8.24
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	10	8.24
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	10	8.24
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	9	8.24
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	9	8.24
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	9	8.24
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	9	8.24
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	9	8.24
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	9	8.24
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	9	8.24
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	9	8.24
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	9	8.24
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	10	8.24
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	10	8.24
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	10	8.24
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	10	8.24
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	10	8.24
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	10	8.24
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	10	8.24
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	10	8.24
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	10	8.24
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	3	8.14
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	3	8.14
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	3	8.14
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	3	8.14
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	3	8.14
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	3	8.14
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	3	8.14
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	3	8.14
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	3	8.14
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	3	8.14
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	3	8.14
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	3	8.14
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	3	8.14
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	3	8.14
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	3	8.14
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	3	8.14
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	3	8.14
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	3	8.14
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD2	8	8.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD3	8	8.11
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD2	8	8.11
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD3	8	8.11
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	5	8.03
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	5	8.03
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	5	8.03
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	5	8.03
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	5	8.03
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	5	8.03
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	5	8.03
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	5	8.03
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	5	8.03
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	5	8.03
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	5	8.03
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	5	8.03
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	5	8.03
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	5	8.03
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	5	8.03
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	5	8.03
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	5	8.03
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	5	8.03
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD2	11	7.97
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD3	11	7.97
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD2	11	7.97
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD3	11	7.97
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	14	7.87
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	14	7.87
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	14	7.87
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	14	7.87
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	14	7.87
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	14	7.87
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	14	7.87
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	14	7.87
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	14	7.87
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	14	7.87
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	14	7.87
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	14	7.87
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	14	7.87
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	14	7.87
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	14	7.87
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	14	7.87
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	14	7.87

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	14	7.87
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	8	7.8
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	8	7.8
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	8	7.8
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	8	7.8
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	8	7.8
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	8	7.8
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	8	7.8
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	8	7.8
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	8	7.8
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	8	7.8
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	8	7.8
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	8	7.8
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	8	7.8
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	8	7.8
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	8	7.8
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	8	7.8
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	8	7.8
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	8	7.8
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	13	7.68
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	13	7.68
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	13	7.68
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	13	7.68
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	13	7.68
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	13	7.68
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	13	7.68
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	13	7.68
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	13	7.68
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	13	7.68
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	13	7.68
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	13	7.68
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	13	7.68
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	13	7.68
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	13	7.68
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	13	7.68
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	13	7.68
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	13	7.68
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD2	2	7.47
(1,14)	1:67:A:GLY:H	1:109:A:ARG:HD3	2	7.47
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD2	2	7.47
(1,13)	1:67:A:GLY:H	1:109:A:ARG:HD3	2	7.47
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB1	12	7.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB2	12	7.34
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB3	12	7.34
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB1	12	7.34
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB2	12	7.34
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB3	12	7.34
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	12	6.98
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	12	6.98
(1,24)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	12	6.98
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	12	6.98
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	12	6.98
(1,24)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	12	6.98
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	12	6.98
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	12	6.98
(1,24)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	12	6.98
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD21	12	6.98
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD22	12	6.98
(1,23)	1:76:A:LEU:HD21	1:63:A:LEU:HD23	12	6.98
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD21	12	6.98
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD22	12	6.98
(1,23)	1:76:A:LEU:HD22	1:63:A:LEU:HD23	12	6.98
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD21	12	6.98
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD22	12	6.98
(1,23)	1:76:A:LEU:HD23	1:63:A:LEU:HD23	12	6.98
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB1	10	6.52
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB2	10	6.52
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB3	10	6.52
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB1	10	6.52
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB2	10	6.52
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB3	10	6.52
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB1	1	6.32
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB2	1	6.32
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB3	1	6.32
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB1	1	6.32
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB2	1	6.32
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB3	1	6.32
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB1	13	5.98
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB2	13	5.98
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB3	13	5.98
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB1	13	5.98
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB2	13	5.98
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB3	13	5.98
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	1	5.93

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	1	5.93
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	1	5.93
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	1	5.93
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	1	5.93
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	1	5.93
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	1	5.93
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	1	5.93
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	1	5.93
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	1	5.93
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	1	5.93
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	1	5.93
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	1	5.93
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	1	5.93
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	1	5.93
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	1	5.93
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	1	5.93
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	1	5.93
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB1	6	5.59
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB2	6	5.59
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB3	6	5.59
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB1	6	5.59
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB2	6	5.59
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB3	6	5.59
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB1	9	5.52
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB2	9	5.52
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB3	9	5.52
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB1	9	5.52
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB2	9	5.52
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB3	9	5.52
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB1	4	5.46
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB2	4	5.46
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB3	4	5.46
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB1	4	5.46
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB2	4	5.46
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB3	4	5.46
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	12	5.21
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	12	5.21
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	12	5.21
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	12	5.21
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	12	5.21
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	12	5.21
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	12	5.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	12	5.21
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	12	5.21
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	12	5.21
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	12	5.21
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	12	5.21
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	12	5.21
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	12	5.21
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	12	5.21
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	12	5.21
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	12	5.21
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	12	5.21
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	9	5.03
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	9	5.03
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	9	5.03
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	9	5.03
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	9	5.03
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	9	5.03
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	9	5.03
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	9	5.03
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	9	5.03
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	9	5.03
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	9	5.03
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	9	5.03
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	9	5.03
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	9	5.03
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	9	5.03
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	9	5.03
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	9	5.03
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	9	5.03
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	6	4.94
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	6	4.94
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	6	4.94
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	6	4.94
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	6	4.94
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	6	4.94
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	6	4.94
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	6	4.94
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	6	4.94
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	6	4.94
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	6	4.94
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	6	4.94
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	6	4.94

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	6	4.94
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	6	4.94
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	6	4.94
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	6	4.94
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	6	4.94
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	12	4.88
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	12	4.88
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	12	4.88
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	12	4.88
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	12	4.88
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	12	4.88
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	12	4.88
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	12	4.88
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	12	4.88
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	12	4.88
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	12	4.88
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	12	4.88
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB1	5	4.7
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB2	5	4.7
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB3	5	4.7
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB1	5	4.7
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB2	5	4.7
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB3	5	4.7
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	3	4.55
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	3	4.55
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	3	4.55
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	3	4.55
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	3	4.55
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	3	4.55
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	3	4.55
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	3	4.55
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	3	4.55
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	3	4.55
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	3	4.55
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	3	4.55
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	3	4.55
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	3	4.55
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	3	4.55
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	3	4.55
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	3	4.55
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	3	4.55
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	4	4.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	4	4.54
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	4	4.54
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	4	4.54
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	4	4.54
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	4	4.54
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	4	4.54
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	4	4.54
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	4	4.54
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	4	4.54
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	4	4.54
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	4	4.54
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	4	4.54
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	4	4.54
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	4	4.54
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	4	4.54
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	4	4.54
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	4	4.54
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB1	15	4.53
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB2	15	4.53
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB3	15	4.53
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB1	15	4.53
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB2	15	4.53
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB3	15	4.53
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB1	3	4.46
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB2	3	4.46
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB3	3	4.46
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB1	3	4.46
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB2	3	4.46
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB3	3	4.46
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	10	4.37
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	10	4.37
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	10	4.37
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	10	4.37
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	10	4.37
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	10	4.37
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	10	4.37
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	10	4.37
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	10	4.37
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	10	4.37
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	10	4.37
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	10	4.37
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	10	4.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	10	4.37
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	10	4.37
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	10	4.37
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	10	4.37
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	10	4.37
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	15	4.33
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	15	4.33
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	15	4.33
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	15	4.33
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	15	4.33
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	15	4.33
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	15	4.33
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	15	4.33
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	15	4.33
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	15	4.33
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	15	4.33
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	15	4.33
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	15	4.33
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	15	4.33
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	15	4.33
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	15	4.33
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	15	4.33
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	15	4.33
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB1	14	4.33
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB2	14	4.33
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB3	14	4.33
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB1	14	4.33
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB2	14	4.33
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB3	14	4.33
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	5	4.25
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	5	4.25
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	5	4.25
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	5	4.25
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	5	4.25
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	5	4.25
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	5	4.25
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	5	4.25
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	5	4.25
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	5	4.25
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	5	4.25
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	5	4.25
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	5	4.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	5	4.25
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	5	4.25
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	5	4.25
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	5	4.25
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	5	4.25
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB1	8	4.17
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB2	8	4.17
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB3	8	4.17
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB1	8	4.17
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB2	8	4.17
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB3	8	4.17
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	10	4.06
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	10	4.06
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	10	4.06
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	10	4.06
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	10	4.06
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	10	4.06
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	10	4.06
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	10	4.06
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	10	4.06
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	10	4.06
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	10	4.06
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	10	4.06
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	14	4.03
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	14	4.03
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	14	4.03
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	14	4.03
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	14	4.03
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	14	4.03
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	14	4.03
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	14	4.03
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	14	4.03
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	14	4.03
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	14	4.03
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	14	4.03
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	14	4.03
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	14	4.03
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	14	4.03
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	14	4.03
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	14	4.03
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	14	4.03
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	8	4.02

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	8	4.02
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	8	4.02
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	8	4.02
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	8	4.02
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	8	4.02
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	8	4.02
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	8	4.02
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	8	4.02
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	8	4.02
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	8	4.02
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	8	4.02
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	8	4.02
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	8	4.02
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	8	4.02
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	8	4.02
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	8	4.02
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	8	4.02
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB1	11	3.99
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB2	11	3.99
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB3	11	3.99
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB1	11	3.99
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB2	11	3.99
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB3	11	3.99
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	13	3.97
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	13	3.97
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	13	3.97
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	13	3.97
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	13	3.97
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	13	3.97
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	13	3.97
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	13	3.97
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	13	3.97
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	13	3.97
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	13	3.97
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	13	3.97
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	13	3.97
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	13	3.97
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	13	3.97
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	13	3.97
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	13	3.97
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	13	3.97
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	13	3.88

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	13	3.88
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	13	3.88
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	13	3.88
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	13	3.88
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	13	3.88
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	13	3.88
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	13	3.88
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	13	3.88
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	13	3.88
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	13	3.88
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	13	3.88
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	1	3.82
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	1	3.82
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	1	3.82
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	1	3.82
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	1	3.82
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	1	3.82
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	1	3.82
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	1	3.82
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	1	3.82
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	1	3.82
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	1	3.82
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	1	3.82
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	7	3.79
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	7	3.79
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	7	3.79
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	7	3.79
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	7	3.79
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	7	3.79
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	7	3.79
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	7	3.79
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	7	3.79
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	7	3.79
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	7	3.79
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	7	3.79
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	7	3.79
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	7	3.79
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	7	3.79
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	7	3.79
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	7	3.79
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	7	3.79
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB1	2	3.77

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB2	2	3.77
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB3	2	3.77
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB1	2	3.77
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB2	2	3.77
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB3	2	3.77
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB1	7	3.76
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB2	7	3.76
(1,16)	1:67:A:GLY:H	1:112:A:ALA:HB3	7	3.76
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB1	7	3.76
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB2	7	3.76
(1,15)	1:67:A:GLY:H	1:112:A:ALA:HB3	7	3.76
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	11	3.74
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	11	3.74
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	11	3.74
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	11	3.74
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	11	3.74
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	11	3.74
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	11	3.74
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	11	3.74
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	11	3.74
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	11	3.74
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	11	3.74
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	11	3.74
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	11	3.74
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	11	3.74
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	11	3.74
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	11	3.74
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	11	3.74
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	11	3.74
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	12	3.67
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	12	3.67
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	12	3.67
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	12	3.67
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	12	3.67
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	12	3.67
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	12	3.67
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	12	3.67
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	12	3.67
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	12	3.67
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	12	3.67
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	12	3.67
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	12	3.67

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	12	3.67
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	12	3.67
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	12	3.67
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	12	3.67
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	12	3.67
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	2	3.35
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	2	3.35
(1,50)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	2	3.35
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	2	3.35
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	2	3.35
(1,50)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	2	3.35
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	2	3.35
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	2	3.35
(1,50)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	2	3.35
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD21	2	3.35
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD22	2	3.35
(1,49)	1:112:A:ALA:HB1	1:63:A:LEU:HD23	2	3.35
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD21	2	3.35
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD22	2	3.35
(1,49)	1:112:A:ALA:HB2	1:63:A:LEU:HD23	2	3.35
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD21	2	3.35
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD22	2	3.35
(1,49)	1:112:A:ALA:HB3	1:63:A:LEU:HD23	2	3.35
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	10	3.1
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	10	3.1
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	10	3.1
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	10	3.1
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	10	3.1
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	10	3.1
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	10	3.1
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	10	3.1
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	10	3.1
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	10	3.1
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	10	3.1
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	10	3.1
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	10	3.1
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	10	3.1
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	10	3.1
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	10	3.1
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	10	3.1
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	10	3.1
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	1	3.0

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	1	3.0
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	1	3.0
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	1	3.0
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	1	3.0
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	1	3.0
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	1	3.0
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	1	3.0
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	1	3.0
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	1	3.0
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	1	3.0
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	1	3.0
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	1	3.0
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	1	3.0
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	1	3.0
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	1	3.0
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	1	3.0
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	1	3.0
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	6	2.96
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	6	2.96
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	6	2.96
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	6	2.96
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	6	2.96
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	6	2.96
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	6	2.96
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	6	2.96
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	6	2.96
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	6	2.96
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	6	2.96
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	6	2.96
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	4	2.95
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	4	2.95
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	4	2.95
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	4	2.95
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	4	2.95
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	4	2.95
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	4	2.95
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	4	2.95
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	4	2.95
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	4	2.95
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	4	2.95
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	4	2.95
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	4	2.95

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	4	2.95
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	4	2.95
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	4	2.95
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	4	2.95
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	4	2.95
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	4	2.91
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	4	2.91
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	4	2.91
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	4	2.91
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	4	2.91
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	4	2.91
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	9	2.91
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	9	2.91
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	9	2.91
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	9	2.91
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	9	2.91
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	9	2.91
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	4	2.91
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	4	2.91
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	4	2.91
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	4	2.91
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	4	2.91
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	4	2.91
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	9	2.91
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	9	2.91
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	9	2.91
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	9	2.91
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	9	2.91
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	9	2.91
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	6	2.86
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	6	2.86
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	6	2.86
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	6	2.86
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	6	2.86
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	6	2.86
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	6	2.86
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	6	2.86
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	6	2.86
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	6	2.86
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	6	2.86
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	6	2.86
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	6	2.86

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	6	2.86
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	6	2.86
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	6	2.86
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	6	2.86
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	6	2.86
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	9	2.73
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	9	2.73
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	9	2.73
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	9	2.73
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	9	2.73
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	9	2.73
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	9	2.73
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	9	2.73
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	9	2.73
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	9	2.73
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	9	2.73
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	9	2.73
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	9	2.73
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	9	2.73
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	9	2.73
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	9	2.73
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	9	2.73
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	9	2.73
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	13	2.69
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	13	2.69
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	13	2.69
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	13	2.69
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	13	2.69
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	13	2.69
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	13	2.69
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	13	2.69
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	13	2.69
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	13	2.69
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	13	2.69
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	13	2.69
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	13	2.69
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	13	2.69
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	13	2.69
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	13	2.69
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	13	2.69
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	13	2.69
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	15	2.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	15	2.6
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	15	2.6
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	15	2.6
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	15	2.6
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	15	2.6
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	15	2.6
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	15	2.6
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	15	2.6
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	15	2.6
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	15	2.6
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	15	2.6
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	15	2.6
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	15	2.6
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	15	2.6
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	15	2.6
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	15	2.6
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	15	2.6
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	3	2.5
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	3	2.5
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	3	2.5
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	3	2.5
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	3	2.5
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	3	2.5
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	3	2.5
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	3	2.5
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	3	2.5
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	3	2.5
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	3	2.5
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	3	2.5
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	3	2.5
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	3	2.5
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	3	2.5
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	3	2.5
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	3	2.5
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	3	2.5
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	5	2.44
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	5	2.44
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	5	2.44
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	5	2.44
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	5	2.44
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	5	2.44
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	5	2.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	5	2.44
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	5	2.44
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	5	2.44
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	5	2.44
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	5	2.44
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	5	2.44
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	5	2.44
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	5	2.44
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	5	2.44
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	5	2.44
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	5	2.44
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	14	2.27
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	14	2.27
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	14	2.27
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	14	2.27
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	14	2.27
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	14	2.27
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	14	2.27
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	14	2.27
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	14	2.27
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	14	2.27
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	14	2.27
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	14	2.27
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	14	2.27
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	14	2.27
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	14	2.27
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	14	2.27
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	14	2.27
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	14	2.27
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	4	2.23
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	4	2.23
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	4	2.23
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	4	2.23
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	4	2.23
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	4	2.23
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	4	2.23
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	4	2.23
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	4	2.23
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	4	2.23
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	4	2.23
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	4	2.23
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG21	4	2.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG22	4	2.22
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG23	4	2.22
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG21	4	2.22
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG22	4	2.22
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG23	4	2.22
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	13	2.17
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	13	2.17
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	13	2.17
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	13	2.17
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	13	2.17
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	13	2.17
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	13	2.17
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	13	2.17
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	13	2.17
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	13	2.17
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	13	2.17
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	13	2.17
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	5	2.13
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	5	2.13
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	5	2.13
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	5	2.13
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	5	2.13
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	5	2.13
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	5	2.13
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	5	2.13
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	5	2.13
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	5	2.13
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	5	2.13
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	5	2.13
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	8	1.97
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	8	1.97
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	8	1.97
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	8	1.97
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	8	1.97
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	8	1.97
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	8	1.97
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	8	1.97
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	8	1.97
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	8	1.97
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	8	1.97
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	8	1.97
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	8	1.97

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	8	1.97
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	8	1.97
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	8	1.97
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	8	1.97
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	8	1.97
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG21	13	1.95
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG22	13	1.95
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG23	13	1.95
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG21	13	1.95
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG22	13	1.95
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG23	13	1.95
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	15	1.94
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	15	1.94
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	15	1.94
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	15	1.94
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	15	1.94
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	15	1.94
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	15	1.94
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	15	1.94
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	15	1.94
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	15	1.94
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	15	1.94
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	15	1.94
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG21	10	1.87
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG22	10	1.87
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG23	10	1.87
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG21	10	1.87
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG22	10	1.87
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG23	10	1.87
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	3	1.83
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	3	1.83
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	3	1.83
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	3	1.83
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	3	1.83
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	3	1.83
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	3	1.83
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	3	1.83
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	3	1.83
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	3	1.83
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	3	1.83
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	3	1.83
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG21	3	1.82

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG22	3	1.82
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG23	3	1.82
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG21	3	1.82
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG22	3	1.82
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG23	3	1.82
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	14	1.82
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	14	1.82
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	14	1.82
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	14	1.82
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	14	1.82
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	14	1.82
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	14	1.82
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	14	1.82
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	14	1.82
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	14	1.82
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	14	1.82
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	14	1.82
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	11	1.82
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	11	1.82
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	11	1.82
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	11	1.82
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	11	1.82
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	11	1.82
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	11	1.82
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	11	1.82
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	11	1.82
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	11	1.82
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	11	1.82
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	11	1.82
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	11	1.82
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	11	1.82
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	11	1.82
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	11	1.82
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	11	1.82
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	11	1.82
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG21	8	1.81
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG22	8	1.81
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG23	8	1.81
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG21	8	1.81
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG22	8	1.81
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG23	8	1.81
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	3	1.81

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	3	1.81
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	3	1.81
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	3	1.81
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	3	1.81
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	3	1.81
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	3	1.81
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	3	1.81
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	3	1.81
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	3	1.81
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	3	1.81
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	3	1.81
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG21	9	1.79
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG22	9	1.79
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG23	9	1.79
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG21	9	1.79
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG22	9	1.79
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG23	9	1.79
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	12	1.77
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	12	1.77
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	12	1.77
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	12	1.77
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	12	1.77
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	12	1.77
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	12	1.77
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	12	1.77
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	12	1.77
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	12	1.77
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	12	1.77
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	12	1.77
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG21	7	1.73
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG22	7	1.73
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG23	7	1.73
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG21	7	1.73
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG22	7	1.73
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG23	7	1.73
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG21	5	1.72
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG22	5	1.72
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG23	5	1.72
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG21	5	1.72
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG22	5	1.72
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG23	5	1.72
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG21	14	1.71

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG22	14	1.71
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG23	14	1.71
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG21	14	1.71
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG22	14	1.71
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG23	14	1.71
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	10	1.71
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	10	1.71
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	10	1.71
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	10	1.71
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	10	1.71
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	10	1.71
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	10	1.71
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	10	1.71
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	10	1.71
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	10	1.71
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	10	1.71
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	10	1.71
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	8	1.69
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	8	1.69
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	8	1.69
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	8	1.69
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	8	1.69
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	8	1.69
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	8	1.69
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	8	1.69
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	8	1.69
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	8	1.69
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	8	1.69
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	8	1.69
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	2	1.69
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	2	1.69
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	2	1.69
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	2	1.69
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	2	1.69
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	2	1.69
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	2	1.69
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	2	1.69
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	2	1.69
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	2	1.69
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	2	1.69
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	2	1.69
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	2	1.69

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	2	1.69
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	2	1.69
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	2	1.69
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	2	1.69
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	2	1.69
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG21	2	1.67
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG22	2	1.67
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG23	2	1.67
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG21	2	1.67
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG22	2	1.67
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG23	2	1.67
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	8	1.64
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	8	1.64
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	8	1.64
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	8	1.64
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	8	1.64
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	8	1.64
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	8	1.64
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	8	1.64
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	8	1.64
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	8	1.64
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	8	1.64
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	8	1.64
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	11	1.61
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	11	1.61
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	11	1.61
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	11	1.61
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	11	1.61
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	11	1.61
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	11	1.61
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	11	1.61
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	11	1.61
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	11	1.61
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	11	1.61
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	11	1.61
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG21	1	1.6
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG22	1	1.6
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG23	1	1.6
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG21	1	1.6
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG22	1	1.6
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG23	1	1.6
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG21	15	1.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG22	15	1.59
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG23	15	1.59
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG21	15	1.59
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG22	15	1.59
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG23	15	1.59
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG21	12	1.55
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG22	12	1.55
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG23	12	1.55
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG21	12	1.55
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG22	12	1.55
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG23	12	1.55
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	7	1.54
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	7	1.54
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	7	1.54
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	7	1.54
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	7	1.54
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	7	1.54
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	7	1.54
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	7	1.54
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	7	1.54
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	7	1.54
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	7	1.54
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	7	1.54
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	9	1.5
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	9	1.5
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	9	1.5
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	9	1.5
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	9	1.5
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	9	1.5
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	9	1.5
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	9	1.5
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	9	1.5
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	9	1.5
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	9	1.5
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	9	1.5
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	15	1.48
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	15	1.48
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	15	1.48
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	15	1.48
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	15	1.48
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	15	1.48
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	15	1.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	15	1.48
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	15	1.48
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	15	1.48
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	15	1.48
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	15	1.48
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG21	11	1.46
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG22	11	1.46
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG23	11	1.46
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG21	11	1.46
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG22	11	1.46
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG23	11	1.46
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	14	1.43
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	14	1.43
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	14	1.43
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	14	1.43
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	14	1.43
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	14	1.43
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	14	1.43
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	14	1.43
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	14	1.43
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	14	1.43
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	14	1.43
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	14	1.43
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	7	1.39
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	7	1.39
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	7	1.39
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	7	1.39
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	7	1.39
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	7	1.39
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	7	1.39
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	7	1.39
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	7	1.39
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	7	1.39
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	7	1.39
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	7	1.39
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	2	1.38
(1,52)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	2	1.38
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	2	1.38
(1,52)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	2	1.38
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	2	1.38
(1,52)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	2	1.38
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA2	2	1.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:112:A:ALA:HB1	1:67:A:GLY:HA3	2	1.38
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA2	2	1.38
(1,51)	1:112:A:ALA:HB2	1:67:A:GLY:HA3	2	1.38
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA2	2	1.38
(1,51)	1:112:A:ALA:HB3	1:67:A:GLY:HA3	2	1.38
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	7	1.38
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	7	1.38
(1,10)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	7	1.38
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	7	1.38
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	7	1.38
(1,10)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	7	1.38
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	7	1.38
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	7	1.38
(1,10)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	7	1.38
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB1	7	1.38
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB2	7	1.38
(1,9)	1:66:A:ILE:HG21	1:112:A:ALA:HB3	7	1.38
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB1	7	1.38
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB2	7	1.38
(1,9)	1:66:A:ILE:HG22	1:112:A:ALA:HB3	7	1.38
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB1	7	1.38
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB2	7	1.38
(1,9)	1:66:A:ILE:HG23	1:112:A:ALA:HB3	7	1.38
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG21	6	1.37
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG22	6	1.37
(1,56)	1:115:A:TYR:H	1:111:A:VAL:HG23	6	1.37
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG21	6	1.37
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG22	6	1.37
(1,55)	1:115:A:TYR:H	1:111:A:VAL:HG23	6	1.37
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	5	1.35
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	5	1.35
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	5	1.35
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	5	1.35
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	5	1.35
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	5	1.35
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	5	1.35
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	5	1.35
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	5	1.35
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	5	1.35
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	5	1.35
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	5	1.35
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	2	1.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	2	1.27
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	2	1.27
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	2	1.27
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	2	1.27
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	2	1.27
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	2	1.27
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	2	1.27
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	2	1.27
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	2	1.27
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	2	1.27
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	2	1.27
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	1	1.26
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	1	1.26
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	1	1.26
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	1	1.26
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	1	1.26
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	1	1.26
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	1	1.26
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	1	1.26
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	1	1.26
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	1	1.26
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	1	1.26
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	1	1.26
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	11	1.23
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	11	1.23
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	11	1.23
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	11	1.23
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	11	1.23
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	11	1.23
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	11	1.23
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	11	1.23
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	11	1.23
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	11	1.23
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	11	1.23
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	11	1.23
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	6	1.11
(1,46)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	6	1.11
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	6	1.11
(1,46)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	6	1.11
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	6	1.11
(1,46)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	6	1.11
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB2	6	1.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:111:A:VAL:HG21	1:115:A:TYR:HB3	6	1.11
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB2	6	1.11
(1,45)	1:111:A:VAL:HG22	1:115:A:TYR:HB3	6	1.11
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB2	6	1.11
(1,45)	1:111:A:VAL:HG23	1:115:A:TYR:HB3	6	1.11
(3,686)	1:126:A:SER:H	1:125:A:LEU:HG	3	0.94
(3,685)	1:126:A:SER:H	1:125:A:LEU:HG	3	0.94
(2,686)	1:126:A:SER:H	1:125:A:LEU:HG	3	0.94
(2,685)	1:126:A:SER:H	1:125:A:LEU:HG	3	0.94
(3,614)	1:121:A:VAL:H	1:120:A:LEU:HG	13	0.79
(3,613)	1:121:A:VAL:H	1:120:A:LEU:HG	13	0.79
(2,614)	1:121:A:VAL:H	1:120:A:LEU:HG	13	0.79
(2,613)	1:121:A:VAL:H	1:120:A:LEU:HG	13	0.79
(3,280)	1:85:A:THR:H	1:85:A:THR:HG21	15	0.78
(3,280)	1:85:A:THR:H	1:85:A:THR:HG22	15	0.78
(3,280)	1:85:A:THR:H	1:85:A:THR:HG23	15	0.78
(3,279)	1:85:A:THR:H	1:85:A:THR:HG21	15	0.78
(3,279)	1:85:A:THR:H	1:85:A:THR:HG22	15	0.78
(3,279)	1:85:A:THR:H	1:85:A:THR:HG23	15	0.78
(2,280)	1:85:A:THR:H	1:85:A:THR:HG21	15	0.78
(2,280)	1:85:A:THR:H	1:85:A:THR:HG22	15	0.78
(2,280)	1:85:A:THR:H	1:85:A:THR:HG23	15	0.78
(2,279)	1:85:A:THR:H	1:85:A:THR:HG21	15	0.78
(2,279)	1:85:A:THR:H	1:85:A:THR:HG22	15	0.78
(2,279)	1:85:A:THR:H	1:85:A:THR:HG23	15	0.78
(3,492)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	13	0.64
(3,491)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	13	0.64
(2,492)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	13	0.64
(2,491)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	13	0.64
(3,492)	1:110:A:VAL:HG12	1:107:A:TRP:HZ3	6	0.63
(3,491)	1:110:A:VAL:HG12	1:107:A:TRP:HZ3	6	0.63
(2,492)	1:110:A:VAL:HG12	1:107:A:TRP:HZ3	6	0.63
(2,491)	1:110:A:VAL:HG12	1:107:A:TRP:HZ3	6	0.63
(3,572)	1:118:A:SER:H	1:113:A:LEU:HA	9	0.54
(3,571)	1:118:A:SER:H	1:113:A:LEU:HA	9	0.54
(2,572)	1:118:A:SER:H	1:113:A:LEU:HA	9	0.54
(2,571)	1:118:A:SER:H	1:113:A:LEU:HA	9	0.54
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG21	2	0.51
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG22	2	0.51
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG23	2	0.51
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG21	2	0.51
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG22	2	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG23	2	0.51
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG21	5	0.5
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG22	5	0.5
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG23	5	0.5
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG21	9	0.5
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG22	9	0.5
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG23	9	0.5
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG21	5	0.5
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG22	5	0.5
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG23	5	0.5
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG21	9	0.5
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG22	9	0.5
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG23	9	0.5
(3,572)	1:118:A:SER:H	1:113:A:LEU:HA	13	0.48
(3,571)	1:118:A:SER:H	1:113:A:LEU:HA	13	0.48
(2,572)	1:118:A:SER:H	1:113:A:LEU:HA	13	0.48
(2,571)	1:118:A:SER:H	1:113:A:LEU:HA	13	0.48
(3,572)	1:118:A:SER:H	1:113:A:LEU:HA	8	0.44
(3,571)	1:118:A:SER:H	1:113:A:LEU:HA	8	0.44
(3,492)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	5	0.44
(3,491)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	5	0.44
(2,572)	1:118:A:SER:H	1:113:A:LEU:HA	8	0.44
(2,571)	1:118:A:SER:H	1:113:A:LEU:HA	8	0.44
(2,492)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	5	0.44
(2,491)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	5	0.44
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG21	14	0.44
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG22	14	0.44
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG23	14	0.44
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG21	14	0.44
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG22	14	0.44
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG23	14	0.44
(3,492)	1:110:A:VAL:HG12	1:107:A:TRP:HZ3	10	0.43
(3,491)	1:110:A:VAL:HG12	1:107:A:TRP:HZ3	10	0.43
(2,492)	1:110:A:VAL:HG12	1:107:A:TRP:HZ3	10	0.43
(2,491)	1:110:A:VAL:HG12	1:107:A:TRP:HZ3	10	0.43
(3,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	6	0.41
(3,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	6	0.41
(3,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	6	0.41
(3,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	6	0.41
(3,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	6	0.41
(3,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	6	0.41
(3,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	6	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	6	0.41
(3,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	6	0.41
(3,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	6	0.41
(3,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	6	0.41
(3,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	6	0.41
(2,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	6	0.41
(2,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	6	0.41
(2,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	6	0.41
(2,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	6	0.41
(2,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	6	0.41
(2,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	6	0.41
(2,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	6	0.41
(2,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	6	0.41
(2,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	6	0.41
(2,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	6	0.41
(2,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	6	0.41
(2,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	6	0.41
(3,694)	1:127:A:THR:H	1:128:A:LYS:H	5	0.4
(3,693)	1:127:A:THR:H	1:128:A:LYS:H	5	0.4
(3,572)	1:118:A:SER:H	1:113:A:LEU:HA	10	0.4
(3,571)	1:118:A:SER:H	1:113:A:LEU:HA	10	0.4
(3,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	10	0.4
(3,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	10	0.4
(3,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	10	0.4
(3,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	10	0.4
(3,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	10	0.4
(3,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	10	0.4
(3,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	10	0.4
(3,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	10	0.4
(3,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	10	0.4
(3,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	10	0.4
(3,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	10	0.4
(3,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	10	0.4
(3,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	5	0.4
(3,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	5	0.4
(3,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	5	0.4
(3,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	6	0.4
(3,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	6	0.4
(3,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	6	0.4
(3,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	5	0.4
(3,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	5	0.4
(3,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	5	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	6	0.4
(3,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	6	0.4
(3,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	6	0.4
(2,694)	1:127:A:THR:H	1:128:A:LYS:H	5	0.4
(2,693)	1:127:A:THR:H	1:128:A:LYS:H	5	0.4
(2,572)	1:118:A:SER:H	1:113:A:LEU:HA	10	0.4
(2,571)	1:118:A:SER:H	1:113:A:LEU:HA	10	0.4
(2,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	10	0.4
(2,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	10	0.4
(2,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	10	0.4
(2,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	10	0.4
(2,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	10	0.4
(2,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	10	0.4
(2,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	10	0.4
(2,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	10	0.4
(2,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	10	0.4
(2,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	10	0.4
(2,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	10	0.4
(2,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	10	0.4
(2,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	5	0.4
(2,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	5	0.4
(2,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	5	0.4
(2,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	6	0.4
(2,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	6	0.4
(2,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	6	0.4
(2,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	5	0.4
(2,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	5	0.4
(2,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	5	0.4
(2,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	6	0.4
(2,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	6	0.4
(2,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	6	0.4
(3,572)	1:118:A:SER:H	1:113:A:LEU:HA	2	0.39
(3,571)	1:118:A:SER:H	1:113:A:LEU:HA	2	0.39
(3,492)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	11	0.39
(3,491)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	11	0.39
(2,572)	1:118:A:SER:H	1:113:A:LEU:HA	2	0.39
(2,571)	1:118:A:SER:H	1:113:A:LEU:HA	2	0.39
(2,492)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	11	0.39
(2,491)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	11	0.39
(3,572)	1:118:A:SER:H	1:113:A:LEU:HA	5	0.38
(3,571)	1:118:A:SER:H	1:113:A:LEU:HA	5	0.38
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	14	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	14	0.38
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	14	0.38
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	14	0.38
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	14	0.38
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	14	0.38
(3,174)	1:71:A:ASP:H	1:70:A:LEU:HG	14	0.38
(3,173)	1:71:A:ASP:H	1:70:A:LEU:HG	14	0.38
(2,572)	1:118:A:SER:H	1:113:A:LEU:HA	5	0.38
(2,571)	1:118:A:SER:H	1:113:A:LEU:HA	5	0.38
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	14	0.38
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	14	0.38
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	14	0.38
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	14	0.38
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	14	0.38
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	14	0.38
(2,174)	1:71:A:ASP:H	1:70:A:LEU:HG	14	0.38
(2,173)	1:71:A:ASP:H	1:70:A:LEU:HG	14	0.38
(3,694)	1:127:A:THR:H	1:128:A:LYS:H	4	0.37
(3,693)	1:127:A:THR:H	1:128:A:LYS:H	4	0.37
(3,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	7	0.37
(3,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	7	0.37
(3,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	7	0.37
(3,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	7	0.37
(3,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	7	0.37
(3,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	7	0.37
(3,272)	1:84:A:ASP:H	1:85:A:THR:HA	8	0.37
(3,271)	1:84:A:ASP:H	1:85:A:THR:HA	8	0.37
(3,174)	1:71:A:ASP:H	1:70:A:LEU:HG	1	0.37
(3,174)	1:71:A:ASP:H	1:70:A:LEU:HG	2	0.37
(3,174)	1:71:A:ASP:H	1:70:A:LEU:HG	6	0.37
(3,173)	1:71:A:ASP:H	1:70:A:LEU:HG	1	0.37
(3,173)	1:71:A:ASP:H	1:70:A:LEU:HG	2	0.37
(3,173)	1:71:A:ASP:H	1:70:A:LEU:HG	6	0.37
(2,694)	1:127:A:THR:H	1:128:A:LYS:H	4	0.37
(2,693)	1:127:A:THR:H	1:128:A:LYS:H	4	0.37
(2,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	7	0.37
(2,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	7	0.37
(2,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	7	0.37
(2,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	7	0.37
(2,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	7	0.37
(2,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	7	0.37
(2,272)	1:84:A:ASP:H	1:85:A:THR:HA	8	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,271)	1:84:A:ASP:H	1:85:A:THR:HA	8	0.37
(2,174)	1:71:A:ASP:H	1:70:A:LEU:HG	1	0.37
(2,174)	1:71:A:ASP:H	1:70:A:LEU:HG	2	0.37
(2,174)	1:71:A:ASP:H	1:70:A:LEU:HG	6	0.37
(2,173)	1:71:A:ASP:H	1:70:A:LEU:HG	1	0.37
(2,173)	1:71:A:ASP:H	1:70:A:LEU:HG	2	0.37
(2,173)	1:71:A:ASP:H	1:70:A:LEU:HG	6	0.37
(3,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	8	0.36
(3,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	8	0.36
(3,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	8	0.36
(3,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	11	0.36
(3,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	11	0.36
(3,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	11	0.36
(3,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	8	0.36
(3,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	8	0.36
(3,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	8	0.36
(3,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	11	0.36
(3,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	11	0.36
(3,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	11	0.36
(2,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	8	0.36
(2,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	8	0.36
(2,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	8	0.36
(2,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	11	0.36
(2,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	11	0.36
(2,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	11	0.36
(2,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	8	0.36
(2,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	8	0.36
(2,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	8	0.36
(2,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	11	0.36
(2,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	11	0.36
(2,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	11	0.36
(3,572)	1:118:A:SER:H	1:113:A:LEU:HA	3	0.35
(3,572)	1:118:A:SER:H	1:113:A:LEU:HA	7	0.35
(3,572)	1:118:A:SER:H	1:113:A:LEU:HA	14	0.35
(3,571)	1:118:A:SER:H	1:113:A:LEU:HA	3	0.35
(3,571)	1:118:A:SER:H	1:113:A:LEU:HA	7	0.35
(3,571)	1:118:A:SER:H	1:113:A:LEU:HA	14	0.35
(3,492)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	1	0.35
(3,491)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	1	0.35
(3,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	3	0.35
(3,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	3	0.35
(3,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	3	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	14	0.35
(3,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	14	0.35
(3,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	14	0.35
(3,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	3	0.35
(3,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	3	0.35
(3,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	3	0.35
(3,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	14	0.35
(3,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	14	0.35
(3,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	14	0.35
(3,246)	1:83:A:VAL:H	1:82:A:ALA:HA	8	0.35
(3,245)	1:83:A:VAL:H	1:82:A:ALA:HA	8	0.35
(2,572)	1:118:A:SER:H	1:113:A:LEU:HA	3	0.35
(2,572)	1:118:A:SER:H	1:113:A:LEU:HA	7	0.35
(2,572)	1:118:A:SER:H	1:113:A:LEU:HA	14	0.35
(2,571)	1:118:A:SER:H	1:113:A:LEU:HA	3	0.35
(2,571)	1:118:A:SER:H	1:113:A:LEU:HA	7	0.35
(2,571)	1:118:A:SER:H	1:113:A:LEU:HA	14	0.35
(2,492)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	1	0.35
(2,491)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	1	0.35
(2,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	3	0.35
(2,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	3	0.35
(2,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	3	0.35
(2,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	14	0.35
(2,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	14	0.35
(2,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	14	0.35
(2,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	3	0.35
(2,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	3	0.35
(2,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	3	0.35
(2,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	14	0.35
(2,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	14	0.35
(2,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	14	0.35
(2,246)	1:83:A:VAL:H	1:82:A:ALA:HA	8	0.35
(2,245)	1:83:A:VAL:H	1:82:A:ALA:HA	8	0.35
(3,572)	1:118:A:SER:H	1:113:A:LEU:HA	4	0.34
(3,572)	1:118:A:SER:H	1:113:A:LEU:HA	6	0.34
(3,572)	1:118:A:SER:H	1:113:A:LEU:HA	11	0.34
(3,571)	1:118:A:SER:H	1:113:A:LEU:HA	4	0.34
(3,571)	1:118:A:SER:H	1:113:A:LEU:HA	6	0.34
(3,571)	1:118:A:SER:H	1:113:A:LEU:HA	11	0.34
(3,492)	1:110:A:VAL:HG12	1:107:A:TRP:HZ3	12	0.34
(3,491)	1:110:A:VAL:HG12	1:107:A:TRP:HZ3	12	0.34
(3,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	12	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	12	0.34
(3,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	12	0.34
(3,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	12	0.34
(3,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	12	0.34
(3,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	12	0.34
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	1	0.34
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	1	0.34
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	1	0.34
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	1	0.34
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	1	0.34
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	1	0.34
(3,246)	1:83:A:VAL:H	1:82:A:ALA:HA	5	0.34
(3,245)	1:83:A:VAL:H	1:82:A:ALA:HA	5	0.34
(3,174)	1:71:A:ASP:H	1:70:A:LEU:HG	5	0.34
(3,173)	1:71:A:ASP:H	1:70:A:LEU:HG	5	0.34
(3,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	15	0.34
(3,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	15	0.34
(3,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	15	0.34
(3,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	15	0.34
(3,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	15	0.34
(3,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	15	0.34
(2,572)	1:118:A:SER:H	1:113:A:LEU:HA	4	0.34
(2,572)	1:118:A:SER:H	1:113:A:LEU:HA	6	0.34
(2,572)	1:118:A:SER:H	1:113:A:LEU:HA	11	0.34
(2,571)	1:118:A:SER:H	1:113:A:LEU:HA	4	0.34
(2,571)	1:118:A:SER:H	1:113:A:LEU:HA	6	0.34
(2,571)	1:118:A:SER:H	1:113:A:LEU:HA	11	0.34
(2,492)	1:110:A:VAL:HG12	1:107:A:TRP:HZ3	12	0.34
(2,491)	1:110:A:VAL:HG12	1:107:A:TRP:HZ3	12	0.34
(2,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	12	0.34
(2,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	12	0.34
(2,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	12	0.34
(2,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	12	0.34
(2,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	12	0.34
(2,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	12	0.34
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	1	0.34
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	1	0.34
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	1	0.34
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	1	0.34
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	1	0.34
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	1	0.34
(2,246)	1:83:A:VAL:H	1:82:A:ALA:HA	5	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,245)	1:83:A:VAL:H	1:82:A:ALA:HA	5	0.34
(2,174)	1:71:A:ASP:H	1:70:A:LEU:HG	5	0.34
(2,173)	1:71:A:ASP:H	1:70:A:LEU:HG	5	0.34
(2,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	15	0.34
(2,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	15	0.34
(2,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	15	0.34
(2,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	15	0.34
(2,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	15	0.34
(2,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	15	0.34
(3,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	13	0.33
(3,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	13	0.33
(3,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	13	0.33
(3,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	13	0.33
(3,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	13	0.33
(3,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	13	0.33
(3,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	13	0.33
(3,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	13	0.33
(3,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	13	0.33
(3,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	13	0.33
(3,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	13	0.33
(3,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	13	0.33
(3,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	4	0.33
(3,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	4	0.33
(3,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	4	0.33
(3,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	4	0.33
(3,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	4	0.33
(3,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	4	0.33
(3,302)	1:90:A:GLU:H	1:89:A:ARG:HD2	6	0.33
(3,302)	1:90:A:GLU:H	1:89:A:ARG:HD3	6	0.33
(3,301)	1:90:A:GLU:H	1:89:A:ARG:HD2	6	0.33
(3,301)	1:90:A:GLU:H	1:89:A:ARG:HD3	6	0.33
(3,246)	1:83:A:VAL:H	1:82:A:ALA:HA	4	0.33
(3,245)	1:83:A:VAL:H	1:82:A:ALA:HA	4	0.33
(3,174)	1:71:A:ASP:H	1:70:A:LEU:HG	3	0.33
(3,174)	1:71:A:ASP:H	1:70:A:LEU:HG	7	0.33
(3,173)	1:71:A:ASP:H	1:70:A:LEU:HG	3	0.33
(3,173)	1:71:A:ASP:H	1:70:A:LEU:HG	7	0.33
(2,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	13	0.33
(2,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	13	0.33
(2,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	13	0.33
(2,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	13	0.33
(2,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	13	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	13	0.33
(2,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	13	0.33
(2,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	13	0.33
(2,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	13	0.33
(2,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	13	0.33
(2,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	13	0.33
(2,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	13	0.33
(2,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	4	0.33
(2,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	4	0.33
(2,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	4	0.33
(2,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	4	0.33
(2,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	4	0.33
(2,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	4	0.33
(2,302)	1:90:A:GLU:H	1:89:A:ARG:HD2	6	0.33
(2,302)	1:90:A:GLU:H	1:89:A:ARG:HD3	6	0.33
(2,301)	1:90:A:GLU:H	1:89:A:ARG:HD2	6	0.33
(2,301)	1:90:A:GLU:H	1:89:A:ARG:HD3	6	0.33
(2,246)	1:83:A:VAL:H	1:82:A:ALA:HA	4	0.33
(2,245)	1:83:A:VAL:H	1:82:A:ALA:HA	4	0.33
(2,174)	1:71:A:ASP:H	1:70:A:LEU:HG	3	0.33
(2,174)	1:71:A:ASP:H	1:70:A:LEU:HG	7	0.33
(2,173)	1:71:A:ASP:H	1:70:A:LEU:HG	3	0.33
(2,173)	1:71:A:ASP:H	1:70:A:LEU:HG	7	0.33
(3,246)	1:83:A:VAL:H	1:82:A:ALA:HA	7	0.32
(3,245)	1:83:A:VAL:H	1:82:A:ALA:HA	7	0.32
(3,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	1	0.32
(3,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	1	0.32
(3,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	1	0.32
(3,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	1	0.32
(3,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	1	0.32
(3,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	1	0.32
(3,174)	1:71:A:ASP:H	1:70:A:LEU:HG	10	0.32
(3,173)	1:71:A:ASP:H	1:70:A:LEU:HG	10	0.32
(2,246)	1:83:A:VAL:H	1:82:A:ALA:HA	7	0.32
(2,245)	1:83:A:VAL:H	1:82:A:ALA:HA	7	0.32
(2,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	1	0.32
(2,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	1	0.32
(2,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	1	0.32
(2,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	1	0.32
(2,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	1	0.32
(2,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	1	0.32
(2,174)	1:71:A:ASP:H	1:70:A:LEU:HG	10	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,173)	1:71:A:ASP:H	1:70:A:LEU:HG	10	0.32
(3,694)	1:127:A:THR:H	1:128:A:LYS:H	15	0.31
(3,693)	1:127:A:THR:H	1:128:A:LYS:H	15	0.31
(3,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	9	0.31
(3,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	9	0.31
(3,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	9	0.31
(3,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	9	0.31
(3,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	9	0.31
(3,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	9	0.31
(3,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	9	0.31
(3,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	9	0.31
(3,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	9	0.31
(3,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	9	0.31
(3,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	9	0.31
(3,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	9	0.31
(3,480)	1:103:A:GLY:H	1:102:A:ASP:HB2	7	0.31
(3,480)	1:103:A:GLY:H	1:102:A:ASP:HB3	7	0.31
(3,479)	1:103:A:GLY:H	1:102:A:ASP:HB2	7	0.31
(3,479)	1:103:A:GLY:H	1:102:A:ASP:HB3	7	0.31
(3,384)	1:96:A:ALA:H	1:95:A:VAL:HG11	2	0.31
(3,384)	1:96:A:ALA:H	1:95:A:VAL:HG12	2	0.31
(3,384)	1:96:A:ALA:H	1:95:A:VAL:HG13	2	0.31
(3,383)	1:96:A:ALA:H	1:95:A:VAL:HG11	2	0.31
(3,383)	1:96:A:ALA:H	1:95:A:VAL:HG12	2	0.31
(3,383)	1:96:A:ALA:H	1:95:A:VAL:HG13	2	0.31
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	11	0.31
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	11	0.31
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	11	0.31
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	11	0.31
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	11	0.31
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	11	0.31
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	11	0.31
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	11	0.31
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	11	0.31
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	11	0.31
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	11	0.31
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	11	0.31
(3,274)	1:85:A:THR:H	1:84:A:ASP:HB2	15	0.31
(3,274)	1:85:A:THR:H	1:84:A:ASP:HB3	15	0.31
(3,273)	1:85:A:THR:H	1:84:A:ASP:HB2	15	0.31
(3,273)	1:85:A:THR:H	1:84:A:ASP:HB3	15	0.31
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	9	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	9	0.31
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	9	0.31
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	9	0.31
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	9	0.31
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	9	0.31
(3,246)	1:83:A:VAL:H	1:82:A:ALA:HA	3	0.31
(3,246)	1:83:A:VAL:H	1:82:A:ALA:HA	14	0.31
(3,245)	1:83:A:VAL:H	1:82:A:ALA:HA	3	0.31
(3,245)	1:83:A:VAL:H	1:82:A:ALA:HA	14	0.31
(3,209)	1:77:A:GLN:H	1:76:A:LEU:HG	2	0.31
(3,206)	1:77:A:GLN:H	1:76:A:LEU:HG	2	0.31
(3,174)	1:71:A:ASP:H	1:70:A:LEU:HG	13	0.31
(3,173)	1:71:A:ASP:H	1:70:A:LEU:HG	13	0.31
(2,694)	1:127:A:THR:H	1:128:A:LYS:H	15	0.31
(2,693)	1:127:A:THR:H	1:128:A:LYS:H	15	0.31
(2,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	9	0.31
(2,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	9	0.31
(2,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	9	0.31
(2,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	9	0.31
(2,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	9	0.31
(2,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	9	0.31
(2,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	9	0.31
(2,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	9	0.31
(2,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	9	0.31
(2,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	9	0.31
(2,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	9	0.31
(2,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	9	0.31
(2,480)	1:103:A:GLY:H	1:102:A:ASP:HB2	7	0.31
(2,480)	1:103:A:GLY:H	1:102:A:ASP:HB3	7	0.31
(2,479)	1:103:A:GLY:H	1:102:A:ASP:HB2	7	0.31
(2,479)	1:103:A:GLY:H	1:102:A:ASP:HB3	7	0.31
(2,384)	1:96:A:ALA:H	1:95:A:VAL:HG11	2	0.31
(2,384)	1:96:A:ALA:H	1:95:A:VAL:HG12	2	0.31
(2,384)	1:96:A:ALA:H	1:95:A:VAL:HG13	2	0.31
(2,383)	1:96:A:ALA:H	1:95:A:VAL:HG11	2	0.31
(2,383)	1:96:A:ALA:H	1:95:A:VAL:HG12	2	0.31
(2,383)	1:96:A:ALA:H	1:95:A:VAL:HG13	2	0.31
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	11	0.31
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	11	0.31
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	11	0.31
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	11	0.31
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	11	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	11	0.31
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	11	0.31
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	11	0.31
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	11	0.31
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	11	0.31
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	11	0.31
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	11	0.31
(2,274)	1:85:A:THR:H	1:84:A:ASP:HB2	15	0.31
(2,274)	1:85:A:THR:H	1:84:A:ASP:HB3	15	0.31
(2,273)	1:85:A:THR:H	1:84:A:ASP:HB2	15	0.31
(2,273)	1:85:A:THR:H	1:84:A:ASP:HB3	15	0.31
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	9	0.31
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	9	0.31
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	9	0.31
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	9	0.31
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	9	0.31
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	9	0.31
(2,246)	1:83:A:VAL:H	1:82:A:ALA:HA	3	0.31
(2,246)	1:83:A:VAL:H	1:82:A:ALA:HA	14	0.31
(2,245)	1:83:A:VAL:H	1:82:A:ALA:HA	3	0.31
(2,245)	1:83:A:VAL:H	1:82:A:ALA:HA	14	0.31
(2,209)	1:77:A:GLN:H	1:76:A:LEU:HG	2	0.31
(2,206)	1:77:A:GLN:H	1:76:A:LEU:HG	2	0.31
(2,174)	1:71:A:ASP:H	1:70:A:LEU:HG	13	0.31
(2,173)	1:71:A:ASP:H	1:70:A:LEU:HG	13	0.31
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG21	1	0.31
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG22	1	0.31
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG23	1	0.31
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG21	1	0.31
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG22	1	0.31
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG23	1	0.31
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	6	0.3
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	6	0.3
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	6	0.3
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	6	0.3
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	6	0.3
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	6	0.3
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	6	0.3
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	6	0.3
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	6	0.3
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	6	0.3
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	6	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	6	0.3
(3,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	2	0.3
(3,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	2	0.3
(3,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	2	0.3
(3,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	2	0.3
(3,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	2	0.3
(3,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	2	0.3
(3,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	11	0.3
(3,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	11	0.3
(3,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	11	0.3
(3,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	11	0.3
(3,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	11	0.3
(3,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	11	0.3
(3,286)	1:86:A:ASP:H	1:85:A:THR:HG21	14	0.3
(3,286)	1:86:A:ASP:H	1:85:A:THR:HG22	14	0.3
(3,286)	1:86:A:ASP:H	1:85:A:THR:HG23	14	0.3
(3,285)	1:86:A:ASP:H	1:85:A:THR:HG21	14	0.3
(3,285)	1:86:A:ASP:H	1:85:A:THR:HG22	14	0.3
(3,285)	1:86:A:ASP:H	1:85:A:THR:HG23	14	0.3
(3,282)	1:85:A:THR:HG21	1:86:A:ASP:H	14	0.3
(3,282)	1:85:A:THR:HG22	1:86:A:ASP:H	14	0.3
(3,282)	1:85:A:THR:HG23	1:86:A:ASP:H	14	0.3
(3,281)	1:85:A:THR:HG21	1:86:A:ASP:H	14	0.3
(3,281)	1:85:A:THR:HG22	1:86:A:ASP:H	14	0.3
(3,281)	1:85:A:THR:HG23	1:86:A:ASP:H	14	0.3
(3,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	9	0.3
(3,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	9	0.3
(3,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	9	0.3
(3,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	9	0.3
(3,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	9	0.3
(3,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	9	0.3
(3,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	9	0.3
(3,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	9	0.3
(3,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	9	0.3
(3,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	9	0.3
(3,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	9	0.3
(3,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	9	0.3
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	6	0.3
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	6	0.3
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	6	0.3
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	6	0.3
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	6	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	6	0.3
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	6	0.3
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	6	0.3
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	6	0.3
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	6	0.3
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	6	0.3
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	6	0.3
(2,324)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	2	0.3
(2,324)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	2	0.3
(2,324)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	2	0.3
(2,323)	1:91:A:VAL:HG21	1:92:A:PHE:HD1	2	0.3
(2,323)	1:91:A:VAL:HG22	1:92:A:PHE:HD1	2	0.3
(2,323)	1:91:A:VAL:HG23	1:92:A:PHE:HD1	2	0.3
(2,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	11	0.3
(2,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	11	0.3
(2,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	11	0.3
(2,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	11	0.3
(2,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	11	0.3
(2,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	11	0.3
(2,286)	1:86:A:ASP:H	1:85:A:THR:HG21	14	0.3
(2,286)	1:86:A:ASP:H	1:85:A:THR:HG22	14	0.3
(2,286)	1:86:A:ASP:H	1:85:A:THR:HG23	14	0.3
(2,285)	1:86:A:ASP:H	1:85:A:THR:HG21	14	0.3
(2,285)	1:86:A:ASP:H	1:85:A:THR:HG22	14	0.3
(2,285)	1:86:A:ASP:H	1:85:A:THR:HG23	14	0.3
(2,282)	1:85:A:THR:HG21	1:86:A:ASP:H	14	0.3
(2,282)	1:85:A:THR:HG22	1:86:A:ASP:H	14	0.3
(2,282)	1:85:A:THR:HG23	1:86:A:ASP:H	14	0.3
(2,281)	1:85:A:THR:HG21	1:86:A:ASP:H	14	0.3
(2,281)	1:85:A:THR:HG22	1:86:A:ASP:H	14	0.3
(2,281)	1:85:A:THR:HG23	1:86:A:ASP:H	14	0.3
(2,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	9	0.3
(2,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	9	0.3
(2,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	9	0.3
(2,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	9	0.3
(2,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	9	0.3
(2,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	9	0.3
(2,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	9	0.3
(2,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	9	0.3
(2,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	9	0.3
(2,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	9	0.3
(2,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	9	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	9	0.3
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG21	7	0.3
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG22	7	0.3
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG23	7	0.3
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG21	7	0.3
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG22	7	0.3
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG23	7	0.3
(3,700)	1:127:A:THR:HG21	1:128:A:LYS:H	7	0.29
(3,700)	1:127:A:THR:HG22	1:128:A:LYS:H	7	0.29
(3,700)	1:127:A:THR:HG23	1:128:A:LYS:H	7	0.29
(3,699)	1:127:A:THR:HG21	1:128:A:LYS:H	7	0.29
(3,699)	1:127:A:THR:HG22	1:128:A:LYS:H	7	0.29
(3,699)	1:127:A:THR:HG23	1:128:A:LYS:H	7	0.29
(3,638)	1:122:A:LEU:HD11	1:118:A:SER:HA	13	0.29
(3,638)	1:122:A:LEU:HD12	1:118:A:SER:HA	13	0.29
(3,638)	1:122:A:LEU:HD13	1:118:A:SER:HA	13	0.29
(3,637)	1:122:A:LEU:HD11	1:118:A:SER:HA	13	0.29
(3,637)	1:122:A:LEU:HD12	1:118:A:SER:HA	13	0.29
(3,637)	1:122:A:LEU:HD13	1:118:A:SER:HA	13	0.29
(3,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	6	0.29
(3,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	6	0.29
(3,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	6	0.29
(3,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	6	0.29
(3,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	6	0.29
(3,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	6	0.29
(3,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	6	0.29
(3,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	6	0.29
(3,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	6	0.29
(3,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	6	0.29
(3,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	6	0.29
(3,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	6	0.29
(3,622)	1:121:A:VAL:HG21	1:117:A:ALA:HB1	6	0.29
(3,622)	1:121:A:VAL:HG21	1:117:A:ALA:HB2	6	0.29
(3,622)	1:121:A:VAL:HG21	1:117:A:ALA:HB3	6	0.29
(3,622)	1:121:A:VAL:HG22	1:117:A:ALA:HB1	6	0.29
(3,622)	1:121:A:VAL:HG22	1:117:A:ALA:HB2	6	0.29
(3,622)	1:121:A:VAL:HG22	1:117:A:ALA:HB3	6	0.29
(3,622)	1:121:A:VAL:HG23	1:117:A:ALA:HB1	6	0.29
(3,622)	1:121:A:VAL:HG23	1:117:A:ALA:HB2	6	0.29
(3,622)	1:121:A:VAL:HG23	1:117:A:ALA:HB3	6	0.29
(3,621)	1:121:A:VAL:HG21	1:117:A:ALA:HB1	6	0.29
(3,621)	1:121:A:VAL:HG21	1:117:A:ALA:HB2	6	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,621)	1:121:A:VAL:HG21	1:117:A:ALA:HB3	6	0.29
(3,621)	1:121:A:VAL:HG22	1:117:A:ALA:HB1	6	0.29
(3,621)	1:121:A:VAL:HG22	1:117:A:ALA:HB2	6	0.29
(3,621)	1:121:A:VAL:HG22	1:117:A:ALA:HB3	6	0.29
(3,621)	1:121:A:VAL:HG23	1:117:A:ALA:HB1	6	0.29
(3,621)	1:121:A:VAL:HG23	1:117:A:ALA:HB2	6	0.29
(3,621)	1:121:A:VAL:HG23	1:117:A:ALA:HB3	6	0.29
(3,446)	1:101:A:SER:H	1:102:A:ASP:H	6	0.29
(3,445)	1:101:A:SER:H	1:102:A:ASP:H	6	0.29
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	2	0.29
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	2	0.29
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	2	0.29
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	2	0.29
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	2	0.29
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	2	0.29
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	8	0.29
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	8	0.29
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	8	0.29
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	8	0.29
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	8	0.29
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	8	0.29
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	2	0.29
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	2	0.29
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	2	0.29
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	2	0.29
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	2	0.29
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	2	0.29
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	8	0.29
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	8	0.29
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	8	0.29
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	8	0.29
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	8	0.29
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	8	0.29
(3,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	6	0.29
(3,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	6	0.29
(3,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	6	0.29
(3,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	6	0.29
(3,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	6	0.29
(3,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	6	0.29
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	11	0.29
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	11	0.29
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	11	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	11	0.29
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	11	0.29
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	11	0.29
(3,209)	1:77:A:GLN:H	1:76:A:LEU:HG	12	0.29
(3,206)	1:77:A:GLN:H	1:76:A:LEU:HG	12	0.29
(2,700)	1:127:A:THR:HG21	1:128:A:LYS:H	7	0.29
(2,700)	1:127:A:THR:HG22	1:128:A:LYS:H	7	0.29
(2,700)	1:127:A:THR:HG23	1:128:A:LYS:H	7	0.29
(2,699)	1:127:A:THR:HG21	1:128:A:LYS:H	7	0.29
(2,699)	1:127:A:THR:HG22	1:128:A:LYS:H	7	0.29
(2,699)	1:127:A:THR:HG23	1:128:A:LYS:H	7	0.29
(2,638)	1:122:A:LEU:HD11	1:118:A:SER:HA	13	0.29
(2,638)	1:122:A:LEU:HD12	1:118:A:SER:HA	13	0.29
(2,638)	1:122:A:LEU:HD13	1:118:A:SER:HA	13	0.29
(2,637)	1:122:A:LEU:HD11	1:118:A:SER:HA	13	0.29
(2,637)	1:122:A:LEU:HD12	1:118:A:SER:HA	13	0.29
(2,637)	1:122:A:LEU:HD13	1:118:A:SER:HA	13	0.29
(2,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	6	0.29
(2,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	6	0.29
(2,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	6	0.29
(2,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	6	0.29
(2,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	6	0.29
(2,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	6	0.29
(2,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	6	0.29
(2,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	6	0.29
(2,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	6	0.29
(2,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	6	0.29
(2,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	6	0.29
(2,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	6	0.29
(2,622)	1:121:A:VAL:HG21	1:117:A:ALA:HB1	6	0.29
(2,622)	1:121:A:VAL:HG21	1:117:A:ALA:HB2	6	0.29
(2,622)	1:121:A:VAL:HG21	1:117:A:ALA:HB3	6	0.29
(2,622)	1:121:A:VAL:HG22	1:117:A:ALA:HB1	6	0.29
(2,622)	1:121:A:VAL:HG22	1:117:A:ALA:HB2	6	0.29
(2,622)	1:121:A:VAL:HG22	1:117:A:ALA:HB3	6	0.29
(2,622)	1:121:A:VAL:HG23	1:117:A:ALA:HB1	6	0.29
(2,622)	1:121:A:VAL:HG23	1:117:A:ALA:HB2	6	0.29
(2,622)	1:121:A:VAL:HG23	1:117:A:ALA:HB3	6	0.29
(2,621)	1:121:A:VAL:HG21	1:117:A:ALA:HB1	6	0.29
(2,621)	1:121:A:VAL:HG21	1:117:A:ALA:HB2	6	0.29
(2,621)	1:121:A:VAL:HG21	1:117:A:ALA:HB3	6	0.29
(2,621)	1:121:A:VAL:HG22	1:117:A:ALA:HB1	6	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,621)	1:121:A:VAL:HG22	1:117:A:ALA:HB2	6	0.29
(2,621)	1:121:A:VAL:HG22	1:117:A:ALA:HB3	6	0.29
(2,621)	1:121:A:VAL:HG23	1:117:A:ALA:HB1	6	0.29
(2,621)	1:121:A:VAL:HG23	1:117:A:ALA:HB2	6	0.29
(2,621)	1:121:A:VAL:HG23	1:117:A:ALA:HB3	6	0.29
(2,446)	1:101:A:SER:H	1:102:A:ASP:H	6	0.29
(2,445)	1:101:A:SER:H	1:102:A:ASP:H	6	0.29
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	2	0.29
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	2	0.29
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	2	0.29
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	2	0.29
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	2	0.29
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	2	0.29
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	8	0.29
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	8	0.29
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	8	0.29
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	8	0.29
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	8	0.29
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	8	0.29
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	2	0.29
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	2	0.29
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	2	0.29
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	2	0.29
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	2	0.29
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	2	0.29
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	8	0.29
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	8	0.29
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	8	0.29
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	8	0.29
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	8	0.29
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	8	0.29
(2,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	6	0.29
(2,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	6	0.29
(2,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	6	0.29
(2,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	6	0.29
(2,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	6	0.29
(2,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	6	0.29
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	11	0.29
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	11	0.29
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	11	0.29
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	11	0.29
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	11	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	11	0.29
(2,209)	1:77:A:GLN:H	1:76:A:LEU:HG	12	0.29
(2,206)	1:77:A:GLN:H	1:76:A:LEU:HG	12	0.29
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG21	4	0.29
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG22	4	0.29
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG23	4	0.29
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG21	4	0.29
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG22	4	0.29
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG23	4	0.29
(3,686)	1:126:A:SER:H	1:125:A:LEU:HG	1	0.28
(3,685)	1:126:A:SER:H	1:125:A:LEU:HG	1	0.28
(3,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	12	0.28
(3,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	12	0.28
(3,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	12	0.28
(3,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	12	0.28
(3,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	12	0.28
(3,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	12	0.28
(3,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	12	0.28
(3,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	12	0.28
(3,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	12	0.28
(3,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	12	0.28
(3,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	12	0.28
(3,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	12	0.28
(3,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	1	0.28
(3,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	1	0.28
(3,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	1	0.28
(3,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	1	0.28
(3,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	1	0.28
(3,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	1	0.28
(3,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	1	0.28
(3,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	1	0.28
(3,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	1	0.28
(3,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	1	0.28
(3,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	1	0.28
(3,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	1	0.28
(3,572)	1:118:A:SER:H	1:113:A:LEU:HA	1	0.28
(3,572)	1:118:A:SER:H	1:113:A:LEU:HA	15	0.28
(3,571)	1:118:A:SER:H	1:113:A:LEU:HA	1	0.28
(3,571)	1:118:A:SER:H	1:113:A:LEU:HA	15	0.28
(3,548)	1:116:A:PHE:H	1:115:A:TYR:H	12	0.28
(3,547)	1:116:A:PHE:H	1:115:A:TYR:H	12	0.28
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	5	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	5	0.28
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	5	0.28
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	5	0.28
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	5	0.28
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	5	0.28
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	5	0.28
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	5	0.28
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	5	0.28
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	5	0.28
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	5	0.28
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	5	0.28
(3,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	2	0.28
(3,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	2	0.28
(3,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	2	0.28
(3,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	8	0.28
(3,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	8	0.28
(3,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	8	0.28
(3,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	2	0.28
(3,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	2	0.28
(3,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	2	0.28
(3,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	8	0.28
(3,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	8	0.28
(3,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	8	0.28
(3,292)	1:87:A:SER:H	1:86:A:ASP:HA	10	0.28
(3,292)	1:87:A:SER:H	1:86:A:ASP:HA	15	0.28
(3,291)	1:87:A:SER:H	1:86:A:ASP:HA	10	0.28
(3,291)	1:87:A:SER:H	1:86:A:ASP:HA	15	0.28
(3,272)	1:84:A:ASP:H	1:85:A:THR:HA	13	0.28
(3,271)	1:84:A:ASP:H	1:85:A:THR:HA	13	0.28
(3,174)	1:71:A:ASP:H	1:70:A:LEU:HG	15	0.28
(3,173)	1:71:A:ASP:H	1:70:A:LEU:HG	15	0.28
(3,82)	1:60:A:SER:H	1:59:A:LEU:HG	9	0.28
(3,81)	1:60:A:SER:H	1:59:A:LEU:HG	9	0.28
(2,686)	1:126:A:SER:H	1:125:A:LEU:HG	1	0.28
(2,685)	1:126:A:SER:H	1:125:A:LEU:HG	1	0.28
(2,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	12	0.28
(2,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	12	0.28
(2,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	12	0.28
(2,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	12	0.28
(2,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	12	0.28
(2,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	12	0.28
(2,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	12	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	12	0.28
(2,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	12	0.28
(2,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	12	0.28
(2,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	12	0.28
(2,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	12	0.28
(2,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	1	0.28
(2,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	1	0.28
(2,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	1	0.28
(2,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	1	0.28
(2,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	1	0.28
(2,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	1	0.28
(2,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	1	0.28
(2,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	1	0.28
(2,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	1	0.28
(2,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	1	0.28
(2,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	1	0.28
(2,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	1	0.28
(2,572)	1:118:A:SER:H	1:113:A:LEU:HA	1	0.28
(2,572)	1:118:A:SER:H	1:113:A:LEU:HA	15	0.28
(2,571)	1:118:A:SER:H	1:113:A:LEU:HA	1	0.28
(2,571)	1:118:A:SER:H	1:113:A:LEU:HA	15	0.28
(2,548)	1:116:A:PHE:H	1:115:A:TYR:H	12	0.28
(2,547)	1:116:A:PHE:H	1:115:A:TYR:H	12	0.28
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	5	0.28
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	5	0.28
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	5	0.28
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	5	0.28
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	5	0.28
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	5	0.28
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	5	0.28
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	5	0.28
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	5	0.28
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	5	0.28
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	5	0.28
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	5	0.28
(2,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	2	0.28
(2,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	2	0.28
(2,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	2	0.28
(2,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	8	0.28
(2,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	8	0.28
(2,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	8	0.28
(2,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	2	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	2	0.28
(2,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	2	0.28
(2,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	8	0.28
(2,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	8	0.28
(2,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	8	0.28
(2,292)	1:87:A:SER:H	1:86:A:ASP:HA	10	0.28
(2,292)	1:87:A:SER:H	1:86:A:ASP:HA	15	0.28
(2,291)	1:87:A:SER:H	1:86:A:ASP:HA	10	0.28
(2,291)	1:87:A:SER:H	1:86:A:ASP:HA	15	0.28
(2,272)	1:84:A:ASP:H	1:85:A:THR:HA	13	0.28
(2,271)	1:84:A:ASP:H	1:85:A:THR:HA	13	0.28
(2,174)	1:71:A:ASP:H	1:70:A:LEU:HG	15	0.28
(2,173)	1:71:A:ASP:H	1:70:A:LEU:HG	15	0.28
(2,82)	1:60:A:SER:H	1:59:A:LEU:HG	9	0.28
(2,81)	1:60:A:SER:H	1:59:A:LEU:HG	9	0.28
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG21	8	0.28
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG22	8	0.28
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG23	8	0.28
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG21	8	0.28
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG22	8	0.28
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG23	8	0.28
(3,572)	1:118:A:SER:H	1:113:A:LEU:HA	12	0.27
(3,571)	1:118:A:SER:H	1:113:A:LEU:HA	12	0.27
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	3	0.27
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	3	0.27
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	3	0.27
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	3	0.27
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	3	0.27
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	3	0.27
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	3	0.27
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	3	0.27
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	3	0.27
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	3	0.27
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	3	0.27
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	3	0.27
(3,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	5	0.27
(3,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	5	0.27
(3,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	5	0.27
(3,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	5	0.27
(3,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	5	0.27
(3,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	5	0.27
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	9	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	9	0.27
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	9	0.27
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	9	0.27
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	9	0.27
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	9	0.27
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	9	0.27
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	9	0.27
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	9	0.27
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	9	0.27
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	9	0.27
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	9	0.27
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	9	0.27
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	9	0.27
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	9	0.27
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	9	0.27
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	9	0.27
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	9	0.27
(3,292)	1:87:A:SER:H	1:86:A:ASP:HA	14	0.27
(3,291)	1:87:A:SER:H	1:86:A:ASP:HA	14	0.27
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	7	0.27
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	7	0.27
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	7	0.27
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	7	0.27
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	7	0.27
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	7	0.27
(3,260)	1:83:A:VAL:HG11	1:84:A:ASP:H	8	0.27
(3,260)	1:83:A:VAL:HG12	1:84:A:ASP:H	8	0.27
(3,260)	1:83:A:VAL:HG13	1:84:A:ASP:H	8	0.27
(3,260)	1:83:A:VAL:HG21	1:84:A:ASP:H	8	0.27
(3,260)	1:83:A:VAL:HG22	1:84:A:ASP:H	8	0.27
(3,260)	1:83:A:VAL:HG23	1:84:A:ASP:H	8	0.27
(3,259)	1:83:A:VAL:HG11	1:84:A:ASP:H	8	0.27
(3,259)	1:83:A:VAL:HG12	1:84:A:ASP:H	8	0.27
(3,259)	1:83:A:VAL:HG13	1:84:A:ASP:H	8	0.27
(3,259)	1:83:A:VAL:HG21	1:84:A:ASP:H	8	0.27
(3,259)	1:83:A:VAL:HG22	1:84:A:ASP:H	8	0.27
(3,259)	1:83:A:VAL:HG23	1:84:A:ASP:H	8	0.27
(3,246)	1:83:A:VAL:H	1:82:A:ALA:HA	15	0.27
(3,245)	1:83:A:VAL:H	1:82:A:ALA:HA	15	0.27
(3,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	6	0.27
(3,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	6	0.27
(3,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	6	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	6	0.27
(3,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	6	0.27
(3,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	6	0.27
(3,174)	1:71:A:ASP:H	1:70:A:LEU:HG	11	0.27
(3,173)	1:71:A:ASP:H	1:70:A:LEU:HG	11	0.27
(3,34)	1:56:A:THR:H	1:55:A:SER:HB2	11	0.27
(3,34)	1:56:A:THR:H	1:55:A:SER:HB3	11	0.27
(3,33)	1:56:A:THR:H	1:55:A:SER:HB2	11	0.27
(3,33)	1:56:A:THR:H	1:55:A:SER:HB3	11	0.27
(2,572)	1:118:A:SER:H	1:113:A:LEU:HA	12	0.27
(2,571)	1:118:A:SER:H	1:113:A:LEU:HA	12	0.27
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	3	0.27
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	3	0.27
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	3	0.27
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	3	0.27
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	3	0.27
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	3	0.27
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	3	0.27
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	3	0.27
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	3	0.27
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	3	0.27
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	3	0.27
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	3	0.27
(2,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	5	0.27
(2,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	5	0.27
(2,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	5	0.27
(2,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	5	0.27
(2,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	5	0.27
(2,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	5	0.27
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	9	0.27
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	9	0.27
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	9	0.27
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	9	0.27
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	9	0.27
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	9	0.27
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	9	0.27
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	9	0.27
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	9	0.27
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	9	0.27
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	9	0.27
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	9	0.27
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	9	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	9	0.27
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	9	0.27
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	9	0.27
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	9	0.27
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	9	0.27
(2,292)	1:87:A:SER:H	1:86:A:ASP:HA	14	0.27
(2,291)	1:87:A:SER:H	1:86:A:ASP:HA	14	0.27
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	7	0.27
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	7	0.27
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	7	0.27
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	7	0.27
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	7	0.27
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	7	0.27
(2,260)	1:83:A:VAL:HG11	1:84:A:ASP:H	8	0.27
(2,260)	1:83:A:VAL:HG12	1:84:A:ASP:H	8	0.27
(2,260)	1:83:A:VAL:HG13	1:84:A:ASP:H	8	0.27
(2,260)	1:83:A:VAL:HG21	1:84:A:ASP:H	8	0.27
(2,260)	1:83:A:VAL:HG22	1:84:A:ASP:H	8	0.27
(2,260)	1:83:A:VAL:HG23	1:84:A:ASP:H	8	0.27
(2,259)	1:83:A:VAL:HG11	1:84:A:ASP:H	8	0.27
(2,259)	1:83:A:VAL:HG12	1:84:A:ASP:H	8	0.27
(2,259)	1:83:A:VAL:HG13	1:84:A:ASP:H	8	0.27
(2,259)	1:83:A:VAL:HG21	1:84:A:ASP:H	8	0.27
(2,259)	1:83:A:VAL:HG22	1:84:A:ASP:H	8	0.27
(2,259)	1:83:A:VAL:HG23	1:84:A:ASP:H	8	0.27
(2,246)	1:83:A:VAL:H	1:82:A:ALA:HA	15	0.27
(2,245)	1:83:A:VAL:H	1:82:A:ALA:HA	15	0.27
(2,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	6	0.27
(2,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	6	0.27
(2,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	6	0.27
(2,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	6	0.27
(2,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	6	0.27
(2,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	6	0.27
(2,174)	1:71:A:ASP:H	1:70:A:LEU:HG	11	0.27
(2,173)	1:71:A:ASP:H	1:70:A:LEU:HG	11	0.27
(2,34)	1:56:A:THR:H	1:55:A:SER:HB2	11	0.27
(2,34)	1:56:A:THR:H	1:55:A:SER:HB3	11	0.27
(2,33)	1:56:A:THR:H	1:55:A:SER:HB2	11	0.27
(2,33)	1:56:A:THR:H	1:55:A:SER:HB3	11	0.27
(3,700)	1:127:A:THR:HG21	1:128:A:LYS:H	11	0.26
(3,700)	1:127:A:THR:HG22	1:128:A:LYS:H	11	0.26
(3,700)	1:127:A:THR:HG23	1:128:A:LYS:H	11	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,699)	1:127:A:THR:HG21	1:128:A:LYS:H	11	0.26
(3,699)	1:127:A:THR:HG22	1:128:A:LYS:H	11	0.26
(3,699)	1:127:A:THR:HG23	1:128:A:LYS:H	11	0.26
(3,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	1	0.26
(3,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	1	0.26
(3,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	1	0.26
(3,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	1	0.26
(3,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	1	0.26
(3,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	1	0.26
(3,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	5	0.26
(3,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	5	0.26
(3,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	5	0.26
(3,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	5	0.26
(3,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	5	0.26
(3,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	5	0.26
(3,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	1	0.26
(3,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	1	0.26
(3,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	1	0.26
(3,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	1	0.26
(3,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	1	0.26
(3,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	1	0.26
(3,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	5	0.26
(3,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	5	0.26
(3,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	5	0.26
(3,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	5	0.26
(3,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	5	0.26
(3,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	5	0.26
(3,530)	1:113:A:LEU:HD11	1:99:A:MET:HE1	14	0.26
(3,530)	1:113:A:LEU:HD11	1:99:A:MET:HE2	14	0.26
(3,530)	1:113:A:LEU:HD11	1:99:A:MET:HE3	14	0.26
(3,530)	1:113:A:LEU:HD12	1:99:A:MET:HE1	14	0.26
(3,530)	1:113:A:LEU:HD12	1:99:A:MET:HE2	14	0.26
(3,530)	1:113:A:LEU:HD12	1:99:A:MET:HE3	14	0.26
(3,530)	1:113:A:LEU:HD13	1:99:A:MET:HE1	14	0.26
(3,530)	1:113:A:LEU:HD13	1:99:A:MET:HE2	14	0.26
(3,530)	1:113:A:LEU:HD13	1:99:A:MET:HE3	14	0.26
(3,530)	1:113:A:LEU:HD21	1:99:A:MET:HE1	14	0.26
(3,530)	1:113:A:LEU:HD21	1:99:A:MET:HE2	14	0.26
(3,530)	1:113:A:LEU:HD21	1:99:A:MET:HE3	14	0.26
(3,530)	1:113:A:LEU:HD22	1:99:A:MET:HE1	14	0.26
(3,530)	1:113:A:LEU:HD22	1:99:A:MET:HE2	14	0.26
(3,530)	1:113:A:LEU:HD22	1:99:A:MET:HE3	14	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,530)	1:113:A:LEU:HD23	1:99:A:MET:HE1	14	0.26
(3,530)	1:113:A:LEU:HD23	1:99:A:MET:HE2	14	0.26
(3,530)	1:113:A:LEU:HD23	1:99:A:MET:HE3	14	0.26
(3,526)	1:113:A:LEU:HD11	1:99:A:MET:HE1	14	0.26
(3,526)	1:113:A:LEU:HD11	1:99:A:MET:HE2	14	0.26
(3,526)	1:113:A:LEU:HD11	1:99:A:MET:HE3	14	0.26
(3,526)	1:113:A:LEU:HD12	1:99:A:MET:HE1	14	0.26
(3,526)	1:113:A:LEU:HD12	1:99:A:MET:HE2	14	0.26
(3,526)	1:113:A:LEU:HD12	1:99:A:MET:HE3	14	0.26
(3,526)	1:113:A:LEU:HD13	1:99:A:MET:HE1	14	0.26
(3,526)	1:113:A:LEU:HD13	1:99:A:MET:HE2	14	0.26
(3,526)	1:113:A:LEU:HD13	1:99:A:MET:HE3	14	0.26
(3,526)	1:113:A:LEU:HD21	1:99:A:MET:HE1	14	0.26
(3,526)	1:113:A:LEU:HD21	1:99:A:MET:HE2	14	0.26
(3,526)	1:113:A:LEU:HD21	1:99:A:MET:HE3	14	0.26
(3,526)	1:113:A:LEU:HD22	1:99:A:MET:HE1	14	0.26
(3,526)	1:113:A:LEU:HD22	1:99:A:MET:HE2	14	0.26
(3,526)	1:113:A:LEU:HD22	1:99:A:MET:HE3	14	0.26
(3,526)	1:113:A:LEU:HD23	1:99:A:MET:HE1	14	0.26
(3,526)	1:113:A:LEU:HD23	1:99:A:MET:HE2	14	0.26
(3,526)	1:113:A:LEU:HD23	1:99:A:MET:HE3	14	0.26
(3,446)	1:101:A:SER:H	1:102:A:ASP:H	5	0.26
(3,445)	1:101:A:SER:H	1:102:A:ASP:H	5	0.26
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	4	0.26
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	4	0.26
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	4	0.26
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	4	0.26
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	4	0.26
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	4	0.26
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	4	0.26
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	4	0.26
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	4	0.26
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	14	0.26
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	14	0.26
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	14	0.26
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	14	0.26
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	14	0.26
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	14	0.26
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	14	0.26
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	14	0.26
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	14	0.26
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	4	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	4	0.26
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	4	0.26
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	4	0.26
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	4	0.26
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	4	0.26
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	4	0.26
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	4	0.26
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	4	0.26
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	14	0.26
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	14	0.26
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	14	0.26
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	14	0.26
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	14	0.26
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	14	0.26
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	14	0.26
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	14	0.26
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	14	0.26
(3,370)	1:95:A:VAL:HG21	1:92:A:PHE:HE2	13	0.26
(3,370)	1:95:A:VAL:HG22	1:92:A:PHE:HE2	13	0.26
(3,370)	1:95:A:VAL:HG23	1:92:A:PHE:HE2	13	0.26
(3,369)	1:95:A:VAL:HG21	1:92:A:PHE:HE2	13	0.26
(3,369)	1:95:A:VAL:HG22	1:92:A:PHE:HE2	13	0.26
(3,369)	1:95:A:VAL:HG23	1:92:A:PHE:HE2	13	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	4	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	4	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	4	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	4	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	4	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	4	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	14	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	14	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	14	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	14	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	14	0.26
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	14	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	4	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	4	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	4	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	4	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	4	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	4	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	14	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	14	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	14	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	14	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	14	0.26
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	14	0.26
(3,272)	1:84:A:ASP:H	1:85:A:THR:HA	10	0.26
(3,271)	1:84:A:ASP:H	1:85:A:THR:HA	10	0.26
(3,136)	1:67:A:GLY:H	1:66:A:ILE:HB	15	0.26
(3,135)	1:67:A:GLY:H	1:66:A:ILE:HB	15	0.26
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG21	15	0.26
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG22	15	0.26
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG23	15	0.26
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG21	15	0.26
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG22	15	0.26
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG23	15	0.26
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB1	9	0.26
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB2	9	0.26
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB3	9	0.26
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB1	9	0.26
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB2	9	0.26
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB3	9	0.26
(2,700)	1:127:A:THR:HG21	1:128:A:LYS:H	11	0.26
(2,700)	1:127:A:THR:HG22	1:128:A:LYS:H	11	0.26
(2,700)	1:127:A:THR:HG23	1:128:A:LYS:H	11	0.26
(2,699)	1:127:A:THR:HG21	1:128:A:LYS:H	11	0.26
(2,699)	1:127:A:THR:HG22	1:128:A:LYS:H	11	0.26
(2,699)	1:127:A:THR:HG23	1:128:A:LYS:H	11	0.26
(2,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	1	0.26
(2,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	1	0.26
(2,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	1	0.26
(2,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	1	0.26
(2,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	1	0.26
(2,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	1	0.26
(2,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	5	0.26
(2,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	5	0.26
(2,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	5	0.26
(2,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	5	0.26
(2,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	5	0.26
(2,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	5	0.26
(2,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	1	0.26
(2,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	1	0.26
(2,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	1	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	1	0.26
(2,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	1	0.26
(2,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	1	0.26
(2,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	5	0.26
(2,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	5	0.26
(2,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	5	0.26
(2,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	5	0.26
(2,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	5	0.26
(2,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	5	0.26
(2,530)	1:113:A:LEU:HD11	1:99:A:MET:HE1	14	0.26
(2,530)	1:113:A:LEU:HD11	1:99:A:MET:HE2	14	0.26
(2,530)	1:113:A:LEU:HD11	1:99:A:MET:HE3	14	0.26
(2,530)	1:113:A:LEU:HD12	1:99:A:MET:HE1	14	0.26
(2,530)	1:113:A:LEU:HD12	1:99:A:MET:HE2	14	0.26
(2,530)	1:113:A:LEU:HD12	1:99:A:MET:HE3	14	0.26
(2,530)	1:113:A:LEU:HD13	1:99:A:MET:HE1	14	0.26
(2,530)	1:113:A:LEU:HD13	1:99:A:MET:HE2	14	0.26
(2,530)	1:113:A:LEU:HD13	1:99:A:MET:HE3	14	0.26
(2,530)	1:113:A:LEU:HD21	1:99:A:MET:HE1	14	0.26
(2,530)	1:113:A:LEU:HD21	1:99:A:MET:HE2	14	0.26
(2,530)	1:113:A:LEU:HD21	1:99:A:MET:HE3	14	0.26
(2,530)	1:113:A:LEU:HD22	1:99:A:MET:HE1	14	0.26
(2,530)	1:113:A:LEU:HD22	1:99:A:MET:HE2	14	0.26
(2,530)	1:113:A:LEU:HD22	1:99:A:MET:HE3	14	0.26
(2,530)	1:113:A:LEU:HD23	1:99:A:MET:HE1	14	0.26
(2,530)	1:113:A:LEU:HD23	1:99:A:MET:HE2	14	0.26
(2,530)	1:113:A:LEU:HD23	1:99:A:MET:HE3	14	0.26
(2,526)	1:113:A:LEU:HD11	1:99:A:MET:HE1	14	0.26
(2,526)	1:113:A:LEU:HD11	1:99:A:MET:HE2	14	0.26
(2,526)	1:113:A:LEU:HD11	1:99:A:MET:HE3	14	0.26
(2,526)	1:113:A:LEU:HD12	1:99:A:MET:HE1	14	0.26
(2,526)	1:113:A:LEU:HD12	1:99:A:MET:HE2	14	0.26
(2,526)	1:113:A:LEU:HD12	1:99:A:MET:HE3	14	0.26
(2,526)	1:113:A:LEU:HD13	1:99:A:MET:HE1	14	0.26
(2,526)	1:113:A:LEU:HD13	1:99:A:MET:HE2	14	0.26
(2,526)	1:113:A:LEU:HD13	1:99:A:MET:HE3	14	0.26
(2,526)	1:113:A:LEU:HD21	1:99:A:MET:HE1	14	0.26
(2,526)	1:113:A:LEU:HD21	1:99:A:MET:HE2	14	0.26
(2,526)	1:113:A:LEU:HD21	1:99:A:MET:HE3	14	0.26
(2,526)	1:113:A:LEU:HD22	1:99:A:MET:HE1	14	0.26
(2,526)	1:113:A:LEU:HD22	1:99:A:MET:HE2	14	0.26
(2,526)	1:113:A:LEU:HD22	1:99:A:MET:HE3	14	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,526)	1:113:A:LEU:HD23	1:99:A:MET:HE1	14	0.26
(2,526)	1:113:A:LEU:HD23	1:99:A:MET:HE2	14	0.26
(2,526)	1:113:A:LEU:HD23	1:99:A:MET:HE3	14	0.26
(2,446)	1:101:A:SER:H	1:102:A:ASP:H	5	0.26
(2,445)	1:101:A:SER:H	1:102:A:ASP:H	5	0.26
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	4	0.26
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	4	0.26
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	4	0.26
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	4	0.26
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	4	0.26
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	4	0.26
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	4	0.26
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	4	0.26
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	4	0.26
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	14	0.26
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	14	0.26
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	14	0.26
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	14	0.26
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	14	0.26
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	14	0.26
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	14	0.26
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	14	0.26
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	14	0.26
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	4	0.26
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	4	0.26
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	4	0.26
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	4	0.26
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	4	0.26
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	4	0.26
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	4	0.26
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	4	0.26
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	4	0.26
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	14	0.26
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	14	0.26
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	14	0.26
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	14	0.26
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	14	0.26
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	14	0.26
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	14	0.26
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	14	0.26
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	14	0.26
(2,370)	1:95:A:VAL:HG21	1:92:A:PHE:HE2	13	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,370)	1:95:A:VAL:HG22	1:92:A:PHE:HE2	13	0.26
(2,370)	1:95:A:VAL:HG23	1:92:A:PHE:HE2	13	0.26
(2,369)	1:95:A:VAL:HG21	1:92:A:PHE:HE2	13	0.26
(2,369)	1:95:A:VAL:HG22	1:92:A:PHE:HE2	13	0.26
(2,369)	1:95:A:VAL:HG23	1:92:A:PHE:HE2	13	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	4	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	4	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	4	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	4	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	4	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	4	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	14	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	14	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	14	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	14	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	14	0.26
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	14	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	4	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	4	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	4	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	4	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	4	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	4	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	14	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	14	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	14	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	14	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	14	0.26
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	14	0.26
(2,272)	1:84:A:ASP:H	1:85:A:THR:HA	10	0.26
(2,271)	1:84:A:ASP:H	1:85:A:THR:HA	10	0.26
(2,136)	1:67:A:GLY:H	1:66:A:ILE:HB	15	0.26
(2,135)	1:67:A:GLY:H	1:66:A:ILE:HB	15	0.26
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG21	15	0.26
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG22	15	0.26
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG23	15	0.26
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG21	15	0.26
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG22	15	0.26
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG23	15	0.26
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB1	9	0.26
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB2	9	0.26
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB3	9	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB1	9	0.26
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB2	9	0.26
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB3	9	0.26
(3,700)	1:127:A:THR:HG21	1:128:A:LYS:H	12	0.25
(3,700)	1:127:A:THR:HG22	1:128:A:LYS:H	12	0.25
(3,700)	1:127:A:THR:HG23	1:128:A:LYS:H	12	0.25
(3,699)	1:127:A:THR:HG21	1:128:A:LYS:H	12	0.25
(3,699)	1:127:A:THR:HG22	1:128:A:LYS:H	12	0.25
(3,699)	1:127:A:THR:HG23	1:128:A:LYS:H	12	0.25
(3,696)	1:127:A:THR:H	1:126:A:SER:H	3	0.25
(3,695)	1:127:A:THR:H	1:126:A:SER:H	3	0.25
(3,694)	1:127:A:THR:H	1:128:A:LYS:H	7	0.25
(3,693)	1:127:A:THR:H	1:128:A:LYS:H	7	0.25
(3,686)	1:126:A:SER:H	1:125:A:LEU:HG	9	0.25
(3,685)	1:126:A:SER:H	1:125:A:LEU:HG	9	0.25
(3,678)	1:126:A:SER:H	1:127:A:THR:H	3	0.25
(3,677)	1:126:A:SER:H	1:127:A:THR:H	3	0.25
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	9	0.25
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	9	0.25
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	9	0.25
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	9	0.25
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	9	0.25
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	9	0.25
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	9	0.25
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	9	0.25
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	9	0.25
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	9	0.25
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	9	0.25
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	9	0.25
(3,446)	1:101:A:SER:H	1:102:A:ASP:H	2	0.25
(3,446)	1:101:A:SER:H	1:102:A:ASP:H	13	0.25
(3,446)	1:101:A:SER:H	1:102:A:ASP:H	14	0.25
(3,445)	1:101:A:SER:H	1:102:A:ASP:H	2	0.25
(3,445)	1:101:A:SER:H	1:102:A:ASP:H	13	0.25
(3,445)	1:101:A:SER:H	1:102:A:ASP:H	14	0.25
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	3	0.25
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	3	0.25
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	3	0.25
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	3	0.25
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	3	0.25
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	3	0.25
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	3	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	3	0.25
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	3	0.25
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	9	0.25
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	9	0.25
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	9	0.25
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	9	0.25
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	9	0.25
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	9	0.25
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	9	0.25
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	9	0.25
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	9	0.25
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	3	0.25
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	3	0.25
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	3	0.25
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	3	0.25
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	3	0.25
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	3	0.25
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	3	0.25
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	3	0.25
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	3	0.25
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	9	0.25
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	9	0.25
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	9	0.25
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	9	0.25
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	9	0.25
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	9	0.25
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	9	0.25
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	9	0.25
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	9	0.25
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	7	0.25
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	7	0.25
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	7	0.25
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	7	0.25
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	7	0.25
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	7	0.25
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	7	0.25
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	7	0.25
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	7	0.25
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	7	0.25
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	7	0.25
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	7	0.25
(3,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	3	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	3	0.25
(3,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	3	0.25
(3,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	3	0.25
(3,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	3	0.25
(3,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	3	0.25
(3,272)	1:84:A:ASP:H	1:85:A:THR:HA	3	0.25
(3,272)	1:84:A:ASP:H	1:85:A:THR:HA	9	0.25
(3,271)	1:84:A:ASP:H	1:85:A:THR:HA	3	0.25
(3,271)	1:84:A:ASP:H	1:85:A:THR:HA	9	0.25
(3,260)	1:83:A:VAL:HG11	1:84:A:ASP:H	10	0.25
(3,260)	1:83:A:VAL:HG12	1:84:A:ASP:H	10	0.25
(3,260)	1:83:A:VAL:HG13	1:84:A:ASP:H	10	0.25
(3,260)	1:83:A:VAL:HG21	1:84:A:ASP:H	10	0.25
(3,260)	1:83:A:VAL:HG22	1:84:A:ASP:H	10	0.25
(3,260)	1:83:A:VAL:HG23	1:84:A:ASP:H	10	0.25
(3,259)	1:83:A:VAL:HG11	1:84:A:ASP:H	10	0.25
(3,259)	1:83:A:VAL:HG12	1:84:A:ASP:H	10	0.25
(3,259)	1:83:A:VAL:HG13	1:84:A:ASP:H	10	0.25
(3,259)	1:83:A:VAL:HG21	1:84:A:ASP:H	10	0.25
(3,259)	1:83:A:VAL:HG22	1:84:A:ASP:H	10	0.25
(3,259)	1:83:A:VAL:HG23	1:84:A:ASP:H	10	0.25
(3,246)	1:83:A:VAL:H	1:82:A:ALA:HA	12	0.25
(3,245)	1:83:A:VAL:H	1:82:A:ALA:HA	12	0.25
(3,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	11	0.25
(3,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	11	0.25
(3,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	11	0.25
(3,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	11	0.25
(3,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	11	0.25
(3,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	11	0.25
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	9	0.25
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	9	0.25
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	9	0.25
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	9	0.25
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	9	0.25
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	9	0.25
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	9	0.25
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	9	0.25
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	9	0.25
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	9	0.25
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	9	0.25
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	9	0.25
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG21	2	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG22	2	0.25
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG23	2	0.25
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG21	14	0.25
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG22	14	0.25
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG23	14	0.25
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG21	2	0.25
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG22	2	0.25
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG23	2	0.25
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG21	14	0.25
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG22	14	0.25
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG23	14	0.25
(2,700)	1:127:A:THR:HG21	1:128:A:LYS:H	12	0.25
(2,700)	1:127:A:THR:HG22	1:128:A:LYS:H	12	0.25
(2,700)	1:127:A:THR:HG23	1:128:A:LYS:H	12	0.25
(2,699)	1:127:A:THR:HG21	1:128:A:LYS:H	12	0.25
(2,699)	1:127:A:THR:HG22	1:128:A:LYS:H	12	0.25
(2,699)	1:127:A:THR:HG23	1:128:A:LYS:H	12	0.25
(2,696)	1:127:A:THR:H	1:126:A:SER:H	3	0.25
(2,695)	1:127:A:THR:H	1:126:A:SER:H	3	0.25
(2,694)	1:127:A:THR:H	1:128:A:LYS:H	7	0.25
(2,693)	1:127:A:THR:H	1:128:A:LYS:H	7	0.25
(2,686)	1:126:A:SER:H	1:125:A:LEU:HG	9	0.25
(2,685)	1:126:A:SER:H	1:125:A:LEU:HG	9	0.25
(2,678)	1:126:A:SER:H	1:127:A:THR:H	3	0.25
(2,677)	1:126:A:SER:H	1:127:A:THR:H	3	0.25
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	9	0.25
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	9	0.25
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	9	0.25
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	9	0.25
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	9	0.25
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	9	0.25
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	9	0.25
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	9	0.25
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	9	0.25
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	9	0.25
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	9	0.25
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	9	0.25
(2,446)	1:101:A:SER:H	1:102:A:ASP:H	2	0.25
(2,446)	1:101:A:SER:H	1:102:A:ASP:H	13	0.25
(2,446)	1:101:A:SER:H	1:102:A:ASP:H	14	0.25
(2,445)	1:101:A:SER:H	1:102:A:ASP:H	2	0.25
(2,445)	1:101:A:SER:H	1:102:A:ASP:H	13	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,445)	1:101:A:SER:H	1:102:A:ASP:H	14	0.25
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	3	0.25
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	3	0.25
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	3	0.25
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	3	0.25
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	3	0.25
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	3	0.25
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	3	0.25
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	3	0.25
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	3	0.25
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	9	0.25
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	9	0.25
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	9	0.25
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	9	0.25
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	9	0.25
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	9	0.25
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	9	0.25
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	9	0.25
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	9	0.25
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	3	0.25
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	3	0.25
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	3	0.25
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	3	0.25
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	3	0.25
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	3	0.25
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	3	0.25
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	3	0.25
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	3	0.25
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	9	0.25
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	9	0.25
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	9	0.25
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	9	0.25
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	9	0.25
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	9	0.25
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	9	0.25
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	9	0.25
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	9	0.25
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	7	0.25
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	7	0.25
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	7	0.25
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	7	0.25
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	7	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	7	0.25
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	7	0.25
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	7	0.25
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	7	0.25
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	7	0.25
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	7	0.25
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	7	0.25
(2,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	3	0.25
(2,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	3	0.25
(2,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	3	0.25
(2,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	3	0.25
(2,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	3	0.25
(2,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	3	0.25
(2,272)	1:84:A:ASP:H	1:85:A:THR:HA	3	0.25
(2,272)	1:84:A:ASP:H	1:85:A:THR:HA	9	0.25
(2,271)	1:84:A:ASP:H	1:85:A:THR:HA	3	0.25
(2,271)	1:84:A:ASP:H	1:85:A:THR:HA	9	0.25
(2,260)	1:83:A:VAL:HG11	1:84:A:ASP:H	10	0.25
(2,260)	1:83:A:VAL:HG12	1:84:A:ASP:H	10	0.25
(2,260)	1:83:A:VAL:HG13	1:84:A:ASP:H	10	0.25
(2,260)	1:83:A:VAL:HG21	1:84:A:ASP:H	10	0.25
(2,260)	1:83:A:VAL:HG22	1:84:A:ASP:H	10	0.25
(2,260)	1:83:A:VAL:HG23	1:84:A:ASP:H	10	0.25
(2,259)	1:83:A:VAL:HG11	1:84:A:ASP:H	10	0.25
(2,259)	1:83:A:VAL:HG12	1:84:A:ASP:H	10	0.25
(2,259)	1:83:A:VAL:HG13	1:84:A:ASP:H	10	0.25
(2,259)	1:83:A:VAL:HG21	1:84:A:ASP:H	10	0.25
(2,259)	1:83:A:VAL:HG22	1:84:A:ASP:H	10	0.25
(2,259)	1:83:A:VAL:HG23	1:84:A:ASP:H	10	0.25
(2,246)	1:83:A:VAL:H	1:82:A:ALA:HA	12	0.25
(2,245)	1:83:A:VAL:H	1:82:A:ALA:HA	12	0.25
(2,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	11	0.25
(2,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	11	0.25
(2,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	11	0.25
(2,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	11	0.25
(2,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	11	0.25
(2,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	11	0.25
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	9	0.25
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	9	0.25
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	9	0.25
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	9	0.25
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	9	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	9	0.25
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	9	0.25
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	9	0.25
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	9	0.25
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	9	0.25
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	9	0.25
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	9	0.25
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG21	2	0.25
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG22	2	0.25
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG23	2	0.25
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG21	14	0.25
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG22	14	0.25
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG23	14	0.25
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG21	2	0.25
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG22	2	0.25
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG23	2	0.25
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG21	14	0.25
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG22	14	0.25
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG23	14	0.25
(3,702)	1:128:A:LYS:H	1:127:A:THR:HB	6	0.24
(3,701)	1:128:A:LYS:H	1:127:A:THR:HB	6	0.24
(3,700)	1:127:A:THR:HG21	1:128:A:LYS:H	4	0.24
(3,700)	1:127:A:THR:HG22	1:128:A:LYS:H	4	0.24
(3,700)	1:127:A:THR:HG23	1:128:A:LYS:H	4	0.24
(3,700)	1:127:A:THR:HG21	1:128:A:LYS:H	5	0.24
(3,700)	1:127:A:THR:HG22	1:128:A:LYS:H	5	0.24
(3,700)	1:127:A:THR:HG23	1:128:A:LYS:H	5	0.24
(3,700)	1:127:A:THR:HG21	1:128:A:LYS:H	15	0.24
(3,700)	1:127:A:THR:HG22	1:128:A:LYS:H	15	0.24
(3,700)	1:127:A:THR:HG23	1:128:A:LYS:H	15	0.24
(3,699)	1:127:A:THR:HG21	1:128:A:LYS:H	4	0.24
(3,699)	1:127:A:THR:HG22	1:128:A:LYS:H	4	0.24
(3,699)	1:127:A:THR:HG23	1:128:A:LYS:H	4	0.24
(3,699)	1:127:A:THR:HG21	1:128:A:LYS:H	5	0.24
(3,699)	1:127:A:THR:HG22	1:128:A:LYS:H	5	0.24
(3,699)	1:127:A:THR:HG23	1:128:A:LYS:H	5	0.24
(3,699)	1:127:A:THR:HG21	1:128:A:LYS:H	15	0.24
(3,699)	1:127:A:THR:HG22	1:128:A:LYS:H	15	0.24
(3,699)	1:127:A:THR:HG23	1:128:A:LYS:H	15	0.24
(3,672)	1:125:A:LEU:H	1:126:A:SER:HA	3	0.24
(3,671)	1:125:A:LEU:H	1:126:A:SER:HA	3	0.24
(3,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	4	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	4	0.24
(3,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	4	0.24
(3,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	4	0.24
(3,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	4	0.24
(3,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	4	0.24
(3,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	10	0.24
(3,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	10	0.24
(3,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	10	0.24
(3,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	10	0.24
(3,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	10	0.24
(3,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	10	0.24
(3,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	4	0.24
(3,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	4	0.24
(3,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	4	0.24
(3,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	4	0.24
(3,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	4	0.24
(3,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	4	0.24
(3,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	10	0.24
(3,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	10	0.24
(3,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	10	0.24
(3,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	10	0.24
(3,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	10	0.24
(3,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	10	0.24
(3,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	10	0.24
(3,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	10	0.24
(3,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	10	0.24
(3,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	10	0.24
(3,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	10	0.24
(3,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	10	0.24
(3,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	11	0.24
(3,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	11	0.24
(3,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	11	0.24
(3,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	11	0.24
(3,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	11	0.24
(3,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	11	0.24
(3,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	10	0.24
(3,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	10	0.24
(3,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	10	0.24
(3,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	10	0.24
(3,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	10	0.24
(3,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	10	0.24
(3,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	11	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	11	0.24
(3,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	11	0.24
(3,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	11	0.24
(3,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	11	0.24
(3,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	11	0.24
(3,548)	1:116:A:PHE:H	1:115:A:TYR:H	1	0.24
(3,548)	1:116:A:PHE:H	1:115:A:TYR:H	5	0.24
(3,548)	1:116:A:PHE:H	1:115:A:TYR:H	6	0.24
(3,548)	1:116:A:PHE:H	1:115:A:TYR:H	11	0.24
(3,547)	1:116:A:PHE:H	1:115:A:TYR:H	1	0.24
(3,547)	1:116:A:PHE:H	1:115:A:TYR:H	5	0.24
(3,547)	1:116:A:PHE:H	1:115:A:TYR:H	6	0.24
(3,547)	1:116:A:PHE:H	1:115:A:TYR:H	11	0.24
(3,486)	1:106:A:ASN:H	1:105:A:PHE:H	11	0.24
(3,485)	1:106:A:ASN:H	1:105:A:PHE:H	11	0.24
(3,484)	1:105:A:PHE:H	1:106:A:ASN:H	11	0.24
(3,483)	1:105:A:PHE:H	1:106:A:ASN:H	11	0.24
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	12	0.24
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	12	0.24
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	12	0.24
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	12	0.24
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	12	0.24
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	12	0.24
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	12	0.24
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	12	0.24
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	12	0.24
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	12	0.24
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	12	0.24
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	12	0.24
(3,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	4	0.24
(3,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	4	0.24
(3,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	4	0.24
(3,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	7	0.24
(3,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	7	0.24
(3,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	7	0.24
(3,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	14	0.24
(3,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	14	0.24
(3,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	14	0.24
(3,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	4	0.24
(3,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	4	0.24
(3,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	4	0.24
(3,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	7	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	7	0.24
(3,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	7	0.24
(3,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	14	0.24
(3,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	14	0.24
(3,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	14	0.24
(3,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	4	0.24
(3,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	4	0.24
(3,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	4	0.24
(3,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	4	0.24
(3,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	4	0.24
(3,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	4	0.24
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	3	0.24
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	3	0.24
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	3	0.24
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	3	0.24
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	3	0.24
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	3	0.24
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	3	0.24
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	3	0.24
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	3	0.24
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	8	0.24
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	8	0.24
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	8	0.24
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	8	0.24
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	8	0.24
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	8	0.24
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	8	0.24
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	8	0.24
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	8	0.24
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	3	0.24
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	3	0.24
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	3	0.24
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	3	0.24
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	3	0.24
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	3	0.24
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	3	0.24
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	3	0.24
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	3	0.24
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	8	0.24
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	8	0.24
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	8	0.24
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	8	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	8	0.24
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	8	0.24
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	8	0.24
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	8	0.24
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	8	0.24
(3,34)	1:56:A:THR:H	1:55:A:SER:HB2	13	0.24
(3,34)	1:56:A:THR:H	1:55:A:SER:HB3	13	0.24
(3,33)	1:56:A:THR:H	1:55:A:SER:HB2	13	0.24
(3,33)	1:56:A:THR:H	1:55:A:SER:HB3	13	0.24
(3,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	4	0.24
(3,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	4	0.24
(3,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	4	0.24
(3,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	4	0.24
(3,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	4	0.24
(3,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	4	0.24
(2,702)	1:128:A:LYS:H	1:127:A:THR:HB	6	0.24
(2,701)	1:128:A:LYS:H	1:127:A:THR:HB	6	0.24
(2,700)	1:127:A:THR:HG21	1:128:A:LYS:H	4	0.24
(2,700)	1:127:A:THR:HG22	1:128:A:LYS:H	4	0.24
(2,700)	1:127:A:THR:HG23	1:128:A:LYS:H	4	0.24
(2,700)	1:127:A:THR:HG21	1:128:A:LYS:H	5	0.24
(2,700)	1:127:A:THR:HG22	1:128:A:LYS:H	5	0.24
(2,700)	1:127:A:THR:HG23	1:128:A:LYS:H	5	0.24
(2,700)	1:127:A:THR:HG21	1:128:A:LYS:H	15	0.24
(2,700)	1:127:A:THR:HG22	1:128:A:LYS:H	15	0.24
(2,700)	1:127:A:THR:HG23	1:128:A:LYS:H	15	0.24
(2,699)	1:127:A:THR:HG21	1:128:A:LYS:H	4	0.24
(2,699)	1:127:A:THR:HG22	1:128:A:LYS:H	4	0.24
(2,699)	1:127:A:THR:HG23	1:128:A:LYS:H	4	0.24
(2,699)	1:127:A:THR:HG21	1:128:A:LYS:H	5	0.24
(2,699)	1:127:A:THR:HG22	1:128:A:LYS:H	5	0.24
(2,699)	1:127:A:THR:HG23	1:128:A:LYS:H	5	0.24
(2,699)	1:127:A:THR:HG21	1:128:A:LYS:H	15	0.24
(2,699)	1:127:A:THR:HG22	1:128:A:LYS:H	15	0.24
(2,699)	1:127:A:THR:HG23	1:128:A:LYS:H	15	0.24
(2,672)	1:125:A:LEU:H	1:126:A:SER:HA	3	0.24
(2,671)	1:125:A:LEU:H	1:126:A:SER:HA	3	0.24
(2,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	4	0.24
(2,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	4	0.24
(2,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	4	0.24
(2,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	4	0.24
(2,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	4	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	4	0.24
(2,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	10	0.24
(2,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	10	0.24
(2,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	10	0.24
(2,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	10	0.24
(2,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	10	0.24
(2,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	10	0.24
(2,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	4	0.24
(2,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	4	0.24
(2,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	4	0.24
(2,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	4	0.24
(2,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	4	0.24
(2,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	4	0.24
(2,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	10	0.24
(2,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	10	0.24
(2,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	10	0.24
(2,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	10	0.24
(2,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	10	0.24
(2,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	10	0.24
(2,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	10	0.24
(2,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	10	0.24
(2,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	10	0.24
(2,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	10	0.24
(2,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	10	0.24
(2,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	10	0.24
(2,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	11	0.24
(2,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	11	0.24
(2,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	11	0.24
(2,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	11	0.24
(2,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	11	0.24
(2,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	11	0.24
(2,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	10	0.24
(2,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	10	0.24
(2,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	10	0.24
(2,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	10	0.24
(2,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	10	0.24
(2,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	10	0.24
(2,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	11	0.24
(2,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	11	0.24
(2,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	11	0.24
(2,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	11	0.24
(2,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	11	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	11	0.24
(2,548)	1:116:A:PHE:H	1:115:A:TYR:H	1	0.24
(2,548)	1:116:A:PHE:H	1:115:A:TYR:H	5	0.24
(2,548)	1:116:A:PHE:H	1:115:A:TYR:H	6	0.24
(2,548)	1:116:A:PHE:H	1:115:A:TYR:H	11	0.24
(2,547)	1:116:A:PHE:H	1:115:A:TYR:H	1	0.24
(2,547)	1:116:A:PHE:H	1:115:A:TYR:H	5	0.24
(2,547)	1:116:A:PHE:H	1:115:A:TYR:H	6	0.24
(2,547)	1:116:A:PHE:H	1:115:A:TYR:H	11	0.24
(2,486)	1:106:A:ASN:H	1:105:A:PHE:H	11	0.24
(2,485)	1:106:A:ASN:H	1:105:A:PHE:H	11	0.24
(2,484)	1:105:A:PHE:H	1:106:A:ASN:H	11	0.24
(2,483)	1:105:A:PHE:H	1:106:A:ASN:H	11	0.24
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	12	0.24
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	12	0.24
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	12	0.24
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	12	0.24
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	12	0.24
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	12	0.24
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	12	0.24
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	12	0.24
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	12	0.24
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	12	0.24
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	12	0.24
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	12	0.24
(2,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	4	0.24
(2,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	4	0.24
(2,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	4	0.24
(2,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	7	0.24
(2,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	7	0.24
(2,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	7	0.24
(2,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	14	0.24
(2,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	14	0.24
(2,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	14	0.24
(2,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	4	0.24
(2,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	4	0.24
(2,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	4	0.24
(2,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	7	0.24
(2,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	7	0.24
(2,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	7	0.24
(2,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	14	0.24
(2,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	14	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	14	0.24
(2,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	4	0.24
(2,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	4	0.24
(2,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	4	0.24
(2,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	4	0.24
(2,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	4	0.24
(2,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	4	0.24
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	3	0.24
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	3	0.24
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	3	0.24
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	3	0.24
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	3	0.24
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	3	0.24
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	3	0.24
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	3	0.24
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	3	0.24
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	8	0.24
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	8	0.24
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	8	0.24
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	8	0.24
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	8	0.24
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	8	0.24
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	8	0.24
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	8	0.24
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	8	0.24
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	3	0.24
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	3	0.24
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	3	0.24
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	3	0.24
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	3	0.24
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	3	0.24
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	3	0.24
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	3	0.24
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	3	0.24
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	8	0.24
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	8	0.24
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	8	0.24
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	8	0.24
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	8	0.24
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	8	0.24
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	8	0.24
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	8	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	8	0.24
(2,34)	1:56:A:THR:H	1:55:A:SER:HB2	13	0.24
(2,34)	1:56:A:THR:H	1:55:A:SER:HB3	13	0.24
(2,33)	1:56:A:THR:H	1:55:A:SER:HB2	13	0.24
(2,33)	1:56:A:THR:H	1:55:A:SER:HB3	13	0.24
(2,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	4	0.24
(2,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	4	0.24
(2,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	4	0.24
(2,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	4	0.24
(2,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	4	0.24
(2,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	4	0.24
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG21	3	0.24
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG22	3	0.24
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG23	3	0.24
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG21	3	0.24
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG22	3	0.24
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG23	3	0.24
(3,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	2	0.23
(3,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	2	0.23
(3,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	2	0.23
(3,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	2	0.23
(3,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	2	0.23
(3,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	2	0.23
(3,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	7	0.23
(3,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	7	0.23
(3,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	7	0.23
(3,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	7	0.23
(3,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	7	0.23
(3,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	7	0.23
(3,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	8	0.23
(3,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	8	0.23
(3,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	8	0.23
(3,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	8	0.23
(3,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	8	0.23
(3,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	8	0.23
(3,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	2	0.23
(3,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	2	0.23
(3,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	2	0.23
(3,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	2	0.23
(3,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	2	0.23
(3,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	2	0.23
(3,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	7	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	7	0.23
(3,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	7	0.23
(3,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	7	0.23
(3,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	7	0.23
(3,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	7	0.23
(3,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	8	0.23
(3,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	8	0.23
(3,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	8	0.23
(3,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	8	0.23
(3,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	8	0.23
(3,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	8	0.23
(3,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	5	0.23
(3,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	5	0.23
(3,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	5	0.23
(3,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	5	0.23
(3,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	5	0.23
(3,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	5	0.23
(3,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	5	0.23
(3,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	5	0.23
(3,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	5	0.23
(3,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	5	0.23
(3,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	5	0.23
(3,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	5	0.23
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	5	0.23
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	5	0.23
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	5	0.23
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	5	0.23
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	5	0.23
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	5	0.23
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	12	0.23
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	12	0.23
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	12	0.23
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	12	0.23
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	12	0.23
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	12	0.23
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	5	0.23
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	5	0.23
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	5	0.23
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	5	0.23
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	5	0.23
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	5	0.23
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	12	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	12	0.23
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	12	0.23
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	12	0.23
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	12	0.23
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	12	0.23
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	9	0.23
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	9	0.23
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	9	0.23
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	9	0.23
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	9	0.23
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	9	0.23
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	9	0.23
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	9	0.23
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	9	0.23
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	9	0.23
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	9	0.23
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	9	0.23
(3,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	12	0.23
(3,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	12	0.23
(3,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	12	0.23
(3,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	12	0.23
(3,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	12	0.23
(3,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	12	0.23
(3,292)	1:87:A:SER:H	1:86:A:ASP:HA	11	0.23
(3,291)	1:87:A:SER:H	1:86:A:ASP:HA	11	0.23
(3,272)	1:84:A:ASP:H	1:85:A:THR:HA	7	0.23
(3,272)	1:84:A:ASP:H	1:85:A:THR:HA	11	0.23
(3,271)	1:84:A:ASP:H	1:85:A:THR:HA	7	0.23
(3,271)	1:84:A:ASP:H	1:85:A:THR:HA	11	0.23
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	3	0.23
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	3	0.23
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	3	0.23
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	13	0.23
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	13	0.23
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	13	0.23
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	3	0.23
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	3	0.23
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	3	0.23
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	13	0.23
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	13	0.23
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	13	0.23
(3,246)	1:83:A:VAL:H	1:82:A:ALA:HA	2	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,245)	1:83:A:VAL:H	1:82:A:ALA:HA	2	0.23
(3,209)	1:77:A:GLN:H	1:76:A:LEU:HG	10	0.23
(3,206)	1:77:A:GLN:H	1:76:A:LEU:HG	10	0.23
(3,174)	1:71:A:ASP:H	1:70:A:LEU:HG	9	0.23
(3,173)	1:71:A:ASP:H	1:70:A:LEU:HG	9	0.23
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG21	3	0.23
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG22	3	0.23
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG23	3	0.23
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG21	11	0.23
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG22	11	0.23
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG23	11	0.23
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG21	3	0.23
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG22	3	0.23
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG23	3	0.23
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG21	11	0.23
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG22	11	0.23
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG23	11	0.23
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	2	0.23
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	2	0.23
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	2	0.23
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	2	0.23
(3,82)	1:60:A:SER:H	1:59:A:LEU:HG	6	0.23
(3,81)	1:60:A:SER:H	1:59:A:LEU:HG	6	0.23
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB1	15	0.23
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB2	15	0.23
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB3	15	0.23
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB1	15	0.23
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB2	15	0.23
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB3	15	0.23
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB1	1	0.23
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB2	1	0.23
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB3	1	0.23
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB1	1	0.23
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB2	1	0.23
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB3	1	0.23
(2,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	2	0.23
(2,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	2	0.23
(2,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	2	0.23
(2,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	2	0.23
(2,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	2	0.23
(2,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	2	0.23
(2,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	7	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	7	0.23
(2,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	7	0.23
(2,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	7	0.23
(2,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	7	0.23
(2,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	7	0.23
(2,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	8	0.23
(2,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	8	0.23
(2,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	8	0.23
(2,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	8	0.23
(2,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	8	0.23
(2,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	8	0.23
(2,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	2	0.23
(2,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	2	0.23
(2,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	2	0.23
(2,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	2	0.23
(2,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	2	0.23
(2,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	2	0.23
(2,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	7	0.23
(2,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	7	0.23
(2,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	7	0.23
(2,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	7	0.23
(2,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	7	0.23
(2,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	7	0.23
(2,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	8	0.23
(2,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	8	0.23
(2,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	8	0.23
(2,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	8	0.23
(2,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	8	0.23
(2,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	8	0.23
(2,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	5	0.23
(2,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	5	0.23
(2,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	5	0.23
(2,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	5	0.23
(2,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	5	0.23
(2,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	5	0.23
(2,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	5	0.23
(2,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	5	0.23
(2,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	5	0.23
(2,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	5	0.23
(2,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	5	0.23
(2,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	5	0.23
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	5	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	5	0.23
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	5	0.23
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	5	0.23
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	5	0.23
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	5	0.23
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	12	0.23
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	12	0.23
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	12	0.23
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	12	0.23
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	12	0.23
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	12	0.23
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	5	0.23
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	5	0.23
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	5	0.23
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	5	0.23
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	5	0.23
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	5	0.23
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	12	0.23
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	12	0.23
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	12	0.23
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	12	0.23
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	12	0.23
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	12	0.23
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	9	0.23
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	9	0.23
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	9	0.23
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	9	0.23
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	9	0.23
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	9	0.23
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	9	0.23
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	9	0.23
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	9	0.23
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	9	0.23
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	9	0.23
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	9	0.23
(2,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	12	0.23
(2,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	12	0.23
(2,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	12	0.23
(2,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	12	0.23
(2,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	12	0.23
(2,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	12	0.23
(2,292)	1:87:A:SER:H	1:86:A:ASP:HA	11	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,291)	1:87:A:SER:H	1:86:A:ASP:HA	11	0.23
(2,272)	1:84:A:ASP:H	1:85:A:THR:HA	7	0.23
(2,272)	1:84:A:ASP:H	1:85:A:THR:HA	11	0.23
(2,271)	1:84:A:ASP:H	1:85:A:THR:HA	7	0.23
(2,271)	1:84:A:ASP:H	1:85:A:THR:HA	11	0.23
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	3	0.23
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	3	0.23
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	3	0.23
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	13	0.23
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	13	0.23
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	13	0.23
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	3	0.23
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	3	0.23
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	3	0.23
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	13	0.23
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	13	0.23
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	13	0.23
(2,246)	1:83:A:VAL:H	1:82:A:ALA:HA	2	0.23
(2,245)	1:83:A:VAL:H	1:82:A:ALA:HA	2	0.23
(2,209)	1:77:A:GLN:H	1:76:A:LEU:HG	10	0.23
(2,206)	1:77:A:GLN:H	1:76:A:LEU:HG	10	0.23
(2,174)	1:71:A:ASP:H	1:70:A:LEU:HG	9	0.23
(2,173)	1:71:A:ASP:H	1:70:A:LEU:HG	9	0.23
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG21	3	0.23
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG22	3	0.23
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG23	3	0.23
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG21	11	0.23
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG22	11	0.23
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG23	11	0.23
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG21	3	0.23
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG22	3	0.23
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG23	3	0.23
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG21	11	0.23
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG22	11	0.23
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG23	11	0.23
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	2	0.23
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	2	0.23
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	2	0.23
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	2	0.23
(2,82)	1:60:A:SER:H	1:59:A:LEU:HG	6	0.23
(2,81)	1:60:A:SER:H	1:59:A:LEU:HG	6	0.23
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB1	15	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB2	15	0.23
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB3	15	0.23
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB1	15	0.23
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB2	15	0.23
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB3	15	0.23
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB1	1	0.23
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB2	1	0.23
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB3	1	0.23
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB1	1	0.23
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB2	1	0.23
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB3	1	0.23
(3,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	3	0.22
(3,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	3	0.22
(3,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	3	0.22
(3,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	3	0.22
(3,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	3	0.22
(3,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	3	0.22
(3,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	14	0.22
(3,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	14	0.22
(3,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	14	0.22
(3,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	14	0.22
(3,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	14	0.22
(3,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	14	0.22
(3,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	15	0.22
(3,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	15	0.22
(3,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	15	0.22
(3,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	15	0.22
(3,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	15	0.22
(3,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	15	0.22
(3,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	3	0.22
(3,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	3	0.22
(3,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	3	0.22
(3,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	3	0.22
(3,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	3	0.22
(3,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	3	0.22
(3,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	14	0.22
(3,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	14	0.22
(3,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	14	0.22
(3,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	14	0.22
(3,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	14	0.22
(3,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	14	0.22
(3,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	15	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	15	0.22
(3,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	15	0.22
(3,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	15	0.22
(3,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	15	0.22
(3,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	15	0.22
(3,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	3	0.22
(3,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	3	0.22
(3,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	3	0.22
(3,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	3	0.22
(3,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	3	0.22
(3,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	3	0.22
(3,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	3	0.22
(3,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	3	0.22
(3,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	3	0.22
(3,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	3	0.22
(3,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	3	0.22
(3,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	3	0.22
(3,560)	1:117:A:ALA:H	1:113:A:LEU:HD11	9	0.22
(3,560)	1:117:A:ALA:H	1:113:A:LEU:HD12	9	0.22
(3,560)	1:117:A:ALA:H	1:113:A:LEU:HD13	9	0.22
(3,560)	1:117:A:ALA:H	1:113:A:LEU:HD21	9	0.22
(3,560)	1:117:A:ALA:H	1:113:A:LEU:HD22	9	0.22
(3,560)	1:117:A:ALA:H	1:113:A:LEU:HD23	9	0.22
(3,559)	1:117:A:ALA:H	1:113:A:LEU:HD11	9	0.22
(3,559)	1:117:A:ALA:H	1:113:A:LEU:HD12	9	0.22
(3,559)	1:117:A:ALA:H	1:113:A:LEU:HD13	9	0.22
(3,559)	1:117:A:ALA:H	1:113:A:LEU:HD21	9	0.22
(3,559)	1:117:A:ALA:H	1:113:A:LEU:HD22	9	0.22
(3,559)	1:117:A:ALA:H	1:113:A:LEU:HD23	9	0.22
(3,548)	1:116:A:PHE:H	1:115:A:TYR:H	2	0.22
(3,548)	1:116:A:PHE:H	1:115:A:TYR:H	10	0.22
(3,547)	1:116:A:PHE:H	1:115:A:TYR:H	2	0.22
(3,547)	1:116:A:PHE:H	1:115:A:TYR:H	10	0.22
(3,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	12	0.22
(3,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	12	0.22
(3,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	12	0.22
(3,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	12	0.22
(3,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	12	0.22
(3,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	12	0.22
(3,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	12	0.22
(3,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	12	0.22
(3,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	12	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	12	0.22
(3,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	12	0.22
(3,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	12	0.22
(3,486)	1:106:A:ASN:H	1:105:A:PHE:H	3	0.22
(3,485)	1:106:A:ASN:H	1:105:A:PHE:H	3	0.22
(3,484)	1:105:A:PHE:H	1:106:A:ASN:H	3	0.22
(3,483)	1:105:A:PHE:H	1:106:A:ASN:H	3	0.22
(3,446)	1:101:A:SER:H	1:102:A:ASP:H	4	0.22
(3,446)	1:101:A:SER:H	1:102:A:ASP:H	10	0.22
(3,445)	1:101:A:SER:H	1:102:A:ASP:H	4	0.22
(3,445)	1:101:A:SER:H	1:102:A:ASP:H	10	0.22
(3,370)	1:95:A:VAL:HG21	1:92:A:PHE:HE2	15	0.22
(3,370)	1:95:A:VAL:HG22	1:92:A:PHE:HE2	15	0.22
(3,370)	1:95:A:VAL:HG23	1:92:A:PHE:HE2	15	0.22
(3,369)	1:95:A:VAL:HG21	1:92:A:PHE:HE2	15	0.22
(3,369)	1:95:A:VAL:HG22	1:92:A:PHE:HE2	15	0.22
(3,369)	1:95:A:VAL:HG23	1:92:A:PHE:HE2	15	0.22
(3,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	9	0.22
(3,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	9	0.22
(3,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	9	0.22
(3,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	9	0.22
(3,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	9	0.22
(3,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	9	0.22
(3,292)	1:87:A:SER:H	1:86:A:ASP:HA	3	0.22
(3,292)	1:87:A:SER:H	1:86:A:ASP:HA	4	0.22
(3,291)	1:87:A:SER:H	1:86:A:ASP:HA	3	0.22
(3,291)	1:87:A:SER:H	1:86:A:ASP:HA	4	0.22
(3,272)	1:84:A:ASP:H	1:85:A:THR:HA	1	0.22
(3,271)	1:84:A:ASP:H	1:85:A:THR:HA	1	0.22
(3,262)	1:84:A:ASP:H	1:83:A:VAL:H	15	0.22
(3,261)	1:84:A:ASP:H	1:83:A:VAL:H	15	0.22
(3,248)	1:83:A:VAL:H	1:84:A:ASP:H	15	0.22
(3,247)	1:83:A:VAL:H	1:84:A:ASP:H	15	0.22
(3,246)	1:83:A:VAL:H	1:82:A:ALA:HA	9	0.22
(3,246)	1:83:A:VAL:H	1:82:A:ALA:HA	11	0.22
(3,245)	1:83:A:VAL:H	1:82:A:ALA:HA	9	0.22
(3,245)	1:83:A:VAL:H	1:82:A:ALA:HA	11	0.22
(3,209)	1:77:A:GLN:H	1:76:A:LEU:HG	4	0.22
(3,209)	1:77:A:GLN:H	1:76:A:LEU:HG	13	0.22
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	6	0.22
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	6	0.22
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	6	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,206)	1:77:A:GLN:H	1:76:A:LEU:HG	4	0.22
(3,206)	1:77:A:GLN:H	1:76:A:LEU:HG	13	0.22
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	6	0.22
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	6	0.22
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	6	0.22
(3,188)	1:73:A:ASN:H	1:74:A:MET:H	12	0.22
(3,188)	1:73:A:ASN:H	1:74:A:MET:H	13	0.22
(3,185)	1:73:A:ASN:H	1:74:A:MET:H	12	0.22
(3,185)	1:73:A:ASN:H	1:74:A:MET:H	13	0.22
(2,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	3	0.22
(2,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	3	0.22
(2,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	3	0.22
(2,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	3	0.22
(2,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	3	0.22
(2,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	3	0.22
(2,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	14	0.22
(2,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	14	0.22
(2,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	14	0.22
(2,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	14	0.22
(2,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	14	0.22
(2,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	14	0.22
(2,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	15	0.22
(2,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	15	0.22
(2,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	15	0.22
(2,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	15	0.22
(2,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	15	0.22
(2,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	15	0.22
(2,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	3	0.22
(2,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	3	0.22
(2,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	3	0.22
(2,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	3	0.22
(2,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	3	0.22
(2,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	3	0.22
(2,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	14	0.22
(2,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	14	0.22
(2,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	14	0.22
(2,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	14	0.22
(2,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	14	0.22
(2,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	14	0.22
(2,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	15	0.22
(2,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	15	0.22
(2,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	15	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	15	0.22
(2,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	15	0.22
(2,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	15	0.22
(2,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	3	0.22
(2,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	3	0.22
(2,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	3	0.22
(2,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	3	0.22
(2,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	3	0.22
(2,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	3	0.22
(2,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	3	0.22
(2,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	3	0.22
(2,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	3	0.22
(2,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	3	0.22
(2,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	3	0.22
(2,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	3	0.22
(2,560)	1:117:A:ALA:H	1:113:A:LEU:HD11	9	0.22
(2,560)	1:117:A:ALA:H	1:113:A:LEU:HD12	9	0.22
(2,560)	1:117:A:ALA:H	1:113:A:LEU:HD13	9	0.22
(2,560)	1:117:A:ALA:H	1:113:A:LEU:HD21	9	0.22
(2,560)	1:117:A:ALA:H	1:113:A:LEU:HD22	9	0.22
(2,560)	1:117:A:ALA:H	1:113:A:LEU:HD23	9	0.22
(2,559)	1:117:A:ALA:H	1:113:A:LEU:HD11	9	0.22
(2,559)	1:117:A:ALA:H	1:113:A:LEU:HD12	9	0.22
(2,559)	1:117:A:ALA:H	1:113:A:LEU:HD13	9	0.22
(2,559)	1:117:A:ALA:H	1:113:A:LEU:HD21	9	0.22
(2,559)	1:117:A:ALA:H	1:113:A:LEU:HD22	9	0.22
(2,559)	1:117:A:ALA:H	1:113:A:LEU:HD23	9	0.22
(2,548)	1:116:A:PHE:H	1:115:A:TYR:H	2	0.22
(2,548)	1:116:A:PHE:H	1:115:A:TYR:H	10	0.22
(2,547)	1:116:A:PHE:H	1:115:A:TYR:H	2	0.22
(2,547)	1:116:A:PHE:H	1:115:A:TYR:H	10	0.22
(2,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	12	0.22
(2,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	12	0.22
(2,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	12	0.22
(2,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	12	0.22
(2,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	12	0.22
(2,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	12	0.22
(2,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	12	0.22
(2,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	12	0.22
(2,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	12	0.22
(2,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	12	0.22
(2,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	12	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	12	0.22
(2,486)	1:106:A:ASN:H	1:105:A:PHE:H	3	0.22
(2,485)	1:106:A:ASN:H	1:105:A:PHE:H	3	0.22
(2,484)	1:105:A:PHE:H	1:106:A:ASN:H	3	0.22
(2,483)	1:105:A:PHE:H	1:106:A:ASN:H	3	0.22
(2,446)	1:101:A:SER:H	1:102:A:ASP:H	4	0.22
(2,446)	1:101:A:SER:H	1:102:A:ASP:H	10	0.22
(2,445)	1:101:A:SER:H	1:102:A:ASP:H	4	0.22
(2,445)	1:101:A:SER:H	1:102:A:ASP:H	10	0.22
(2,370)	1:95:A:VAL:HG21	1:92:A:PHE:HE2	15	0.22
(2,370)	1:95:A:VAL:HG22	1:92:A:PHE:HE2	15	0.22
(2,370)	1:95:A:VAL:HG23	1:92:A:PHE:HE2	15	0.22
(2,369)	1:95:A:VAL:HG21	1:92:A:PHE:HE2	15	0.22
(2,369)	1:95:A:VAL:HG22	1:92:A:PHE:HE2	15	0.22
(2,369)	1:95:A:VAL:HG23	1:92:A:PHE:HE2	15	0.22
(2,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	9	0.22
(2,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	9	0.22
(2,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	9	0.22
(2,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	9	0.22
(2,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	9	0.22
(2,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	9	0.22
(2,292)	1:87:A:SER:H	1:86:A:ASP:HA	3	0.22
(2,292)	1:87:A:SER:H	1:86:A:ASP:HA	4	0.22
(2,291)	1:87:A:SER:H	1:86:A:ASP:HA	3	0.22
(2,291)	1:87:A:SER:H	1:86:A:ASP:HA	4	0.22
(2,272)	1:84:A:ASP:H	1:85:A:THR:HA	1	0.22
(2,271)	1:84:A:ASP:H	1:85:A:THR:HA	1	0.22
(2,262)	1:84:A:ASP:H	1:83:A:VAL:H	15	0.22
(2,261)	1:84:A:ASP:H	1:83:A:VAL:H	15	0.22
(2,248)	1:83:A:VAL:H	1:84:A:ASP:H	15	0.22
(2,247)	1:83:A:VAL:H	1:84:A:ASP:H	15	0.22
(2,246)	1:83:A:VAL:H	1:82:A:ALA:HA	9	0.22
(2,246)	1:83:A:VAL:H	1:82:A:ALA:HA	11	0.22
(2,245)	1:83:A:VAL:H	1:82:A:ALA:HA	9	0.22
(2,245)	1:83:A:VAL:H	1:82:A:ALA:HA	11	0.22
(2,209)	1:77:A:GLN:H	1:76:A:LEU:HG	4	0.22
(2,209)	1:77:A:GLN:H	1:76:A:LEU:HG	13	0.22
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	6	0.22
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	6	0.22
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	6	0.22
(2,206)	1:77:A:GLN:H	1:76:A:LEU:HG	4	0.22
(2,206)	1:77:A:GLN:H	1:76:A:LEU:HG	13	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	6	0.22
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	6	0.22
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	6	0.22
(2,188)	1:73:A:ASN:H	1:74:A:MET:H	12	0.22
(2,188)	1:73:A:ASN:H	1:74:A:MET:H	13	0.22
(2,185)	1:73:A:ASN:H	1:74:A:MET:H	12	0.22
(2,185)	1:73:A:ASN:H	1:74:A:MET:H	13	0.22
(3,694)	1:127:A:THR:H	1:128:A:LYS:H	11	0.21
(3,693)	1:127:A:THR:H	1:128:A:LYS:H	11	0.21
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	9	0.21
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	9	0.21
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	9	0.21
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	9	0.21
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	9	0.21
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	9	0.21
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	9	0.21
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	9	0.21
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	9	0.21
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	9	0.21
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	9	0.21
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	9	0.21
(3,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	11	0.21
(3,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	11	0.21
(3,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	11	0.21
(3,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	11	0.21
(3,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	11	0.21
(3,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	11	0.21
(3,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	11	0.21
(3,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	11	0.21
(3,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	11	0.21
(3,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	11	0.21
(3,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	11	0.21
(3,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	11	0.21
(3,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	2	0.21
(3,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	2	0.21
(3,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	2	0.21
(3,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	2	0.21
(3,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	2	0.21
(3,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	2	0.21
(3,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	4	0.21
(3,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	4	0.21
(3,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	4	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	4	0.21
(3,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	4	0.21
(3,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	4	0.21
(3,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	8	0.21
(3,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	8	0.21
(3,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	8	0.21
(3,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	8	0.21
(3,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	8	0.21
(3,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	8	0.21
(3,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	2	0.21
(3,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	2	0.21
(3,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	2	0.21
(3,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	2	0.21
(3,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	2	0.21
(3,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	2	0.21
(3,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	4	0.21
(3,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	4	0.21
(3,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	4	0.21
(3,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	4	0.21
(3,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	4	0.21
(3,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	4	0.21
(3,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	8	0.21
(3,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	8	0.21
(3,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	8	0.21
(3,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	8	0.21
(3,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	8	0.21
(3,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	8	0.21
(3,618)	1:121:A:VAL:HG11	1:117:A:ALA:HA	6	0.21
(3,618)	1:121:A:VAL:HG12	1:117:A:ALA:HA	6	0.21
(3,618)	1:121:A:VAL:HG13	1:117:A:ALA:HA	6	0.21
(3,617)	1:121:A:VAL:HG11	1:117:A:ALA:HA	6	0.21
(3,617)	1:121:A:VAL:HG12	1:117:A:ALA:HA	6	0.21
(3,617)	1:121:A:VAL:HG13	1:117:A:ALA:HA	6	0.21
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	9	0.21
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	9	0.21
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	9	0.21
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	9	0.21
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	9	0.21
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	9	0.21
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	9	0.21
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	9	0.21
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	9	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	9	0.21
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	9	0.21
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	9	0.21
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	9	0.21
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	9	0.21
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	9	0.21
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	9	0.21
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	9	0.21
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	9	0.21
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	1	0.21
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	1	0.21
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	1	0.21
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	1	0.21
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	1	0.21
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	1	0.21
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	2	0.21
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	2	0.21
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	2	0.21
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	2	0.21
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	2	0.21
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	2	0.21
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	1	0.21
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	1	0.21
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	1	0.21
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	1	0.21
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	1	0.21
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	1	0.21
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	2	0.21
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	2	0.21
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	2	0.21
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	2	0.21
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	2	0.21
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	2	0.21
(3,548)	1:116:A:PHE:H	1:115:A:TYR:H	15	0.21
(3,547)	1:116:A:PHE:H	1:115:A:TYR:H	15	0.21
(3,531)	1:113:A:LEU:HD21	1:96:A:ALA:HA	14	0.21
(3,531)	1:113:A:LEU:HD22	1:96:A:ALA:HA	14	0.21
(3,531)	1:113:A:LEU:HD23	1:96:A:ALA:HA	14	0.21
(3,527)	1:113:A:LEU:HD21	1:96:A:ALA:HA	14	0.21
(3,527)	1:113:A:LEU:HD22	1:96:A:ALA:HA	14	0.21
(3,527)	1:113:A:LEU:HD23	1:96:A:ALA:HA	14	0.21
(3,494)	1:110:A:VAL:HG21	1:113:A:LEU:HD11	10	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,494)	1:110:A:VAL:HG21	1:113:A:LEU:HD12	10	0.21
(3,494)	1:110:A:VAL:HG21	1:113:A:LEU:HD13	10	0.21
(3,494)	1:110:A:VAL:HG21	1:113:A:LEU:HD21	10	0.21
(3,494)	1:110:A:VAL:HG21	1:113:A:LEU:HD22	10	0.21
(3,494)	1:110:A:VAL:HG21	1:113:A:LEU:HD23	10	0.21
(3,494)	1:110:A:VAL:HG22	1:113:A:LEU:HD11	10	0.21
(3,494)	1:110:A:VAL:HG22	1:113:A:LEU:HD12	10	0.21
(3,494)	1:110:A:VAL:HG22	1:113:A:LEU:HD13	10	0.21
(3,494)	1:110:A:VAL:HG22	1:113:A:LEU:HD21	10	0.21
(3,494)	1:110:A:VAL:HG22	1:113:A:LEU:HD22	10	0.21
(3,494)	1:110:A:VAL:HG22	1:113:A:LEU:HD23	10	0.21
(3,494)	1:110:A:VAL:HG23	1:113:A:LEU:HD11	10	0.21
(3,494)	1:110:A:VAL:HG23	1:113:A:LEU:HD12	10	0.21
(3,494)	1:110:A:VAL:HG23	1:113:A:LEU:HD13	10	0.21
(3,494)	1:110:A:VAL:HG23	1:113:A:LEU:HD21	10	0.21
(3,494)	1:110:A:VAL:HG23	1:113:A:LEU:HD22	10	0.21
(3,494)	1:110:A:VAL:HG23	1:113:A:LEU:HD23	10	0.21
(3,493)	1:110:A:VAL:HG21	1:113:A:LEU:HD11	10	0.21
(3,493)	1:110:A:VAL:HG21	1:113:A:LEU:HD12	10	0.21
(3,493)	1:110:A:VAL:HG21	1:113:A:LEU:HD13	10	0.21
(3,493)	1:110:A:VAL:HG21	1:113:A:LEU:HD21	10	0.21
(3,493)	1:110:A:VAL:HG21	1:113:A:LEU:HD22	10	0.21
(3,493)	1:110:A:VAL:HG21	1:113:A:LEU:HD23	10	0.21
(3,493)	1:110:A:VAL:HG22	1:113:A:LEU:HD11	10	0.21
(3,493)	1:110:A:VAL:HG22	1:113:A:LEU:HD12	10	0.21
(3,493)	1:110:A:VAL:HG22	1:113:A:LEU:HD13	10	0.21
(3,493)	1:110:A:VAL:HG22	1:113:A:LEU:HD21	10	0.21
(3,493)	1:110:A:VAL:HG22	1:113:A:LEU:HD22	10	0.21
(3,493)	1:110:A:VAL:HG22	1:113:A:LEU:HD23	10	0.21
(3,493)	1:110:A:VAL:HG23	1:113:A:LEU:HD11	10	0.21
(3,493)	1:110:A:VAL:HG23	1:113:A:LEU:HD12	10	0.21
(3,493)	1:110:A:VAL:HG23	1:113:A:LEU:HD13	10	0.21
(3,493)	1:110:A:VAL:HG23	1:113:A:LEU:HD21	10	0.21
(3,493)	1:110:A:VAL:HG23	1:113:A:LEU:HD22	10	0.21
(3,493)	1:110:A:VAL:HG23	1:113:A:LEU:HD23	10	0.21
(3,486)	1:106:A:ASN:H	1:105:A:PHE:H	5	0.21
(3,485)	1:106:A:ASN:H	1:105:A:PHE:H	5	0.21
(3,484)	1:105:A:PHE:H	1:106:A:ASN:H	5	0.21
(3,483)	1:105:A:PHE:H	1:106:A:ASN:H	5	0.21
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	6	0.21
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	6	0.21
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	6	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	6	0.21
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	6	0.21
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	6	0.21
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	6	0.21
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	6	0.21
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	6	0.21
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	6	0.21
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	6	0.21
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	6	0.21
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	6	0.21
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	6	0.21
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	6	0.21
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	6	0.21
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	6	0.21
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	6	0.21
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	13	0.21
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	13	0.21
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	13	0.21
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	13	0.21
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	13	0.21
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	13	0.21
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	13	0.21
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	13	0.21
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	13	0.21
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	13	0.21
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	13	0.21
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	13	0.21
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	6	0.21
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	6	0.21
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	6	0.21
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	6	0.21
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	6	0.21
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	6	0.21
(3,188)	1:73:A:ASN:H	1:74:A:MET:H	8	0.21
(3,185)	1:73:A:ASN:H	1:74:A:MET:H	8	0.21
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	4	0.21
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	4	0.21
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	4	0.21
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	4	0.21
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	4	0.21
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	4	0.21
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	4	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	4	0.21
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	4	0.21
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	4	0.21
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	4	0.21
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	4	0.21
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	4	0.21
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	4	0.21
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	4	0.21
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	4	0.21
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	4	0.21
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	4	0.21
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	13	0.21
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	13	0.21
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	13	0.21
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	13	0.21
(3,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	3	0.21
(3,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	3	0.21
(3,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	3	0.21
(3,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	3	0.21
(3,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	3	0.21
(3,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	3	0.21
(2,694)	1:127:A:THR:H	1:128:A:LYS:H	11	0.21
(2,693)	1:127:A:THR:H	1:128:A:LYS:H	11	0.21
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	9	0.21
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	9	0.21
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	9	0.21
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	9	0.21
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	9	0.21
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	9	0.21
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	9	0.21
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	9	0.21
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	9	0.21
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	9	0.21
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	9	0.21
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	9	0.21
(2,630)	1:121:A:VAL:HG11	1:122:A:LEU:H	11	0.21
(2,630)	1:121:A:VAL:HG12	1:122:A:LEU:H	11	0.21
(2,630)	1:121:A:VAL:HG13	1:122:A:LEU:H	11	0.21
(2,630)	1:121:A:VAL:HG21	1:122:A:LEU:H	11	0.21
(2,630)	1:121:A:VAL:HG22	1:122:A:LEU:H	11	0.21
(2,630)	1:121:A:VAL:HG23	1:122:A:LEU:H	11	0.21
(2,629)	1:121:A:VAL:HG11	1:122:A:LEU:H	11	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,629)	1:121:A:VAL:HG12	1:122:A:LEU:H	11	0.21
(2,629)	1:121:A:VAL:HG13	1:122:A:LEU:H	11	0.21
(2,629)	1:121:A:VAL:HG21	1:122:A:LEU:H	11	0.21
(2,629)	1:121:A:VAL:HG22	1:122:A:LEU:H	11	0.21
(2,629)	1:121:A:VAL:HG23	1:122:A:LEU:H	11	0.21
(2,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	2	0.21
(2,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	2	0.21
(2,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	2	0.21
(2,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	2	0.21
(2,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	2	0.21
(2,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	2	0.21
(2,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	4	0.21
(2,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	4	0.21
(2,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	4	0.21
(2,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	4	0.21
(2,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	4	0.21
(2,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	4	0.21
(2,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	8	0.21
(2,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	8	0.21
(2,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	8	0.21
(2,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	8	0.21
(2,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	8	0.21
(2,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	8	0.21
(2,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	2	0.21
(2,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	2	0.21
(2,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	2	0.21
(2,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	2	0.21
(2,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	2	0.21
(2,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	2	0.21
(2,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	4	0.21
(2,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	4	0.21
(2,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	4	0.21
(2,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	4	0.21
(2,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	4	0.21
(2,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	4	0.21
(2,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	8	0.21
(2,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	8	0.21
(2,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	8	0.21
(2,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	8	0.21
(2,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	8	0.21
(2,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	8	0.21
(2,618)	1:121:A:VAL:HG11	1:117:A:ALA:HA	6	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,618)	1:121:A:VAL:HG12	1:117:A:ALA:HA	6	0.21
(2,618)	1:121:A:VAL:HG13	1:117:A:ALA:HA	6	0.21
(2,617)	1:121:A:VAL:HG11	1:117:A:ALA:HA	6	0.21
(2,617)	1:121:A:VAL:HG12	1:117:A:ALA:HA	6	0.21
(2,617)	1:121:A:VAL:HG13	1:117:A:ALA:HA	6	0.21
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	9	0.21
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	9	0.21
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	9	0.21
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	9	0.21
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	9	0.21
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	9	0.21
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	9	0.21
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	9	0.21
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	9	0.21
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	9	0.21
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	9	0.21
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	9	0.21
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	9	0.21
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	9	0.21
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	9	0.21
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	9	0.21
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	9	0.21
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	9	0.21
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	1	0.21
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	1	0.21
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	1	0.21
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	1	0.21
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	1	0.21
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	1	0.21
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	2	0.21
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	2	0.21
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	2	0.21
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	2	0.21
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	2	0.21
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	2	0.21
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	1	0.21
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	1	0.21
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	1	0.21
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	1	0.21
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	1	0.21
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	1	0.21
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	2	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	2	0.21
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	2	0.21
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	2	0.21
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	2	0.21
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	2	0.21
(2,548)	1:116:A:PHE:H	1:115:A:TYR:H	15	0.21
(2,547)	1:116:A:PHE:H	1:115:A:TYR:H	15	0.21
(2,531)	1:113:A:LEU:HD21	1:96:A:ALA:HA	14	0.21
(2,531)	1:113:A:LEU:HD22	1:96:A:ALA:HA	14	0.21
(2,531)	1:113:A:LEU:HD23	1:96:A:ALA:HA	14	0.21
(2,527)	1:113:A:LEU:HD21	1:96:A:ALA:HA	14	0.21
(2,527)	1:113:A:LEU:HD22	1:96:A:ALA:HA	14	0.21
(2,527)	1:113:A:LEU:HD23	1:96:A:ALA:HA	14	0.21
(2,494)	1:110:A:VAL:HG21	1:113:A:LEU:HD11	10	0.21
(2,494)	1:110:A:VAL:HG21	1:113:A:LEU:HD12	10	0.21
(2,494)	1:110:A:VAL:HG21	1:113:A:LEU:HD13	10	0.21
(2,494)	1:110:A:VAL:HG21	1:113:A:LEU:HD21	10	0.21
(2,494)	1:110:A:VAL:HG21	1:113:A:LEU:HD22	10	0.21
(2,494)	1:110:A:VAL:HG21	1:113:A:LEU:HD23	10	0.21
(2,494)	1:110:A:VAL:HG22	1:113:A:LEU:HD11	10	0.21
(2,494)	1:110:A:VAL:HG22	1:113:A:LEU:HD12	10	0.21
(2,494)	1:110:A:VAL:HG22	1:113:A:LEU:HD13	10	0.21
(2,494)	1:110:A:VAL:HG22	1:113:A:LEU:HD21	10	0.21
(2,494)	1:110:A:VAL:HG22	1:113:A:LEU:HD22	10	0.21
(2,494)	1:110:A:VAL:HG22	1:113:A:LEU:HD23	10	0.21
(2,494)	1:110:A:VAL:HG23	1:113:A:LEU:HD11	10	0.21
(2,494)	1:110:A:VAL:HG23	1:113:A:LEU:HD12	10	0.21
(2,494)	1:110:A:VAL:HG23	1:113:A:LEU:HD13	10	0.21
(2,494)	1:110:A:VAL:HG23	1:113:A:LEU:HD21	10	0.21
(2,494)	1:110:A:VAL:HG23	1:113:A:LEU:HD22	10	0.21
(2,494)	1:110:A:VAL:HG23	1:113:A:LEU:HD23	10	0.21
(2,493)	1:110:A:VAL:HG21	1:113:A:LEU:HD11	10	0.21
(2,493)	1:110:A:VAL:HG21	1:113:A:LEU:HD12	10	0.21
(2,493)	1:110:A:VAL:HG21	1:113:A:LEU:HD13	10	0.21
(2,493)	1:110:A:VAL:HG21	1:113:A:LEU:HD21	10	0.21
(2,493)	1:110:A:VAL:HG21	1:113:A:LEU:HD22	10	0.21
(2,493)	1:110:A:VAL:HG21	1:113:A:LEU:HD23	10	0.21
(2,493)	1:110:A:VAL:HG22	1:113:A:LEU:HD11	10	0.21
(2,493)	1:110:A:VAL:HG22	1:113:A:LEU:HD12	10	0.21
(2,493)	1:110:A:VAL:HG22	1:113:A:LEU:HD13	10	0.21
(2,493)	1:110:A:VAL:HG22	1:113:A:LEU:HD21	10	0.21
(2,493)	1:110:A:VAL:HG22	1:113:A:LEU:HD22	10	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,493)	1:110:A:VAL:HG22	1:113:A:LEU:HD23	10	0.21
(2,493)	1:110:A:VAL:HG23	1:113:A:LEU:HD11	10	0.21
(2,493)	1:110:A:VAL:HG23	1:113:A:LEU:HD12	10	0.21
(2,493)	1:110:A:VAL:HG23	1:113:A:LEU:HD13	10	0.21
(2,493)	1:110:A:VAL:HG23	1:113:A:LEU:HD21	10	0.21
(2,493)	1:110:A:VAL:HG23	1:113:A:LEU:HD22	10	0.21
(2,493)	1:110:A:VAL:HG23	1:113:A:LEU:HD23	10	0.21
(2,486)	1:106:A:ASN:H	1:105:A:PHE:H	5	0.21
(2,485)	1:106:A:ASN:H	1:105:A:PHE:H	5	0.21
(2,484)	1:105:A:PHE:H	1:106:A:ASN:H	5	0.21
(2,483)	1:105:A:PHE:H	1:106:A:ASN:H	5	0.21
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	6	0.21
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	6	0.21
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	6	0.21
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	6	0.21
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	6	0.21
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	6	0.21
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	6	0.21
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	6	0.21
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	6	0.21
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	6	0.21
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	6	0.21
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	6	0.21
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	6	0.21
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	6	0.21
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	6	0.21
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	6	0.21
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	6	0.21
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	6	0.21
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	13	0.21
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	13	0.21
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	13	0.21
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	13	0.21
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	13	0.21
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	13	0.21
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	13	0.21
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	13	0.21
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	13	0.21
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	13	0.21
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	13	0.21
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	13	0.21
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	6	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	6	0.21
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	6	0.21
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	6	0.21
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	6	0.21
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	6	0.21
(2,188)	1:73:A:ASN:H	1:74:A:MET:H	8	0.21
(2,185)	1:73:A:ASN:H	1:74:A:MET:H	8	0.21
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	4	0.21
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	4	0.21
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	4	0.21
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	4	0.21
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	4	0.21
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	4	0.21
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	4	0.21
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	4	0.21
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	4	0.21
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	4	0.21
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	4	0.21
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	4	0.21
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	4	0.21
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	4	0.21
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	4	0.21
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	4	0.21
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	4	0.21
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	4	0.21
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	13	0.21
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	13	0.21
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	13	0.21
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	13	0.21
(2,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	3	0.21
(2,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	3	0.21
(2,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	3	0.21
(2,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	3	0.21
(2,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	3	0.21
(2,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	3	0.21
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG21	11	0.21
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG22	11	0.21
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG23	11	0.21
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG21	11	0.21
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG22	11	0.21
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG23	11	0.21
(3,686)	1:126:A:SER:H	1:125:A:LEU:HG	8	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,685)	1:126:A:SER:H	1:125:A:LEU:HG	8	0.2
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	4	0.2
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	4	0.2
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	4	0.2
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	4	0.2
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	4	0.2
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	4	0.2
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	4	0.2
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	4	0.2
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	4	0.2
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	4	0.2
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	4	0.2
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	4	0.2
(3,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	7	0.2
(3,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	7	0.2
(3,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	7	0.2
(3,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	7	0.2
(3,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	7	0.2
(3,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	7	0.2
(3,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	9	0.2
(3,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	9	0.2
(3,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	9	0.2
(3,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	9	0.2
(3,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	9	0.2
(3,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	9	0.2
(3,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	12	0.2
(3,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	12	0.2
(3,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	12	0.2
(3,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	12	0.2
(3,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	12	0.2
(3,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	12	0.2
(3,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	7	0.2
(3,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	7	0.2
(3,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	7	0.2
(3,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	7	0.2
(3,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	7	0.2
(3,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	7	0.2
(3,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	9	0.2
(3,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	9	0.2
(3,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	9	0.2
(3,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	9	0.2
(3,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	9	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	9	0.2
(3,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	12	0.2
(3,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	12	0.2
(3,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	12	0.2
(3,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	12	0.2
(3,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	12	0.2
(3,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	12	0.2
(3,548)	1:116:A:PHE:H	1:115:A:TYR:H	9	0.2
(3,548)	1:116:A:PHE:H	1:115:A:TYR:H	13	0.2
(3,547)	1:116:A:PHE:H	1:115:A:TYR:H	9	0.2
(3,547)	1:116:A:PHE:H	1:115:A:TYR:H	13	0.2
(3,518)	1:112:A:ALA:HB1	1:115:A:TYR:HD1	10	0.2
(3,518)	1:112:A:ALA:HB1	1:115:A:TYR:HD2	10	0.2
(3,518)	1:112:A:ALA:HB2	1:115:A:TYR:HD1	10	0.2
(3,518)	1:112:A:ALA:HB2	1:115:A:TYR:HD2	10	0.2
(3,518)	1:112:A:ALA:HB3	1:115:A:TYR:HD1	10	0.2
(3,518)	1:112:A:ALA:HB3	1:115:A:TYR:HD2	10	0.2
(3,517)	1:112:A:ALA:HB1	1:115:A:TYR:HD1	10	0.2
(3,517)	1:112:A:ALA:HB1	1:115:A:TYR:HD2	10	0.2
(3,517)	1:112:A:ALA:HB2	1:115:A:TYR:HD1	10	0.2
(3,517)	1:112:A:ALA:HB2	1:115:A:TYR:HD2	10	0.2
(3,517)	1:112:A:ALA:HB3	1:115:A:TYR:HD1	10	0.2
(3,517)	1:112:A:ALA:HB3	1:115:A:TYR:HD2	10	0.2
(3,470)	1:102:A:ASP:H	1:101:A:SER:HB2	8	0.2
(3,470)	1:102:A:ASP:H	1:101:A:SER:HB3	8	0.2
(3,469)	1:102:A:ASP:H	1:101:A:SER:HB2	8	0.2
(3,469)	1:102:A:ASP:H	1:101:A:SER:HB3	8	0.2
(3,446)	1:101:A:SER:H	1:102:A:ASP:H	3	0.2
(3,446)	1:101:A:SER:H	1:102:A:ASP:H	9	0.2
(3,445)	1:101:A:SER:H	1:102:A:ASP:H	3	0.2
(3,445)	1:101:A:SER:H	1:102:A:ASP:H	9	0.2
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	5	0.2
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	5	0.2
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	5	0.2
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	5	0.2
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	5	0.2
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	5	0.2
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	5	0.2
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	5	0.2
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	5	0.2
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	11	0.2
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	11	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	11	0.2
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	11	0.2
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	11	0.2
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	11	0.2
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	11	0.2
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	11	0.2
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	11	0.2
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	5	0.2
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	5	0.2
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	5	0.2
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	5	0.2
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	5	0.2
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	5	0.2
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	5	0.2
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	5	0.2
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	5	0.2
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	11	0.2
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	11	0.2
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	11	0.2
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	11	0.2
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	11	0.2
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	11	0.2
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	11	0.2
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	11	0.2
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	11	0.2
(3,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	13	0.2
(3,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	13	0.2
(3,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	13	0.2
(3,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	13	0.2
(3,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	13	0.2
(3,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	13	0.2
(3,292)	1:87:A:SER:H	1:86:A:ASP:HA	6	0.2
(3,291)	1:87:A:SER:H	1:86:A:ASP:HA	6	0.2
(3,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	2	0.2
(3,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	2	0.2
(3,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	2	0.2
(3,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	2	0.2
(3,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	2	0.2
(3,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	2	0.2
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	5	0.2
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	5	0.2
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	5	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	5	0.2
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	5	0.2
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	5	0.2
(3,188)	1:73:A:ASN:H	1:74:A:MET:H	5	0.2
(3,188)	1:73:A:ASN:H	1:74:A:MET:H	11	0.2
(3,186)	1:73:A:ASN:H	1:72:A:SER:HB2	11	0.2
(3,186)	1:73:A:ASN:H	1:72:A:SER:HB3	11	0.2
(3,185)	1:73:A:ASN:H	1:74:A:MET:H	5	0.2
(3,185)	1:73:A:ASN:H	1:74:A:MET:H	11	0.2
(3,183)	1:73:A:ASN:H	1:72:A:SER:HB2	11	0.2
(3,183)	1:73:A:ASN:H	1:72:A:SER:HB3	11	0.2
(3,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	5	0.2
(3,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	5	0.2
(3,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	5	0.2
(3,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	5	0.2
(3,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	5	0.2
(3,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	5	0.2
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	15	0.2
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	15	0.2
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	15	0.2
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	15	0.2
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	15	0.2
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	15	0.2
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	15	0.2
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	15	0.2
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	15	0.2
(3,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	5	0.2
(3,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	5	0.2
(3,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	5	0.2
(3,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	5	0.2
(3,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	5	0.2
(3,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	5	0.2
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	15	0.2
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	15	0.2
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	15	0.2
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	15	0.2
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	15	0.2
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	15	0.2
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	15	0.2
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	15	0.2
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	15	0.2
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG21	5	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG22	5	0.2
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG23	5	0.2
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG21	5	0.2
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG22	5	0.2
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG23	5	0.2
(3,118)	1:63:A:LEU:H	1:63:A:LEU:HG	1	0.2
(3,117)	1:63:A:LEU:H	1:63:A:LEU:HG	1	0.2
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	14	0.2
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	14	0.2
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	14	0.2
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	14	0.2
(3,82)	1:60:A:SER:H	1:59:A:LEU:HG	4	0.2
(3,81)	1:60:A:SER:H	1:59:A:LEU:HG	4	0.2
(3,34)	1:56:A:THR:H	1:55:A:SER:HB2	1	0.2
(3,34)	1:56:A:THR:H	1:55:A:SER:HB3	1	0.2
(3,33)	1:56:A:THR:H	1:55:A:SER:HB2	1	0.2
(3,33)	1:56:A:THR:H	1:55:A:SER:HB3	1	0.2
(3,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	5	0.2
(3,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	5	0.2
(3,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	5	0.2
(3,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	5	0.2
(3,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	5	0.2
(3,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	5	0.2
(3,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	5	0.2
(3,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	5	0.2
(3,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	5	0.2
(3,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	5	0.2
(3,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	5	0.2
(3,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	5	0.2
(2,686)	1:126:A:SER:H	1:125:A:LEU:HG	8	0.2
(2,685)	1:126:A:SER:H	1:125:A:LEU:HG	8	0.2
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	4	0.2
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	4	0.2
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	4	0.2
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	4	0.2
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	4	0.2
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	4	0.2
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	4	0.2
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	4	0.2
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	4	0.2
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	4	0.2
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	4	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	4	0.2
(2,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	7	0.2
(2,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	7	0.2
(2,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	7	0.2
(2,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	7	0.2
(2,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	7	0.2
(2,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	7	0.2
(2,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	9	0.2
(2,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	9	0.2
(2,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	9	0.2
(2,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	9	0.2
(2,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	9	0.2
(2,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	9	0.2
(2,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	12	0.2
(2,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	12	0.2
(2,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	12	0.2
(2,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	12	0.2
(2,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	12	0.2
(2,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	12	0.2
(2,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	7	0.2
(2,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	7	0.2
(2,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	7	0.2
(2,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	7	0.2
(2,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	7	0.2
(2,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	7	0.2
(2,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	9	0.2
(2,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	9	0.2
(2,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	9	0.2
(2,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	9	0.2
(2,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	9	0.2
(2,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	9	0.2
(2,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	12	0.2
(2,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	12	0.2
(2,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	12	0.2
(2,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	12	0.2
(2,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	12	0.2
(2,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	12	0.2
(2,548)	1:116:A:PHE:H	1:115:A:TYR:H	9	0.2
(2,548)	1:116:A:PHE:H	1:115:A:TYR:H	13	0.2
(2,547)	1:116:A:PHE:H	1:115:A:TYR:H	9	0.2
(2,547)	1:116:A:PHE:H	1:115:A:TYR:H	13	0.2
(2,518)	1:112:A:ALA:HB1	1:115:A:TYR:HD1	10	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,518)	1:112:A:ALA:HB1	1:115:A:TYR:HD2	10	0.2
(2,518)	1:112:A:ALA:HB2	1:115:A:TYR:HD1	10	0.2
(2,518)	1:112:A:ALA:HB2	1:115:A:TYR:HD2	10	0.2
(2,518)	1:112:A:ALA:HB3	1:115:A:TYR:HD1	10	0.2
(2,518)	1:112:A:ALA:HB3	1:115:A:TYR:HD2	10	0.2
(2,517)	1:112:A:ALA:HB1	1:115:A:TYR:HD1	10	0.2
(2,517)	1:112:A:ALA:HB1	1:115:A:TYR:HD2	10	0.2
(2,517)	1:112:A:ALA:HB2	1:115:A:TYR:HD1	10	0.2
(2,517)	1:112:A:ALA:HB2	1:115:A:TYR:HD2	10	0.2
(2,517)	1:112:A:ALA:HB3	1:115:A:TYR:HD1	10	0.2
(2,517)	1:112:A:ALA:HB3	1:115:A:TYR:HD2	10	0.2
(2,470)	1:102:A:ASP:H	1:101:A:SER:HB2	8	0.2
(2,470)	1:102:A:ASP:H	1:101:A:SER:HB3	8	0.2
(2,469)	1:102:A:ASP:H	1:101:A:SER:HB2	8	0.2
(2,469)	1:102:A:ASP:H	1:101:A:SER:HB3	8	0.2
(2,446)	1:101:A:SER:H	1:102:A:ASP:H	3	0.2
(2,446)	1:101:A:SER:H	1:102:A:ASP:H	9	0.2
(2,445)	1:101:A:SER:H	1:102:A:ASP:H	3	0.2
(2,445)	1:101:A:SER:H	1:102:A:ASP:H	9	0.2
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	5	0.2
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	5	0.2
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	5	0.2
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	5	0.2
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	5	0.2
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	5	0.2
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	5	0.2
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	5	0.2
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	5	0.2
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	11	0.2
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	11	0.2
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	11	0.2
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	11	0.2
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	11	0.2
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	11	0.2
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	11	0.2
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	11	0.2
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	11	0.2
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	5	0.2
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	5	0.2
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	5	0.2
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	5	0.2
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	5	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	5	0.2
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	5	0.2
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	5	0.2
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	5	0.2
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	11	0.2
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	11	0.2
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	11	0.2
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	11	0.2
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	11	0.2
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	11	0.2
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	11	0.2
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	11	0.2
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	11	0.2
(2,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	13	0.2
(2,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	13	0.2
(2,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	13	0.2
(2,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	13	0.2
(2,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	13	0.2
(2,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	13	0.2
(2,292)	1:87:A:SER:H	1:86:A:ASP:HA	6	0.2
(2,291)	1:87:A:SER:H	1:86:A:ASP:HA	6	0.2
(2,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	2	0.2
(2,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	2	0.2
(2,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	2	0.2
(2,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	2	0.2
(2,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	2	0.2
(2,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	2	0.2
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	5	0.2
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	5	0.2
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	5	0.2
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	5	0.2
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	5	0.2
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	5	0.2
(2,188)	1:73:A:ASN:H	1:74:A:MET:H	5	0.2
(2,188)	1:73:A:ASN:H	1:74:A:MET:H	11	0.2
(2,186)	1:73:A:ASN:H	1:72:A:SER:HB2	11	0.2
(2,186)	1:73:A:ASN:H	1:72:A:SER:HB3	11	0.2
(2,185)	1:73:A:ASN:H	1:74:A:MET:H	5	0.2
(2,185)	1:73:A:ASN:H	1:74:A:MET:H	11	0.2
(2,183)	1:73:A:ASN:H	1:72:A:SER:HB2	11	0.2
(2,183)	1:73:A:ASN:H	1:72:A:SER:HB3	11	0.2
(2,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	5	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	5	0.2
(2,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	5	0.2
(2,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	5	0.2
(2,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	5	0.2
(2,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	5	0.2
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	15	0.2
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	15	0.2
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	15	0.2
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	15	0.2
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	15	0.2
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	15	0.2
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	15	0.2
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	15	0.2
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	15	0.2
(2,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	5	0.2
(2,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	5	0.2
(2,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	5	0.2
(2,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	5	0.2
(2,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	5	0.2
(2,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	5	0.2
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	15	0.2
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	15	0.2
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	15	0.2
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	15	0.2
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	15	0.2
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	15	0.2
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	15	0.2
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	15	0.2
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	15	0.2
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG21	5	0.2
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG22	5	0.2
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG23	5	0.2
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG21	5	0.2
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG22	5	0.2
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG23	5	0.2
(2,118)	1:63:A:LEU:H	1:63:A:LEU:HG	1	0.2
(2,117)	1:63:A:LEU:H	1:63:A:LEU:HG	1	0.2
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	14	0.2
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	14	0.2
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	14	0.2
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	14	0.2
(2,82)	1:60:A:SER:H	1:59:A:LEU:HG	4	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,81)	1:60:A:SER:H	1:59:A:LEU:HG	4	0.2
(2,34)	1:56:A:THR:H	1:55:A:SER:HB2	1	0.2
(2,34)	1:56:A:THR:H	1:55:A:SER:HB3	1	0.2
(2,33)	1:56:A:THR:H	1:55:A:SER:HB2	1	0.2
(2,33)	1:56:A:THR:H	1:55:A:SER:HB3	1	0.2
(2,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	5	0.2
(2,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	5	0.2
(2,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	5	0.2
(2,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	5	0.2
(2,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	5	0.2
(2,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	5	0.2
(2,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	5	0.2
(2,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	5	0.2
(2,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	5	0.2
(2,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	5	0.2
(2,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	5	0.2
(2,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	5	0.2
(3,702)	1:128:A:LYS:H	1:127:A:THR:HB	8	0.19
(3,701)	1:128:A:LYS:H	1:127:A:THR:HB	8	0.19
(3,694)	1:127:A:THR:H	1:128:A:LYS:H	2	0.19
(3,693)	1:127:A:THR:H	1:128:A:LYS:H	2	0.19
(3,686)	1:126:A:SER:H	1:125:A:LEU:HG	4	0.19
(3,685)	1:126:A:SER:H	1:125:A:LEU:HG	4	0.19
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	12	0.19
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	12	0.19
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	12	0.19
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	12	0.19
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	12	0.19
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	12	0.19
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	12	0.19
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	12	0.19
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	12	0.19
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	12	0.19
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	12	0.19
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	12	0.19
(3,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	15	0.19
(3,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	15	0.19
(3,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	15	0.19
(3,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	15	0.19
(3,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	15	0.19
(3,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	15	0.19
(3,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	15	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	15	0.19
(3,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	15	0.19
(3,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	15	0.19
(3,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	15	0.19
(3,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	15	0.19
(3,624)	1:121:A:VAL:HG21	1:122:A:LEU:HG	6	0.19
(3,624)	1:121:A:VAL:HG22	1:122:A:LEU:HG	6	0.19
(3,624)	1:121:A:VAL:HG23	1:122:A:LEU:HG	6	0.19
(3,623)	1:121:A:VAL:HG21	1:122:A:LEU:HG	6	0.19
(3,623)	1:121:A:VAL:HG22	1:122:A:LEU:HG	6	0.19
(3,623)	1:121:A:VAL:HG23	1:122:A:LEU:HG	6	0.19
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	8	0.19
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	8	0.19
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	8	0.19
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	8	0.19
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	8	0.19
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	8	0.19
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	8	0.19
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	8	0.19
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	8	0.19
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	8	0.19
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	8	0.19
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	8	0.19
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB2	6	0.19
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB3	6	0.19
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB2	6	0.19
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB3	6	0.19
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	6	0.19
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	6	0.19
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	6	0.19
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	6	0.19
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	6	0.19
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	6	0.19
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	6	0.19
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	6	0.19
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	6	0.19
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	6	0.19
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	6	0.19
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	6	0.19
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	6	0.19
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	6	0.19
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	6	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	6	0.19
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	6	0.19
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	6	0.19
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD11	15	0.19
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD12	15	0.19
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD13	15	0.19
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD11	15	0.19
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD12	15	0.19
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD13	15	0.19
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD11	15	0.19
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD12	15	0.19
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD13	15	0.19
(3,226)	1:81:A:ALA:H	1:83:A:VAL:H	3	0.19
(3,226)	1:81:A:ALA:H	1:83:A:VAL:H	7	0.19
(3,226)	1:81:A:ALA:H	1:83:A:VAL:H	8	0.19
(3,222)	1:81:A:ALA:H	1:83:A:VAL:H	3	0.19
(3,222)	1:81:A:ALA:H	1:83:A:VAL:H	7	0.19
(3,222)	1:81:A:ALA:H	1:83:A:VAL:H	8	0.19
(3,218)	1:80:A:ILE:HD11	1:116:A:PHE:HE1	3	0.19
(3,218)	1:80:A:ILE:HD11	1:116:A:PHE:HE2	3	0.19
(3,218)	1:80:A:ILE:HD12	1:116:A:PHE:HE1	3	0.19
(3,218)	1:80:A:ILE:HD12	1:116:A:PHE:HE2	3	0.19
(3,218)	1:80:A:ILE:HD13	1:116:A:PHE:HE1	3	0.19
(3,218)	1:80:A:ILE:HD13	1:116:A:PHE:HE2	3	0.19
(3,217)	1:80:A:ILE:HD11	1:116:A:PHE:HE1	3	0.19
(3,217)	1:80:A:ILE:HD11	1:116:A:PHE:HE2	3	0.19
(3,217)	1:80:A:ILE:HD12	1:116:A:PHE:HE1	3	0.19
(3,217)	1:80:A:ILE:HD12	1:116:A:PHE:HE2	3	0.19
(3,217)	1:80:A:ILE:HD13	1:116:A:PHE:HE1	3	0.19
(3,217)	1:80:A:ILE:HD13	1:116:A:PHE:HE2	3	0.19
(3,209)	1:77:A:GLN:H	1:76:A:LEU:HG	8	0.19
(3,206)	1:77:A:GLN:H	1:76:A:LEU:HG	8	0.19
(3,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	7	0.19
(3,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	7	0.19
(3,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	7	0.19
(3,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	7	0.19
(3,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	7	0.19
(3,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	7	0.19
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	13	0.19
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	13	0.19
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	13	0.19
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	13	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	13	0.19
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	13	0.19
(3,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	7	0.19
(3,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	7	0.19
(3,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	7	0.19
(3,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	7	0.19
(3,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	7	0.19
(3,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	7	0.19
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	13	0.19
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	13	0.19
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	13	0.19
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	13	0.19
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	13	0.19
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	13	0.19
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB1	11	0.19
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB2	11	0.19
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB3	11	0.19
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB1	12	0.19
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB2	12	0.19
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB3	12	0.19
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB1	11	0.19
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB2	11	0.19
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB3	11	0.19
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB1	12	0.19
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB2	12	0.19
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB3	12	0.19
(3,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	6	0.19
(3,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	6	0.19
(3,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	6	0.19
(3,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	6	0.19
(3,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	6	0.19
(3,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	6	0.19
(3,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	13	0.19
(3,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	13	0.19
(3,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	13	0.19
(3,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	13	0.19
(3,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	13	0.19
(3,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	13	0.19
(3,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	6	0.19
(3,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	6	0.19
(3,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	6	0.19
(3,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	6	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	6	0.19
(3,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	6	0.19
(3,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	13	0.19
(3,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	13	0.19
(3,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	13	0.19
(3,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	13	0.19
(3,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	13	0.19
(3,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	13	0.19
(3,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	5	0.19
(3,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	5	0.19
(3,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	5	0.19
(3,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	5	0.19
(3,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	5	0.19
(3,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	5	0.19
(2,702)	1:128:A:LYS:H	1:127:A:THR:HB	8	0.19
(2,701)	1:128:A:LYS:H	1:127:A:THR:HB	8	0.19
(2,694)	1:127:A:THR:H	1:128:A:LYS:H	2	0.19
(2,693)	1:127:A:THR:H	1:128:A:LYS:H	2	0.19
(2,686)	1:126:A:SER:H	1:125:A:LEU:HG	4	0.19
(2,685)	1:126:A:SER:H	1:125:A:LEU:HG	4	0.19
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	12	0.19
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	12	0.19
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	12	0.19
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	12	0.19
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	12	0.19
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	12	0.19
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	12	0.19
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	12	0.19
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	12	0.19
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	12	0.19
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	12	0.19
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	12	0.19
(2,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	15	0.19
(2,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	15	0.19
(2,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	15	0.19
(2,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	15	0.19
(2,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	15	0.19
(2,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	15	0.19
(2,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	15	0.19
(2,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	15	0.19
(2,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	15	0.19
(2,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	15	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	15	0.19
(2,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	15	0.19
(2,624)	1:121:A:VAL:HG21	1:122:A:LEU:HG	6	0.19
(2,624)	1:121:A:VAL:HG22	1:122:A:LEU:HG	6	0.19
(2,624)	1:121:A:VAL:HG23	1:122:A:LEU:HG	6	0.19
(2,623)	1:121:A:VAL:HG21	1:122:A:LEU:HG	6	0.19
(2,623)	1:121:A:VAL:HG22	1:122:A:LEU:HG	6	0.19
(2,623)	1:121:A:VAL:HG23	1:122:A:LEU:HG	6	0.19
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	8	0.19
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	8	0.19
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	8	0.19
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	8	0.19
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	8	0.19
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	8	0.19
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	8	0.19
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	8	0.19
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	8	0.19
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	8	0.19
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	8	0.19
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	8	0.19
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB2	6	0.19
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB3	6	0.19
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB2	6	0.19
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB3	6	0.19
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	6	0.19
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	6	0.19
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	6	0.19
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	6	0.19
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	6	0.19
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	6	0.19
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	6	0.19
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	6	0.19
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	6	0.19
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	6	0.19
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	6	0.19
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	6	0.19
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	6	0.19
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	6	0.19
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	6	0.19
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	6	0.19
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	6	0.19
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	6	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD11	15	0.19
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD12	15	0.19
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD13	15	0.19
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD11	15	0.19
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD12	15	0.19
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD13	15	0.19
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD11	15	0.19
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD12	15	0.19
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD13	15	0.19
(2,226)	1:81:A:ALA:H	1:83:A:VAL:H	3	0.19
(2,226)	1:81:A:ALA:H	1:83:A:VAL:H	7	0.19
(2,226)	1:81:A:ALA:H	1:83:A:VAL:H	8	0.19
(2,222)	1:81:A:ALA:H	1:83:A:VAL:H	3	0.19
(2,222)	1:81:A:ALA:H	1:83:A:VAL:H	7	0.19
(2,222)	1:81:A:ALA:H	1:83:A:VAL:H	8	0.19
(2,218)	1:80:A:ILE:HD11	1:116:A:PHE:HE1	3	0.19
(2,218)	1:80:A:ILE:HD11	1:116:A:PHE:HE2	3	0.19
(2,218)	1:80:A:ILE:HD12	1:116:A:PHE:HE1	3	0.19
(2,218)	1:80:A:ILE:HD12	1:116:A:PHE:HE2	3	0.19
(2,218)	1:80:A:ILE:HD13	1:116:A:PHE:HE1	3	0.19
(2,218)	1:80:A:ILE:HD13	1:116:A:PHE:HE2	3	0.19
(2,217)	1:80:A:ILE:HD11	1:116:A:PHE:HE1	3	0.19
(2,217)	1:80:A:ILE:HD11	1:116:A:PHE:HE2	3	0.19
(2,217)	1:80:A:ILE:HD12	1:116:A:PHE:HE1	3	0.19
(2,217)	1:80:A:ILE:HD12	1:116:A:PHE:HE2	3	0.19
(2,217)	1:80:A:ILE:HD13	1:116:A:PHE:HE1	3	0.19
(2,217)	1:80:A:ILE:HD13	1:116:A:PHE:HE2	3	0.19
(2,209)	1:77:A:GLN:H	1:76:A:LEU:HG	8	0.19
(2,206)	1:77:A:GLN:H	1:76:A:LEU:HG	8	0.19
(2,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	7	0.19
(2,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	7	0.19
(2,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	7	0.19
(2,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	7	0.19
(2,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	7	0.19
(2,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	7	0.19
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	13	0.19
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	13	0.19
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	13	0.19
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	13	0.19
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	13	0.19
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	13	0.19
(2,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	7	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	7	0.19
(2,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	7	0.19
(2,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	7	0.19
(2,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	7	0.19
(2,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	7	0.19
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	13	0.19
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	13	0.19
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	13	0.19
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	13	0.19
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	13	0.19
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	13	0.19
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB1	11	0.19
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB2	11	0.19
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB3	11	0.19
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB1	12	0.19
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB2	12	0.19
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB3	12	0.19
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB1	11	0.19
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB2	11	0.19
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB3	11	0.19
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB1	12	0.19
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB2	12	0.19
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB3	12	0.19
(2,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	6	0.19
(2,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	6	0.19
(2,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	6	0.19
(2,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	6	0.19
(2,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	6	0.19
(2,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	6	0.19
(2,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	13	0.19
(2,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	13	0.19
(2,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	13	0.19
(2,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	13	0.19
(2,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	13	0.19
(2,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	13	0.19
(2,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	6	0.19
(2,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	6	0.19
(2,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	6	0.19
(2,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	6	0.19
(2,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	6	0.19
(2,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	6	0.19
(2,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	13	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	13	0.19
(2,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	13	0.19
(2,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	13	0.19
(2,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	13	0.19
(2,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	13	0.19
(2,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	5	0.19
(2,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	5	0.19
(2,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	5	0.19
(2,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	5	0.19
(2,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	5	0.19
(2,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	5	0.19
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG21	10	0.19
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG22	10	0.19
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG23	10	0.19
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG21	10	0.19
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG22	10	0.19
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG23	10	0.19
(3,700)	1:127:A:THR:HG21	1:128:A:LYS:H	1	0.18
(3,700)	1:127:A:THR:HG22	1:128:A:LYS:H	1	0.18
(3,700)	1:127:A:THR:HG23	1:128:A:LYS:H	1	0.18
(3,699)	1:127:A:THR:HG21	1:128:A:LYS:H	1	0.18
(3,699)	1:127:A:THR:HG22	1:128:A:LYS:H	1	0.18
(3,699)	1:127:A:THR:HG23	1:128:A:LYS:H	1	0.18
(3,686)	1:126:A:SER:H	1:125:A:LEU:HG	10	0.18
(3,685)	1:126:A:SER:H	1:125:A:LEU:HG	10	0.18
(3,672)	1:125:A:LEU:H	1:126:A:SER:HA	2	0.18
(3,672)	1:125:A:LEU:H	1:126:A:SER:HA	15	0.18
(3,671)	1:125:A:LEU:H	1:126:A:SER:HA	2	0.18
(3,671)	1:125:A:LEU:H	1:126:A:SER:HA	15	0.18
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	7	0.18
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	7	0.18
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	7	0.18
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	7	0.18
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	7	0.18
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	7	0.18
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	14	0.18
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	14	0.18
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	14	0.18
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	14	0.18
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	14	0.18
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	14	0.18
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	7	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	7	0.18
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	7	0.18
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	7	0.18
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	7	0.18
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	7	0.18
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	14	0.18
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	14	0.18
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	14	0.18
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	14	0.18
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	14	0.18
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	14	0.18
(3,446)	1:101:A:SER:H	1:102:A:ASP:H	7	0.18
(3,446)	1:101:A:SER:H	1:102:A:ASP:H	12	0.18
(3,446)	1:101:A:SER:H	1:102:A:ASP:H	15	0.18
(3,445)	1:101:A:SER:H	1:102:A:ASP:H	7	0.18
(3,445)	1:101:A:SER:H	1:102:A:ASP:H	12	0.18
(3,445)	1:101:A:SER:H	1:102:A:ASP:H	15	0.18
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	10	0.18
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	10	0.18
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	10	0.18
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	10	0.18
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	10	0.18
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	10	0.18
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	15	0.18
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	15	0.18
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	15	0.18
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	15	0.18
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	15	0.18
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	15	0.18
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	10	0.18
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	10	0.18
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	10	0.18
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	10	0.18
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	10	0.18
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	10	0.18
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	15	0.18
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	15	0.18
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	15	0.18
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	15	0.18
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	15	0.18
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	15	0.18
(3,300)	1:90:A:GLU:H	1:89:A:ARG:HB2	6	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,300)	1:90:A:GLU:H	1:89:A:ARG:HB3	6	0.18
(3,299)	1:90:A:GLU:H	1:89:A:ARG:HB2	6	0.18
(3,299)	1:90:A:GLU:H	1:89:A:ARG:HB3	6	0.18
(3,292)	1:87:A:SER:H	1:86:A:ASP:HA	7	0.18
(3,292)	1:87:A:SER:H	1:86:A:ASP:HA	12	0.18
(3,291)	1:87:A:SER:H	1:86:A:ASP:HA	7	0.18
(3,291)	1:87:A:SER:H	1:86:A:ASP:HA	12	0.18
(3,272)	1:84:A:ASP:H	1:85:A:THR:HA	6	0.18
(3,271)	1:84:A:ASP:H	1:85:A:THR:HA	6	0.18
(3,246)	1:83:A:VAL:H	1:82:A:ALA:HA	6	0.18
(3,245)	1:83:A:VAL:H	1:82:A:ALA:HA	6	0.18
(3,226)	1:81:A:ALA:H	1:83:A:VAL:H	15	0.18
(3,222)	1:81:A:ALA:H	1:83:A:VAL:H	15	0.18
(3,186)	1:73:A:ASN:H	1:72:A:SER:HB2	12	0.18
(3,186)	1:73:A:ASN:H	1:72:A:SER:HB3	12	0.18
(3,183)	1:73:A:ASN:H	1:72:A:SER:HB2	12	0.18
(3,183)	1:73:A:ASN:H	1:72:A:SER:HB3	12	0.18
(3,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	6	0.18
(3,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	6	0.18
(3,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	6	0.18
(3,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	6	0.18
(3,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	6	0.18
(3,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	6	0.18
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	10	0.18
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	10	0.18
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	10	0.18
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	10	0.18
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	10	0.18
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	10	0.18
(3,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	6	0.18
(3,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	6	0.18
(3,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	6	0.18
(3,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	6	0.18
(3,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	6	0.18
(3,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	6	0.18
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	10	0.18
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	10	0.18
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	10	0.18
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	10	0.18
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	10	0.18
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	10	0.18
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	10	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	10	0.18
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	10	0.18
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	10	0.18
(3,82)	1:60:A:SER:H	1:59:A:LEU:HG	15	0.18
(3,81)	1:60:A:SER:H	1:59:A:LEU:HG	15	0.18
(3,34)	1:56:A:THR:H	1:55:A:SER:HB2	5	0.18
(3,34)	1:56:A:THR:H	1:55:A:SER:HB3	5	0.18
(3,34)	1:56:A:THR:H	1:55:A:SER:HB2	10	0.18
(3,34)	1:56:A:THR:H	1:55:A:SER:HB3	10	0.18
(3,33)	1:56:A:THR:H	1:55:A:SER:HB2	5	0.18
(3,33)	1:56:A:THR:H	1:55:A:SER:HB3	5	0.18
(3,33)	1:56:A:THR:H	1:55:A:SER:HB2	10	0.18
(3,33)	1:56:A:THR:H	1:55:A:SER:HB3	10	0.18
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB1	1	0.18
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB2	1	0.18
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB3	1	0.18
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB1	9	0.18
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB2	9	0.18
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB3	9	0.18
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB1	1	0.18
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB2	1	0.18
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB3	1	0.18
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB1	9	0.18
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB2	9	0.18
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB3	9	0.18
(3,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	11	0.18
(3,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	11	0.18
(3,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	11	0.18
(3,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	13	0.18
(3,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	13	0.18
(3,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	13	0.18
(3,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	11	0.18
(3,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	11	0.18
(3,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	11	0.18
(3,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	13	0.18
(3,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	13	0.18
(3,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	13	0.18
(2,700)	1:127:A:THR:HG21	1:128:A:LYS:H	1	0.18
(2,700)	1:127:A:THR:HG22	1:128:A:LYS:H	1	0.18
(2,700)	1:127:A:THR:HG23	1:128:A:LYS:H	1	0.18
(2,699)	1:127:A:THR:HG21	1:128:A:LYS:H	1	0.18
(2,699)	1:127:A:THR:HG22	1:128:A:LYS:H	1	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,699)	1:127:A:THR:HG23	1:128:A:LYS:H	1	0.18
(2,686)	1:126:A:SER:H	1:125:A:LEU:HG	10	0.18
(2,685)	1:126:A:SER:H	1:125:A:LEU:HG	10	0.18
(2,672)	1:125:A:LEU:H	1:126:A:SER:HA	2	0.18
(2,672)	1:125:A:LEU:H	1:126:A:SER:HA	15	0.18
(2,671)	1:125:A:LEU:H	1:126:A:SER:HA	2	0.18
(2,671)	1:125:A:LEU:H	1:126:A:SER:HA	15	0.18
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	7	0.18
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	7	0.18
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	7	0.18
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	7	0.18
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	7	0.18
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	7	0.18
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	14	0.18
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	14	0.18
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	14	0.18
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	14	0.18
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	14	0.18
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	14	0.18
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	7	0.18
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	7	0.18
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	7	0.18
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	7	0.18
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	7	0.18
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	7	0.18
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	14	0.18
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	14	0.18
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	14	0.18
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	14	0.18
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	14	0.18
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	14	0.18
(2,446)	1:101:A:SER:H	1:102:A:ASP:H	7	0.18
(2,446)	1:101:A:SER:H	1:102:A:ASP:H	12	0.18
(2,446)	1:101:A:SER:H	1:102:A:ASP:H	15	0.18
(2,445)	1:101:A:SER:H	1:102:A:ASP:H	7	0.18
(2,445)	1:101:A:SER:H	1:102:A:ASP:H	12	0.18
(2,445)	1:101:A:SER:H	1:102:A:ASP:H	15	0.18
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	10	0.18
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	10	0.18
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	10	0.18
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	10	0.18
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	10	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	10	0.18
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	15	0.18
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	15	0.18
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	15	0.18
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	15	0.18
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	15	0.18
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	15	0.18
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	10	0.18
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	10	0.18
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	10	0.18
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	10	0.18
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	10	0.18
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	10	0.18
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	15	0.18
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	15	0.18
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	15	0.18
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	15	0.18
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	15	0.18
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	15	0.18
(2,300)	1:90:A:GLU:H	1:89:A:ARG:HB2	6	0.18
(2,300)	1:90:A:GLU:H	1:89:A:ARG:HB3	6	0.18
(2,299)	1:90:A:GLU:H	1:89:A:ARG:HB2	6	0.18
(2,299)	1:90:A:GLU:H	1:89:A:ARG:HB3	6	0.18
(2,292)	1:87:A:SER:H	1:86:A:ASP:HA	7	0.18
(2,292)	1:87:A:SER:H	1:86:A:ASP:HA	12	0.18
(2,291)	1:87:A:SER:H	1:86:A:ASP:HA	7	0.18
(2,291)	1:87:A:SER:H	1:86:A:ASP:HA	12	0.18
(2,272)	1:84:A:ASP:H	1:85:A:THR:HA	6	0.18
(2,271)	1:84:A:ASP:H	1:85:A:THR:HA	6	0.18
(2,246)	1:83:A:VAL:H	1:82:A:ALA:HA	6	0.18
(2,245)	1:83:A:VAL:H	1:82:A:ALA:HA	6	0.18
(2,226)	1:81:A:ALA:H	1:83:A:VAL:H	15	0.18
(2,222)	1:81:A:ALA:H	1:83:A:VAL:H	15	0.18
(2,186)	1:73:A:ASN:H	1:72:A:SER:HB2	12	0.18
(2,186)	1:73:A:ASN:H	1:72:A:SER:HB3	12	0.18
(2,183)	1:73:A:ASN:H	1:72:A:SER:HB2	12	0.18
(2,183)	1:73:A:ASN:H	1:72:A:SER:HB3	12	0.18
(2,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	6	0.18
(2,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	6	0.18
(2,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	6	0.18
(2,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	6	0.18
(2,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	6	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	6	0.18
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	10	0.18
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	10	0.18
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	10	0.18
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	10	0.18
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	10	0.18
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	10	0.18
(2,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	6	0.18
(2,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	6	0.18
(2,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	6	0.18
(2,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	6	0.18
(2,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	6	0.18
(2,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	6	0.18
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	10	0.18
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	10	0.18
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	10	0.18
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	10	0.18
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	10	0.18
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	10	0.18
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	10	0.18
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	10	0.18
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	10	0.18
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	10	0.18
(2,82)	1:60:A:SER:H	1:59:A:LEU:HG	15	0.18
(2,81)	1:60:A:SER:H	1:59:A:LEU:HG	15	0.18
(2,34)	1:56:A:THR:H	1:55:A:SER:HB2	5	0.18
(2,34)	1:56:A:THR:H	1:55:A:SER:HB3	5	0.18
(2,34)	1:56:A:THR:H	1:55:A:SER:HB2	10	0.18
(2,34)	1:56:A:THR:H	1:55:A:SER:HB3	10	0.18
(2,33)	1:56:A:THR:H	1:55:A:SER:HB2	5	0.18
(2,33)	1:56:A:THR:H	1:55:A:SER:HB3	5	0.18
(2,33)	1:56:A:THR:H	1:55:A:SER:HB2	10	0.18
(2,33)	1:56:A:THR:H	1:55:A:SER:HB3	10	0.18
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB1	1	0.18
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB2	1	0.18
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB3	1	0.18
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB1	9	0.18
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB2	9	0.18
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB3	9	0.18
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB1	1	0.18
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB2	1	0.18
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB3	1	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB1	9	0.18
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB2	9	0.18
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB3	9	0.18
(2,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	11	0.18
(2,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	11	0.18
(2,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	11	0.18
(2,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	13	0.18
(2,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	13	0.18
(2,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	13	0.18
(2,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	11	0.18
(2,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	11	0.18
(2,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	11	0.18
(2,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	13	0.18
(2,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	13	0.18
(2,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	13	0.18
(3,672)	1:125:A:LEU:H	1:126:A:SER:HA	13	0.17
(3,671)	1:125:A:LEU:H	1:126:A:SER:HA	13	0.17
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	12	0.17
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	12	0.17
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	12	0.17
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	12	0.17
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	12	0.17
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	12	0.17
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	12	0.17
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	12	0.17
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	12	0.17
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	12	0.17
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	12	0.17
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	12	0.17
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	12	0.17
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	12	0.17
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	12	0.17
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	12	0.17
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	12	0.17
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	12	0.17
(3,548)	1:116:A:PHE:H	1:115:A:TYR:H	4	0.17
(3,548)	1:116:A:PHE:H	1:115:A:TYR:H	7	0.17
(3,547)	1:116:A:PHE:H	1:115:A:TYR:H	4	0.17
(3,547)	1:116:A:PHE:H	1:115:A:TYR:H	7	0.17
(3,531)	1:113:A:LEU:HD21	1:96:A:ALA:HA	8	0.17
(3,531)	1:113:A:LEU:HD22	1:96:A:ALA:HA	8	0.17
(3,531)	1:113:A:LEU:HD23	1:96:A:ALA:HA	8	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,527)	1:113:A:LEU:HD21	1:96:A:ALA:HA	8	0.17
(3,527)	1:113:A:LEU:HD22	1:96:A:ALA:HA	8	0.17
(3,527)	1:113:A:LEU:HD23	1:96:A:ALA:HA	8	0.17
(3,486)	1:106:A:ASN:H	1:105:A:PHE:H	8	0.17
(3,485)	1:106:A:ASN:H	1:105:A:PHE:H	8	0.17
(3,484)	1:105:A:PHE:H	1:106:A:ASN:H	8	0.17
(3,483)	1:105:A:PHE:H	1:106:A:ASN:H	8	0.17
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB2	2	0.17
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB3	2	0.17
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB2	13	0.17
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB3	13	0.17
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB2	2	0.17
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB3	2	0.17
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB2	13	0.17
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB3	13	0.17
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	2	0.17
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	2	0.17
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	2	0.17
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	3	0.17
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	3	0.17
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	3	0.17
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	2	0.17
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	2	0.17
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	2	0.17
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	3	0.17
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	3	0.17
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	3	0.17
(3,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	10	0.17
(3,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	10	0.17
(3,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	10	0.17
(3,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	15	0.17
(3,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	15	0.17
(3,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	15	0.17
(3,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	10	0.17
(3,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	10	0.17
(3,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	10	0.17
(3,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	15	0.17
(3,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	15	0.17
(3,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	15	0.17
(3,300)	1:90:A:GLU:H	1:89:A:ARG:HB2	9	0.17
(3,300)	1:90:A:GLU:H	1:89:A:ARG:HB3	9	0.17
(3,299)	1:90:A:GLU:H	1:89:A:ARG:HB2	9	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,299)	1:90:A:GLU:H	1:89:A:ARG:HB3	9	0.17
(3,274)	1:85:A:THR:H	1:84:A:ASP:HB2	5	0.17
(3,274)	1:85:A:THR:H	1:84:A:ASP:HB3	5	0.17
(3,273)	1:85:A:THR:H	1:84:A:ASP:HB2	5	0.17
(3,273)	1:85:A:THR:H	1:84:A:ASP:HB3	5	0.17
(3,272)	1:84:A:ASP:H	1:85:A:THR:HA	14	0.17
(3,271)	1:84:A:ASP:H	1:85:A:THR:HA	14	0.17
(3,262)	1:84:A:ASP:H	1:83:A:VAL:H	2	0.17
(3,261)	1:84:A:ASP:H	1:83:A:VAL:H	2	0.17
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD11	6	0.17
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD12	6	0.17
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD13	6	0.17
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD11	6	0.17
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD12	6	0.17
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD13	6	0.17
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD11	6	0.17
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD12	6	0.17
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD13	6	0.17
(3,248)	1:83:A:VAL:H	1:84:A:ASP:H	2	0.17
(3,247)	1:83:A:VAL:H	1:84:A:ASP:H	2	0.17
(3,244)	1:83:A:VAL:H	1:82:A:ALA:HB1	10	0.17
(3,244)	1:83:A:VAL:H	1:82:A:ALA:HB2	10	0.17
(3,244)	1:83:A:VAL:H	1:82:A:ALA:HB3	10	0.17
(3,243)	1:83:A:VAL:H	1:82:A:ALA:HB1	10	0.17
(3,243)	1:83:A:VAL:H	1:82:A:ALA:HB2	10	0.17
(3,243)	1:83:A:VAL:H	1:82:A:ALA:HB3	10	0.17
(3,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	9	0.17
(3,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	9	0.17
(3,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	9	0.17
(3,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	12	0.17
(3,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	12	0.17
(3,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	12	0.17
(3,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	13	0.17
(3,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	13	0.17
(3,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	13	0.17
(3,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	9	0.17
(3,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	9	0.17
(3,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	9	0.17
(3,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	12	0.17
(3,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	12	0.17
(3,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	12	0.17
(3,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	13	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	13	0.17
(3,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	13	0.17
(3,226)	1:81:A:ALA:H	1:83:A:VAL:H	14	0.17
(3,222)	1:81:A:ALA:H	1:83:A:VAL:H	14	0.17
(3,188)	1:73:A:ASN:H	1:74:A:MET:H	14	0.17
(3,185)	1:73:A:ASN:H	1:74:A:MET:H	14	0.17
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG21	8	0.17
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG22	8	0.17
(3,134)	1:67:A:GLY:H	1:66:A:ILE:HG23	8	0.17
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG21	8	0.17
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG22	8	0.17
(3,133)	1:67:A:GLY:H	1:66:A:ILE:HG23	8	0.17
(3,34)	1:56:A:THR:H	1:55:A:SER:HB2	4	0.17
(3,34)	1:56:A:THR:H	1:55:A:SER:HB3	4	0.17
(3,34)	1:56:A:THR:H	1:55:A:SER:HB2	8	0.17
(3,34)	1:56:A:THR:H	1:55:A:SER:HB3	8	0.17
(3,33)	1:56:A:THR:H	1:55:A:SER:HB2	4	0.17
(3,33)	1:56:A:THR:H	1:55:A:SER:HB3	4	0.17
(3,33)	1:56:A:THR:H	1:55:A:SER:HB2	8	0.17
(3,33)	1:56:A:THR:H	1:55:A:SER:HB3	8	0.17
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB1	5	0.17
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB2	5	0.17
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB3	5	0.17
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB1	6	0.17
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB2	6	0.17
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB3	6	0.17
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB1	7	0.17
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB2	7	0.17
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB3	7	0.17
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB1	5	0.17
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB2	5	0.17
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB3	5	0.17
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB1	6	0.17
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB2	6	0.17
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB3	6	0.17
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB1	7	0.17
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB2	7	0.17
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB3	7	0.17
(3,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	10	0.17
(3,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	10	0.17
(3,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	10	0.17
(3,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	10	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	10	0.17
(3,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	10	0.17
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB1	12	0.17
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB2	12	0.17
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB3	12	0.17
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB1	12	0.17
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB2	12	0.17
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB3	12	0.17
(2,672)	1:125:A:LEU:H	1:126:A:SER:HA	13	0.17
(2,671)	1:125:A:LEU:H	1:126:A:SER:HA	13	0.17
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	12	0.17
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	12	0.17
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	12	0.17
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	12	0.17
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	12	0.17
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	12	0.17
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	12	0.17
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	12	0.17
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	12	0.17
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	12	0.17
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	12	0.17
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	12	0.17
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	12	0.17
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	12	0.17
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	12	0.17
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	12	0.17
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	12	0.17
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	12	0.17
(2,548)	1:116:A:PHE:H	1:115:A:TYR:H	4	0.17
(2,548)	1:116:A:PHE:H	1:115:A:TYR:H	7	0.17
(2,547)	1:116:A:PHE:H	1:115:A:TYR:H	4	0.17
(2,547)	1:116:A:PHE:H	1:115:A:TYR:H	7	0.17
(2,531)	1:113:A:LEU:HD21	1:96:A:ALA:HA	8	0.17
(2,531)	1:113:A:LEU:HD22	1:96:A:ALA:HA	8	0.17
(2,531)	1:113:A:LEU:HD23	1:96:A:ALA:HA	8	0.17
(2,527)	1:113:A:LEU:HD21	1:96:A:ALA:HA	8	0.17
(2,527)	1:113:A:LEU:HD22	1:96:A:ALA:HA	8	0.17
(2,527)	1:113:A:LEU:HD23	1:96:A:ALA:HA	8	0.17
(2,486)	1:106:A:ASN:H	1:105:A:PHE:H	8	0.17
(2,485)	1:106:A:ASN:H	1:105:A:PHE:H	8	0.17
(2,484)	1:105:A:PHE:H	1:106:A:ASN:H	8	0.17
(2,483)	1:105:A:PHE:H	1:106:A:ASN:H	8	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB2	2	0.17
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB3	2	0.17
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB2	13	0.17
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB3	13	0.17
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB2	2	0.17
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB3	2	0.17
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB2	13	0.17
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB3	13	0.17
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	2	0.17
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	2	0.17
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	2	0.17
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	3	0.17
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	3	0.17
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	3	0.17
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	2	0.17
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	2	0.17
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	2	0.17
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	3	0.17
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	3	0.17
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	3	0.17
(2,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	10	0.17
(2,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	10	0.17
(2,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	10	0.17
(2,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	15	0.17
(2,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	15	0.17
(2,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	15	0.17
(2,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	10	0.17
(2,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	10	0.17
(2,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	10	0.17
(2,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	15	0.17
(2,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	15	0.17
(2,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	15	0.17
(2,300)	1:90:A:GLU:H	1:89:A:ARG:HB2	9	0.17
(2,300)	1:90:A:GLU:H	1:89:A:ARG:HB3	9	0.17
(2,299)	1:90:A:GLU:H	1:89:A:ARG:HB2	9	0.17
(2,299)	1:90:A:GLU:H	1:89:A:ARG:HB3	9	0.17
(2,274)	1:85:A:THR:H	1:84:A:ASP:HB2	5	0.17
(2,274)	1:85:A:THR:H	1:84:A:ASP:HB3	5	0.17
(2,273)	1:85:A:THR:H	1:84:A:ASP:HB2	5	0.17
(2,273)	1:85:A:THR:H	1:84:A:ASP:HB3	5	0.17
(2,272)	1:84:A:ASP:H	1:85:A:THR:HA	14	0.17
(2,271)	1:84:A:ASP:H	1:85:A:THR:HA	14	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,262)	1:84:A:ASP:H	1:83:A:VAL:H	2	0.17
(2,261)	1:84:A:ASP:H	1:83:A:VAL:H	2	0.17
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD11	6	0.17
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD12	6	0.17
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD13	6	0.17
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD11	6	0.17
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD12	6	0.17
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD13	6	0.17
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD11	6	0.17
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD12	6	0.17
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD13	6	0.17
(2,248)	1:83:A:VAL:H	1:84:A:ASP:H	2	0.17
(2,247)	1:83:A:VAL:H	1:84:A:ASP:H	2	0.17
(2,244)	1:83:A:VAL:H	1:82:A:ALA:HB1	10	0.17
(2,244)	1:83:A:VAL:H	1:82:A:ALA:HB2	10	0.17
(2,244)	1:83:A:VAL:H	1:82:A:ALA:HB3	10	0.17
(2,243)	1:83:A:VAL:H	1:82:A:ALA:HB1	10	0.17
(2,243)	1:83:A:VAL:H	1:82:A:ALA:HB2	10	0.17
(2,243)	1:83:A:VAL:H	1:82:A:ALA:HB3	10	0.17
(2,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	9	0.17
(2,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	9	0.17
(2,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	9	0.17
(2,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	12	0.17
(2,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	12	0.17
(2,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	12	0.17
(2,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	13	0.17
(2,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	13	0.17
(2,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	13	0.17
(2,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	9	0.17
(2,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	9	0.17
(2,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	9	0.17
(2,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	12	0.17
(2,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	12	0.17
(2,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	12	0.17
(2,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	13	0.17
(2,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	13	0.17
(2,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	13	0.17
(2,226)	1:81:A:ALA:H	1:83:A:VAL:H	14	0.17
(2,222)	1:81:A:ALA:H	1:83:A:VAL:H	14	0.17
(2,188)	1:73:A:ASN:H	1:74:A:MET:H	14	0.17
(2,185)	1:73:A:ASN:H	1:74:A:MET:H	14	0.17
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG21	8	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG22	8	0.17
(2,134)	1:67:A:GLY:H	1:66:A:ILE:HG23	8	0.17
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG21	8	0.17
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG22	8	0.17
(2,133)	1:67:A:GLY:H	1:66:A:ILE:HG23	8	0.17
(2,34)	1:56:A:THR:H	1:55:A:SER:HB2	4	0.17
(2,34)	1:56:A:THR:H	1:55:A:SER:HB3	4	0.17
(2,34)	1:56:A:THR:H	1:55:A:SER:HB2	8	0.17
(2,34)	1:56:A:THR:H	1:55:A:SER:HB3	8	0.17
(2,33)	1:56:A:THR:H	1:55:A:SER:HB2	4	0.17
(2,33)	1:56:A:THR:H	1:55:A:SER:HB3	4	0.17
(2,33)	1:56:A:THR:H	1:55:A:SER:HB2	8	0.17
(2,33)	1:56:A:THR:H	1:55:A:SER:HB3	8	0.17
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB1	5	0.17
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB2	5	0.17
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB3	5	0.17
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB1	6	0.17
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB2	6	0.17
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB3	6	0.17
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB1	7	0.17
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB2	7	0.17
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB3	7	0.17
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB1	5	0.17
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB2	5	0.17
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB3	5	0.17
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB1	6	0.17
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB2	6	0.17
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB3	6	0.17
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB1	7	0.17
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB2	7	0.17
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB3	7	0.17
(2,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	10	0.17
(2,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	10	0.17
(2,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	10	0.17
(2,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	10	0.17
(2,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	10	0.17
(2,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	10	0.17
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB1	12	0.17
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB2	12	0.17
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB3	12	0.17
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB1	12	0.17
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB2	12	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB3	12	0.17
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG21	6	0.17
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG22	6	0.17
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG23	6	0.17
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG21	6	0.17
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG22	6	0.17
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG23	6	0.17
(1,20)	1:70:A:LEU:HD11	1:66:A:ILE:HG21	2	0.17
(1,20)	1:70:A:LEU:HD11	1:66:A:ILE:HG22	2	0.17
(1,20)	1:70:A:LEU:HD11	1:66:A:ILE:HG23	2	0.17
(1,20)	1:70:A:LEU:HD12	1:66:A:ILE:HG21	2	0.17
(1,20)	1:70:A:LEU:HD12	1:66:A:ILE:HG22	2	0.17
(1,20)	1:70:A:LEU:HD12	1:66:A:ILE:HG23	2	0.17
(1,20)	1:70:A:LEU:HD13	1:66:A:ILE:HG21	2	0.17
(1,20)	1:70:A:LEU:HD13	1:66:A:ILE:HG22	2	0.17
(1,20)	1:70:A:LEU:HD13	1:66:A:ILE:HG23	2	0.17
(1,20)	1:70:A:LEU:HD11	1:66:A:ILE:HG21	5	0.17
(1,20)	1:70:A:LEU:HD11	1:66:A:ILE:HG22	5	0.17
(1,20)	1:70:A:LEU:HD11	1:66:A:ILE:HG23	5	0.17
(1,20)	1:70:A:LEU:HD12	1:66:A:ILE:HG21	5	0.17
(1,20)	1:70:A:LEU:HD12	1:66:A:ILE:HG22	5	0.17
(1,20)	1:70:A:LEU:HD12	1:66:A:ILE:HG23	5	0.17
(1,20)	1:70:A:LEU:HD13	1:66:A:ILE:HG21	5	0.17
(1,20)	1:70:A:LEU:HD13	1:66:A:ILE:HG22	5	0.17
(1,20)	1:70:A:LEU:HD13	1:66:A:ILE:HG23	5	0.17
(1,19)	1:70:A:LEU:HD11	1:66:A:ILE:HG21	2	0.17
(1,19)	1:70:A:LEU:HD11	1:66:A:ILE:HG22	2	0.17
(1,19)	1:70:A:LEU:HD11	1:66:A:ILE:HG23	2	0.17
(1,19)	1:70:A:LEU:HD12	1:66:A:ILE:HG21	2	0.17
(1,19)	1:70:A:LEU:HD12	1:66:A:ILE:HG22	2	0.17
(1,19)	1:70:A:LEU:HD12	1:66:A:ILE:HG23	2	0.17
(1,19)	1:70:A:LEU:HD13	1:66:A:ILE:HG21	2	0.17
(1,19)	1:70:A:LEU:HD13	1:66:A:ILE:HG22	2	0.17
(1,19)	1:70:A:LEU:HD13	1:66:A:ILE:HG23	2	0.17
(1,19)	1:70:A:LEU:HD11	1:66:A:ILE:HG21	5	0.17
(1,19)	1:70:A:LEU:HD11	1:66:A:ILE:HG22	5	0.17
(1,19)	1:70:A:LEU:HD11	1:66:A:ILE:HG23	5	0.17
(1,19)	1:70:A:LEU:HD12	1:66:A:ILE:HG21	5	0.17
(1,19)	1:70:A:LEU:HD12	1:66:A:ILE:HG22	5	0.17
(1,19)	1:70:A:LEU:HD12	1:66:A:ILE:HG23	5	0.17
(1,19)	1:70:A:LEU:HD13	1:66:A:ILE:HG21	5	0.17
(1,19)	1:70:A:LEU:HD13	1:66:A:ILE:HG22	5	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:70:A:LEU:HD13	1:66:A:ILE:HG23	5	0.17
(1,12)	1:66:A:ILE:HG21	1:70:A:LEU:HD11	2	0.17
(1,12)	1:66:A:ILE:HG21	1:70:A:LEU:HD12	2	0.17
(1,12)	1:66:A:ILE:HG21	1:70:A:LEU:HD13	2	0.17
(1,12)	1:66:A:ILE:HG22	1:70:A:LEU:HD11	2	0.17
(1,12)	1:66:A:ILE:HG22	1:70:A:LEU:HD12	2	0.17
(1,12)	1:66:A:ILE:HG22	1:70:A:LEU:HD13	2	0.17
(1,12)	1:66:A:ILE:HG23	1:70:A:LEU:HD11	2	0.17
(1,12)	1:66:A:ILE:HG23	1:70:A:LEU:HD12	2	0.17
(1,12)	1:66:A:ILE:HG23	1:70:A:LEU:HD13	2	0.17
(1,12)	1:66:A:ILE:HG21	1:70:A:LEU:HD11	5	0.17
(1,12)	1:66:A:ILE:HG21	1:70:A:LEU:HD12	5	0.17
(1,12)	1:66:A:ILE:HG21	1:70:A:LEU:HD13	5	0.17
(1,12)	1:66:A:ILE:HG22	1:70:A:LEU:HD11	5	0.17
(1,12)	1:66:A:ILE:HG22	1:70:A:LEU:HD12	5	0.17
(1,12)	1:66:A:ILE:HG22	1:70:A:LEU:HD13	5	0.17
(1,12)	1:66:A:ILE:HG23	1:70:A:LEU:HD11	5	0.17
(1,12)	1:66:A:ILE:HG23	1:70:A:LEU:HD12	5	0.17
(1,12)	1:66:A:ILE:HG23	1:70:A:LEU:HD13	5	0.17
(1,11)	1:66:A:ILE:HG21	1:70:A:LEU:HD11	2	0.17
(1,11)	1:66:A:ILE:HG21	1:70:A:LEU:HD12	2	0.17
(1,11)	1:66:A:ILE:HG21	1:70:A:LEU:HD13	2	0.17
(1,11)	1:66:A:ILE:HG22	1:70:A:LEU:HD11	2	0.17
(1,11)	1:66:A:ILE:HG22	1:70:A:LEU:HD12	2	0.17
(1,11)	1:66:A:ILE:HG22	1:70:A:LEU:HD13	2	0.17
(1,11)	1:66:A:ILE:HG23	1:70:A:LEU:HD11	2	0.17
(1,11)	1:66:A:ILE:HG23	1:70:A:LEU:HD12	2	0.17
(1,11)	1:66:A:ILE:HG23	1:70:A:LEU:HD13	2	0.17
(1,11)	1:66:A:ILE:HG21	1:70:A:LEU:HD11	5	0.17
(1,11)	1:66:A:ILE:HG21	1:70:A:LEU:HD12	5	0.17
(1,11)	1:66:A:ILE:HG21	1:70:A:LEU:HD13	5	0.17
(1,11)	1:66:A:ILE:HG22	1:70:A:LEU:HD11	5	0.17
(1,11)	1:66:A:ILE:HG22	1:70:A:LEU:HD12	5	0.17
(1,11)	1:66:A:ILE:HG22	1:70:A:LEU:HD13	5	0.17
(1,11)	1:66:A:ILE:HG23	1:70:A:LEU:HD11	5	0.17
(1,11)	1:66:A:ILE:HG23	1:70:A:LEU:HD12	5	0.17
(1,11)	1:66:A:ILE:HG23	1:70:A:LEU:HD13	5	0.17
(3,686)	1:126:A:SER:H	1:125:A:LEU:HG	14	0.16
(3,685)	1:126:A:SER:H	1:125:A:LEU:HG	14	0.16
(3,672)	1:125:A:LEU:H	1:126:A:SER:HA	5	0.16
(3,672)	1:125:A:LEU:H	1:126:A:SER:HA	7	0.16
(3,671)	1:125:A:LEU:H	1:126:A:SER:HA	5	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,671)	1:125:A:LEU:H	1:126:A:SER:HA	7	0.16
(3,470)	1:102:A:ASP:H	1:101:A:SER:HB2	3	0.16
(3,470)	1:102:A:ASP:H	1:101:A:SER:HB3	3	0.16
(3,470)	1:102:A:ASP:H	1:101:A:SER:HB2	6	0.16
(3,470)	1:102:A:ASP:H	1:101:A:SER:HB3	6	0.16
(3,470)	1:102:A:ASP:H	1:101:A:SER:HB2	11	0.16
(3,470)	1:102:A:ASP:H	1:101:A:SER:HB3	11	0.16
(3,469)	1:102:A:ASP:H	1:101:A:SER:HB2	3	0.16
(3,469)	1:102:A:ASP:H	1:101:A:SER:HB3	3	0.16
(3,469)	1:102:A:ASP:H	1:101:A:SER:HB2	6	0.16
(3,469)	1:102:A:ASP:H	1:101:A:SER:HB3	6	0.16
(3,469)	1:102:A:ASP:H	1:101:A:SER:HB2	11	0.16
(3,469)	1:102:A:ASP:H	1:101:A:SER:HB3	11	0.16
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB2	14	0.16
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB3	14	0.16
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB2	14	0.16
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB3	14	0.16
(3,446)	1:101:A:SER:H	1:102:A:ASP:H	8	0.16
(3,446)	1:101:A:SER:H	1:102:A:ASP:H	11	0.16
(3,445)	1:101:A:SER:H	1:102:A:ASP:H	8	0.16
(3,445)	1:101:A:SER:H	1:102:A:ASP:H	11	0.16
(3,436)	1:99:A:MET:H	1:97:A:ALA:HA	6	0.16
(3,435)	1:99:A:MET:H	1:97:A:ALA:HA	6	0.16
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	14	0.16
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	14	0.16
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	14	0.16
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	14	0.16
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	14	0.16
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	14	0.16
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	1	0.16
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	1	0.16
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	1	0.16
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	1	0.16
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	1	0.16
(3,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	1	0.16
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	1	0.16
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	1	0.16
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	1	0.16
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	1	0.16
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	1	0.16
(3,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	1	0.16
(3,264)	1:84:A:ASP:H	1:83:A:VAL:HG11	8	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,264)	1:84:A:ASP:H	1:83:A:VAL:HG12	8	0.16
(3,264)	1:84:A:ASP:H	1:83:A:VAL:HG13	8	0.16
(3,263)	1:84:A:ASP:H	1:83:A:VAL:HG11	8	0.16
(3,263)	1:84:A:ASP:H	1:83:A:VAL:HG12	8	0.16
(3,263)	1:84:A:ASP:H	1:83:A:VAL:HG13	8	0.16
(3,226)	1:81:A:ALA:H	1:83:A:VAL:H	4	0.16
(3,222)	1:81:A:ALA:H	1:83:A:VAL:H	4	0.16
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	12	0.16
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	12	0.16
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	12	0.16
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	12	0.16
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	12	0.16
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	12	0.16
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	7	0.16
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	7	0.16
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	7	0.16
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	7	0.16
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	7	0.16
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	7	0.16
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	7	0.16
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	7	0.16
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	7	0.16
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	7	0.16
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	7	0.16
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	7	0.16
(3,82)	1:60:A:SER:H	1:59:A:LEU:HG	1	0.16
(3,81)	1:60:A:SER:H	1:59:A:LEU:HG	1	0.16
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB1	4	0.16
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB2	4	0.16
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB3	4	0.16
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB1	10	0.16
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB2	10	0.16
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB3	10	0.16
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB1	13	0.16
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB2	13	0.16
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB3	13	0.16
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB1	4	0.16
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB2	4	0.16
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB3	4	0.16
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB1	10	0.16
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB2	10	0.16
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB3	10	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB1	13	0.16
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB2	13	0.16
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB3	13	0.16
(3,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	2	0.16
(3,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	2	0.16
(3,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	2	0.16
(3,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	6	0.16
(3,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	6	0.16
(3,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	6	0.16
(3,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	7	0.16
(3,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	7	0.16
(3,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	7	0.16
(3,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	8	0.16
(3,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	8	0.16
(3,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	8	0.16
(3,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	2	0.16
(3,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	2	0.16
(3,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	2	0.16
(3,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	6	0.16
(3,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	6	0.16
(3,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	6	0.16
(3,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	7	0.16
(3,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	7	0.16
(3,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	7	0.16
(3,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	8	0.16
(3,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	8	0.16
(3,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	8	0.16
(2,686)	1:126:A:SER:H	1:125:A:LEU:HG	14	0.16
(2,685)	1:126:A:SER:H	1:125:A:LEU:HG	14	0.16
(2,672)	1:125:A:LEU:H	1:126:A:SER:HA	5	0.16
(2,672)	1:125:A:LEU:H	1:126:A:SER:HA	7	0.16
(2,671)	1:125:A:LEU:H	1:126:A:SER:HA	5	0.16
(2,671)	1:125:A:LEU:H	1:126:A:SER:HA	7	0.16
(2,470)	1:102:A:ASP:H	1:101:A:SER:HB2	3	0.16
(2,470)	1:102:A:ASP:H	1:101:A:SER:HB3	3	0.16
(2,470)	1:102:A:ASP:H	1:101:A:SER:HB2	6	0.16
(2,470)	1:102:A:ASP:H	1:101:A:SER:HB3	6	0.16
(2,470)	1:102:A:ASP:H	1:101:A:SER:HB2	11	0.16
(2,470)	1:102:A:ASP:H	1:101:A:SER:HB3	11	0.16
(2,469)	1:102:A:ASP:H	1:101:A:SER:HB2	3	0.16
(2,469)	1:102:A:ASP:H	1:101:A:SER:HB3	3	0.16
(2,469)	1:102:A:ASP:H	1:101:A:SER:HB2	6	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,469)	1:102:A:ASP:H	1:101:A:SER:HB3	6	0.16
(2,469)	1:102:A:ASP:H	1:101:A:SER:HB2	11	0.16
(2,469)	1:102:A:ASP:H	1:101:A:SER:HB3	11	0.16
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB2	14	0.16
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB3	14	0.16
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB2	14	0.16
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB3	14	0.16
(2,446)	1:101:A:SER:H	1:102:A:ASP:H	8	0.16
(2,446)	1:101:A:SER:H	1:102:A:ASP:H	11	0.16
(2,445)	1:101:A:SER:H	1:102:A:ASP:H	8	0.16
(2,445)	1:101:A:SER:H	1:102:A:ASP:H	11	0.16
(2,436)	1:99:A:MET:H	1:97:A:ALA:HA	6	0.16
(2,435)	1:99:A:MET:H	1:97:A:ALA:HA	6	0.16
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	14	0.16
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	14	0.16
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	14	0.16
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	14	0.16
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	14	0.16
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	14	0.16
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG11	1	0.16
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG12	1	0.16
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG13	1	0.16
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG21	1	0.16
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG22	1	0.16
(2,330)	1:92:A:PHE:H	1:91:A:VAL:HG23	1	0.16
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG11	1	0.16
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG12	1	0.16
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG13	1	0.16
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG21	1	0.16
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG22	1	0.16
(2,329)	1:92:A:PHE:H	1:91:A:VAL:HG23	1	0.16
(2,264)	1:84:A:ASP:H	1:83:A:VAL:HG11	8	0.16
(2,264)	1:84:A:ASP:H	1:83:A:VAL:HG12	8	0.16
(2,264)	1:84:A:ASP:H	1:83:A:VAL:HG13	8	0.16
(2,263)	1:84:A:ASP:H	1:83:A:VAL:HG11	8	0.16
(2,263)	1:84:A:ASP:H	1:83:A:VAL:HG12	8	0.16
(2,263)	1:84:A:ASP:H	1:83:A:VAL:HG13	8	0.16
(2,226)	1:81:A:ALA:H	1:83:A:VAL:H	4	0.16
(2,222)	1:81:A:ALA:H	1:83:A:VAL:H	4	0.16
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	12	0.16
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	12	0.16
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	12	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	12	0.16
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	12	0.16
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	12	0.16
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	7	0.16
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	7	0.16
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	7	0.16
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	7	0.16
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	7	0.16
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	7	0.16
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	7	0.16
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	7	0.16
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	7	0.16
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	7	0.16
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	7	0.16
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	7	0.16
(2,82)	1:60:A:SER:H	1:59:A:LEU:HG	1	0.16
(2,81)	1:60:A:SER:H	1:59:A:LEU:HG	1	0.16
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB1	4	0.16
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB2	4	0.16
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB3	4	0.16
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB1	10	0.16
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB2	10	0.16
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB3	10	0.16
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB1	13	0.16
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB2	13	0.16
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB3	13	0.16
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB1	4	0.16
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB2	4	0.16
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB3	4	0.16
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB1	10	0.16
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB2	10	0.16
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB3	10	0.16
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB1	13	0.16
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB2	13	0.16
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB3	13	0.16
(2,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	2	0.16
(2,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	2	0.16
(2,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	2	0.16
(2,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	6	0.16
(2,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	6	0.16
(2,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	6	0.16
(2,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	7	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	7	0.16
(2,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	7	0.16
(2,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	8	0.16
(2,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	8	0.16
(2,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	8	0.16
(2,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	2	0.16
(2,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	2	0.16
(2,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	2	0.16
(2,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	6	0.16
(2,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	6	0.16
(2,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	6	0.16
(2,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	7	0.16
(2,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	7	0.16
(2,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	7	0.16
(2,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	8	0.16
(2,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	8	0.16
(2,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	8	0.16
(3,686)	1:126:A:SER:H	1:125:A:LEU:HG	7	0.15
(3,685)	1:126:A:SER:H	1:125:A:LEU:HG	7	0.15
(3,672)	1:125:A:LEU:H	1:126:A:SER:HA	9	0.15
(3,672)	1:125:A:LEU:H	1:126:A:SER:HA	10	0.15
(3,671)	1:125:A:LEU:H	1:126:A:SER:HA	9	0.15
(3,671)	1:125:A:LEU:H	1:126:A:SER:HA	10	0.15
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	8	0.15
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	8	0.15
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	8	0.15
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	8	0.15
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	8	0.15
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	8	0.15
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	8	0.15
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	8	0.15
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	8	0.15
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	8	0.15
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	8	0.15
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	8	0.15
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	6	0.15
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	6	0.15
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	6	0.15
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	6	0.15
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	6	0.15
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	6	0.15
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	6	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	6	0.15
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	6	0.15
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	15	0.15
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	15	0.15
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	15	0.15
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	15	0.15
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	15	0.15
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	15	0.15
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	15	0.15
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	15	0.15
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	15	0.15
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	6	0.15
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	6	0.15
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	6	0.15
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	6	0.15
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	6	0.15
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	6	0.15
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	6	0.15
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	6	0.15
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	6	0.15
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	15	0.15
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	15	0.15
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	15	0.15
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	15	0.15
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	15	0.15
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	15	0.15
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	15	0.15
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	15	0.15
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	15	0.15
(3,586)	1:120:A:LEU:H	1:117:A:ALA:HA	1	0.15
(3,585)	1:120:A:LEU:H	1:117:A:ALA:HA	1	0.15
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	4	0.15
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	4	0.15
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	4	0.15
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	4	0.15
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	4	0.15
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	4	0.15
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	4	0.15
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	4	0.15
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	4	0.15
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	4	0.15
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	4	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	4	0.15
(3,548)	1:116:A:PHE:H	1:115:A:TYR:H	3	0.15
(3,548)	1:116:A:PHE:H	1:115:A:TYR:H	14	0.15
(3,547)	1:116:A:PHE:H	1:115:A:TYR:H	3	0.15
(3,547)	1:116:A:PHE:H	1:115:A:TYR:H	14	0.15
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	11	0.15
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	11	0.15
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	11	0.15
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	11	0.15
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	11	0.15
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	11	0.15
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	13	0.15
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	13	0.15
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	13	0.15
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	13	0.15
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	13	0.15
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	13	0.15
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	11	0.15
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	11	0.15
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	11	0.15
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	11	0.15
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	11	0.15
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	11	0.15
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	13	0.15
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	13	0.15
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	13	0.15
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	13	0.15
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	13	0.15
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	13	0.15
(3,486)	1:106:A:ASN:H	1:105:A:PHE:H	9	0.15
(3,485)	1:106:A:ASN:H	1:105:A:PHE:H	9	0.15
(3,484)	1:105:A:PHE:H	1:106:A:ASN:H	9	0.15
(3,483)	1:105:A:PHE:H	1:106:A:ASN:H	9	0.15
(3,470)	1:102:A:ASP:H	1:101:A:SER:HB2	10	0.15
(3,470)	1:102:A:ASP:H	1:101:A:SER:HB3	10	0.15
(3,469)	1:102:A:ASP:H	1:101:A:SER:HB2	10	0.15
(3,469)	1:102:A:ASP:H	1:101:A:SER:HB3	10	0.15
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	8	0.15
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	8	0.15
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	8	0.15
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	8	0.15
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	8	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	8	0.15
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	8	0.15
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	8	0.15
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	8	0.15
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	8	0.15
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	8	0.15
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	8	0.15
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	8	0.15
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	8	0.15
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	8	0.15
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	8	0.15
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	8	0.15
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	8	0.15
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	5	0.15
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	5	0.15
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	5	0.15
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	5	0.15
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	5	0.15
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	5	0.15
(3,316)	1:91:A:VAL:HG11	1:83:A:VAL:HA	13	0.15
(3,316)	1:91:A:VAL:HG12	1:83:A:VAL:HA	13	0.15
(3,316)	1:91:A:VAL:HG13	1:83:A:VAL:HA	13	0.15
(3,316)	1:91:A:VAL:HG11	1:83:A:VAL:HA	15	0.15
(3,316)	1:91:A:VAL:HG12	1:83:A:VAL:HA	15	0.15
(3,316)	1:91:A:VAL:HG13	1:83:A:VAL:HA	15	0.15
(3,315)	1:91:A:VAL:HG11	1:83:A:VAL:HA	13	0.15
(3,315)	1:91:A:VAL:HG12	1:83:A:VAL:HA	13	0.15
(3,315)	1:91:A:VAL:HG13	1:83:A:VAL:HA	13	0.15
(3,315)	1:91:A:VAL:HG11	1:83:A:VAL:HA	15	0.15
(3,315)	1:91:A:VAL:HG12	1:83:A:VAL:HA	15	0.15
(3,315)	1:91:A:VAL:HG13	1:83:A:VAL:HA	15	0.15
(3,302)	1:90:A:GLU:H	1:89:A:ARG:HD2	5	0.15
(3,302)	1:90:A:GLU:H	1:89:A:ARG:HD3	5	0.15
(3,301)	1:90:A:GLU:H	1:89:A:ARG:HD2	5	0.15
(3,301)	1:90:A:GLU:H	1:89:A:ARG:HD3	5	0.15
(3,300)	1:90:A:GLU:H	1:89:A:ARG:HB2	2	0.15
(3,300)	1:90:A:GLU:H	1:89:A:ARG:HB3	2	0.15
(3,299)	1:90:A:GLU:H	1:89:A:ARG:HB2	2	0.15
(3,299)	1:90:A:GLU:H	1:89:A:ARG:HB3	2	0.15
(3,254)	1:83:A:VAL:HG21	1:120:A:LEU:HD21	9	0.15
(3,254)	1:83:A:VAL:HG21	1:120:A:LEU:HD22	9	0.15
(3,254)	1:83:A:VAL:HG21	1:120:A:LEU:HD23	9	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,254)	1:83:A:VAL:HG22	1:120:A:LEU:HD21	9	0.15
(3,254)	1:83:A:VAL:HG22	1:120:A:LEU:HD22	9	0.15
(3,254)	1:83:A:VAL:HG22	1:120:A:LEU:HD23	9	0.15
(3,254)	1:83:A:VAL:HG23	1:120:A:LEU:HD21	9	0.15
(3,254)	1:83:A:VAL:HG23	1:120:A:LEU:HD22	9	0.15
(3,254)	1:83:A:VAL:HG23	1:120:A:LEU:HD23	9	0.15
(3,246)	1:83:A:VAL:H	1:82:A:ALA:HA	10	0.15
(3,246)	1:83:A:VAL:H	1:82:A:ALA:HA	13	0.15
(3,245)	1:83:A:VAL:H	1:82:A:ALA:HA	10	0.15
(3,245)	1:83:A:VAL:H	1:82:A:ALA:HA	13	0.15
(3,244)	1:83:A:VAL:H	1:82:A:ALA:HB1	1	0.15
(3,244)	1:83:A:VAL:H	1:82:A:ALA:HB2	1	0.15
(3,244)	1:83:A:VAL:H	1:82:A:ALA:HB3	1	0.15
(3,243)	1:83:A:VAL:H	1:82:A:ALA:HB1	1	0.15
(3,243)	1:83:A:VAL:H	1:82:A:ALA:HB2	1	0.15
(3,243)	1:83:A:VAL:H	1:82:A:ALA:HB3	1	0.15
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	15	0.15
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	15	0.15
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	15	0.15
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	15	0.15
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	15	0.15
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	15	0.15
(3,188)	1:73:A:ASN:H	1:74:A:MET:H	2	0.15
(3,188)	1:73:A:ASN:H	1:74:A:MET:H	3	0.15
(3,188)	1:73:A:ASN:H	1:74:A:MET:H	9	0.15
(3,185)	1:73:A:ASN:H	1:74:A:MET:H	2	0.15
(3,185)	1:73:A:ASN:H	1:74:A:MET:H	3	0.15
(3,185)	1:73:A:ASN:H	1:74:A:MET:H	9	0.15
(3,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	10	0.15
(3,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	10	0.15
(3,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	10	0.15
(3,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	10	0.15
(3,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	10	0.15
(3,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	10	0.15
(3,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	10	0.15
(3,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	10	0.15
(3,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	10	0.15
(3,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	10	0.15
(3,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	10	0.15
(3,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	10	0.15
(3,136)	1:67:A:GLY:H	1:66:A:ILE:HB	3	0.15
(3,136)	1:67:A:GLY:H	1:66:A:ILE:HB	11	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,135)	1:67:A:GLY:H	1:66:A:ILE:HB	3	0.15
(3,135)	1:67:A:GLY:H	1:66:A:ILE:HB	11	0.15
(3,34)	1:56:A:THR:H	1:55:A:SER:HB2	7	0.15
(3,34)	1:56:A:THR:H	1:55:A:SER:HB3	7	0.15
(3,33)	1:56:A:THR:H	1:55:A:SER:HB2	7	0.15
(3,33)	1:56:A:THR:H	1:55:A:SER:HB3	7	0.15
(3,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	3	0.15
(3,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	3	0.15
(3,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	3	0.15
(3,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	3	0.15
(3,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	3	0.15
(3,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	3	0.15
(3,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	3	0.15
(3,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	3	0.15
(3,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	3	0.15
(3,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	3	0.15
(3,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	3	0.15
(3,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	3	0.15
(3,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	12	0.15
(3,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	12	0.15
(3,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	12	0.15
(3,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	12	0.15
(3,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	12	0.15
(3,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	12	0.15
(2,686)	1:126:A:SER:H	1:125:A:LEU:HG	7	0.15
(2,685)	1:126:A:SER:H	1:125:A:LEU:HG	7	0.15
(2,672)	1:125:A:LEU:H	1:126:A:SER:HA	9	0.15
(2,672)	1:125:A:LEU:H	1:126:A:SER:HA	10	0.15
(2,671)	1:125:A:LEU:H	1:126:A:SER:HA	9	0.15
(2,671)	1:125:A:LEU:H	1:126:A:SER:HA	10	0.15
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	8	0.15
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	8	0.15
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	8	0.15
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	8	0.15
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	8	0.15
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	8	0.15
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	8	0.15
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	8	0.15
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	8	0.15
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	8	0.15
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	8	0.15
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	8	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	6	0.15
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	6	0.15
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	6	0.15
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	6	0.15
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	6	0.15
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	6	0.15
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	6	0.15
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	6	0.15
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	6	0.15
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	15	0.15
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	15	0.15
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	15	0.15
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	15	0.15
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	15	0.15
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	15	0.15
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	15	0.15
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	15	0.15
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	15	0.15
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	6	0.15
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	6	0.15
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	6	0.15
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	6	0.15
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	6	0.15
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	6	0.15
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	6	0.15
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	6	0.15
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	6	0.15
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	15	0.15
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	15	0.15
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	15	0.15
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	15	0.15
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	15	0.15
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	15	0.15
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	15	0.15
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	15	0.15
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	15	0.15
(2,586)	1:120:A:LEU:H	1:117:A:ALA:HA	1	0.15
(2,585)	1:120:A:LEU:H	1:117:A:ALA:HA	1	0.15
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	4	0.15
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	4	0.15
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	4	0.15
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	4	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	4	0.15
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	4	0.15
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	4	0.15
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	4	0.15
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	4	0.15
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	4	0.15
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	4	0.15
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	4	0.15
(2,548)	1:116:A:PHE:H	1:115:A:TYR:H	3	0.15
(2,548)	1:116:A:PHE:H	1:115:A:TYR:H	14	0.15
(2,547)	1:116:A:PHE:H	1:115:A:TYR:H	3	0.15
(2,547)	1:116:A:PHE:H	1:115:A:TYR:H	14	0.15
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	11	0.15
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	11	0.15
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	11	0.15
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	11	0.15
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	11	0.15
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	11	0.15
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	13	0.15
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	13	0.15
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	13	0.15
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	13	0.15
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	13	0.15
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	13	0.15
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	11	0.15
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	11	0.15
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	11	0.15
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	11	0.15
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	11	0.15
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	11	0.15
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	13	0.15
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	13	0.15
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	13	0.15
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	13	0.15
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	13	0.15
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	13	0.15
(2,486)	1:106:A:ASN:H	1:105:A:PHE:H	9	0.15
(2,485)	1:106:A:ASN:H	1:105:A:PHE:H	9	0.15
(2,484)	1:105:A:PHE:H	1:106:A:ASN:H	9	0.15
(2,483)	1:105:A:PHE:H	1:106:A:ASN:H	9	0.15
(2,470)	1:102:A:ASP:H	1:101:A:SER:HB2	10	0.15
(2,470)	1:102:A:ASP:H	1:101:A:SER:HB3	10	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,469)	1:102:A:ASP:H	1:101:A:SER:HB2	10	0.15
(2,469)	1:102:A:ASP:H	1:101:A:SER:HB3	10	0.15
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	8	0.15
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	8	0.15
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	8	0.15
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	8	0.15
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	8	0.15
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	8	0.15
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	8	0.15
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	8	0.15
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	8	0.15
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	8	0.15
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	8	0.15
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	8	0.15
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	8	0.15
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	8	0.15
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	8	0.15
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	8	0.15
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	8	0.15
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	8	0.15
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	5	0.15
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	5	0.15
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	5	0.15
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	5	0.15
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	5	0.15
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	5	0.15
(2,316)	1:91:A:VAL:HG11	1:83:A:VAL:HA	13	0.15
(2,316)	1:91:A:VAL:HG12	1:83:A:VAL:HA	13	0.15
(2,316)	1:91:A:VAL:HG13	1:83:A:VAL:HA	13	0.15
(2,316)	1:91:A:VAL:HG11	1:83:A:VAL:HA	15	0.15
(2,316)	1:91:A:VAL:HG12	1:83:A:VAL:HA	15	0.15
(2,316)	1:91:A:VAL:HG13	1:83:A:VAL:HA	15	0.15
(2,315)	1:91:A:VAL:HG11	1:83:A:VAL:HA	13	0.15
(2,315)	1:91:A:VAL:HG12	1:83:A:VAL:HA	13	0.15
(2,315)	1:91:A:VAL:HG13	1:83:A:VAL:HA	13	0.15
(2,315)	1:91:A:VAL:HG11	1:83:A:VAL:HA	15	0.15
(2,315)	1:91:A:VAL:HG12	1:83:A:VAL:HA	15	0.15
(2,315)	1:91:A:VAL:HG13	1:83:A:VAL:HA	15	0.15
(2,302)	1:90:A:GLU:H	1:89:A:ARG:HD2	5	0.15
(2,302)	1:90:A:GLU:H	1:89:A:ARG:HD3	5	0.15
(2,301)	1:90:A:GLU:H	1:89:A:ARG:HD2	5	0.15
(2,301)	1:90:A:GLU:H	1:89:A:ARG:HD3	5	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,300)	1:90:A:GLU:H	1:89:A:ARG:HB2	2	0.15
(2,300)	1:90:A:GLU:H	1:89:A:ARG:HB3	2	0.15
(2,299)	1:90:A:GLU:H	1:89:A:ARG:HB2	2	0.15
(2,299)	1:90:A:GLU:H	1:89:A:ARG:HB3	2	0.15
(2,254)	1:83:A:VAL:HG21	1:120:A:LEU:HD21	9	0.15
(2,254)	1:83:A:VAL:HG21	1:120:A:LEU:HD22	9	0.15
(2,254)	1:83:A:VAL:HG21	1:120:A:LEU:HD23	9	0.15
(2,254)	1:83:A:VAL:HG22	1:120:A:LEU:HD21	9	0.15
(2,254)	1:83:A:VAL:HG22	1:120:A:LEU:HD22	9	0.15
(2,254)	1:83:A:VAL:HG22	1:120:A:LEU:HD23	9	0.15
(2,254)	1:83:A:VAL:HG23	1:120:A:LEU:HD21	9	0.15
(2,254)	1:83:A:VAL:HG23	1:120:A:LEU:HD22	9	0.15
(2,254)	1:83:A:VAL:HG23	1:120:A:LEU:HD23	9	0.15
(2,246)	1:83:A:VAL:H	1:82:A:ALA:HA	10	0.15
(2,246)	1:83:A:VAL:H	1:82:A:ALA:HA	13	0.15
(2,245)	1:83:A:VAL:H	1:82:A:ALA:HA	10	0.15
(2,245)	1:83:A:VAL:H	1:82:A:ALA:HA	13	0.15
(2,244)	1:83:A:VAL:H	1:82:A:ALA:HB1	1	0.15
(2,244)	1:83:A:VAL:H	1:82:A:ALA:HB2	1	0.15
(2,244)	1:83:A:VAL:H	1:82:A:ALA:HB3	1	0.15
(2,243)	1:83:A:VAL:H	1:82:A:ALA:HB1	1	0.15
(2,243)	1:83:A:VAL:H	1:82:A:ALA:HB2	1	0.15
(2,243)	1:83:A:VAL:H	1:82:A:ALA:HB3	1	0.15
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	15	0.15
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	15	0.15
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	15	0.15
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	15	0.15
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	15	0.15
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	15	0.15
(2,188)	1:73:A:ASN:H	1:74:A:MET:H	2	0.15
(2,188)	1:73:A:ASN:H	1:74:A:MET:H	3	0.15
(2,188)	1:73:A:ASN:H	1:74:A:MET:H	9	0.15
(2,185)	1:73:A:ASN:H	1:74:A:MET:H	2	0.15
(2,185)	1:73:A:ASN:H	1:74:A:MET:H	3	0.15
(2,185)	1:73:A:ASN:H	1:74:A:MET:H	9	0.15
(2,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	10	0.15
(2,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	10	0.15
(2,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	10	0.15
(2,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	10	0.15
(2,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	10	0.15
(2,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	10	0.15
(2,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	10	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	10	0.15
(2,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	10	0.15
(2,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	10	0.15
(2,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	10	0.15
(2,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	10	0.15
(2,136)	1:67:A:GLY:H	1:66:A:ILE:HB	3	0.15
(2,136)	1:67:A:GLY:H	1:66:A:ILE:HB	11	0.15
(2,135)	1:67:A:GLY:H	1:66:A:ILE:HB	3	0.15
(2,135)	1:67:A:GLY:H	1:66:A:ILE:HB	11	0.15
(2,34)	1:56:A:THR:H	1:55:A:SER:HB2	7	0.15
(2,34)	1:56:A:THR:H	1:55:A:SER:HB3	7	0.15
(2,33)	1:56:A:THR:H	1:55:A:SER:HB2	7	0.15
(2,33)	1:56:A:THR:H	1:55:A:SER:HB3	7	0.15
(2,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	3	0.15
(2,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	3	0.15
(2,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	3	0.15
(2,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	3	0.15
(2,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	3	0.15
(2,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	3	0.15
(2,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	3	0.15
(2,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	3	0.15
(2,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	3	0.15
(2,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	3	0.15
(2,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	3	0.15
(2,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	3	0.15
(2,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	12	0.15
(2,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	12	0.15
(2,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	12	0.15
(2,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	12	0.15
(2,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	12	0.15
(2,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	12	0.15
(1,20)	1:70:A:LEU:HD11	1:66:A:ILE:HG21	11	0.15
(1,20)	1:70:A:LEU:HD11	1:66:A:ILE:HG22	11	0.15
(1,20)	1:70:A:LEU:HD11	1:66:A:ILE:HG23	11	0.15
(1,20)	1:70:A:LEU:HD12	1:66:A:ILE:HG21	11	0.15
(1,20)	1:70:A:LEU:HD12	1:66:A:ILE:HG22	11	0.15
(1,20)	1:70:A:LEU:HD12	1:66:A:ILE:HG23	11	0.15
(1,20)	1:70:A:LEU:HD13	1:66:A:ILE:HG21	11	0.15
(1,20)	1:70:A:LEU:HD13	1:66:A:ILE:HG22	11	0.15
(1,20)	1:70:A:LEU:HD13	1:66:A:ILE:HG23	11	0.15
(1,19)	1:70:A:LEU:HD11	1:66:A:ILE:HG21	11	0.15
(1,19)	1:70:A:LEU:HD11	1:66:A:ILE:HG22	11	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:70:A:LEU:HD11	1:66:A:ILE:HG23	11	0.15
(1,19)	1:70:A:LEU:HD12	1:66:A:ILE:HG21	11	0.15
(1,19)	1:70:A:LEU:HD12	1:66:A:ILE:HG22	11	0.15
(1,19)	1:70:A:LEU:HD12	1:66:A:ILE:HG23	11	0.15
(1,19)	1:70:A:LEU:HD13	1:66:A:ILE:HG21	11	0.15
(1,19)	1:70:A:LEU:HD13	1:66:A:ILE:HG22	11	0.15
(1,19)	1:70:A:LEU:HD13	1:66:A:ILE:HG23	11	0.15
(1,12)	1:66:A:ILE:HG21	1:70:A:LEU:HD11	11	0.15
(1,12)	1:66:A:ILE:HG21	1:70:A:LEU:HD12	11	0.15
(1,12)	1:66:A:ILE:HG21	1:70:A:LEU:HD13	11	0.15
(1,12)	1:66:A:ILE:HG22	1:70:A:LEU:HD11	11	0.15
(1,12)	1:66:A:ILE:HG22	1:70:A:LEU:HD12	11	0.15
(1,12)	1:66:A:ILE:HG22	1:70:A:LEU:HD13	11	0.15
(1,12)	1:66:A:ILE:HG23	1:70:A:LEU:HD11	11	0.15
(1,12)	1:66:A:ILE:HG23	1:70:A:LEU:HD12	11	0.15
(1,12)	1:66:A:ILE:HG23	1:70:A:LEU:HD13	11	0.15
(1,11)	1:66:A:ILE:HG21	1:70:A:LEU:HD11	11	0.15
(1,11)	1:66:A:ILE:HG21	1:70:A:LEU:HD12	11	0.15
(1,11)	1:66:A:ILE:HG21	1:70:A:LEU:HD13	11	0.15
(1,11)	1:66:A:ILE:HG22	1:70:A:LEU:HD11	11	0.15
(1,11)	1:66:A:ILE:HG22	1:70:A:LEU:HD12	11	0.15
(1,11)	1:66:A:ILE:HG22	1:70:A:LEU:HD13	11	0.15
(1,11)	1:66:A:ILE:HG23	1:70:A:LEU:HD11	11	0.15
(1,11)	1:66:A:ILE:HG23	1:70:A:LEU:HD12	11	0.15
(1,11)	1:66:A:ILE:HG23	1:70:A:LEU:HD13	11	0.15
(3,686)	1:126:A:SER:H	1:125:A:LEU:HG	5	0.14
(3,686)	1:126:A:SER:H	1:125:A:LEU:HG	11	0.14
(3,686)	1:126:A:SER:H	1:125:A:LEU:HG	13	0.14
(3,685)	1:126:A:SER:H	1:125:A:LEU:HG	5	0.14
(3,685)	1:126:A:SER:H	1:125:A:LEU:HG	11	0.14
(3,685)	1:126:A:SER:H	1:125:A:LEU:HG	13	0.14
(3,672)	1:125:A:LEU:H	1:126:A:SER:HA	4	0.14
(3,672)	1:125:A:LEU:H	1:126:A:SER:HA	8	0.14
(3,672)	1:125:A:LEU:H	1:126:A:SER:HA	11	0.14
(3,672)	1:125:A:LEU:H	1:126:A:SER:HA	12	0.14
(3,672)	1:125:A:LEU:H	1:126:A:SER:HA	14	0.14
(3,671)	1:125:A:LEU:H	1:126:A:SER:HA	4	0.14
(3,671)	1:125:A:LEU:H	1:126:A:SER:HA	8	0.14
(3,671)	1:125:A:LEU:H	1:126:A:SER:HA	11	0.14
(3,671)	1:125:A:LEU:H	1:126:A:SER:HA	12	0.14
(3,671)	1:125:A:LEU:H	1:126:A:SER:HA	14	0.14
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	11	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	11	0.14
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	11	0.14
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	11	0.14
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	11	0.14
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	11	0.14
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	13	0.14
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	13	0.14
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	13	0.14
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	13	0.14
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	13	0.14
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	13	0.14
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	11	0.14
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	11	0.14
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	11	0.14
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	11	0.14
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	11	0.14
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	11	0.14
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	13	0.14
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	13	0.14
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	13	0.14
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	13	0.14
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	13	0.14
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	13	0.14
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	5	0.14
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	5	0.14
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	5	0.14
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	5	0.14
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	5	0.14
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	5	0.14
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	5	0.14
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	5	0.14
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	5	0.14
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	14	0.14
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	14	0.14
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	14	0.14
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	14	0.14
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	14	0.14
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	14	0.14
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	14	0.14
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	14	0.14
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	14	0.14
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	5	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	5	0.14
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	5	0.14
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	5	0.14
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	5	0.14
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	5	0.14
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	5	0.14
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	5	0.14
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	5	0.14
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	14	0.14
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	14	0.14
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	14	0.14
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	14	0.14
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	14	0.14
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	14	0.14
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	14	0.14
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	14	0.14
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	14	0.14
(3,531)	1:113:A:LEU:HD21	1:96:A:ALA:HA	5	0.14
(3,531)	1:113:A:LEU:HD22	1:96:A:ALA:HA	5	0.14
(3,531)	1:113:A:LEU:HD23	1:96:A:ALA:HA	5	0.14
(3,527)	1:113:A:LEU:HD21	1:96:A:ALA:HA	5	0.14
(3,527)	1:113:A:LEU:HD22	1:96:A:ALA:HA	5	0.14
(3,527)	1:113:A:LEU:HD23	1:96:A:ALA:HA	5	0.14
(3,470)	1:102:A:ASP:H	1:101:A:SER:HB2	1	0.14
(3,470)	1:102:A:ASP:H	1:101:A:SER:HB3	1	0.14
(3,470)	1:102:A:ASP:H	1:101:A:SER:HB2	7	0.14
(3,470)	1:102:A:ASP:H	1:101:A:SER:HB3	7	0.14
(3,469)	1:102:A:ASP:H	1:101:A:SER:HB2	1	0.14
(3,469)	1:102:A:ASP:H	1:101:A:SER:HB3	1	0.14
(3,469)	1:102:A:ASP:H	1:101:A:SER:HB2	7	0.14
(3,469)	1:102:A:ASP:H	1:101:A:SER:HB3	7	0.14
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	7	0.14
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	7	0.14
(3,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	7	0.14
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	7	0.14
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	7	0.14
(3,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	7	0.14
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	7	0.14
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	7	0.14
(3,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	7	0.14
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	7	0.14
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	7	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	7	0.14
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	7	0.14
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	7	0.14
(3,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	7	0.14
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	7	0.14
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	7	0.14
(3,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	7	0.14
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	8	0.14
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	8	0.14
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	8	0.14
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	8	0.14
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	8	0.14
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	8	0.14
(3,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	1	0.14
(3,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	1	0.14
(3,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	1	0.14
(3,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	1	0.14
(3,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	1	0.14
(3,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	1	0.14
(3,316)	1:91:A:VAL:HG11	1:83:A:VAL:HA	2	0.14
(3,316)	1:91:A:VAL:HG12	1:83:A:VAL:HA	2	0.14
(3,316)	1:91:A:VAL:HG13	1:83:A:VAL:HA	2	0.14
(3,316)	1:91:A:VAL:HG11	1:83:A:VAL:HA	12	0.14
(3,316)	1:91:A:VAL:HG12	1:83:A:VAL:HA	12	0.14
(3,316)	1:91:A:VAL:HG13	1:83:A:VAL:HA	12	0.14
(3,315)	1:91:A:VAL:HG11	1:83:A:VAL:HA	2	0.14
(3,315)	1:91:A:VAL:HG12	1:83:A:VAL:HA	2	0.14
(3,315)	1:91:A:VAL:HG13	1:83:A:VAL:HA	2	0.14
(3,315)	1:91:A:VAL:HG11	1:83:A:VAL:HA	12	0.14
(3,315)	1:91:A:VAL:HG12	1:83:A:VAL:HA	12	0.14
(3,315)	1:91:A:VAL:HG13	1:83:A:VAL:HA	12	0.14
(3,308)	1:90:A:GLU:H	1:90:A:GLU:HB2	12	0.14
(3,308)	1:90:A:GLU:H	1:90:A:GLU:HB3	12	0.14
(3,307)	1:90:A:GLU:H	1:90:A:GLU:HB2	12	0.14
(3,307)	1:90:A:GLU:H	1:90:A:GLU:HB3	12	0.14
(3,278)	1:85:A:THR:H	1:86:A:ASP:HB2	9	0.14
(3,278)	1:85:A:THR:H	1:86:A:ASP:HB3	9	0.14
(3,277)	1:85:A:THR:H	1:86:A:ASP:HB2	9	0.14
(3,277)	1:85:A:THR:H	1:86:A:ASP:HB3	9	0.14
(3,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD21	5	0.14
(3,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD22	5	0.14
(3,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD23	5	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD21	5	0.14
(3,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD22	5	0.14
(3,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD23	5	0.14
(3,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD21	5	0.14
(3,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD22	5	0.14
(3,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD23	5	0.14
(3,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	5	0.14
(3,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	5	0.14
(3,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	5	0.14
(3,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	15	0.14
(3,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	15	0.14
(3,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	15	0.14
(3,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	5	0.14
(3,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	5	0.14
(3,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	5	0.14
(3,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	15	0.14
(3,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	15	0.14
(3,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	15	0.14
(3,209)	1:77:A:GLN:H	1:76:A:LEU:HG	11	0.14
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	14	0.14
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	14	0.14
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	14	0.14
(3,206)	1:77:A:GLN:H	1:76:A:LEU:HG	11	0.14
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	14	0.14
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	14	0.14
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	14	0.14
(3,188)	1:73:A:ASN:H	1:74:A:MET:H	4	0.14
(3,188)	1:73:A:ASN:H	1:74:A:MET:H	15	0.14
(3,185)	1:73:A:ASN:H	1:74:A:MET:H	4	0.14
(3,185)	1:73:A:ASN:H	1:74:A:MET:H	15	0.14
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	4	0.14
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	4	0.14
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	4	0.14
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	4	0.14
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	4	0.14
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	4	0.14
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	4	0.14
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	4	0.14
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	4	0.14
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	4	0.14
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	4	0.14
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	4	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,148)	1:68:A:ASP:H	1:65:A:ARG:HA	10	0.14
(3,147)	1:68:A:ASP:H	1:65:A:ARG:HA	10	0.14
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB1	3	0.14
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB2	3	0.14
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB3	3	0.14
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB1	3	0.14
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB2	3	0.14
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB3	3	0.14
(3,16)	1:54:A:ALA:HB1	1:52:A:MET:HA	11	0.14
(3,16)	1:54:A:ALA:HB2	1:52:A:MET:HA	11	0.14
(3,16)	1:54:A:ALA:HB3	1:52:A:MET:HA	11	0.14
(3,15)	1:54:A:ALA:HB1	1:52:A:MET:HA	11	0.14
(3,15)	1:54:A:ALA:HB2	1:52:A:MET:HA	11	0.14
(3,15)	1:54:A:ALA:HB3	1:52:A:MET:HA	11	0.14
(3,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	7	0.14
(3,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	7	0.14
(3,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	7	0.14
(3,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	7	0.14
(3,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	7	0.14
(3,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	7	0.14
(3,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	7	0.14
(3,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	7	0.14
(3,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	7	0.14
(3,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	7	0.14
(3,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	7	0.14
(3,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	7	0.14
(3,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	14	0.14
(3,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	14	0.14
(3,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	14	0.14
(3,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	14	0.14
(3,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	14	0.14
(3,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	14	0.14
(2,686)	1:126:A:SER:H	1:125:A:LEU:HG	5	0.14
(2,686)	1:126:A:SER:H	1:125:A:LEU:HG	11	0.14
(2,686)	1:126:A:SER:H	1:125:A:LEU:HG	13	0.14
(2,685)	1:126:A:SER:H	1:125:A:LEU:HG	5	0.14
(2,685)	1:126:A:SER:H	1:125:A:LEU:HG	11	0.14
(2,685)	1:126:A:SER:H	1:125:A:LEU:HG	13	0.14
(2,672)	1:125:A:LEU:H	1:126:A:SER:HA	4	0.14
(2,672)	1:125:A:LEU:H	1:126:A:SER:HA	8	0.14
(2,672)	1:125:A:LEU:H	1:126:A:SER:HA	11	0.14
(2,672)	1:125:A:LEU:H	1:126:A:SER:HA	12	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,672)	1:125:A:LEU:H	1:126:A:SER:HA	14	0.14
(2,671)	1:125:A:LEU:H	1:126:A:SER:HA	4	0.14
(2,671)	1:125:A:LEU:H	1:126:A:SER:HA	8	0.14
(2,671)	1:125:A:LEU:H	1:126:A:SER:HA	11	0.14
(2,671)	1:125:A:LEU:H	1:126:A:SER:HA	12	0.14
(2,671)	1:125:A:LEU:H	1:126:A:SER:HA	14	0.14
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	11	0.14
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	11	0.14
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	11	0.14
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	11	0.14
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	11	0.14
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	11	0.14
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	13	0.14
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	13	0.14
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	13	0.14
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	13	0.14
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	13	0.14
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	13	0.14
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	11	0.14
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	11	0.14
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	11	0.14
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	11	0.14
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	11	0.14
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	11	0.14
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	13	0.14
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	13	0.14
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	13	0.14
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	13	0.14
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	13	0.14
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	13	0.14
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	5	0.14
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	5	0.14
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	5	0.14
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	5	0.14
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	5	0.14
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	5	0.14
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	5	0.14
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	5	0.14
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	5	0.14
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	14	0.14
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	14	0.14
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	14	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	14	0.14
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	14	0.14
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	14	0.14
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	14	0.14
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	14	0.14
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	14	0.14
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	5	0.14
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	5	0.14
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	5	0.14
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	5	0.14
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	5	0.14
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	5	0.14
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	5	0.14
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	5	0.14
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	5	0.14
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	14	0.14
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	14	0.14
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	14	0.14
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	14	0.14
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	14	0.14
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	14	0.14
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	14	0.14
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	14	0.14
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	14	0.14
(2,531)	1:113:A:LEU:HD21	1:96:A:ALA:HA	5	0.14
(2,531)	1:113:A:LEU:HD22	1:96:A:ALA:HA	5	0.14
(2,531)	1:113:A:LEU:HD23	1:96:A:ALA:HA	5	0.14
(2,527)	1:113:A:LEU:HD21	1:96:A:ALA:HA	5	0.14
(2,527)	1:113:A:LEU:HD22	1:96:A:ALA:HA	5	0.14
(2,527)	1:113:A:LEU:HD23	1:96:A:ALA:HA	5	0.14
(2,470)	1:102:A:ASP:H	1:101:A:SER:HB2	1	0.14
(2,470)	1:102:A:ASP:H	1:101:A:SER:HB3	1	0.14
(2,470)	1:102:A:ASP:H	1:101:A:SER:HB2	7	0.14
(2,470)	1:102:A:ASP:H	1:101:A:SER:HB3	7	0.14
(2,469)	1:102:A:ASP:H	1:101:A:SER:HB2	1	0.14
(2,469)	1:102:A:ASP:H	1:101:A:SER:HB3	1	0.14
(2,469)	1:102:A:ASP:H	1:101:A:SER:HB2	7	0.14
(2,469)	1:102:A:ASP:H	1:101:A:SER:HB3	7	0.14
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	7	0.14
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	7	0.14
(2,396)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	7	0.14
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	7	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	7	0.14
(2,396)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	7	0.14
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	7	0.14
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	7	0.14
(2,396)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	7	0.14
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG21	7	0.14
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG22	7	0.14
(2,395)	1:96:A:ALA:HB1	1:95:A:VAL:HG23	7	0.14
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG21	7	0.14
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG22	7	0.14
(2,395)	1:96:A:ALA:HB2	1:95:A:VAL:HG23	7	0.14
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG21	7	0.14
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG22	7	0.14
(2,395)	1:96:A:ALA:HB3	1:95:A:VAL:HG23	7	0.14
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	8	0.14
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	8	0.14
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	8	0.14
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	8	0.14
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	8	0.14
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	8	0.14
(2,322)	1:91:A:VAL:HG21	1:92:A:PHE:H	1	0.14
(2,322)	1:91:A:VAL:HG22	1:92:A:PHE:H	1	0.14
(2,322)	1:91:A:VAL:HG23	1:92:A:PHE:H	1	0.14
(2,321)	1:91:A:VAL:HG21	1:92:A:PHE:H	1	0.14
(2,321)	1:91:A:VAL:HG22	1:92:A:PHE:H	1	0.14
(2,321)	1:91:A:VAL:HG23	1:92:A:PHE:H	1	0.14
(2,316)	1:91:A:VAL:HG11	1:83:A:VAL:HA	2	0.14
(2,316)	1:91:A:VAL:HG12	1:83:A:VAL:HA	2	0.14
(2,316)	1:91:A:VAL:HG13	1:83:A:VAL:HA	2	0.14
(2,316)	1:91:A:VAL:HG11	1:83:A:VAL:HA	12	0.14
(2,316)	1:91:A:VAL:HG12	1:83:A:VAL:HA	12	0.14
(2,316)	1:91:A:VAL:HG13	1:83:A:VAL:HA	12	0.14
(2,315)	1:91:A:VAL:HG11	1:83:A:VAL:HA	2	0.14
(2,315)	1:91:A:VAL:HG12	1:83:A:VAL:HA	2	0.14
(2,315)	1:91:A:VAL:HG13	1:83:A:VAL:HA	2	0.14
(2,315)	1:91:A:VAL:HG11	1:83:A:VAL:HA	12	0.14
(2,315)	1:91:A:VAL:HG12	1:83:A:VAL:HA	12	0.14
(2,315)	1:91:A:VAL:HG13	1:83:A:VAL:HA	12	0.14
(2,308)	1:90:A:GLU:H	1:90:A:GLU:HB2	12	0.14
(2,308)	1:90:A:GLU:H	1:90:A:GLU:HB3	12	0.14
(2,307)	1:90:A:GLU:H	1:90:A:GLU:HB2	12	0.14
(2,307)	1:90:A:GLU:H	1:90:A:GLU:HB3	12	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,278)	1:85:A:THR:H	1:86:A:ASP:HB2	9	0.14
(2,278)	1:85:A:THR:H	1:86:A:ASP:HB3	9	0.14
(2,277)	1:85:A:THR:H	1:86:A:ASP:HB2	9	0.14
(2,277)	1:85:A:THR:H	1:86:A:ASP:HB3	9	0.14
(2,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD21	5	0.14
(2,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD22	5	0.14
(2,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD23	5	0.14
(2,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD21	5	0.14
(2,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD22	5	0.14
(2,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD23	5	0.14
(2,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD21	5	0.14
(2,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD22	5	0.14
(2,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD23	5	0.14
(2,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	5	0.14
(2,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	5	0.14
(2,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	5	0.14
(2,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	15	0.14
(2,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	15	0.14
(2,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	15	0.14
(2,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	5	0.14
(2,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	5	0.14
(2,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	5	0.14
(2,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	15	0.14
(2,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	15	0.14
(2,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	15	0.14
(2,209)	1:77:A:GLN:H	1:76:A:LEU:HG	11	0.14
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	14	0.14
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	14	0.14
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	14	0.14
(2,206)	1:77:A:GLN:H	1:76:A:LEU:HG	11	0.14
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	14	0.14
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	14	0.14
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	14	0.14
(2,188)	1:73:A:ASN:H	1:74:A:MET:H	4	0.14
(2,188)	1:73:A:ASN:H	1:74:A:MET:H	15	0.14
(2,185)	1:73:A:ASN:H	1:74:A:MET:H	4	0.14
(2,185)	1:73:A:ASN:H	1:74:A:MET:H	15	0.14
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	4	0.14
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	4	0.14
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	4	0.14
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	4	0.14
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	4	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	4	0.14
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	4	0.14
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	4	0.14
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	4	0.14
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	4	0.14
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	4	0.14
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	4	0.14
(2,148)	1:68:A:ASP:H	1:65:A:ARG:HA	10	0.14
(2,147)	1:68:A:ASP:H	1:65:A:ARG:HA	10	0.14
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB1	3	0.14
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB2	3	0.14
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB3	3	0.14
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB1	3	0.14
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB2	3	0.14
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB3	3	0.14
(2,16)	1:54:A:ALA:HB1	1:52:A:MET:HA	11	0.14
(2,16)	1:54:A:ALA:HB2	1:52:A:MET:HA	11	0.14
(2,16)	1:54:A:ALA:HB3	1:52:A:MET:HA	11	0.14
(2,15)	1:54:A:ALA:HB1	1:52:A:MET:HA	11	0.14
(2,15)	1:54:A:ALA:HB2	1:52:A:MET:HA	11	0.14
(2,15)	1:54:A:ALA:HB3	1:52:A:MET:HA	11	0.14
(2,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	7	0.14
(2,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	7	0.14
(2,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	7	0.14
(2,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	7	0.14
(2,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	7	0.14
(2,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	7	0.14
(2,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	7	0.14
(2,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	7	0.14
(2,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	7	0.14
(2,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	7	0.14
(2,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	7	0.14
(2,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	7	0.14
(2,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	14	0.14
(2,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	14	0.14
(2,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	14	0.14
(2,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	14	0.14
(2,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	14	0.14
(2,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	14	0.14
(3,702)	1:128:A:LYS:H	1:127:A:THR:HB	9	0.13
(3,701)	1:128:A:LYS:H	1:127:A:THR:HB	9	0.13
(3,686)	1:126:A:SER:H	1:125:A:LEU:HG	12	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,685)	1:126:A:SER:H	1:125:A:LEU:HG	12	0.13
(3,654)	1:124:A:ALA:H	1:120:A:LEU:HA	6	0.13
(3,654)	1:124:A:ALA:H	1:120:A:LEU:HA	12	0.13
(3,653)	1:124:A:ALA:H	1:120:A:LEU:HA	6	0.13
(3,653)	1:124:A:ALA:H	1:120:A:LEU:HA	12	0.13
(3,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	13	0.13
(3,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	13	0.13
(3,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	13	0.13
(3,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	13	0.13
(3,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	13	0.13
(3,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	13	0.13
(3,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	13	0.13
(3,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	13	0.13
(3,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	13	0.13
(3,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	13	0.13
(3,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	13	0.13
(3,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	13	0.13
(3,548)	1:116:A:PHE:H	1:115:A:TYR:H	8	0.13
(3,547)	1:116:A:PHE:H	1:115:A:TYR:H	8	0.13
(3,531)	1:113:A:LEU:HD21	1:96:A:ALA:HA	3	0.13
(3,531)	1:113:A:LEU:HD22	1:96:A:ALA:HA	3	0.13
(3,531)	1:113:A:LEU:HD23	1:96:A:ALA:HA	3	0.13
(3,527)	1:113:A:LEU:HD21	1:96:A:ALA:HA	3	0.13
(3,527)	1:113:A:LEU:HD22	1:96:A:ALA:HA	3	0.13
(3,527)	1:113:A:LEU:HD23	1:96:A:ALA:HA	3	0.13
(3,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	1	0.13
(3,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	1	0.13
(3,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	1	0.13
(3,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	1	0.13
(3,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	1	0.13
(3,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	1	0.13
(3,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	15	0.13
(3,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	15	0.13
(3,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	15	0.13
(3,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	15	0.13
(3,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	15	0.13
(3,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	15	0.13
(3,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	1	0.13
(3,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	1	0.13
(3,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	1	0.13
(3,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	1	0.13
(3,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	1	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	1	0.13
(3,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	15	0.13
(3,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	15	0.13
(3,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	15	0.13
(3,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	15	0.13
(3,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	15	0.13
(3,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	15	0.13
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	15	0.13
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	15	0.13
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	15	0.13
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	15	0.13
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	15	0.13
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	15	0.13
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	15	0.13
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	15	0.13
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	15	0.13
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	15	0.13
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	15	0.13
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	15	0.13
(3,492)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	8	0.13
(3,491)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	8	0.13
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB2	10	0.13
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB3	10	0.13
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB2	10	0.13
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB3	10	0.13
(3,446)	1:101:A:SER:H	1:102:A:ASP:H	1	0.13
(3,445)	1:101:A:SER:H	1:102:A:ASP:H	1	0.13
(3,386)	1:96:A:ALA:H	1:95:A:VAL:HG21	2	0.13
(3,386)	1:96:A:ALA:H	1:95:A:VAL:HG22	2	0.13
(3,386)	1:96:A:ALA:H	1:95:A:VAL:HG23	2	0.13
(3,386)	1:96:A:ALA:H	1:95:A:VAL:HG21	3	0.13
(3,386)	1:96:A:ALA:H	1:95:A:VAL:HG22	3	0.13
(3,386)	1:96:A:ALA:H	1:95:A:VAL:HG23	3	0.13
(3,385)	1:96:A:ALA:H	1:95:A:VAL:HG21	2	0.13
(3,385)	1:96:A:ALA:H	1:95:A:VAL:HG22	2	0.13
(3,385)	1:96:A:ALA:H	1:95:A:VAL:HG23	2	0.13
(3,385)	1:96:A:ALA:H	1:95:A:VAL:HG21	3	0.13
(3,385)	1:96:A:ALA:H	1:95:A:VAL:HG22	3	0.13
(3,385)	1:96:A:ALA:H	1:95:A:VAL:HG23	3	0.13
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	1	0.13
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	1	0.13
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	1	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	11	0.13
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	11	0.13
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	11	0.13
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	13	0.13
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	13	0.13
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	13	0.13
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	1	0.13
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	1	0.13
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	1	0.13
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	11	0.13
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	11	0.13
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	11	0.13
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	13	0.13
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	13	0.13
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	13	0.13
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	3	0.13
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	3	0.13
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	3	0.13
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	3	0.13
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	3	0.13
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	3	0.13
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	3	0.13
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	3	0.13
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	3	0.13
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	3	0.13
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	3	0.13
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	3	0.13
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	3	0.13
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	3	0.13
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	3	0.13
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	3	0.13
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	3	0.13
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	3	0.13
(3,290)	1:87:A:SER:H	1:86:A:ASP:HB2	5	0.13
(3,290)	1:87:A:SER:H	1:86:A:ASP:HB3	5	0.13
(3,289)	1:87:A:SER:H	1:86:A:ASP:HB2	5	0.13
(3,289)	1:87:A:SER:H	1:86:A:ASP:HB3	5	0.13
(3,284)	1:86:A:ASP:H	1:85:A:THR:H	5	0.13
(3,283)	1:86:A:ASP:H	1:85:A:THR:H	5	0.13
(3,278)	1:85:A:THR:H	1:86:A:ASP:HB2	14	0.13
(3,278)	1:85:A:THR:H	1:86:A:ASP:HB3	14	0.13
(3,277)	1:85:A:THR:H	1:86:A:ASP:HB2	14	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,277)	1:85:A:THR:H	1:86:A:ASP:HB3	14	0.13
(3,276)	1:85:A:THR:H	1:86:A:ASP:H	5	0.13
(3,275)	1:85:A:THR:H	1:86:A:ASP:H	5	0.13
(3,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD21	12	0.13
(3,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD22	12	0.13
(3,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD23	12	0.13
(3,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD21	12	0.13
(3,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD22	12	0.13
(3,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD23	12	0.13
(3,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD21	12	0.13
(3,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD22	12	0.13
(3,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD23	12	0.13
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD11	14	0.13
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD12	14	0.13
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD13	14	0.13
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD11	14	0.13
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD12	14	0.13
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD13	14	0.13
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD11	14	0.13
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD12	14	0.13
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD13	14	0.13
(3,246)	1:83:A:VAL:H	1:82:A:ALA:HA	1	0.13
(3,245)	1:83:A:VAL:H	1:82:A:ALA:HA	1	0.13
(3,238)	1:82:A:ALA:H	1:80:A:ILE:HB	12	0.13
(3,237)	1:82:A:ALA:H	1:80:A:ILE:HB	12	0.13
(3,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	8	0.13
(3,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	8	0.13
(3,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	8	0.13
(3,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	8	0.13
(3,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	8	0.13
(3,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	8	0.13
(3,209)	1:77:A:GLN:H	1:76:A:LEU:HG	3	0.13
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	9	0.13
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	9	0.13
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	9	0.13
(3,206)	1:77:A:GLN:H	1:76:A:LEU:HG	3	0.13
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	9	0.13
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	9	0.13
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	9	0.13
(3,188)	1:73:A:ASN:H	1:74:A:MET:H	10	0.13
(3,185)	1:73:A:ASN:H	1:74:A:MET:H	10	0.13
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	6	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	6	0.13
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	6	0.13
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	6	0.13
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	6	0.13
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	6	0.13
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	6	0.13
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	6	0.13
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	6	0.13
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	6	0.13
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	6	0.13
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	6	0.13
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	5	0.13
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	5	0.13
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	5	0.13
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	5	0.13
(3,34)	1:56:A:THR:H	1:55:A:SER:HB2	15	0.13
(3,34)	1:56:A:THR:H	1:55:A:SER:HB3	15	0.13
(3,33)	1:56:A:THR:H	1:55:A:SER:HB2	15	0.13
(3,33)	1:56:A:THR:H	1:55:A:SER:HB3	15	0.13
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB1	14	0.13
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB2	14	0.13
(3,30)	1:55:A:SER:H	1:54:A:ALA:HB3	14	0.13
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB1	14	0.13
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB2	14	0.13
(3,29)	1:55:A:SER:H	1:54:A:ALA:HB3	14	0.13
(3,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	8	0.13
(3,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	8	0.13
(3,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	8	0.13
(3,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	8	0.13
(3,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	8	0.13
(3,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	8	0.13
(3,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	8	0.13
(3,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	8	0.13
(3,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	8	0.13
(3,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	8	0.13
(3,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	8	0.13
(3,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	8	0.13
(2,702)	1:128:A:LYS:H	1:127:A:THR:HB	9	0.13
(2,701)	1:128:A:LYS:H	1:127:A:THR:HB	9	0.13
(2,686)	1:126:A:SER:H	1:125:A:LEU:HG	12	0.13
(2,685)	1:126:A:SER:H	1:125:A:LEU:HG	12	0.13
(2,654)	1:124:A:ALA:H	1:120:A:LEU:HA	6	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,654)	1:124:A:ALA:H	1:120:A:LEU:HA	12	0.13
(2,653)	1:124:A:ALA:H	1:120:A:LEU:HA	6	0.13
(2,653)	1:124:A:ALA:H	1:120:A:LEU:HA	12	0.13
(2,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	13	0.13
(2,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	13	0.13
(2,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	13	0.13
(2,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	13	0.13
(2,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	13	0.13
(2,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	13	0.13
(2,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	13	0.13
(2,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	13	0.13
(2,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	13	0.13
(2,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	13	0.13
(2,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	13	0.13
(2,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	13	0.13
(2,548)	1:116:A:PHE:H	1:115:A:TYR:H	8	0.13
(2,547)	1:116:A:PHE:H	1:115:A:TYR:H	8	0.13
(2,531)	1:113:A:LEU:HD21	1:96:A:ALA:HA	3	0.13
(2,531)	1:113:A:LEU:HD22	1:96:A:ALA:HA	3	0.13
(2,531)	1:113:A:LEU:HD23	1:96:A:ALA:HA	3	0.13
(2,527)	1:113:A:LEU:HD21	1:96:A:ALA:HA	3	0.13
(2,527)	1:113:A:LEU:HD22	1:96:A:ALA:HA	3	0.13
(2,527)	1:113:A:LEU:HD23	1:96:A:ALA:HA	3	0.13
(2,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	1	0.13
(2,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	1	0.13
(2,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	1	0.13
(2,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	1	0.13
(2,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	1	0.13
(2,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	1	0.13
(2,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	15	0.13
(2,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	15	0.13
(2,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	15	0.13
(2,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	15	0.13
(2,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	15	0.13
(2,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	15	0.13
(2,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	1	0.13
(2,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	1	0.13
(2,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	1	0.13
(2,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	1	0.13
(2,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	1	0.13
(2,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	1	0.13
(2,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	15	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	15	0.13
(2,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	15	0.13
(2,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	15	0.13
(2,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	15	0.13
(2,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	15	0.13
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	15	0.13
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	15	0.13
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	15	0.13
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	15	0.13
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	15	0.13
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	15	0.13
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	15	0.13
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	15	0.13
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	15	0.13
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	15	0.13
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	15	0.13
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	15	0.13
(2,492)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	8	0.13
(2,491)	1:110:A:VAL:HG11	1:107:A:TRP:HZ3	8	0.13
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB2	10	0.13
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB3	10	0.13
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB2	10	0.13
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB3	10	0.13
(2,446)	1:101:A:SER:H	1:102:A:ASP:H	1	0.13
(2,445)	1:101:A:SER:H	1:102:A:ASP:H	1	0.13
(2,386)	1:96:A:ALA:H	1:95:A:VAL:HG21	2	0.13
(2,386)	1:96:A:ALA:H	1:95:A:VAL:HG22	2	0.13
(2,386)	1:96:A:ALA:H	1:95:A:VAL:HG23	2	0.13
(2,386)	1:96:A:ALA:H	1:95:A:VAL:HG21	3	0.13
(2,386)	1:96:A:ALA:H	1:95:A:VAL:HG22	3	0.13
(2,386)	1:96:A:ALA:H	1:95:A:VAL:HG23	3	0.13
(2,385)	1:96:A:ALA:H	1:95:A:VAL:HG21	2	0.13
(2,385)	1:96:A:ALA:H	1:95:A:VAL:HG22	2	0.13
(2,385)	1:96:A:ALA:H	1:95:A:VAL:HG23	2	0.13
(2,385)	1:96:A:ALA:H	1:95:A:VAL:HG21	3	0.13
(2,385)	1:96:A:ALA:H	1:95:A:VAL:HG22	3	0.13
(2,385)	1:96:A:ALA:H	1:95:A:VAL:HG23	3	0.13
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	1	0.13
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	1	0.13
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	1	0.13
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	11	0.13
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	11	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	11	0.13
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	13	0.13
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	13	0.13
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	13	0.13
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	1	0.13
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	1	0.13
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	1	0.13
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	11	0.13
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	11	0.13
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	11	0.13
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	13	0.13
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	13	0.13
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	13	0.13
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	3	0.13
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	3	0.13
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	3	0.13
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	3	0.13
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	3	0.13
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	3	0.13
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	3	0.13
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	3	0.13
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	3	0.13
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	3	0.13
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	3	0.13
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	3	0.13
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	3	0.13
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	3	0.13
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	3	0.13
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	3	0.13
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	3	0.13
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	3	0.13
(2,290)	1:87:A:SER:H	1:86:A:ASP:HB2	5	0.13
(2,290)	1:87:A:SER:H	1:86:A:ASP:HB3	5	0.13
(2,289)	1:87:A:SER:H	1:86:A:ASP:HB2	5	0.13
(2,289)	1:87:A:SER:H	1:86:A:ASP:HB3	5	0.13
(2,284)	1:86:A:ASP:H	1:85:A:THR:H	5	0.13
(2,283)	1:86:A:ASP:H	1:85:A:THR:H	5	0.13
(2,278)	1:85:A:THR:H	1:86:A:ASP:HB2	14	0.13
(2,278)	1:85:A:THR:H	1:86:A:ASP:HB3	14	0.13
(2,277)	1:85:A:THR:H	1:86:A:ASP:HB2	14	0.13
(2,277)	1:85:A:THR:H	1:86:A:ASP:HB3	14	0.13
(2,276)	1:85:A:THR:H	1:86:A:ASP:H	5	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,275)	1:85:A:THR:H	1:86:A:ASP:H	5	0.13
(2,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD21	12	0.13
(2,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD22	12	0.13
(2,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD23	12	0.13
(2,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD21	12	0.13
(2,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD22	12	0.13
(2,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD23	12	0.13
(2,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD21	12	0.13
(2,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD22	12	0.13
(2,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD23	12	0.13
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD11	14	0.13
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD12	14	0.13
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD13	14	0.13
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD11	14	0.13
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD12	14	0.13
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD13	14	0.13
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD11	14	0.13
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD12	14	0.13
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD13	14	0.13
(2,246)	1:83:A:VAL:H	1:82:A:ALA:HA	1	0.13
(2,245)	1:83:A:VAL:H	1:82:A:ALA:HA	1	0.13
(2,238)	1:82:A:ALA:H	1:80:A:ILE:HB	12	0.13
(2,237)	1:82:A:ALA:H	1:80:A:ILE:HB	12	0.13
(2,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	8	0.13
(2,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	8	0.13
(2,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	8	0.13
(2,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	8	0.13
(2,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	8	0.13
(2,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	8	0.13
(2,209)	1:77:A:GLN:H	1:76:A:LEU:HG	3	0.13
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	9	0.13
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	9	0.13
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	9	0.13
(2,206)	1:77:A:GLN:H	1:76:A:LEU:HG	3	0.13
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	9	0.13
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	9	0.13
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	9	0.13
(2,188)	1:73:A:ASN:H	1:74:A:MET:H	10	0.13
(2,185)	1:73:A:ASN:H	1:74:A:MET:H	10	0.13
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	6	0.13
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	6	0.13
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	6	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	6	0.13
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	6	0.13
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	6	0.13
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	6	0.13
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	6	0.13
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	6	0.13
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	6	0.13
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	6	0.13
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	6	0.13
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	5	0.13
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	5	0.13
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	5	0.13
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	5	0.13
(2,34)	1:56:A:THR:H	1:55:A:SER:HB2	15	0.13
(2,34)	1:56:A:THR:H	1:55:A:SER:HB3	15	0.13
(2,33)	1:56:A:THR:H	1:55:A:SER:HB2	15	0.13
(2,33)	1:56:A:THR:H	1:55:A:SER:HB3	15	0.13
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB1	14	0.13
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB2	14	0.13
(2,30)	1:55:A:SER:H	1:54:A:ALA:HB3	14	0.13
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB1	14	0.13
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB2	14	0.13
(2,29)	1:55:A:SER:H	1:54:A:ALA:HB3	14	0.13
(2,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	8	0.13
(2,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	8	0.13
(2,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	8	0.13
(2,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	8	0.13
(2,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	8	0.13
(2,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	8	0.13
(2,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	8	0.13
(2,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	8	0.13
(2,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	8	0.13
(2,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	8	0.13
(2,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	8	0.13
(2,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	8	0.13
(3,700)	1:127:A:THR:HG21	1:128:A:LYS:H	3	0.12
(3,700)	1:127:A:THR:HG22	1:128:A:LYS:H	3	0.12
(3,700)	1:127:A:THR:HG23	1:128:A:LYS:H	3	0.12
(3,699)	1:127:A:THR:HG21	1:128:A:LYS:H	3	0.12
(3,699)	1:127:A:THR:HG22	1:128:A:LYS:H	3	0.12
(3,699)	1:127:A:THR:HG23	1:128:A:LYS:H	3	0.12
(3,686)	1:126:A:SER:H	1:125:A:LEU:HG	2	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,685)	1:126:A:SER:H	1:125:A:LEU:HG	2	0.12
(3,676)	1:125:A:LEU:HD11	1:122:A:LEU:HA	13	0.12
(3,676)	1:125:A:LEU:HD12	1:122:A:LEU:HA	13	0.12
(3,676)	1:125:A:LEU:HD13	1:122:A:LEU:HA	13	0.12
(3,675)	1:125:A:LEU:HD11	1:122:A:LEU:HA	13	0.12
(3,675)	1:125:A:LEU:HD12	1:122:A:LEU:HA	13	0.12
(3,675)	1:125:A:LEU:HD13	1:122:A:LEU:HA	13	0.12
(3,672)	1:125:A:LEU:H	1:126:A:SER:HA	6	0.12
(3,671)	1:125:A:LEU:H	1:126:A:SER:HA	6	0.12
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	5	0.12
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	5	0.12
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	5	0.12
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	5	0.12
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	5	0.12
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	5	0.12
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	6	0.12
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	6	0.12
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	6	0.12
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	6	0.12
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	6	0.12
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	6	0.12
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	7	0.12
(3,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	7	0.12
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	7	0.12
(3,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	7	0.12
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	7	0.12
(3,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	7	0.12
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	5	0.12
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	5	0.12
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	5	0.12
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	5	0.12
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	5	0.12
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	5	0.12
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	6	0.12
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	6	0.12
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	6	0.12
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	6	0.12
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	6	0.12
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	6	0.12
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	7	0.12
(3,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	7	0.12
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	7	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	7	0.12
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	7	0.12
(3,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	7	0.12
(3,654)	1:124:A:ALA:H	1:120:A:LEU:HA	2	0.12
(3,653)	1:124:A:ALA:H	1:120:A:LEU:HA	2	0.12
(3,638)	1:122:A:LEU:HD11	1:118:A:SER:HA	1	0.12
(3,638)	1:122:A:LEU:HD12	1:118:A:SER:HA	1	0.12
(3,638)	1:122:A:LEU:HD13	1:118:A:SER:HA	1	0.12
(3,637)	1:122:A:LEU:HD11	1:118:A:SER:HA	1	0.12
(3,637)	1:122:A:LEU:HD12	1:118:A:SER:HA	1	0.12
(3,637)	1:122:A:LEU:HD13	1:118:A:SER:HA	1	0.12
(3,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	14	0.12
(3,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	14	0.12
(3,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	14	0.12
(3,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	14	0.12
(3,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	14	0.12
(3,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	14	0.12
(3,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	14	0.12
(3,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	14	0.12
(3,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	14	0.12
(3,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	14	0.12
(3,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	14	0.12
(3,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	14	0.12
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	1	0.12
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	1	0.12
(3,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	1	0.12
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	1	0.12
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	1	0.12
(3,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	1	0.12
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	1	0.12
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	1	0.12
(3,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	1	0.12
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	1	0.12
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	1	0.12
(3,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	1	0.12
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	1	0.12
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	1	0.12
(3,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	1	0.12
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	1	0.12
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	1	0.12
(3,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	1	0.12
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	6	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	6	0.12
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	6	0.12
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	6	0.12
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	6	0.12
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	6	0.12
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	11	0.12
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	11	0.12
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	11	0.12
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	11	0.12
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	11	0.12
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	11	0.12
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	6	0.12
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	6	0.12
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	6	0.12
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	6	0.12
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	6	0.12
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	6	0.12
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	11	0.12
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	11	0.12
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	11	0.12
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	11	0.12
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	11	0.12
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	11	0.12
(3,531)	1:113:A:LEU:HD21	1:96:A:ALA:HA	11	0.12
(3,531)	1:113:A:LEU:HD22	1:96:A:ALA:HA	11	0.12
(3,531)	1:113:A:LEU:HD23	1:96:A:ALA:HA	11	0.12
(3,527)	1:113:A:LEU:HD21	1:96:A:ALA:HA	11	0.12
(3,527)	1:113:A:LEU:HD22	1:96:A:ALA:HA	11	0.12
(3,527)	1:113:A:LEU:HD23	1:96:A:ALA:HA	11	0.12
(3,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	6	0.12
(3,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	6	0.12
(3,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	6	0.12
(3,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	6	0.12
(3,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	6	0.12
(3,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	6	0.12
(3,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	6	0.12
(3,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	6	0.12
(3,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	6	0.12
(3,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	6	0.12
(3,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	6	0.12
(3,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	6	0.12
(3,512)	1:112:A:ALA:H	1:110:A:VAL:H	9	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,511)	1:112:A:ALA:H	1:110:A:VAL:H	9	0.12
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	5	0.12
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	5	0.12
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	5	0.12
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	5	0.12
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	5	0.12
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	5	0.12
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	6	0.12
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	6	0.12
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	6	0.12
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	6	0.12
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	6	0.12
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	6	0.12
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	10	0.12
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	10	0.12
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	10	0.12
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	10	0.12
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	10	0.12
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	10	0.12
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	5	0.12
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	5	0.12
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	5	0.12
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	5	0.12
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	5	0.12
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	5	0.12
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	6	0.12
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	6	0.12
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	6	0.12
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	6	0.12
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	6	0.12
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	6	0.12
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	10	0.12
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	10	0.12
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	10	0.12
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	10	0.12
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	10	0.12
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	10	0.12
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB2	3	0.12
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB3	3	0.12
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB2	5	0.12
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB3	5	0.12
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB2	3	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB3	3	0.12
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB2	5	0.12
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB3	5	0.12
(3,370)	1:95:A:VAL:HG21	1:92:A:PHE:HE2	8	0.12
(3,370)	1:95:A:VAL:HG22	1:92:A:PHE:HE2	8	0.12
(3,370)	1:95:A:VAL:HG23	1:92:A:PHE:HE2	8	0.12
(3,369)	1:95:A:VAL:HG21	1:92:A:PHE:HE2	8	0.12
(3,369)	1:95:A:VAL:HG22	1:92:A:PHE:HE2	8	0.12
(3,369)	1:95:A:VAL:HG23	1:92:A:PHE:HE2	8	0.12
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	7	0.12
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	7	0.12
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	7	0.12
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	7	0.12
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	7	0.12
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	7	0.12
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	1	0.12
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	1	0.12
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	1	0.12
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	1	0.12
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	1	0.12
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	1	0.12
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	1	0.12
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	1	0.12
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	1	0.12
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	4	0.12
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	4	0.12
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	4	0.12
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	4	0.12
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	4	0.12
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	4	0.12
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	4	0.12
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	4	0.12
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	4	0.12
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	1	0.12
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	1	0.12
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	1	0.12
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	1	0.12
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	1	0.12
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	1	0.12
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	1	0.12
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	1	0.12
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	1	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	4	0.12
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	4	0.12
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	4	0.12
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	4	0.12
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	4	0.12
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	4	0.12
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	4	0.12
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	4	0.12
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	4	0.12
(3,292)	1:87:A:SER:H	1:86:A:ASP:HA	1	0.12
(3,291)	1:87:A:SER:H	1:86:A:ASP:HA	1	0.12
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	10	0.12
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	10	0.12
(3,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	10	0.12
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	10	0.12
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	10	0.12
(3,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	10	0.12
(3,244)	1:83:A:VAL:H	1:82:A:ALA:HB1	13	0.12
(3,244)	1:83:A:VAL:H	1:82:A:ALA:HB2	13	0.12
(3,244)	1:83:A:VAL:H	1:82:A:ALA:HB3	13	0.12
(3,243)	1:83:A:VAL:H	1:82:A:ALA:HB1	13	0.12
(3,243)	1:83:A:VAL:H	1:82:A:ALA:HB2	13	0.12
(3,243)	1:83:A:VAL:H	1:82:A:ALA:HB3	13	0.12
(3,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	7	0.12
(3,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	7	0.12
(3,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	7	0.12
(3,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	7	0.12
(3,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	7	0.12
(3,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	7	0.12
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	1	0.12
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	1	0.12
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	1	0.12
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	7	0.12
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	7	0.12
(3,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	7	0.12
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	1	0.12
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	1	0.12
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	1	0.12
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	7	0.12
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	7	0.12
(3,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	7	0.12
(3,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	14	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	14	0.12
(3,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	14	0.12
(3,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	14	0.12
(3,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	14	0.12
(3,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	14	0.12
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	7	0.12
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	7	0.12
(3,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	7	0.12
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	7	0.12
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	7	0.12
(3,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	7	0.12
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	7	0.12
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	7	0.12
(3,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	7	0.12
(3,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	14	0.12
(3,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	14	0.12
(3,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	14	0.12
(3,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	14	0.12
(3,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	14	0.12
(3,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	14	0.12
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	7	0.12
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	7	0.12
(3,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	7	0.12
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	7	0.12
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	7	0.12
(3,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	7	0.12
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	7	0.12
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	7	0.12
(3,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	7	0.12
(3,136)	1:67:A:GLY:H	1:66:A:ILE:HB	8	0.12
(3,136)	1:67:A:GLY:H	1:66:A:ILE:HB	14	0.12
(3,135)	1:67:A:GLY:H	1:66:A:ILE:HB	8	0.12
(3,135)	1:67:A:GLY:H	1:66:A:ILE:HB	14	0.12
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	3	0.12
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	3	0.12
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	11	0.12
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	11	0.12
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	3	0.12
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	3	0.12
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	11	0.12
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	11	0.12
(3,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	9	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	9	0.12
(3,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	9	0.12
(3,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	9	0.12
(3,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	9	0.12
(3,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	9	0.12
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB1	10	0.12
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB2	10	0.12
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB3	10	0.12
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB1	13	0.12
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB2	13	0.12
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB3	13	0.12
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB1	14	0.12
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB2	14	0.12
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB3	14	0.12
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB1	10	0.12
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB2	10	0.12
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB3	10	0.12
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB1	13	0.12
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB2	13	0.12
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB3	13	0.12
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB1	14	0.12
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB2	14	0.12
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB3	14	0.12
(2,700)	1:127:A:THR:HG21	1:128:A:LYS:H	3	0.12
(2,700)	1:127:A:THR:HG22	1:128:A:LYS:H	3	0.12
(2,700)	1:127:A:THR:HG23	1:128:A:LYS:H	3	0.12
(2,699)	1:127:A:THR:HG21	1:128:A:LYS:H	3	0.12
(2,699)	1:127:A:THR:HG22	1:128:A:LYS:H	3	0.12
(2,699)	1:127:A:THR:HG23	1:128:A:LYS:H	3	0.12
(2,686)	1:126:A:SER:H	1:125:A:LEU:HG	2	0.12
(2,685)	1:126:A:SER:H	1:125:A:LEU:HG	2	0.12
(2,676)	1:125:A:LEU:HD11	1:122:A:LEU:HA	13	0.12
(2,676)	1:125:A:LEU:HD12	1:122:A:LEU:HA	13	0.12
(2,676)	1:125:A:LEU:HD13	1:122:A:LEU:HA	13	0.12
(2,675)	1:125:A:LEU:HD11	1:122:A:LEU:HA	13	0.12
(2,675)	1:125:A:LEU:HD12	1:122:A:LEU:HA	13	0.12
(2,675)	1:125:A:LEU:HD13	1:122:A:LEU:HA	13	0.12
(2,672)	1:125:A:LEU:H	1:126:A:SER:HA	6	0.12
(2,671)	1:125:A:LEU:H	1:126:A:SER:HA	6	0.12
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	5	0.12
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	5	0.12
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	5	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	5	0.12
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	5	0.12
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	5	0.12
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	6	0.12
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	6	0.12
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	6	0.12
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	6	0.12
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	6	0.12
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	6	0.12
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	7	0.12
(2,662)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	7	0.12
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	7	0.12
(2,662)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	7	0.12
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	7	0.12
(2,662)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	7	0.12
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	5	0.12
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	5	0.12
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	5	0.12
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	5	0.12
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	5	0.12
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	5	0.12
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	6	0.12
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	6	0.12
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	6	0.12
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	6	0.12
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	6	0.12
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	6	0.12
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB2	7	0.12
(2,661)	1:124:A:ALA:HB1	1:123:A:LYS:HB3	7	0.12
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB2	7	0.12
(2,661)	1:124:A:ALA:HB2	1:123:A:LYS:HB3	7	0.12
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB2	7	0.12
(2,661)	1:124:A:ALA:HB3	1:123:A:LYS:HB3	7	0.12
(2,654)	1:124:A:ALA:H	1:120:A:LEU:HA	2	0.12
(2,653)	1:124:A:ALA:H	1:120:A:LEU:HA	2	0.12
(2,638)	1:122:A:LEU:HD11	1:118:A:SER:HA	1	0.12
(2,638)	1:122:A:LEU:HD12	1:118:A:SER:HA	1	0.12
(2,638)	1:122:A:LEU:HD13	1:118:A:SER:HA	1	0.12
(2,637)	1:122:A:LEU:HD11	1:118:A:SER:HA	1	0.12
(2,637)	1:122:A:LEU:HD12	1:118:A:SER:HA	1	0.12
(2,637)	1:122:A:LEU:HD13	1:118:A:SER:HA	1	0.12
(2,628)	1:121:A:VAL:HG11	1:118:A:SER:HA	14	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,628)	1:121:A:VAL:HG12	1:118:A:SER:HA	14	0.12
(2,628)	1:121:A:VAL:HG13	1:118:A:SER:HA	14	0.12
(2,628)	1:121:A:VAL:HG21	1:118:A:SER:HA	14	0.12
(2,628)	1:121:A:VAL:HG22	1:118:A:SER:HA	14	0.12
(2,628)	1:121:A:VAL:HG23	1:118:A:SER:HA	14	0.12
(2,627)	1:121:A:VAL:HG11	1:118:A:SER:HA	14	0.12
(2,627)	1:121:A:VAL:HG12	1:118:A:SER:HA	14	0.12
(2,627)	1:121:A:VAL:HG13	1:118:A:SER:HA	14	0.12
(2,627)	1:121:A:VAL:HG21	1:118:A:SER:HA	14	0.12
(2,627)	1:121:A:VAL:HG22	1:118:A:SER:HA	14	0.12
(2,627)	1:121:A:VAL:HG23	1:118:A:SER:HA	14	0.12
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	1	0.12
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	1	0.12
(2,596)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	1	0.12
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	1	0.12
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	1	0.12
(2,596)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	1	0.12
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	1	0.12
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	1	0.12
(2,596)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	1	0.12
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG21	1	0.12
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG22	1	0.12
(2,595)	1:120:A:LEU:HD11	1:83:A:VAL:HG23	1	0.12
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG21	1	0.12
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG22	1	0.12
(2,595)	1:120:A:LEU:HD12	1:83:A:VAL:HG23	1	0.12
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG21	1	0.12
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG22	1	0.12
(2,595)	1:120:A:LEU:HD13	1:83:A:VAL:HG23	1	0.12
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	6	0.12
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	6	0.12
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	6	0.12
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	6	0.12
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	6	0.12
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	6	0.12
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	11	0.12
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	11	0.12
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	11	0.12
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	11	0.12
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	11	0.12
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	11	0.12
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	6	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	6	0.12
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	6	0.12
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	6	0.12
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	6	0.12
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	6	0.12
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	11	0.12
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	11	0.12
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	11	0.12
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	11	0.12
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	11	0.12
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	11	0.12
(2,531)	1:113:A:LEU:HD21	1:96:A:ALA:HA	11	0.12
(2,531)	1:113:A:LEU:HD22	1:96:A:ALA:HA	11	0.12
(2,531)	1:113:A:LEU:HD23	1:96:A:ALA:HA	11	0.12
(2,527)	1:113:A:LEU:HD21	1:96:A:ALA:HA	11	0.12
(2,527)	1:113:A:LEU:HD22	1:96:A:ALA:HA	11	0.12
(2,527)	1:113:A:LEU:HD23	1:96:A:ALA:HA	11	0.12
(2,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	6	0.12
(2,516)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	6	0.12
(2,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	6	0.12
(2,516)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	6	0.12
(2,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	6	0.12
(2,516)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	6	0.12
(2,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE1	6	0.12
(2,515)	1:112:A:ALA:HB1	1:115:A:TYR:HE2	6	0.12
(2,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE1	6	0.12
(2,515)	1:112:A:ALA:HB2	1:115:A:TYR:HE2	6	0.12
(2,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE1	6	0.12
(2,515)	1:112:A:ALA:HB3	1:115:A:TYR:HE2	6	0.12
(2,512)	1:112:A:ALA:H	1:110:A:VAL:H	9	0.12
(2,511)	1:112:A:ALA:H	1:110:A:VAL:H	9	0.12
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	5	0.12
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	5	0.12
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	5	0.12
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	5	0.12
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	5	0.12
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	5	0.12
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	6	0.12
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	6	0.12
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	6	0.12
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	6	0.12
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	6	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	6	0.12
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	10	0.12
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	10	0.12
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	10	0.12
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	10	0.12
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	10	0.12
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	10	0.12
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	5	0.12
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	5	0.12
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	5	0.12
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	5	0.12
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	5	0.12
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	5	0.12
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	6	0.12
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	6	0.12
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	6	0.12
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	6	0.12
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	6	0.12
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	6	0.12
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	10	0.12
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	10	0.12
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	10	0.12
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	10	0.12
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	10	0.12
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	10	0.12
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB2	3	0.12
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB3	3	0.12
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB2	5	0.12
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB3	5	0.12
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB2	3	0.12
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB3	3	0.12
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB2	5	0.12
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB3	5	0.12
(2,370)	1:95:A:VAL:HG21	1:92:A:PHE:HE2	8	0.12
(2,370)	1:95:A:VAL:HG22	1:92:A:PHE:HE2	8	0.12
(2,370)	1:95:A:VAL:HG23	1:92:A:PHE:HE2	8	0.12
(2,369)	1:95:A:VAL:HG21	1:92:A:PHE:HE2	8	0.12
(2,369)	1:95:A:VAL:HG22	1:92:A:PHE:HE2	8	0.12
(2,369)	1:95:A:VAL:HG23	1:92:A:PHE:HE2	8	0.12
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	7	0.12
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	7	0.12
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	7	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	7	0.12
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	7	0.12
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	7	0.12
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	1	0.12
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	1	0.12
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	1	0.12
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	1	0.12
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	1	0.12
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	1	0.12
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	1	0.12
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	1	0.12
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	1	0.12
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	4	0.12
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	4	0.12
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	4	0.12
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	4	0.12
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	4	0.12
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	4	0.12
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	4	0.12
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	4	0.12
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	4	0.12
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	1	0.12
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	1	0.12
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	1	0.12
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	1	0.12
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	1	0.12
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	1	0.12
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	1	0.12
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	1	0.12
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	1	0.12
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	4	0.12
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	4	0.12
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	4	0.12
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	4	0.12
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	4	0.12
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	4	0.12
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	4	0.12
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	4	0.12
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	4	0.12
(2,292)	1:87:A:SER:H	1:86:A:ASP:HA	1	0.12
(2,291)	1:87:A:SER:H	1:86:A:ASP:HA	1	0.12
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB1	10	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB2	10	0.12
(2,268)	1:84:A:ASP:H	1:82:A:ALA:HB3	10	0.12
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB1	10	0.12
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB2	10	0.12
(2,267)	1:84:A:ASP:H	1:82:A:ALA:HB3	10	0.12
(2,244)	1:83:A:VAL:H	1:82:A:ALA:HB1	13	0.12
(2,244)	1:83:A:VAL:H	1:82:A:ALA:HB2	13	0.12
(2,244)	1:83:A:VAL:H	1:82:A:ALA:HB3	13	0.12
(2,243)	1:83:A:VAL:H	1:82:A:ALA:HB1	13	0.12
(2,243)	1:83:A:VAL:H	1:82:A:ALA:HB2	13	0.12
(2,243)	1:83:A:VAL:H	1:82:A:ALA:HB3	13	0.12
(2,228)	1:81:A:ALA:HB1	1:80:A:ILE:HB	7	0.12
(2,228)	1:81:A:ALA:HB2	1:80:A:ILE:HB	7	0.12
(2,228)	1:81:A:ALA:HB3	1:80:A:ILE:HB	7	0.12
(2,227)	1:81:A:ALA:HB1	1:80:A:ILE:HB	7	0.12
(2,227)	1:81:A:ALA:HB2	1:80:A:ILE:HB	7	0.12
(2,227)	1:81:A:ALA:HB3	1:80:A:ILE:HB	7	0.12
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	1	0.12
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	1	0.12
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	1	0.12
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD21	7	0.12
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD22	7	0.12
(2,208)	1:77:A:GLN:H	1:76:A:LEU:HD23	7	0.12
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	1	0.12
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	1	0.12
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	1	0.12
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD21	7	0.12
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD22	7	0.12
(2,205)	1:77:A:GLN:H	1:76:A:LEU:HD23	7	0.12
(2,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	14	0.12
(2,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	14	0.12
(2,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	14	0.12
(2,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	14	0.12
(2,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	14	0.12
(2,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	14	0.12
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	7	0.12
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	7	0.12
(2,164)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	7	0.12
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	7	0.12
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	7	0.12
(2,164)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	7	0.12
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	7	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	7	0.12
(2,164)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	7	0.12
(2,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	14	0.12
(2,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	14	0.12
(2,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	14	0.12
(2,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	14	0.12
(2,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	14	0.12
(2,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	14	0.12
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	7	0.12
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	7	0.12
(2,161)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	7	0.12
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	7	0.12
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	7	0.12
(2,161)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	7	0.12
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	7	0.12
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	7	0.12
(2,161)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	7	0.12
(2,136)	1:67:A:GLY:H	1:66:A:ILE:HB	8	0.12
(2,136)	1:67:A:GLY:H	1:66:A:ILE:HB	14	0.12
(2,135)	1:67:A:GLY:H	1:66:A:ILE:HB	8	0.12
(2,135)	1:67:A:GLY:H	1:66:A:ILE:HB	14	0.12
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	3	0.12
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	3	0.12
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	11	0.12
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	11	0.12
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	3	0.12
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	3	0.12
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	11	0.12
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	11	0.12
(2,10)	1:54:A:ALA:HB1	1:53:A:ASP:HA	9	0.12
(2,10)	1:54:A:ALA:HB2	1:53:A:ASP:HA	9	0.12
(2,10)	1:54:A:ALA:HB3	1:53:A:ASP:HA	9	0.12
(2,9)	1:54:A:ALA:HB1	1:53:A:ASP:HA	9	0.12
(2,9)	1:54:A:ALA:HB2	1:53:A:ASP:HA	9	0.12
(2,9)	1:54:A:ALA:HB3	1:53:A:ASP:HA	9	0.12
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB1	10	0.12
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB2	10	0.12
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB3	10	0.12
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB1	13	0.12
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB2	13	0.12
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB3	13	0.12
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB1	14	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB2	14	0.12
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB3	14	0.12
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB1	10	0.12
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB2	10	0.12
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB3	10	0.12
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB1	13	0.12
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB2	13	0.12
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB3	13	0.12
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB1	14	0.12
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB2	14	0.12
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB3	14	0.12
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG21	15	0.12
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG22	15	0.12
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG23	15	0.12
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG21	15	0.12
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG22	15	0.12
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG23	15	0.12
(3,686)	1:126:A:SER:H	1:125:A:LEU:HG	6	0.11
(3,685)	1:126:A:SER:H	1:125:A:LEU:HG	6	0.11
(3,676)	1:125:A:LEU:HD11	1:122:A:LEU:HA	12	0.11
(3,676)	1:125:A:LEU:HD12	1:122:A:LEU:HA	12	0.11
(3,676)	1:125:A:LEU:HD13	1:122:A:LEU:HA	12	0.11
(3,675)	1:125:A:LEU:HD11	1:122:A:LEU:HA	12	0.11
(3,675)	1:125:A:LEU:HD12	1:122:A:LEU:HA	12	0.11
(3,675)	1:125:A:LEU:HD13	1:122:A:LEU:HA	12	0.11
(3,660)	1:124:A:ALA:H	1:123:A:LYS:HB2	6	0.11
(3,660)	1:124:A:ALA:H	1:123:A:LYS:HB3	6	0.11
(3,659)	1:124:A:ALA:H	1:123:A:LYS:HB2	6	0.11
(3,659)	1:124:A:ALA:H	1:123:A:LYS:HB3	6	0.11
(3,586)	1:120:A:LEU:H	1:117:A:ALA:HA	12	0.11
(3,585)	1:120:A:LEU:H	1:117:A:ALA:HA	12	0.11
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	3	0.11
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	3	0.11
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	3	0.11
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	3	0.11
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	3	0.11
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	3	0.11
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	10	0.11
(3,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	10	0.11
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	10	0.11
(3,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	10	0.11
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	10	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	10	0.11
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	3	0.11
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	3	0.11
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	3	0.11
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	3	0.11
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	3	0.11
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	3	0.11
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	10	0.11
(3,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	10	0.11
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	10	0.11
(3,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	10	0.11
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	10	0.11
(3,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	10	0.11
(3,518)	1:112:A:ALA:HB1	1:115:A:TYR:HD1	13	0.11
(3,518)	1:112:A:ALA:HB1	1:115:A:TYR:HD2	13	0.11
(3,518)	1:112:A:ALA:HB2	1:115:A:TYR:HD1	13	0.11
(3,518)	1:112:A:ALA:HB2	1:115:A:TYR:HD2	13	0.11
(3,518)	1:112:A:ALA:HB3	1:115:A:TYR:HD1	13	0.11
(3,518)	1:112:A:ALA:HB3	1:115:A:TYR:HD2	13	0.11
(3,517)	1:112:A:ALA:HB1	1:115:A:TYR:HD1	13	0.11
(3,517)	1:112:A:ALA:HB1	1:115:A:TYR:HD2	13	0.11
(3,517)	1:112:A:ALA:HB2	1:115:A:TYR:HD1	13	0.11
(3,517)	1:112:A:ALA:HB2	1:115:A:TYR:HD2	13	0.11
(3,517)	1:112:A:ALA:HB3	1:115:A:TYR:HD1	13	0.11
(3,517)	1:112:A:ALA:HB3	1:115:A:TYR:HD2	13	0.11
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	8	0.11
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	8	0.11
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	8	0.11
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	8	0.11
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	8	0.11
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	8	0.11
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	14	0.11
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	14	0.11
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	14	0.11
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	14	0.11
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	14	0.11
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	14	0.11
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	8	0.11
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	8	0.11
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	8	0.11
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	8	0.11
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	8	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	8	0.11
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	14	0.11
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	14	0.11
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	14	0.11
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	14	0.11
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	14	0.11
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	14	0.11
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB2	4	0.11
(3,454)	1:101:A:SER:H	1:100:A:PHE:HB3	4	0.11
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB2	4	0.11
(3,453)	1:101:A:SER:H	1:100:A:PHE:HB3	4	0.11
(3,436)	1:99:A:MET:H	1:97:A:ALA:HA	10	0.11
(3,435)	1:99:A:MET:H	1:97:A:ALA:HA	10	0.11
(3,386)	1:96:A:ALA:H	1:95:A:VAL:HG21	4	0.11
(3,386)	1:96:A:ALA:H	1:95:A:VAL:HG22	4	0.11
(3,386)	1:96:A:ALA:H	1:95:A:VAL:HG23	4	0.11
(3,386)	1:96:A:ALA:H	1:95:A:VAL:HG21	14	0.11
(3,386)	1:96:A:ALA:H	1:95:A:VAL:HG22	14	0.11
(3,386)	1:96:A:ALA:H	1:95:A:VAL:HG23	14	0.11
(3,385)	1:96:A:ALA:H	1:95:A:VAL:HG21	4	0.11
(3,385)	1:96:A:ALA:H	1:95:A:VAL:HG22	4	0.11
(3,385)	1:96:A:ALA:H	1:95:A:VAL:HG23	4	0.11
(3,385)	1:96:A:ALA:H	1:95:A:VAL:HG21	14	0.11
(3,385)	1:96:A:ALA:H	1:95:A:VAL:HG22	14	0.11
(3,385)	1:96:A:ALA:H	1:95:A:VAL:HG23	14	0.11
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	4	0.11
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	4	0.11
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	4	0.11
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	12	0.11
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	12	0.11
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	12	0.11
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	15	0.11
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	15	0.11
(3,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	15	0.11
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	4	0.11
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	4	0.11
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	4	0.11
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	12	0.11
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	12	0.11
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	12	0.11
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	15	0.11
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	15	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	15	0.11
(3,300)	1:90:A:GLU:H	1:89:A:ARG:HB2	11	0.11
(3,300)	1:90:A:GLU:H	1:89:A:ARG:HB3	11	0.11
(3,299)	1:90:A:GLU:H	1:89:A:ARG:HB2	11	0.11
(3,299)	1:90:A:GLU:H	1:89:A:ARG:HB3	11	0.11
(3,274)	1:85:A:THR:H	1:84:A:ASP:HB2	6	0.11
(3,274)	1:85:A:THR:H	1:84:A:ASP:HB3	6	0.11
(3,273)	1:85:A:THR:H	1:84:A:ASP:HB2	6	0.11
(3,273)	1:85:A:THR:H	1:84:A:ASP:HB3	6	0.11
(3,264)	1:84:A:ASP:H	1:83:A:VAL:HG11	10	0.11
(3,264)	1:84:A:ASP:H	1:83:A:VAL:HG12	10	0.11
(3,264)	1:84:A:ASP:H	1:83:A:VAL:HG13	10	0.11
(3,263)	1:84:A:ASP:H	1:83:A:VAL:HG11	10	0.11
(3,263)	1:84:A:ASP:H	1:83:A:VAL:HG12	10	0.11
(3,263)	1:84:A:ASP:H	1:83:A:VAL:HG13	10	0.11
(3,262)	1:84:A:ASP:H	1:83:A:VAL:H	12	0.11
(3,261)	1:84:A:ASP:H	1:83:A:VAL:H	12	0.11
(3,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD21	6	0.11
(3,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD22	6	0.11
(3,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD23	6	0.11
(3,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD21	6	0.11
(3,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD22	6	0.11
(3,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD23	6	0.11
(3,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD21	6	0.11
(3,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD22	6	0.11
(3,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD23	6	0.11
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD11	2	0.11
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD12	2	0.11
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD13	2	0.11
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD11	2	0.11
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD12	2	0.11
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD13	2	0.11
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD11	2	0.11
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD12	2	0.11
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD13	2	0.11
(3,248)	1:83:A:VAL:H	1:84:A:ASP:H	12	0.11
(3,247)	1:83:A:VAL:H	1:84:A:ASP:H	12	0.11
(3,238)	1:82:A:ALA:H	1:80:A:ILE:HB	14	0.11
(3,237)	1:82:A:ALA:H	1:80:A:ILE:HB	14	0.11
(3,218)	1:80:A:ILE:HD11	1:116:A:PHE:HE1	1	0.11
(3,218)	1:80:A:ILE:HD11	1:116:A:PHE:HE2	1	0.11
(3,218)	1:80:A:ILE:HD12	1:116:A:PHE:HE1	1	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,218)	1:80:A:ILE:HD12	1:116:A:PHE:HE2	1	0.11
(3,218)	1:80:A:ILE:HD13	1:116:A:PHE:HE1	1	0.11
(3,218)	1:80:A:ILE:HD13	1:116:A:PHE:HE2	1	0.11
(3,218)	1:80:A:ILE:HD11	1:116:A:PHE:HE1	14	0.11
(3,218)	1:80:A:ILE:HD11	1:116:A:PHE:HE2	14	0.11
(3,218)	1:80:A:ILE:HD12	1:116:A:PHE:HE1	14	0.11
(3,218)	1:80:A:ILE:HD12	1:116:A:PHE:HE2	14	0.11
(3,218)	1:80:A:ILE:HD13	1:116:A:PHE:HE1	14	0.11
(3,218)	1:80:A:ILE:HD13	1:116:A:PHE:HE2	14	0.11
(3,217)	1:80:A:ILE:HD11	1:116:A:PHE:HE1	1	0.11
(3,217)	1:80:A:ILE:HD11	1:116:A:PHE:HE2	1	0.11
(3,217)	1:80:A:ILE:HD12	1:116:A:PHE:HE1	1	0.11
(3,217)	1:80:A:ILE:HD12	1:116:A:PHE:HE2	1	0.11
(3,217)	1:80:A:ILE:HD13	1:116:A:PHE:HE1	1	0.11
(3,217)	1:80:A:ILE:HD13	1:116:A:PHE:HE2	1	0.11
(3,217)	1:80:A:ILE:HD11	1:116:A:PHE:HE1	14	0.11
(3,217)	1:80:A:ILE:HD11	1:116:A:PHE:HE2	14	0.11
(3,217)	1:80:A:ILE:HD12	1:116:A:PHE:HE1	14	0.11
(3,217)	1:80:A:ILE:HD12	1:116:A:PHE:HE2	14	0.11
(3,217)	1:80:A:ILE:HD13	1:116:A:PHE:HE1	14	0.11
(3,217)	1:80:A:ILE:HD13	1:116:A:PHE:HE2	14	0.11
(3,174)	1:71:A:ASP:H	1:70:A:LEU:HG	4	0.11
(3,173)	1:71:A:ASP:H	1:70:A:LEU:HG	4	0.11
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	1	0.11
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	1	0.11
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	1	0.11
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	1	0.11
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	1	0.11
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	1	0.11
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	1	0.11
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	1	0.11
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	1	0.11
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	1	0.11
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	1	0.11
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	1	0.11
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	8	0.11
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	8	0.11
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	8	0.11
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	8	0.11
(3,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	1	0.11
(3,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	1	0.11
(3,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	1	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	1	0.11
(3,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	1	0.11
(3,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	1	0.11
(3,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	1	0.11
(3,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	1	0.11
(3,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	1	0.11
(3,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	1	0.11
(3,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	1	0.11
(3,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	1	0.11
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB1	8	0.11
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB2	8	0.11
(3,8)	1:53:A:ASP:H	1:54:A:ALA:HB3	8	0.11
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB1	8	0.11
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB2	8	0.11
(3,7)	1:53:A:ASP:H	1:54:A:ALA:HB3	8	0.11
(2,686)	1:126:A:SER:H	1:125:A:LEU:HG	6	0.11
(2,685)	1:126:A:SER:H	1:125:A:LEU:HG	6	0.11
(2,676)	1:125:A:LEU:HD11	1:122:A:LEU:HA	12	0.11
(2,676)	1:125:A:LEU:HD12	1:122:A:LEU:HA	12	0.11
(2,676)	1:125:A:LEU:HD13	1:122:A:LEU:HA	12	0.11
(2,675)	1:125:A:LEU:HD11	1:122:A:LEU:HA	12	0.11
(2,675)	1:125:A:LEU:HD12	1:122:A:LEU:HA	12	0.11
(2,675)	1:125:A:LEU:HD13	1:122:A:LEU:HA	12	0.11
(2,660)	1:124:A:ALA:H	1:123:A:LYS:HB2	6	0.11
(2,660)	1:124:A:ALA:H	1:123:A:LYS:HB3	6	0.11
(2,659)	1:124:A:ALA:H	1:123:A:LYS:HB2	6	0.11
(2,659)	1:124:A:ALA:H	1:123:A:LYS:HB3	6	0.11
(2,586)	1:120:A:LEU:H	1:117:A:ALA:HA	12	0.11
(2,585)	1:120:A:LEU:H	1:117:A:ALA:HA	12	0.11
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	3	0.11
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	3	0.11
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	3	0.11
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	3	0.11
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	3	0.11
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	3	0.11
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	10	0.11
(2,568)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	10	0.11
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	10	0.11
(2,568)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	10	0.11
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	10	0.11
(2,568)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	10	0.11
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	3	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	3	0.11
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	3	0.11
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	3	0.11
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	3	0.11
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	3	0.11
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD1	10	0.11
(2,567)	1:117:A:ALA:HB1	1:114:A:PHE:HD2	10	0.11
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD1	10	0.11
(2,567)	1:117:A:ALA:HB2	1:114:A:PHE:HD2	10	0.11
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD1	10	0.11
(2,567)	1:117:A:ALA:HB3	1:114:A:PHE:HD2	10	0.11
(2,518)	1:112:A:ALA:HB1	1:115:A:TYR:HD1	13	0.11
(2,518)	1:112:A:ALA:HB1	1:115:A:TYR:HD2	13	0.11
(2,518)	1:112:A:ALA:HB2	1:115:A:TYR:HD1	13	0.11
(2,518)	1:112:A:ALA:HB2	1:115:A:TYR:HD2	13	0.11
(2,518)	1:112:A:ALA:HB3	1:115:A:TYR:HD1	13	0.11
(2,518)	1:112:A:ALA:HB3	1:115:A:TYR:HD2	13	0.11
(2,517)	1:112:A:ALA:HB1	1:115:A:TYR:HD1	13	0.11
(2,517)	1:112:A:ALA:HB1	1:115:A:TYR:HD2	13	0.11
(2,517)	1:112:A:ALA:HB2	1:115:A:TYR:HD1	13	0.11
(2,517)	1:112:A:ALA:HB2	1:115:A:TYR:HD2	13	0.11
(2,517)	1:112:A:ALA:HB3	1:115:A:TYR:HD1	13	0.11
(2,517)	1:112:A:ALA:HB3	1:115:A:TYR:HD2	13	0.11
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	8	0.11
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	8	0.11
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	8	0.11
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	8	0.11
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	8	0.11
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	8	0.11
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	14	0.11
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	14	0.11
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	14	0.11
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	14	0.11
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	14	0.11
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	14	0.11
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	8	0.11
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	8	0.11
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	8	0.11
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	8	0.11
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	8	0.11
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	8	0.11
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	14	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	14	0.11
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	14	0.11
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	14	0.11
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	14	0.11
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	14	0.11
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB2	4	0.11
(2,454)	1:101:A:SER:H	1:100:A:PHE:HB3	4	0.11
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB2	4	0.11
(2,453)	1:101:A:SER:H	1:100:A:PHE:HB3	4	0.11
(2,436)	1:99:A:MET:H	1:97:A:ALA:HA	10	0.11
(2,435)	1:99:A:MET:H	1:97:A:ALA:HA	10	0.11
(2,386)	1:96:A:ALA:H	1:95:A:VAL:HG21	4	0.11
(2,386)	1:96:A:ALA:H	1:95:A:VAL:HG22	4	0.11
(2,386)	1:96:A:ALA:H	1:95:A:VAL:HG23	4	0.11
(2,386)	1:96:A:ALA:H	1:95:A:VAL:HG21	14	0.11
(2,386)	1:96:A:ALA:H	1:95:A:VAL:HG22	14	0.11
(2,386)	1:96:A:ALA:H	1:95:A:VAL:HG23	14	0.11
(2,385)	1:96:A:ALA:H	1:95:A:VAL:HG21	4	0.11
(2,385)	1:96:A:ALA:H	1:95:A:VAL:HG22	4	0.11
(2,385)	1:96:A:ALA:H	1:95:A:VAL:HG23	4	0.11
(2,385)	1:96:A:ALA:H	1:95:A:VAL:HG21	14	0.11
(2,385)	1:96:A:ALA:H	1:95:A:VAL:HG22	14	0.11
(2,385)	1:96:A:ALA:H	1:95:A:VAL:HG23	14	0.11
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	4	0.11
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	4	0.11
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	4	0.11
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	12	0.11
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	12	0.11
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	12	0.11
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB1	15	0.11
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB2	15	0.11
(2,368)	1:95:A:VAL:H	1:96:A:ALA:HB3	15	0.11
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	4	0.11
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	4	0.11
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	4	0.11
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	12	0.11
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	12	0.11
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	12	0.11
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB1	15	0.11
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB2	15	0.11
(2,367)	1:95:A:VAL:H	1:96:A:ALA:HB3	15	0.11
(2,300)	1:90:A:GLU:H	1:89:A:ARG:HB2	11	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,300)	1:90:A:GLU:H	1:89:A:ARG:HB3	11	0.11
(2,299)	1:90:A:GLU:H	1:89:A:ARG:HB2	11	0.11
(2,299)	1:90:A:GLU:H	1:89:A:ARG:HB3	11	0.11
(2,274)	1:85:A:THR:H	1:84:A:ASP:HB2	6	0.11
(2,274)	1:85:A:THR:H	1:84:A:ASP:HB3	6	0.11
(2,273)	1:85:A:THR:H	1:84:A:ASP:HB2	6	0.11
(2,273)	1:85:A:THR:H	1:84:A:ASP:HB3	6	0.11
(2,264)	1:84:A:ASP:H	1:83:A:VAL:HG11	10	0.11
(2,264)	1:84:A:ASP:H	1:83:A:VAL:HG12	10	0.11
(2,264)	1:84:A:ASP:H	1:83:A:VAL:HG13	10	0.11
(2,263)	1:84:A:ASP:H	1:83:A:VAL:HG11	10	0.11
(2,263)	1:84:A:ASP:H	1:83:A:VAL:HG12	10	0.11
(2,263)	1:84:A:ASP:H	1:83:A:VAL:HG13	10	0.11
(2,262)	1:84:A:ASP:H	1:83:A:VAL:H	12	0.11
(2,261)	1:84:A:ASP:H	1:83:A:VAL:H	12	0.11
(2,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD21	6	0.11
(2,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD22	6	0.11
(2,252)	1:83:A:VAL:HG11	1:120:A:LEU:HD23	6	0.11
(2,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD21	6	0.11
(2,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD22	6	0.11
(2,252)	1:83:A:VAL:HG12	1:120:A:LEU:HD23	6	0.11
(2,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD21	6	0.11
(2,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD22	6	0.11
(2,252)	1:83:A:VAL:HG13	1:120:A:LEU:HD23	6	0.11
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD11	2	0.11
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD12	2	0.11
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD13	2	0.11
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD11	2	0.11
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD12	2	0.11
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD13	2	0.11
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD11	2	0.11
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD12	2	0.11
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD13	2	0.11
(2,248)	1:83:A:VAL:H	1:84:A:ASP:H	12	0.11
(2,247)	1:83:A:VAL:H	1:84:A:ASP:H	12	0.11
(2,238)	1:82:A:ALA:H	1:80:A:ILE:HB	14	0.11
(2,237)	1:82:A:ALA:H	1:80:A:ILE:HB	14	0.11
(2,218)	1:80:A:ILE:HD11	1:116:A:PHE:HE1	1	0.11
(2,218)	1:80:A:ILE:HD11	1:116:A:PHE:HE2	1	0.11
(2,218)	1:80:A:ILE:HD12	1:116:A:PHE:HE1	1	0.11
(2,218)	1:80:A:ILE:HD12	1:116:A:PHE:HE2	1	0.11
(2,218)	1:80:A:ILE:HD13	1:116:A:PHE:HE1	1	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,218)	1:80:A:ILE:HD13	1:116:A:PHE:HE2	1	0.11
(2,218)	1:80:A:ILE:HD11	1:116:A:PHE:HE1	14	0.11
(2,218)	1:80:A:ILE:HD11	1:116:A:PHE:HE2	14	0.11
(2,218)	1:80:A:ILE:HD12	1:116:A:PHE:HE1	14	0.11
(2,218)	1:80:A:ILE:HD12	1:116:A:PHE:HE2	14	0.11
(2,218)	1:80:A:ILE:HD13	1:116:A:PHE:HE1	14	0.11
(2,218)	1:80:A:ILE:HD13	1:116:A:PHE:HE2	14	0.11
(2,217)	1:80:A:ILE:HD11	1:116:A:PHE:HE1	1	0.11
(2,217)	1:80:A:ILE:HD11	1:116:A:PHE:HE2	1	0.11
(2,217)	1:80:A:ILE:HD12	1:116:A:PHE:HE1	1	0.11
(2,217)	1:80:A:ILE:HD12	1:116:A:PHE:HE2	1	0.11
(2,217)	1:80:A:ILE:HD13	1:116:A:PHE:HE1	1	0.11
(2,217)	1:80:A:ILE:HD13	1:116:A:PHE:HE2	1	0.11
(2,217)	1:80:A:ILE:HD11	1:116:A:PHE:HE1	14	0.11
(2,217)	1:80:A:ILE:HD11	1:116:A:PHE:HE2	14	0.11
(2,217)	1:80:A:ILE:HD12	1:116:A:PHE:HE1	14	0.11
(2,217)	1:80:A:ILE:HD12	1:116:A:PHE:HE2	14	0.11
(2,217)	1:80:A:ILE:HD13	1:116:A:PHE:HE1	14	0.11
(2,217)	1:80:A:ILE:HD13	1:116:A:PHE:HE2	14	0.11
(2,174)	1:71:A:ASP:H	1:70:A:LEU:HG	4	0.11
(2,173)	1:71:A:ASP:H	1:70:A:LEU:HG	4	0.11
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	1	0.11
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	1	0.11
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	1	0.11
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	1	0.11
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	1	0.11
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	1	0.11
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	1	0.11
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	1	0.11
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	1	0.11
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	1	0.11
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	1	0.11
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	1	0.11
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	8	0.11
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	8	0.11
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	8	0.11
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	8	0.11
(2,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	1	0.11
(2,12)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	1	0.11
(2,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	1	0.11
(2,12)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	1	0.11
(2,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	1	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,12)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	1	0.11
(2,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB2	1	0.11
(2,11)	1:54:A:ALA:HB1	1:53:A:ASP:HB3	1	0.11
(2,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB2	1	0.11
(2,11)	1:54:A:ALA:HB2	1:53:A:ASP:HB3	1	0.11
(2,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB2	1	0.11
(2,11)	1:54:A:ALA:HB3	1:53:A:ASP:HB3	1	0.11
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB1	8	0.11
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB2	8	0.11
(2,8)	1:53:A:ASP:H	1:54:A:ALA:HB3	8	0.11
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB1	8	0.11
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB2	8	0.11
(2,7)	1:53:A:ASP:H	1:54:A:ALA:HB3	8	0.11
(3,654)	1:124:A:ALA:H	1:120:A:LEU:HA	11	0.1
(3,653)	1:124:A:ALA:H	1:120:A:LEU:HA	11	0.1
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	3	0.1
(3,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	3	0.1
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	3	0.1
(3,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	3	0.1
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	3	0.1
(3,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	3	0.1
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	3	0.1
(3,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	3	0.1
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	3	0.1
(3,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	3	0.1
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	3	0.1
(3,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	3	0.1
(3,422)	1:98:A:ASP:H	1:96:A:ALA:HA	7	0.1
(3,421)	1:98:A:ASP:H	1:96:A:ALA:HA	7	0.1
(3,316)	1:91:A:VAL:HG11	1:83:A:VAL:HA	11	0.1
(3,316)	1:91:A:VAL:HG12	1:83:A:VAL:HA	11	0.1
(3,316)	1:91:A:VAL:HG13	1:83:A:VAL:HA	11	0.1
(3,315)	1:91:A:VAL:HG11	1:83:A:VAL:HA	11	0.1
(3,315)	1:91:A:VAL:HG12	1:83:A:VAL:HA	11	0.1
(3,315)	1:91:A:VAL:HG13	1:83:A:VAL:HA	11	0.1
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	7	0.1
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	7	0.1
(3,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	7	0.1
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	7	0.1
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	7	0.1
(3,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	7	0.1
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	7	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	7	0.1
(3,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	7	0.1
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	7	0.1
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	7	0.1
(3,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	7	0.1
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	7	0.1
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	7	0.1
(3,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	7	0.1
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	7	0.1
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	7	0.1
(3,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	7	0.1
(3,284)	1:86:A:ASP:H	1:85:A:THR:H	12	0.1
(3,283)	1:86:A:ASP:H	1:85:A:THR:H	12	0.1
(3,276)	1:85:A:THR:H	1:86:A:ASP:H	12	0.1
(3,275)	1:85:A:THR:H	1:86:A:ASP:H	12	0.1
(3,270)	1:84:A:ASP:H	1:83:A:VAL:HB	9	0.1
(3,270)	1:84:A:ASP:H	1:83:A:VAL:HB	14	0.1
(3,269)	1:84:A:ASP:H	1:83:A:VAL:HB	9	0.1
(3,269)	1:84:A:ASP:H	1:83:A:VAL:HB	14	0.1
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD11	7	0.1
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD12	7	0.1
(3,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD13	7	0.1
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD11	7	0.1
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD12	7	0.1
(3,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD13	7	0.1
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD11	7	0.1
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD12	7	0.1
(3,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD13	7	0.1
(3,188)	1:73:A:ASN:H	1:74:A:MET:H	6	0.1
(3,185)	1:73:A:ASN:H	1:74:A:MET:H	6	0.1
(3,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	13	0.1
(3,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	13	0.1
(3,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	13	0.1
(3,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	13	0.1
(3,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	13	0.1
(3,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	13	0.1
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	14	0.1
(3,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	14	0.1
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	14	0.1
(3,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	14	0.1
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	14	0.1
(3,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	14	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	13	0.1
(3,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	13	0.1
(3,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	13	0.1
(3,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	13	0.1
(3,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	13	0.1
(3,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	13	0.1
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	14	0.1
(3,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	14	0.1
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	14	0.1
(3,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	14	0.1
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	14	0.1
(3,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	14	0.1
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	4	0.1
(3,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	4	0.1
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	4	0.1
(3,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	4	0.1
(2,654)	1:124:A:ALA:H	1:120:A:LEU:HA	11	0.1
(2,653)	1:124:A:ALA:H	1:120:A:LEU:HA	11	0.1
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	3	0.1
(2,496)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	3	0.1
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	3	0.1
(2,496)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	3	0.1
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	3	0.1
(2,496)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	3	0.1
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD1	3	0.1
(2,495)	1:110:A:VAL:HG21	1:105:A:PHE:HD2	3	0.1
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD1	3	0.1
(2,495)	1:110:A:VAL:HG22	1:105:A:PHE:HD2	3	0.1
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD1	3	0.1
(2,495)	1:110:A:VAL:HG23	1:105:A:PHE:HD2	3	0.1
(2,422)	1:98:A:ASP:H	1:96:A:ALA:HA	7	0.1
(2,421)	1:98:A:ASP:H	1:96:A:ALA:HA	7	0.1
(2,316)	1:91:A:VAL:HG11	1:83:A:VAL:HA	11	0.1
(2,316)	1:91:A:VAL:HG12	1:83:A:VAL:HA	11	0.1
(2,316)	1:91:A:VAL:HG13	1:83:A:VAL:HA	11	0.1
(2,315)	1:91:A:VAL:HG11	1:83:A:VAL:HA	11	0.1
(2,315)	1:91:A:VAL:HG12	1:83:A:VAL:HA	11	0.1
(2,315)	1:91:A:VAL:HG13	1:83:A:VAL:HA	11	0.1
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	7	0.1
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	7	0.1
(2,312)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	7	0.1
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	7	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	7	0.1
(2,312)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	7	0.1
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	7	0.1
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	7	0.1
(2,312)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	7	0.1
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG21	7	0.1
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG22	7	0.1
(2,311)	1:91:A:VAL:HG11	1:83:A:VAL:HG23	7	0.1
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG21	7	0.1
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG22	7	0.1
(2,311)	1:91:A:VAL:HG12	1:83:A:VAL:HG23	7	0.1
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG21	7	0.1
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG22	7	0.1
(2,311)	1:91:A:VAL:HG13	1:83:A:VAL:HG23	7	0.1
(2,284)	1:86:A:ASP:H	1:85:A:THR:H	12	0.1
(2,283)	1:86:A:ASP:H	1:85:A:THR:H	12	0.1
(2,276)	1:85:A:THR:H	1:86:A:ASP:H	12	0.1
(2,275)	1:85:A:THR:H	1:86:A:ASP:H	12	0.1
(2,270)	1:84:A:ASP:H	1:83:A:VAL:HB	9	0.1
(2,270)	1:84:A:ASP:H	1:83:A:VAL:HB	14	0.1
(2,269)	1:84:A:ASP:H	1:83:A:VAL:HB	9	0.1
(2,269)	1:84:A:ASP:H	1:83:A:VAL:HB	14	0.1
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD11	7	0.1
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD12	7	0.1
(2,251)	1:83:A:VAL:HG11	1:120:A:LEU:HD13	7	0.1
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD11	7	0.1
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD12	7	0.1
(2,251)	1:83:A:VAL:HG12	1:120:A:LEU:HD13	7	0.1
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD11	7	0.1
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD12	7	0.1
(2,251)	1:83:A:VAL:HG13	1:120:A:LEU:HD13	7	0.1
(2,188)	1:73:A:ASN:H	1:74:A:MET:H	6	0.1
(2,185)	1:73:A:ASN:H	1:74:A:MET:H	6	0.1
(2,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	13	0.1
(2,166)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	13	0.1
(2,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	13	0.1
(2,166)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	13	0.1
(2,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	13	0.1
(2,166)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	13	0.1
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	14	0.1
(2,165)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	14	0.1
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	14	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,165)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	14	0.1
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	14	0.1
(2,165)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	14	0.1
(2,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE1	13	0.1
(2,163)	1:70:A:LEU:HD21	1:115:A:TYR:HE2	13	0.1
(2,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE1	13	0.1
(2,163)	1:70:A:LEU:HD22	1:115:A:TYR:HE2	13	0.1
(2,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE1	13	0.1
(2,163)	1:70:A:LEU:HD23	1:115:A:TYR:HE2	13	0.1
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD1	14	0.1
(2,162)	1:70:A:LEU:HD11	1:115:A:TYR:HD2	14	0.1
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD1	14	0.1
(2,162)	1:70:A:LEU:HD12	1:115:A:TYR:HD2	14	0.1
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD1	14	0.1
(2,162)	1:70:A:LEU:HD13	1:115:A:TYR:HD2	14	0.1
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD2	4	0.1
(2,94)	1:61:A:GLU:H	1:58:A:LYS:HD3	4	0.1
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD2	4	0.1
(2,93)	1:61:A:GLU:H	1:58:A:LYS:HD3	4	0.1
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG21	13	0.1
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG22	13	0.1
(1,54)	1:114:A:PHE:H	1:111:A:VAL:HG23	13	0.1
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG21	13	0.1
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG22	13	0.1
(1,53)	1:114:A:PHE:H	1:111:A:VAL:HG23	13	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found