Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 11:40 AM EDT

PDB ID	:	2LMA
BMRB ID	:	17584
Title	:	Solution structure of CD4+ T cell derived peptide Thp5
Authors	:	Pandey, N.K.; Khan, M.M.; Chatterjee, S.; Dwivedi, V.P.; Tousif, S.; Das, J.; Van Kaer, L.
Deposited on	:	2011-11-29

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

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

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

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

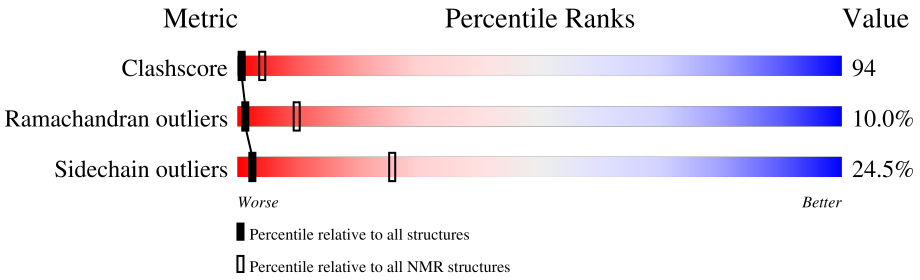
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 64%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	22	27% 18% 5% 50%

2 Ensemble composition and analysis (i)

This entry contains 40 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:12-A:22 (11)	0.16	5

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

Cluster number	Models
1	2, 4, 5, 7, 8, 9, 10, 11, 12, 14, 15, 17, 18, 19, 20, 23, 24, 25, 26, 27, 28, 29, 30, 32
2	1, 3, 6, 13, 16, 21, 22, 31, 35
3	34, 36, 37, 38
4	39, 40
Single-model clusters	33

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 365 atoms, of which 175 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Thp5 peptide.

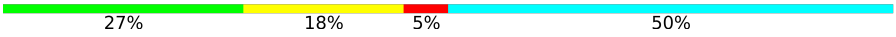
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	22	365	127	175	27	35	1	0

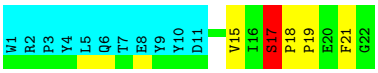
4 Residue-property plots

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: Thp5 peptide

Chain A: 

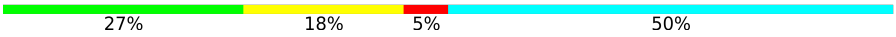


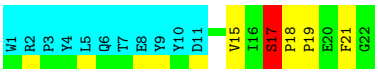
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

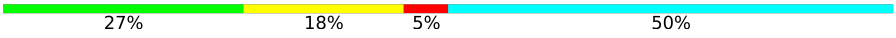
• Molecule 1: Thp5 peptide

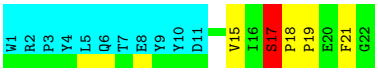
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: Thp5 peptide

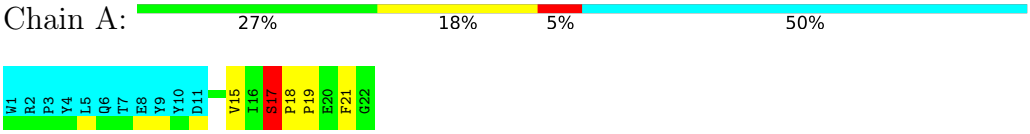
Chain A: 



4.2.3 Score per residue for model 3

• Molecule 1: Thp5 peptide

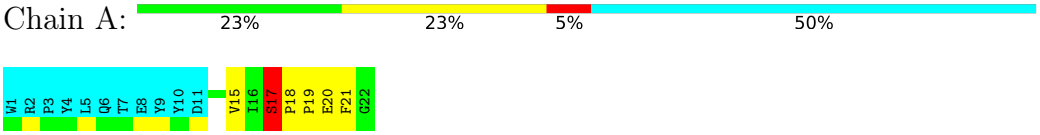
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Thp5 peptide

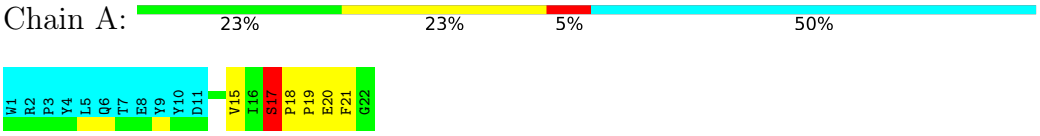
Chain A:



4.2.5 Score per residue for model 5 (medoid)

• Molecule 1: Thp5 peptide

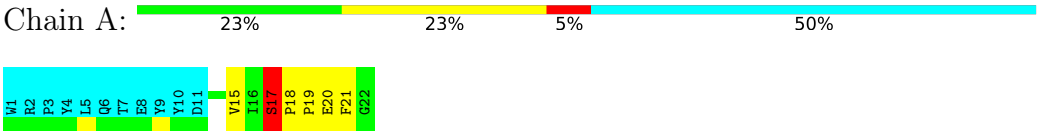
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Thp5 peptide

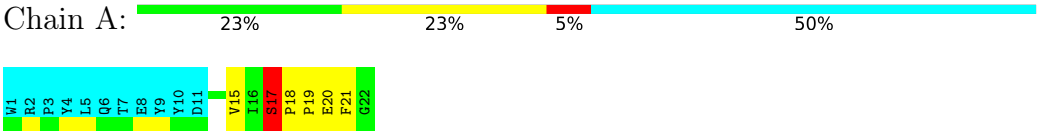
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Thp5 peptide

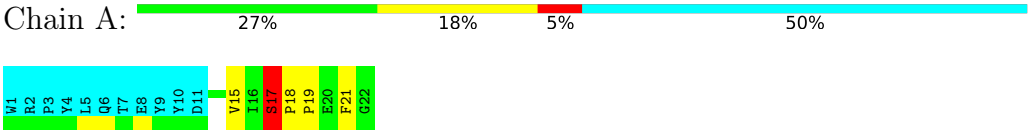
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Thp5 peptide

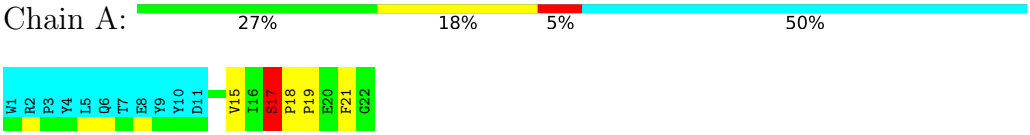
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Thp5 peptide

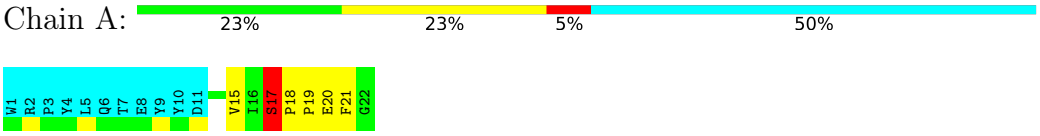
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Thp5 peptide

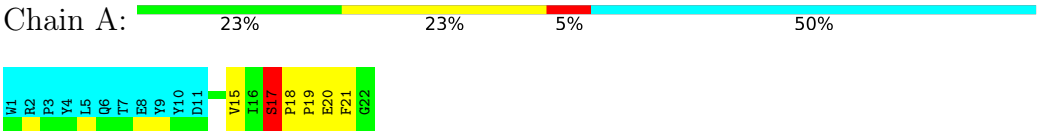
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Thp5 peptide

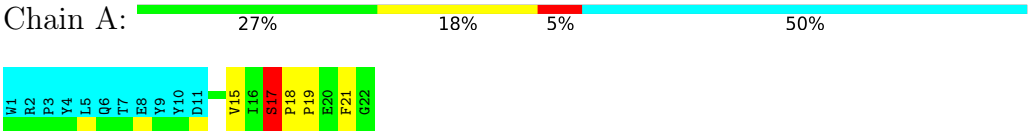
Chain A:



4.2.12 Score per residue for model 12

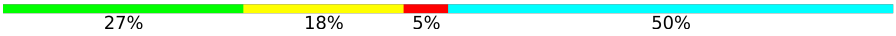
• Molecule 1: Thp5 peptide

Chain A:



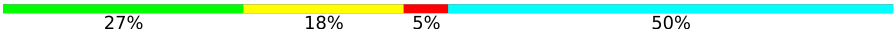
4.2.13 Score per residue for model 13

• Molecule 1: Thp5 peptide

Chain A: 

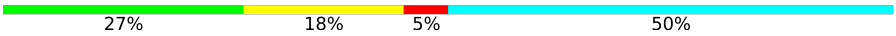
4.2.14 Score per residue for model 14

• Molecule 1: Thp5 peptide

Chain A: 

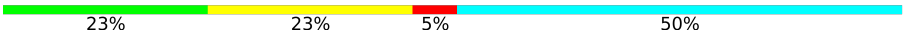
4.2.15 Score per residue for model 15

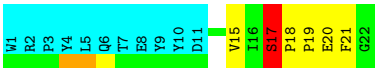
• Molecule 1: Thp5 peptide

Chain A: 

4.2.16 Score per residue for model 16

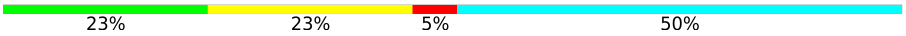
• Molecule 1: Thp5 peptide

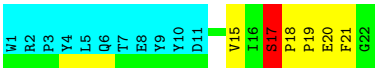
Chain A: 



4.2.17 Score per residue for model 17

• Molecule 1: Thp5 peptide

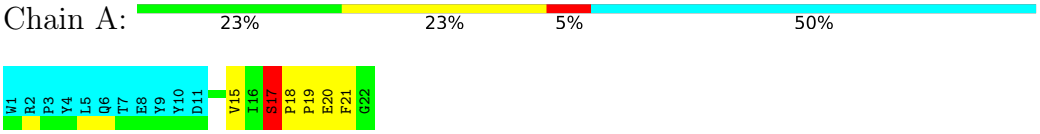
Chain A: 



4.2.18 Score per residue for model 18

• Molecule 1: Thp5 peptide

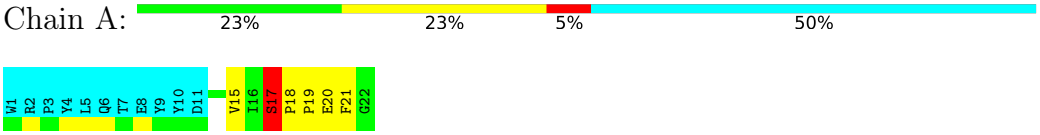
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Thp5 peptide

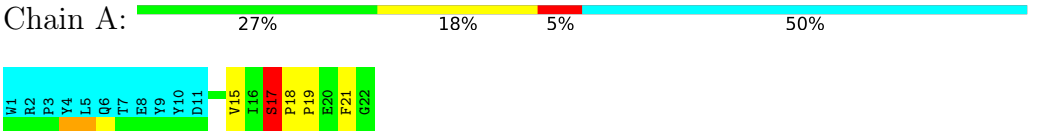
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Thp5 peptide

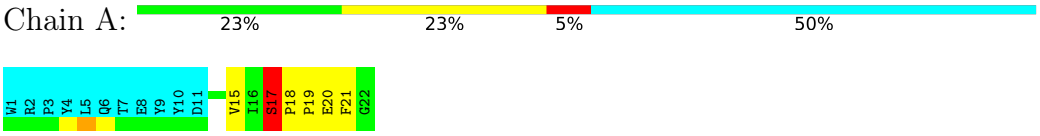
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: Thp5 peptide

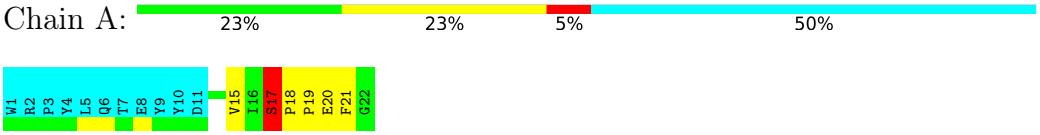
Chain A:



4.2.22 Score per residue for model 22

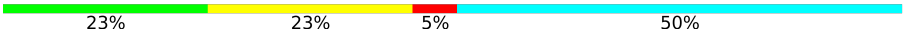
• Molecule 1: Thp5 peptide

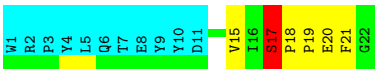
Chain A:



4.2.23 Score per residue for model 23

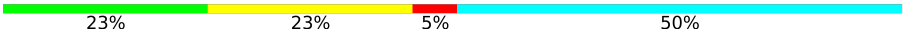
• Molecule 1: Thp5 peptide

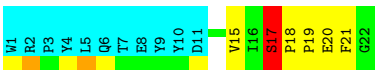
Chain A: 



4.2.24 Score per residue for model 24

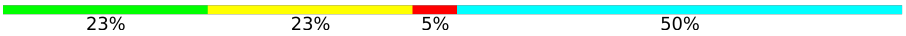
• Molecule 1: Thp5 peptide

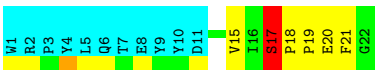
Chain A: 



4.2.25 Score per residue for model 25

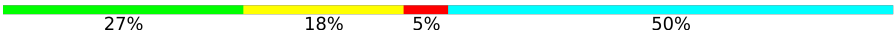
• Molecule 1: Thp5 peptide

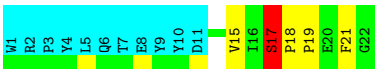
Chain A: 



4.2.26 Score per residue for model 26

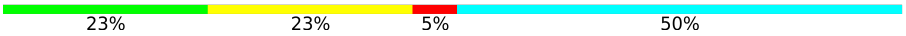
• Molecule 1: Thp5 peptide

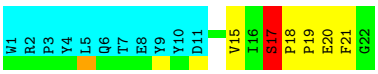
Chain A: 



4.2.27 Score per residue for model 27

• Molecule 1: Thp5 peptide

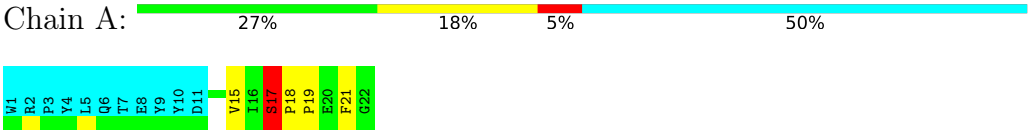
Chain A: 



4.2.28 Score per residue for model 28

• Molecule 1: Thp5 peptide

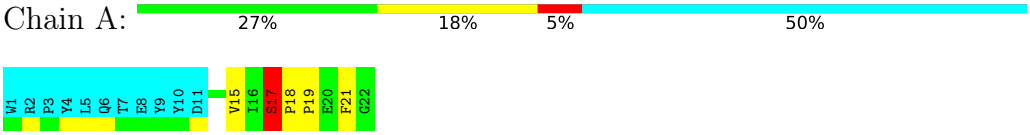
Chain A:



4.2.29 Score per residue for model 29

• Molecule 1: Thp5 peptide

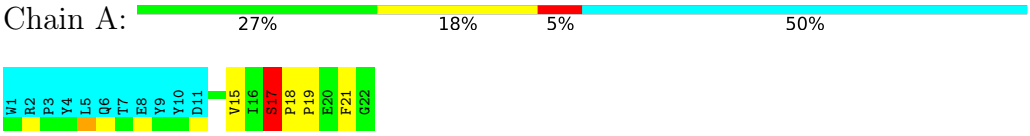
Chain A:



4.2.30 Score per residue for model 30

• Molecule 1: Thp5 peptide

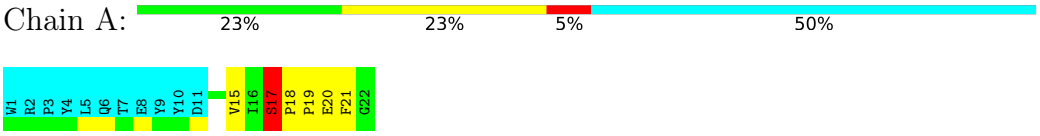
Chain A:



4.2.31 Score per residue for model 31

• Molecule 1: Thp5 peptide

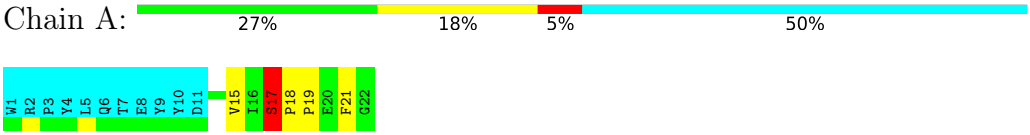
Chain A:



4.2.32 Score per residue for model 32

• Molecule 1: Thp5 peptide

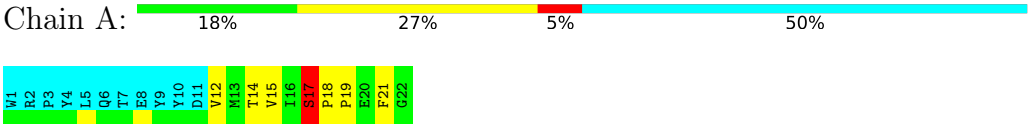
Chain A:



4.2.33 Score per residue for model 33

• Molecule 1: Thp5 peptide

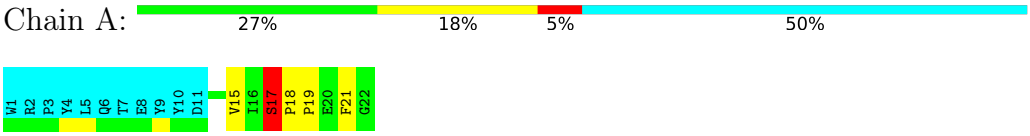
Chain A:



4.2.34 Score per residue for model 34

• Molecule 1: Thp5 peptide

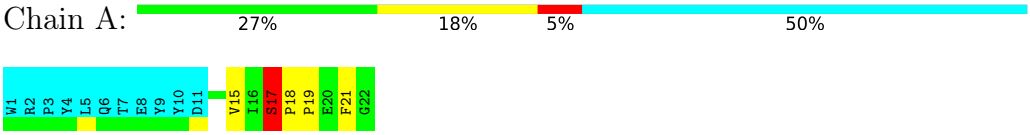
Chain A:



4.2.35 Score per residue for model 35

• Molecule 1: Thp5 peptide

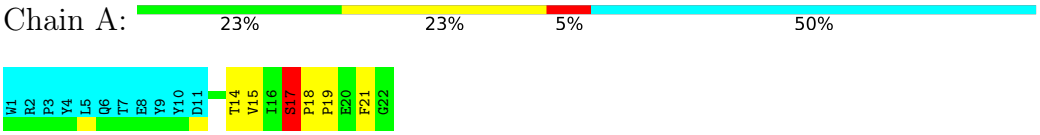
Chain A:



4.2.36 Score per residue for model 36

• Molecule 1: Thp5 peptide

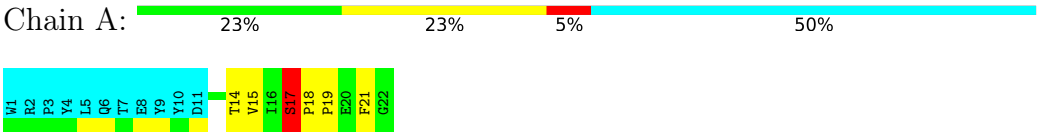
Chain A:



4.2.37 Score per residue for model 37

• Molecule 1: Thp5 peptide

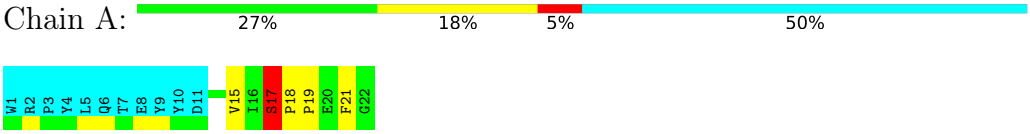
Chain A:



4.2.38 Score per residue for model 38

• Molecule 1: Thp5 peptide

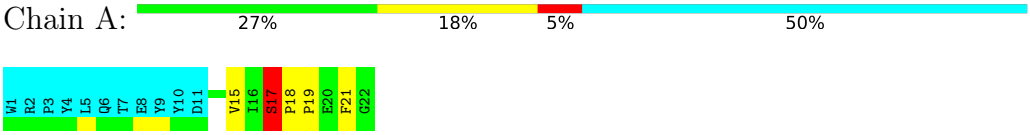
Chain A:



4.2.39 Score per residue for model 39

• Molecule 1: Thp5 peptide

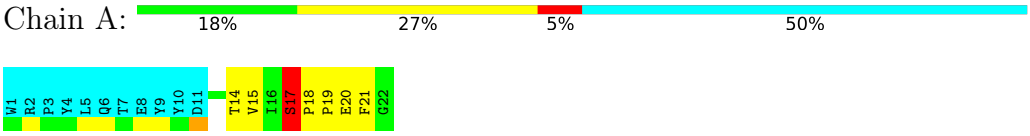
Chain A:



4.2.40 Score per residue for model 40

• Molecule 1: Thp5 peptide

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

Of the 100 calculated structures, 40 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	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	186
Number of shifts mapped to atoms	186
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	64%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	81	82	82	15±1
All	All	3240	3280	3280	613

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 94.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:PRO:N	1:A:19:PRO:HD2	0.88	1.84	40	40
1:A:18:PRO:N	1:A:19:PRO:CD	0.81	2.44	38	40
1:A:18:PRO:CD	1:A:19:PRO:CD	0.73	2.67	35	40
1:A:17:SER:C	1:A:19:PRO:HD2	0.73	2.04	40	40
1:A:18:PRO:HG2	1:A:19:PRO:HD3	0.68	1.66	4	40
1:A:18:PRO:CD	1:A:19:PRO:HD2	0.65	2.22	25	40
1:A:17:SER:CB	1:A:18:PRO:CD	0.62	2.78	22	40
1:A:18:PRO:CG	1:A:19:PRO:HD3	0.62	2.25	35	40
1:A:15:VAL:O	1:A:15:VAL:HG12	0.59	1.98	34	40
1:A:15:VAL:C	1:A:19:PRO:HG3	0.58	2.19	35	40
1:A:17:SER:N	1:A:19:PRO:HD2	0.57	2.14	34	40
1:A:18:PRO:CD	1:A:19:PRO:HD3	0.56	2.31	34	40
1:A:17:SER:CB	1:A:18:PRO:HD3	0.50	2.37	18	40
1:A:18:PRO:HD2	1:A:19:PRO:CD	0.48	2.39	2	40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:PRO:CG	1:A:19:PRO:CD	0.48	2.92	35	40
1:A:14:THR:HG22	1:A:14:THR:O	0.42	2.15	33	1
1:A:15:VAL:O	1:A:15:VAL:CG1	0.42	2.68	38	4
1:A:17:SER:H	1:A:18:PRO:HD2	0.41	1.76	33	4
1:A:18:PRO:HD2	1:A:19:PRO:HD2	0.41	1.93	32	4

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	10/22 (45%)	8±0 (80±0%)	1±0 (10±0%)	1±0 (10±0%)	1	10
All	All	400/880 (45%)	320 (80%)	40 (10%)	40 (10%)	1	10

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	17	SER	40

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	10/21 (48%)	8±0 (76±5%)	2±0 (25±5%)	2	25
All	All	400/840 (48%)	302 (76%)	98 (24%)	2	25

All 3 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	17	SER	40
1	A	21	PHE	40
1	A	20	GLU	18

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 64% for the well-defined parts and 59% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	186
Number of shifts mapped to atoms	186
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

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

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 64%, i.e. 91 atoms were assigned a chemical shift out of a possible 142. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	37/52 (71%)	19/21 (90%)	9/22 (41%)	9/9 (100%)
Sidechain	52/80 (65%)	34/54 (63%)	18/26 (69%)	0/0 (—%)
Aromatic	2/10 (20%)	1/5 (20%)	1/5 (20%)	0/0 (—%)
Overall	91/142 (64%)	54/80 (68%)	28/53 (53%)	9/9 (100%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 59%, i.e. 186 atoms were assigned a chemical shift out of a possible 313. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	71/105 (68%)	37/42 (88%)	16/44 (36%)	18/19 (95%)
Sidechain	93/159 (58%)	61/104 (59%)	32/51 (63%)	0/4 (0%)
Aromatic	22/49 (45%)	11/23 (48%)	10/25 (40%)	1/1 (100%)
Overall	186/313 (59%)	109/169 (64%)	58/120 (48%)	19/24 (79%)

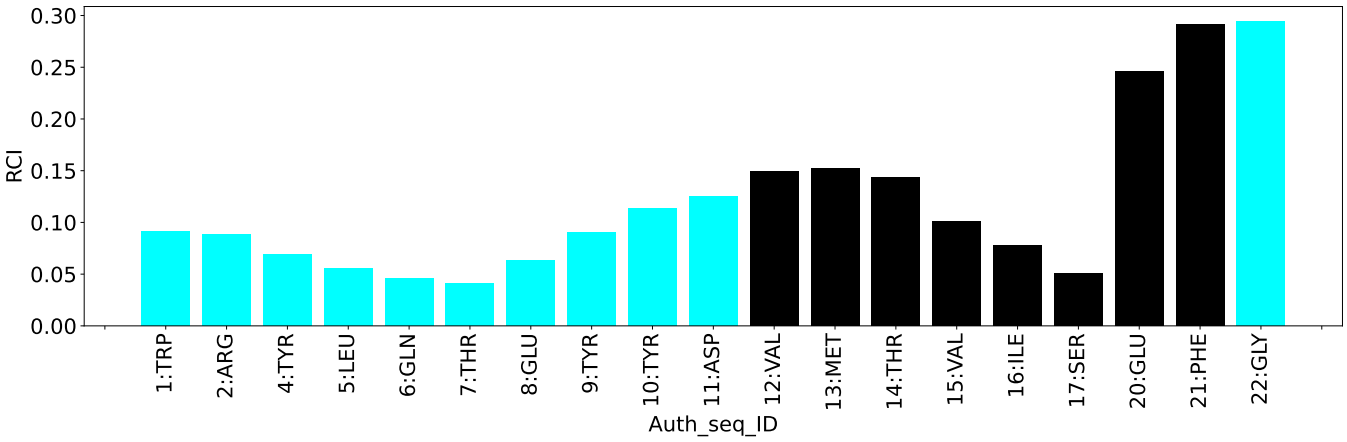
7.1.4 Statistically unusual chemical shifts (i)

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	230
Intra-residue (|i-j|=0)	89
Sequential (|i-j|=1)	68
Medium range (|i-j|>1 and |i-j|<5)	73
Long range (|i-j|≥5)	0
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	10.5
Number of long range restraints per residue[1]	0.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	6.6	0.2
0.2-0.5 (Medium)	10.0	0.49
>0.5 (Large)	3.0	0.9

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 (i)

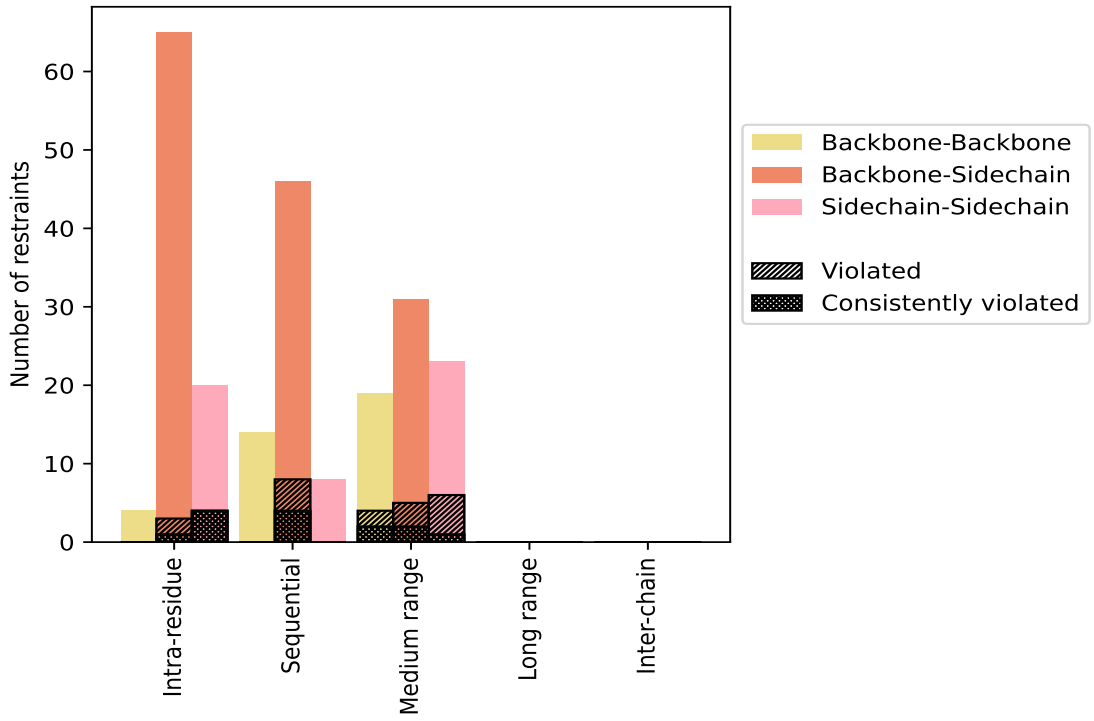
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	89	38.7	7	7.9	3.0	5	5.6	2.2
Backbone-Backbone	4	1.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	65	28.3	3	4.6	1.3	1	1.5	0.4
Sidechain-Sidechain	20	8.7	4	20.0	1.7	4	20.0	1.7
Sequential (|i-j|=1)	68	29.6	8	11.8	3.5	4	5.9	1.7
Backbone-Backbone	14	6.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	46	20.0	8	17.4	3.5	4	8.7	1.7
Sidechain-Sidechain	8	3.5	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	73	31.7	15	20.5	6.5	5	6.8	2.2
Backbone-Backbone	19	8.3	4	21.1	1.7	2	10.5	0.9
Backbone-Sidechain	31	13.5	5	16.1	2.2	2	6.5	0.9
Sidechain-Sidechain	23	10.0	6	26.1	2.6	1	4.3	0.4
Long range (|i-j|≥5)	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
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	230	100.0	30	13.0	13.0	14	6.1	6.1
Backbone-Backbone	37	16.1	4	10.8	1.7	2	5.4	0.9
Backbone-Sidechain	142	61.7	16	11.3	7.0	7	4.9	3.0
Sidechain-Sidechain	51	22.2	10	19.6	4.3	5	9.8	2.2

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	6	7	7	0	0	20	0.32	0.9	0.21	0.27
2	6	7	7	0	0	20	0.32	0.89	0.21	0.28
3	6	7	7	0	0	20	0.32	0.9	0.22	0.28
4	6	7	6	0	0	19	0.33	0.9	0.21	0.29
5	6	7	6	0	0	19	0.33	0.9	0.21	0.29
6	6	7	6	0	0	19	0.33	0.9	0.21	0.29
7	7	7	7	0	0	21	0.31	0.9	0.21	0.25
8	6	7	7	0	0	20	0.32	0.89	0.21	0.27
9	6	7	6	0	0	19	0.33	0.9	0.22	0.3
10	6	7	6	0	0	19	0.33	0.9	0.22	0.3
11	6	7	6	0	0	19	0.33	0.9	0.21	0.29

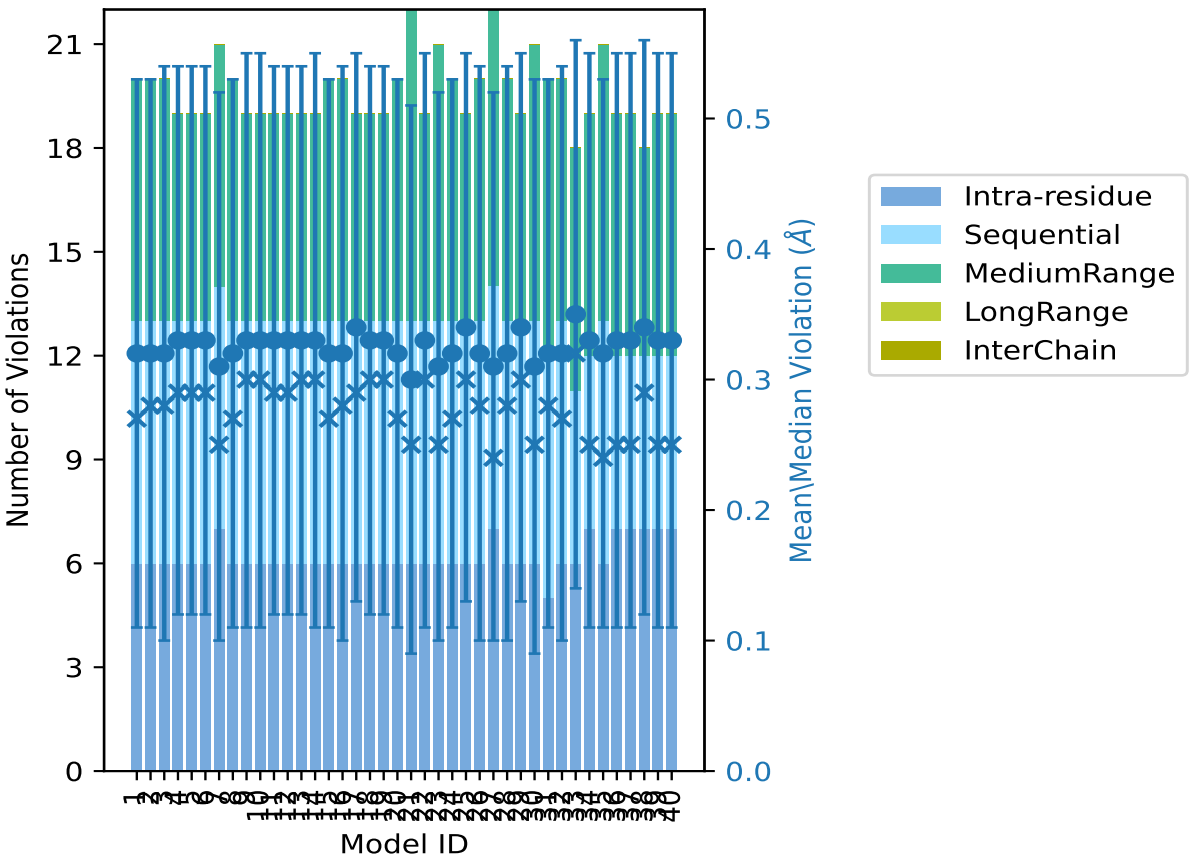
Continued on next page...

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				
12	6	7	6	0	0	19	0.33	0.9	0.21	0.29
13	6	7	6	0	0	19	0.33	0.9	0.21	0.3
14	6	7	6	0	0	19	0.33	0.9	0.22	0.3
15	6	7	7	0	0	20	0.32	0.89	0.21	0.27
16	6	7	7	0	0	20	0.32	0.9	0.22	0.28
17	6	7	6	0	0	19	0.34	0.89	0.21	0.29
18	6	7	6	0	0	19	0.33	0.9	0.21	0.3
19	6	7	6	0	0	19	0.33	0.9	0.21	0.3
20	6	7	7	0	0	20	0.32	0.9	0.21	0.27
21	6	7	9	0	0	22	0.3	0.9	0.21	0.25
22	6	7	6	0	0	19	0.33	0.9	0.22	0.3
23	6	7	8	0	0	21	0.31	0.9	0.21	0.25
24	6	7	7	0	0	20	0.32	0.9	0.21	0.27
25	6	7	6	0	0	19	0.34	0.9	0.21	0.3
26	6	7	7	0	0	20	0.32	0.9	0.22	0.28
27	7	7	8	0	0	22	0.31	0.9	0.21	0.24
28	6	7	7	0	0	20	0.32	0.9	0.22	0.28
29	6	7	6	0	0	19	0.34	0.9	0.21	0.3
30	6	7	8	0	0	21	0.31	0.9	0.22	0.25
31	5	7	8	0	0	20	0.32	0.9	0.21	0.28
32	6	7	7	0	0	20	0.32	0.9	0.22	0.27
33	6	5	7	0	0	18	0.35	0.9	0.21	0.32
34	7	5	7	0	0	19	0.33	0.9	0.22	0.25
35	6	7	8	0	0	21	0.32	0.9	0.21	0.24
36	7	5	7	0	0	19	0.33	0.9	0.22	0.25
37	7	5	7	0	0	19	0.33	0.89	0.22	0.25
38	7	5	6	0	0	18	0.34	0.9	0.22	0.29
39	7	5	7	0	0	19	0.33	0.9	0.22	0.25
40	7	5	7	0	0	19	0.33	0.9	0.22	0.25

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

9.3 Distance violation statistics for the ensemble

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, 200(IR:82, SQ:60, MR:58, LR:0, 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]	%
0	1	4	0	0	5	1	2.5
0	0	1	0	0	1	2	5.0
0	0	1	0	0	1	3	7.5
0	0	0	0	0	0	4	10.0
0	0	1	0	0	1	5	12.5
0	0	1	0	0	1	6	15.0

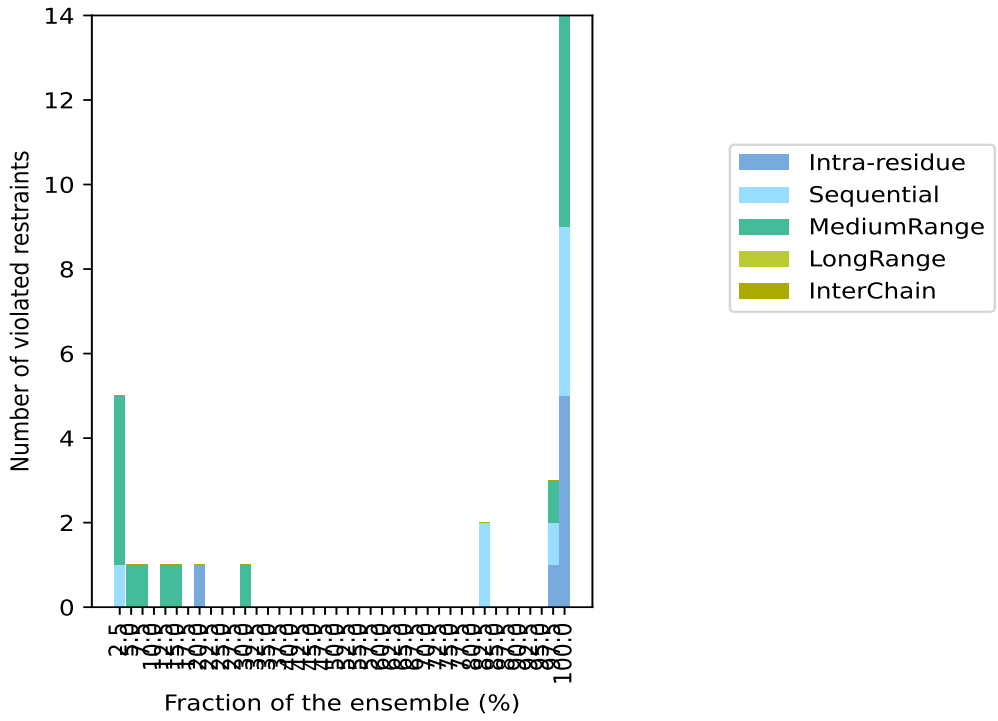
Continued on next page...

Continued from previous page...

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	0	0	7	17.5
1	0	0	0	0	1	8	20.0
0	0	0	0	0	0	9	22.5
0	0	0	0	0	0	10	25.0
0	0	0	0	0	0	11	27.5
0	0	1	0	0	1	12	30.0
0	0	0	0	0	0	13	32.5
0	0	0	0	0	0	14	35.0
0	0	0	0	0	0	15	37.5
0	0	0	0	0	0	16	40.0
0	0	0	0	0	0	17	42.5
0	0	0	0	0	0	18	45.0
0	0	0	0	0	0	19	47.5
0	0	0	0	0	0	20	50.0
0	0	0	0	0	0	21	52.5
0	0	0	0	0	0	22	55.0
0	0	0	0	0	0	23	57.5
0	0	0	0	0	0	24	60.0
0	0	0	0	0	0	25	62.5
0	0	0	0	0	0	26	65.0
0	0	0	0	0	0	27	67.5
0	0	0	0	0	0	28	70.0
0	0	0	0	0	0	29	72.5
0	0	0	0	0	0	30	75.0
0	0	0	0	0	0	31	77.5
0	0	0	0	0	0	32	80.0
0	2	0	0	0	2	33	82.5
0	0	0	0	0	0	34	85.0
0	0	0	0	0	0	35	87.5
0	0	0	0	0	0	36	90.0
0	0	0	0	0	0	37	92.5
0	0	0	0	0	0	38	95.0
1	1	1	0	0	3	39	97.5
5	4	5	0	0	14	40	100.0

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

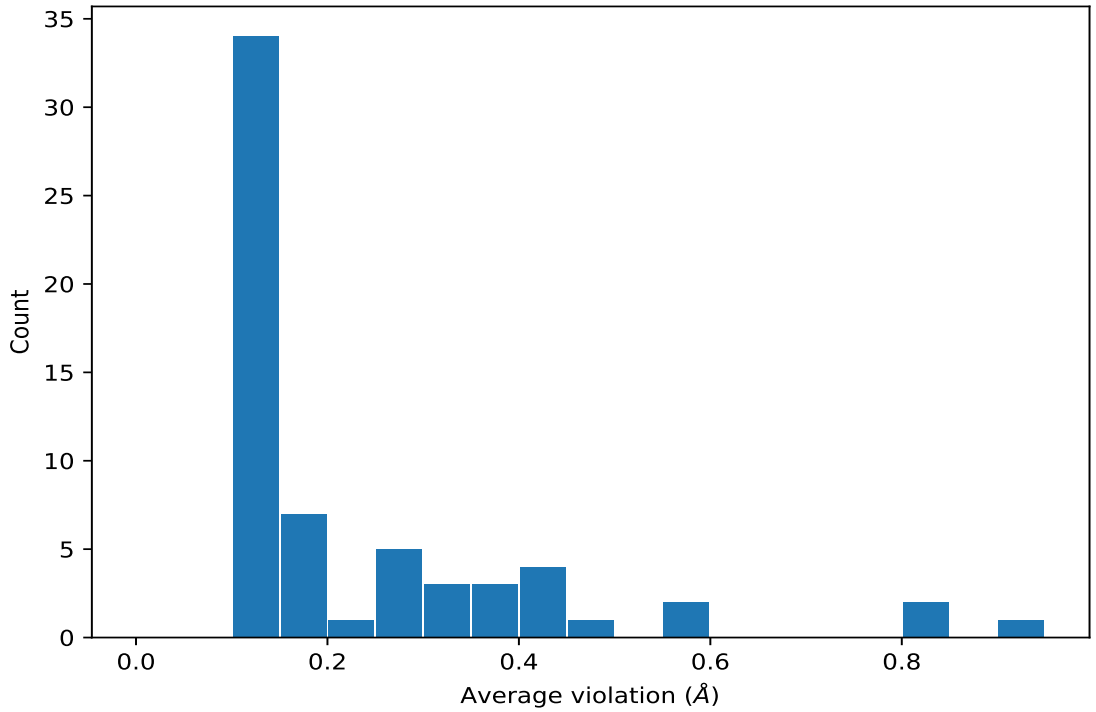
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints (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)
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	40	0.9	0.0	0.9
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	40	0.8	0.0	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	40	0.8	0.0	0.8
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	40	0.55	0.0	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	40	0.55	0.0	0.55
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	40	0.45	0.02	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	40	0.42	0.05	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	40	0.42	0.05	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	40	0.42	0.05	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	40	0.42	0.05	0.44
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	40	0.35	0.02	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	40	0.35	0.02	0.34
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	40	0.35	0.0	0.35
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	40	0.33	0.04	0.31
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	40	0.29	0.02	0.3
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	40	0.28	0.07	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	40	0.16	0.04	0.14
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	40	0.15	0.02	0.15
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	40	0.14	0.04	0.12
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	40	0.13	0.01	0.13
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	39	0.23	0.01	0.23
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	39	0.14	0.01	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	39	0.14	0.01	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	39	0.14	0.01	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	39	0.14	0.01	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	39	0.14	0.01	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	39	0.14	0.01	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	39	0.13	0.01	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	39	0.13	0.01	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	39	0.13	0.01	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	39	0.13	0.01	0.14
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	33	0.33	0.01	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	33	0.33	0.01	0.33
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	33	0.25	0.01	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	33	0.25	0.01	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	33	0.25	0.01	0.25
(1,16)	1:A:13:MET:HA	1:A:16:ILE:H	12	0.11	0.0	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE1	8	0.11	0.01	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE2	8	0.11	0.01	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE3	8	0.11	0.01	0.11
(1,207)	1:A:14:THR:H	1:A:17:SER:HB2	6	0.15	0.01	0.15
(1,207)	1:A:14:THR:H	1:A:17:SER:HB3	6	0.15	0.01	0.15
(1,197)	1:A:5:LEU:HD11	1:A:9:TYR:HB2	5	0.12	0.01	0.11
(1,197)	1:A:5:LEU:HD11	1:A:9:TYR:HB3	5	0.12	0.01	0.11
(1,197)	1:A:5:LEU:HD12	1:A:9:TYR:HB2	5	0.12	0.01	0.11
(1,197)	1:A:5:LEU:HD12	1:A:9:TYR:HB3	5	0.12	0.01	0.11
(1,197)	1:A:5:LEU:HD13	1:A:9:TYR:HB2	5	0.12	0.01	0.11
(1,197)	1:A:5:LEU:HD13	1:A:9:TYR:HB3	5	0.12	0.01	0.11
(1,197)	1:A:5:LEU:HD21	1:A:9:TYR:HB2	5	0.12	0.01	0.11
(1,197)	1:A:5:LEU:HD21	1:A:9:TYR:HB3	5	0.12	0.01	0.11
(1,197)	1:A:5:LEU:HD22	1:A:9:TYR:HB2	5	0.12	0.01	0.11
(1,197)	1:A:5:LEU:HD22	1:A:9:TYR:HB3	5	0.12	0.01	0.11
(1,197)	1:A:5:LEU:HD23	1:A:9:TYR:HB2	5	0.12	0.01	0.11
(1,197)	1:A:5:LEU:HD23	1:A:9:TYR:HB3	5	0.12	0.01	0.11
(1,204)	1:A:13:MET:HE1	1:A:16:ILE:HB	3	0.17	0.06	0.13
(1,204)	1:A:13:MET:HE2	1:A:16:ILE:HB	3	0.17	0.06	0.13
(1,204)	1:A:13:MET:HE3	1:A:16:ILE:HB	3	0.17	0.06	0.13
(1,196)	1:A:5:LEU:HD11	1:A:8:GLU:H	2	0.11	0.0	0.11

Continued on next page...

Continued from previous page...

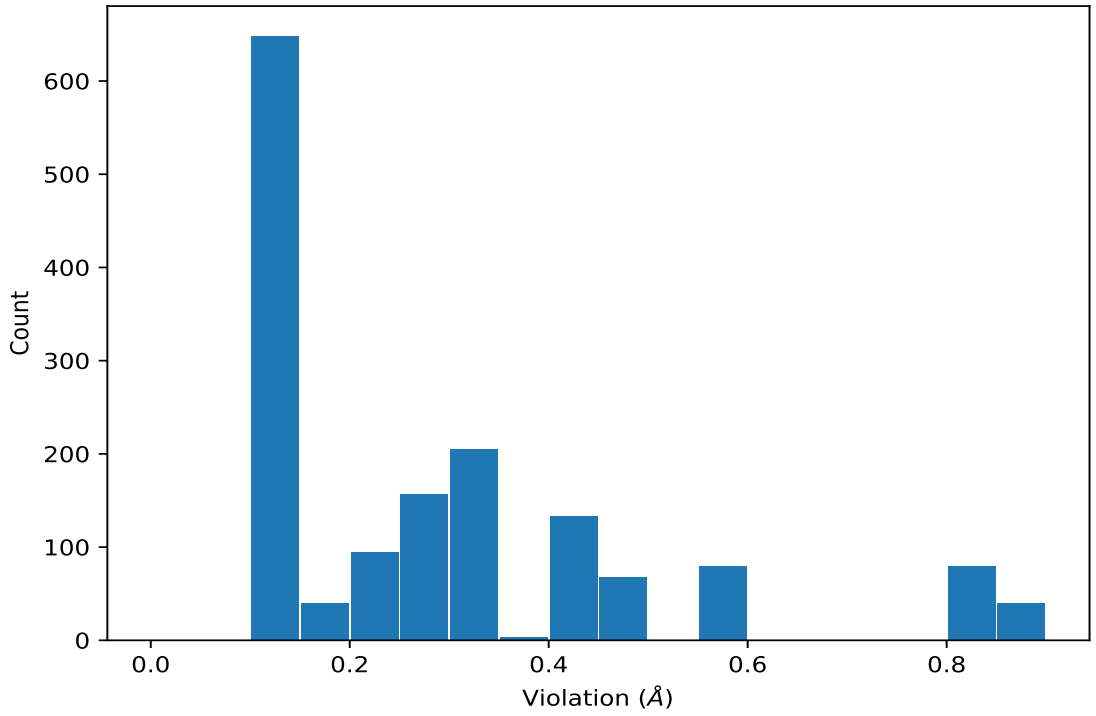
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,196)	1:A:5:LEU:HD12	1:A:8:GLU:H	2	0.11	0.0	0.11
(1,196)	1:A:5:LEU:HD13	1:A:8:GLU:H	2	0.11	0.0	0.11
(1,196)	1:A:5:LEU:HD21	1:A:8:GLU:H	2	0.11	0.0	0.11
(1,196)	1:A:5:LEU:HD22	1:A:8:GLU:H	2	0.11	0.0	0.11
(1,196)	1:A:5:LEU:HD23	1:A:8:GLU:H	2	0.11	0.0	0.11

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	1	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	3	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	4	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	5	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	6	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	7	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	9	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	10	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	11	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	12	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	13	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	14	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	16	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	18	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	19	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	20	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	21	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	22	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	23	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	24	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	25	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	26	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	27	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	28	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	29	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	30	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	31	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	32	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	33	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	34	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	35	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	36	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	38	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	39	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	40	0.9
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	2	0.89
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	8	0.89
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	15	0.89
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	17	0.89
(1,217)	1:A:1:TRP:HE1	1:A:1:TRP:HZ3	37	0.89
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	1	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	1	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	2	0.8

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	2	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	3	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	3	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	4	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	4	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	5	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	5	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	6	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	6	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	7	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	7	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	8	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	8	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	9	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	9	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	10	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	10	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	11	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	11	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	12	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	12	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	13	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	13	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	14	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	14	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	15	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	15	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	16	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	16	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	17	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	17	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	18	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	18	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	19	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	19	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	20	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	20	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	21	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	21	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	22	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	22	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	23	0.8

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	23	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	24	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	24	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	25	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	25	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	26	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	26	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	27	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	27	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	28	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	28	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	29	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	29	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	30	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	30	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	31	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	31	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	32	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	32	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	33	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	33	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	34	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	34	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	35	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	35	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	36	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	36	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	37	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	37	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	38	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	38	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	39	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	39	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB2	40	0.8
(1,225)	1:A:1:TRP:HH2	1:A:1:TRP:HB3	40	0.8
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	1	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	1	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	2	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	2	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	3	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	3	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	4	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	4	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	5	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	5	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	6	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	6	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	7	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	7	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	8	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	8	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	9	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	9	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	10	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	10	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	11	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	11	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	12	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	12	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	13	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	13	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	14	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	14	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	15	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	15	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	16	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	16	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	17	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	17	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	18	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	18	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	19	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	19	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	20	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	20	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	21	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	21	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	22	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	22	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	23	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	23	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	24	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	24	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	25	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	25	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	26	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	26	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	27	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	27	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	28	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	28	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	29	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	29	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	30	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	30	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	31	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	31	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	32	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	32	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	33	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	33	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	34	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	34	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	35	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	35	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	36	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	36	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	37	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	37	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	38	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	38	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	39	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	39	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB2	40	0.55
(1,223)	1:A:1:TRP:HZ2	1:A:1:TRP:HB3	40	0.55
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	34	0.49
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	40	0.49
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	36	0.48
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	37	0.48
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	38	0.48
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	39	0.48
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	2	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	3	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	9	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	10	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	13	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	14	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	16	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	18	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	19	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	21	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	22	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	23	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	25	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	26	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	28	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	29	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	30	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	31	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	32	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	35	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	8	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	8	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	8	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	8	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	12	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	12	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	12	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	12	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	14	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	14	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	14	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	14	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	26	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	26	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	26	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	26	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	28	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	28	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	28	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	28	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	29	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	29	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	29	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	29	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	30	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	30	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	30	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	30	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	32	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	32	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	32	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	32	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	33	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	33	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	33	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	33	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	35	0.46
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	35	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	35	0.46
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	35	0.46
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	12	0.45
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	20	0.45
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	1	0.44
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	4	0.44
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	5	0.44
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	6	0.44
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	8	0.44
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	11	0.44
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	15	0.44
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	17	0.44
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	24	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	1	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	1	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	1	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	1	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	2	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	2	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	2	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	2	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	3	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	3	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	3	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	3	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	4	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	4	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	4	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	4	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	5	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	5	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	5	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	5	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	6	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	6	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	6	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	6	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	7	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	7	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	7	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	7	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	9	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	9	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	9	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	9	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	10	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	10	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	10	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	10	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	11	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	11	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	11	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	11	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	13	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	13	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	13	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	13	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	15	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	15	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	15	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	15	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	16	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	16	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	16	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	16	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	17	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	17	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	17	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	17	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	18	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	18	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	18	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	18	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	19	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	19	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	19	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	19	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	20	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	20	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	20	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	20	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	21	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	21	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	21	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	21	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	22	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	22	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	22	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	22	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	23	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	23	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	23	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	23	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	24	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	24	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	24	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	24	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	25	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	25	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	25	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	25	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	27	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	27	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	27	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	27	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	31	0.44
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	31	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	31	0.44
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	31	0.44
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	34	0.43
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	36	0.43
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	37	0.43
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	38	0.43
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	39	0.43
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	7	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	27	0.43
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	40	0.42
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	33	0.42
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	33	0.4
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	33	0.4
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	34	0.4
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	34	0.4
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	36	0.4
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	36	0.4
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	37	0.4
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	37	0.4
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	38	0.4
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	38	0.4
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	39	0.4
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	39	0.4
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	40	0.4
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	40	0.4
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	34	0.4
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	36	0.4
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	37	0.4
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	38	0.4
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	39	0.4
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	40	0.39
(1,6)	1:A:15:VAL:HA	1:A:19:PRO:HA	33	0.38
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	33	0.37
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	1	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	2	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	3	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	4	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	5	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	6	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	7	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	8	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	9	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	10	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	11	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	12	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	13	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	14	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	15	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	16	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	17	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	18	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	19	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	20	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	21	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	22	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	23	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	24	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	25	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	26	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	27	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	28	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	29	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	30	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	31	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	32	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	33	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	34	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	35	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	36	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	37	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	38	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	39	0.35
(1,221)	1:A:1:TRP:HE1	1:A:1:TRP:HE3	40	0.35
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	1	0.35
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	1	0.35
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	2	0.35
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	2	0.35
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	7	0.35
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	7	0.35
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	8	0.35
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	8	0.35
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	15	0.35
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	15	0.35
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	26	0.35
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	26	0.35
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	27	0.35
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	27	0.35
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	28	0.35
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	28	0.35
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	31	0.35
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	31	0.35
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	5	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	5	0.34
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	9	0.34
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	9	0.34
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	10	0.34
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	10	0.34
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	13	0.34
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	13	0.34
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	14	0.34
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	14	0.34
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	18	0.34
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	18	0.34
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	19	0.34
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	19	0.34
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	20	0.34
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	20	0.34
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	24	0.34
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	24	0.34
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	25	0.34
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	25	0.34
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	29	0.34
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	29	0.34
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	32	0.34
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	32	0.34
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	35	0.34
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	35	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	3	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	3	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	4	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	4	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	5	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	5	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	6	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	6	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	9	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	9	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	10	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	10	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	11	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	11	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	12	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	12	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	13	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	13	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	14	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	14	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	16	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	16	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	17	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	17	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	18	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	18	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	19	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	19	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	20	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	20	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	21	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	21	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	22	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	22	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	23	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	23	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	24	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	24	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	25	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	25	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	29	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	29	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	30	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	30	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	32	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	32	0.34
(1,162)	1:A:13:MET:HG2	1:A:14:THR:H	35	0.34
(1,162)	1:A:13:MET:HG3	1:A:14:THR:H	35	0.34
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	1	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	1	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	2	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	2	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	3	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	3	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	4	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	4	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	6	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	6	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	8	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	8	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	11	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	11	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	12	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	12	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	15	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	15	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	16	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	16	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	17	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	17	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	21	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	21	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	22	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	22	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	23	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	23	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	26	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	26	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	27	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	27	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	28	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	28	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	30	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	30	0.33
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	31	0.33
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	31	0.33
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	38	0.32
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	38	0.32
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	38	0.32
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	38	0.32
(1,163)	1:A:13:MET:HB2	1:A:14:THR:H	7	0.32
(1,163)	1:A:13:MET:HB3	1:A:14:THR:H	7	0.32
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	1	0.32
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	7	0.32
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	8	0.32
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	15	0.32
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	27	0.32
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	2	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	3	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	4	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	5	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	6	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	9	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	11	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	12	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	13	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	14	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	16	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	17	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	20	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	21	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	22	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	23	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	24	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	26	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	28	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	29	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	30	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	31	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	32	0.31
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	35	0.31
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	34	0.3
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	34	0.3
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	34	0.3
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	34	0.3
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	36	0.3
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	36	0.3
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	36	0.3
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	36	0.3
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	37	0.3
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	37	0.3
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	37	0.3
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	37	0.3
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	39	0.3
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	39	0.3
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	39	0.3
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	39	0.3
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB2	40	0.3
(1,28)	1:A:17:SER:HB2	1:A:20:GLU:HB3	40	0.3
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB2	40	0.3
(1,28)	1:A:17:SER:HB3	1:A:20:GLU:HB3	40	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	2	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	3	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	7	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	9	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	10	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	13	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	14	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	16	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	18	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	19	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	21	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	22	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	23	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	25	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	26	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	27	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	28	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	29	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	30	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	31	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	32	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	35	0.3
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	10	0.3
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	18	0.3
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	19	0.3
(1,159)	1:A:15:VAL:HB	1:A:17:SER:H	25	0.3
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	1	0.29
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	4	0.29
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	5	0.29
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	6	0.29
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	8	0.29
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	11	0.29
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	12	0.29
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	15	0.29
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	17	0.29
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	20	0.29
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	24	0.29
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	33	0.28
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	33	0.27
(1,204)	1:A:13:MET:HE1	1:A:16:ILE:HB	33	0.26
(1,204)	1:A:13:MET:HE2	1:A:16:ILE:HB	33	0.26
(1,204)	1:A:13:MET:HE3	1:A:16:ILE:HB	33	0.26
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	34	0.25
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	36	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	37	0.25
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	38	0.25
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	39	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	1	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	2	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	3	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	4	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	6	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	7	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	8	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	11	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	15	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	16	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	17	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	21	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	23	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	24	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	26	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	27	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	28	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	30	0.25
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	31	0.25
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	36	0.25
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	40	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	1	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	1	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	1	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	2	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	2	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	2	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	3	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	3	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	3	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	4	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	4	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	4	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	5	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	5	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	5	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	6	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	6	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	6	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	8	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	8	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	8	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	10	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	10	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	10	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	11	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	11	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	11	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	12	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	12	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	12	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	13	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	13	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	13	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	14	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	14	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	14	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	15	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	15	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	15	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	16	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	16	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	16	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	17	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	17	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	17	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	20	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	20	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	20	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	21	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	21	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	21	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	23	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	23	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	23	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	24	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	24	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	24	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	26	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	26	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	26	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	28	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	28	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	28	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	30	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	30	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	30	0.25
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	31	0.25
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	31	0.25
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	31	0.25
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	40	0.24
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	5	0.24
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	9	0.24
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	10	0.24
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	12	0.24
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	13	0.24
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	14	0.24
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	18	0.24
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	19	0.24
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	20	0.24
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	22	0.24
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	25	0.24
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	29	0.24
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	32	0.24
(1,95)	1:A:14:THR:H	1:A:15:VAL:HB	35	0.24
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	4	0.24
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	5	0.24
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	6	0.24
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	7	0.24
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	11	0.24
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	27	0.24
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	40	0.24
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	34	0.24
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	37	0.24
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	38	0.24
(1,17)	1:A:13:MET:HA	1:A:17:SER:H	39	0.24
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	9	0.24
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	9	0.24
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	9	0.24
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	18	0.24
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	18	0.24
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	18	0.24
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	19	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	19	0.24
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	19	0.24
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	22	0.24
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	22	0.24
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	22	0.24
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	25	0.24
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	25	0.24
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	25	0.24
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	29	0.24
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	29	0.24
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	29	0.24
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	32	0.24
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	32	0.24
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	32	0.24
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	35	0.24
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	35	0.24
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	35	0.24
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	1	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	2	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	3	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	8	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	9	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	10	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	12	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	13	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	14	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	15	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	16	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	17	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	18	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	19	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	20	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	21	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	22	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	23	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	24	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	25	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	26	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	28	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	29	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	30	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	31	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	32	0.23
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	35	0.23
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	34	0.23
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	36	0.23
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	37	0.23
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	38	0.23
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	39	0.23
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	7	0.22
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	7	0.22
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	7	0.22
(1,165)	1:A:13:MET:HE1	1:A:14:THR:H	27	0.22
(1,165)	1:A:13:MET:HE2	1:A:14:THR:H	27	0.22
(1,165)	1:A:13:MET:HE3	1:A:14:THR:H	27	0.22
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	34	0.21
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	36	0.21
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	37	0.21
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	38	0.21
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	39	0.21
(1,90)	1:A:14:THR:HB	1:A:15:VAL:H	40	0.21
(1,91)	1:A:13:MET:HA	1:A:14:THR:HB	33	0.2
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	15	0.19
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	17	0.19
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	18	0.19
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	19	0.19
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	25	0.19
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	29	0.19
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	33	0.18
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	31	0.18
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	35	0.17
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	23	0.17
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	23	0.17
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	23	0.17
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	23	0.17
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	23	0.17
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	23	0.17
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	1	0.16
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	8	0.16
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	15	0.16
(1,207)	1:A:14:THR:H	1:A:17:SER:HB2	36	0.16
(1,207)	1:A:14:THR:H	1:A:17:SER:HB3	36	0.16
(1,207)	1:A:14:THR:H	1:A:17:SER:HB2	40	0.16
(1,207)	1:A:14:THR:H	1:A:17:SER:HB3	40	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	17	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	17	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	17	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	17	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	17	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	17	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	25	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	25	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	25	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	25	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	25	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	25	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	35	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	35	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	35	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	35	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	35	0.16
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	35	0.16
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	7	0.15
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	27	0.15
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	7	0.15
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	27	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	1	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	2	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	3	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	4	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	5	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	6	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	7	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	8	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	9	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	10	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	11	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	12	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	13	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	14	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	27	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	33	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	34	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	36	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	37	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	38	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	39	0.15
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	40	0.15
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	13	0.15
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	13	0.15
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	13	0.15
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	13	0.15
(1,207)	1:A:14:THR:H	1:A:17:SER:HB2	39	0.15
(1,207)	1:A:14:THR:H	1:A:17:SER:HB3	39	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	15	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	15	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	15	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	15	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	15	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	15	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	18	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	18	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	18	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	18	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	18	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	18	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	19	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	19	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	19	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	19	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	19	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	19	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	27	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	27	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	27	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	27	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	27	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	27	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	29	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	29	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	29	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	29	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	29	0.15
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	29	0.15
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	2	0.14
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	3	0.14
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	4	0.14
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	5	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	6	0.14
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	11	0.14
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	12	0.14
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	16	0.14
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	17	0.14
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	20	0.14
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	21	0.14
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	23	0.14
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	24	0.14
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	26	0.14
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	28	0.14
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	30	0.14
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	31	0.14
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	4	0.14
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	5	0.14
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	6	0.14
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	11	0.14
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	12	0.14
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	24	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	1	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	1	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	1	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	1	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	2	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	2	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	2	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	2	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	3	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	3	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	3	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	3	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	4	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	4	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	4	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	4	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	5	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	5	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	5	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	5	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	6	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	6	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	6	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	6	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	7	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	7	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	7	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	7	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	9	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	9	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	9	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	9	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	10	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	10	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	10	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	10	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	11	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	11	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	11	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	11	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	15	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	15	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	15	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	15	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	16	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	16	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	16	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	16	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	17	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	17	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	17	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	17	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	18	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	18	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	18	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	18	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	19	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	19	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	19	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	19	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	20	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	20	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	20	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	20	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	21	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	21	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	21	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	21	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	22	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	22	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	22	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	22	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	23	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	23	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	23	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	23	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	24	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	24	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	24	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	24	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	25	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	25	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	25	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	25	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	27	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	27	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	27	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	27	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	31	0.14
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	31	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	31	0.14
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	31	0.14
(1,33)	1:A:6:GLN:HB2	1:A:8:GLU:HB2	27	0.14
(1,33)	1:A:6:GLN:HB2	1:A:8:GLU:HB3	27	0.14
(1,33)	1:A:6:GLN:HB3	1:A:8:GLU:HB2	27	0.14
(1,33)	1:A:6:GLN:HB3	1:A:8:GLU:HB3	27	0.14
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	9	0.14
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	10	0.14
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	13	0.14
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	14	0.14
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	16	0.14
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	17	0.14
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	18	0.14
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	19	0.14
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	20	0.14
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	22	0.14
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	25	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	29	0.14
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	32	0.14
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	35	0.14
(1,207)	1:A:14:THR:H	1:A:17:SER:HB2	34	0.14
(1,207)	1:A:14:THR:H	1:A:17:SER:HB3	34	0.14
(1,207)	1:A:14:THR:H	1:A:17:SER:HB2	37	0.14
(1,207)	1:A:14:THR:H	1:A:17:SER:HB3	37	0.14
(1,207)	1:A:14:THR:H	1:A:17:SER:HB2	38	0.14
(1,207)	1:A:14:THR:H	1:A:17:SER:HB3	38	0.14
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	13	0.14
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	13	0.14
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	13	0.14
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	13	0.14
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	13	0.14
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	13	0.14
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	21	0.14
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	21	0.14
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	21	0.14
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	21	0.14
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	21	0.14
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	21	0.14
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	9	0.13
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	10	0.13
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	13	0.13
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	14	0.13
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	18	0.13
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	19	0.13
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	22	0.13
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	25	0.13
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	29	0.13
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	32	0.13
(1,96)	1:A:15:VAL:HB	1:A:16:ILE:H	35	0.13
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	1	0.13
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	8	0.13
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	15	0.13
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	17	0.13
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	20	0.13
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	16	0.13
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	20	0.13
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	21	0.13
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	22	0.13
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	23	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	24	0.13
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	26	0.13
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	28	0.13
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	30	0.13
(1,71)	1:A:5:LEU:HA	1:A:5:LEU:HG	32	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	8	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	8	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	8	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	8	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	12	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	12	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	12	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	12	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	14	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	14	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	14	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	14	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	26	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	26	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	26	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	26	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	28	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	28	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	28	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	28	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	29	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	29	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	29	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	29	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	30	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	30	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	30	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	30	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	32	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	32	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	32	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	32	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	33	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	33	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	33	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	33	0.13
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	35	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	35	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	35	0.13
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	35	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	1	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	2	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	3	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	4	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	5	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	6	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	7	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	8	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	11	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	12	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	15	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	21	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	23	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	24	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	26	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	27	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	28	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	30	0.13
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	31	0.13
(1,204)	1:A:13:MET:HE1	1:A:16:ILE:HB	7	0.13
(1,204)	1:A:13:MET:HE2	1:A:16:ILE:HB	7	0.13
(1,204)	1:A:13:MET:HE3	1:A:16:ILE:HB	7	0.13
(1,204)	1:A:13:MET:HE1	1:A:16:ILE:HB	27	0.13
(1,204)	1:A:13:MET:HE2	1:A:16:ILE:HB	27	0.13
(1,204)	1:A:13:MET:HE3	1:A:16:ILE:HB	27	0.13
(1,197)	1:A:5:LEU:HD11	1:A:9:TYR:HB2	35	0.13
(1,197)	1:A:5:LEU:HD11	1:A:9:TYR:HB3	35	0.13
(1,197)	1:A:5:LEU:HD12	1:A:9:TYR:HB2	35	0.13
(1,197)	1:A:5:LEU:HD12	1:A:9:TYR:HB3	35	0.13
(1,197)	1:A:5:LEU:HD13	1:A:9:TYR:HB2	35	0.13
(1,197)	1:A:5:LEU:HD13	1:A:9:TYR:HB3	35	0.13
(1,197)	1:A:5:LEU:HD21	1:A:9:TYR:HB2	35	0.13
(1,197)	1:A:5:LEU:HD21	1:A:9:TYR:HB3	35	0.13
(1,197)	1:A:5:LEU:HD22	1:A:9:TYR:HB2	35	0.13
(1,197)	1:A:5:LEU:HD22	1:A:9:TYR:HB3	35	0.13
(1,197)	1:A:5:LEU:HD23	1:A:9:TYR:HB2	35	0.13
(1,197)	1:A:5:LEU:HD23	1:A:9:TYR:HB3	35	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	1	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	1	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	1	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	1	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	1	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	1	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	2	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	2	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	2	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	2	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	2	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	2	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	3	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	3	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	3	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	3	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	3	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	3	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	4	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	4	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	4	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	4	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	4	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	4	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	5	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	5	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	5	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	5	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	5	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	5	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	6	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	6	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	6	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	6	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	6	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	6	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	7	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	7	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	7	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	7	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	7	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	7	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	8	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	8	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	8	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	8	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	8	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	8	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	9	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	9	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	9	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	9	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	9	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	9	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	10	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	10	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	10	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	10	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	10	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	10	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	11	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	11	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	11	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	11	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	11	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	11	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	12	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	12	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	12	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	12	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	12	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	12	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	14	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	14	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	14	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	14	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	14	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	14	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	16	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	16	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	16	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	16	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	16	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	16	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	20	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	20	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	20	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	20	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	20	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	20	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	32	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	32	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	32	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	32	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	32	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	32	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	33	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	33	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	33	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	33	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	33	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	33	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	34	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	34	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	34	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	34	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	34	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	34	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	36	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	36	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	36	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	36	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	36	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	36	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	37	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	37	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	37	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	37	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	37	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	37	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	38	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	38	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	38	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	38	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	38	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	38	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	39	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	39	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	39	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	39	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	39	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	39	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	40	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	40	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	40	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	40	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	40	0.13
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	40	0.13
(1,180)	1:A:13:MET:H	1:A:13:MET:HE1	36	0.13
(1,180)	1:A:13:MET:H	1:A:13:MET:HE2	36	0.13
(1,180)	1:A:13:MET:H	1:A:13:MET:HE3	36	0.13
(1,153)	1:A:4:TYR:HA	1:A:7:THR:H	35	0.13
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	9	0.12
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	10	0.12
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	13	0.12
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	14	0.12
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	18	0.12
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	19	0.12
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	22	0.12
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	25	0.12
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	29	0.12
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	32	0.12
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	35	0.12
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	33	0.12
(1,197)	1:A:5:LEU:HD11	1:A:9:TYR:HB2	30	0.12
(1,197)	1:A:5:LEU:HD11	1:A:9:TYR:HB3	30	0.12
(1,197)	1:A:5:LEU:HD12	1:A:9:TYR:HB2	30	0.12
(1,197)	1:A:5:LEU:HD12	1:A:9:TYR:HB3	30	0.12
(1,197)	1:A:5:LEU:HD13	1:A:9:TYR:HB2	30	0.12
(1,197)	1:A:5:LEU:HD13	1:A:9:TYR:HB3	30	0.12
(1,197)	1:A:5:LEU:HD21	1:A:9:TYR:HB2	30	0.12
(1,197)	1:A:5:LEU:HD21	1:A:9:TYR:HB3	30	0.12
(1,197)	1:A:5:LEU:HD22	1:A:9:TYR:HB2	30	0.12
(1,197)	1:A:5:LEU:HD22	1:A:9:TYR:HB3	30	0.12
(1,197)	1:A:5:LEU:HD23	1:A:9:TYR:HB2	30	0.12
(1,197)	1:A:5:LEU:HD23	1:A:9:TYR:HB3	30	0.12
(1,195)	1:A:5:LEU:HD11	1:A:7:THR:HG21	31	0.12
(1,195)	1:A:5:LEU:HD11	1:A:7:THR:HG22	31	0.12
(1,195)	1:A:5:LEU:HD11	1:A:7:THR:HG23	31	0.12
(1,195)	1:A:5:LEU:HD12	1:A:7:THR:HG21	31	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,195)	1:A:5:LEU:HD12	1:A:7:THR:HG22	31	0.12
(1,195)	1:A:5:LEU:HD12	1:A:7:THR:HG23	31	0.12
(1,195)	1:A:5:LEU:HD13	1:A:7:THR:HG21	31	0.12
(1,195)	1:A:5:LEU:HD13	1:A:7:THR:HG22	31	0.12
(1,195)	1:A:5:LEU:HD13	1:A:7:THR:HG23	31	0.12
(1,195)	1:A:5:LEU:HD21	1:A:7:THR:HG21	31	0.12
(1,195)	1:A:5:LEU:HD21	1:A:7:THR:HG22	31	0.12
(1,195)	1:A:5:LEU:HD21	1:A:7:THR:HG23	31	0.12
(1,195)	1:A:5:LEU:HD22	1:A:7:THR:HG21	31	0.12
(1,195)	1:A:5:LEU:HD22	1:A:7:THR:HG22	31	0.12
(1,195)	1:A:5:LEU:HD22	1:A:7:THR:HG23	31	0.12
(1,195)	1:A:5:LEU:HD23	1:A:7:THR:HG21	31	0.12
(1,195)	1:A:5:LEU:HD23	1:A:7:THR:HG22	31	0.12
(1,195)	1:A:5:LEU:HD23	1:A:7:THR:HG23	31	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	22	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	22	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	22	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	22	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	22	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	22	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	24	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	24	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	24	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	24	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	24	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	24	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	26	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	26	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	26	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	26	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	26	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	26	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	28	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	28	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	28	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	28	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	28	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	28	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD11	30	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD12	30	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD13	30	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD21	30	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD22	30	0.12
(1,192)	1:A:5:LEU:HA	1:A:5:LEU:HD23	30	0.12
(1,180)	1:A:13:MET:H	1:A:13:MET:HE1	40	0.12
(1,180)	1:A:13:MET:H	1:A:13:MET:HE2	40	0.12
(1,180)	1:A:13:MET:H	1:A:13:MET:HE3	40	0.12
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	2	0.11
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	3	0.11
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	16	0.11
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	21	0.11
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	23	0.11
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	26	0.11
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	28	0.11
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	30	0.11
(1,89)	1:A:14:THR:HB	1:A:17:SER:H	31	0.11
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	34	0.11
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	34	0.11
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	34	0.11
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	34	0.11
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	36	0.11
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	36	0.11
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	36	0.11
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	36	0.11
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	37	0.11
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	37	0.11
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	37	0.11
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	37	0.11
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	39	0.11
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	39	0.11
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	39	0.11
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	39	0.11
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB2	40	0.11
(1,69)	1:A:18:PRO:HB2	1:A:21:PHE:HB3	40	0.11
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB2	40	0.11
(1,69)	1:A:18:PRO:HB3	1:A:21:PHE:HB3	40	0.11
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	34	0.11
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	36	0.11
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	37	0.11
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	38	0.11
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	39	0.11
(1,212)	1:A:16:ILE:HB	1:A:17:SER:H	40	0.11
(1,197)	1:A:5:LEU:HD11	1:A:9:TYR:HB2	20	0.11
(1,197)	1:A:5:LEU:HD11	1:A:9:TYR:HB3	20	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	1:A:5:LEU:HD12	1:A:9:TYR:HB2	20	0.11
(1,197)	1:A:5:LEU:HD12	1:A:9:TYR:HB3	20	0.11
(1,197)	1:A:5:LEU:HD13	1:A:9:TYR:HB2	20	0.11
(1,197)	1:A:5:LEU:HD13	1:A:9:TYR:HB3	20	0.11
(1,197)	1:A:5:LEU:HD21	1:A:9:TYR:HB2	20	0.11
(1,197)	1:A:5:LEU:HD21	1:A:9:TYR:HB3	20	0.11
(1,197)	1:A:5:LEU:HD22	1:A:9:TYR:HB2	20	0.11
(1,197)	1:A:5:LEU:HD22	1:A:9:TYR:HB3	20	0.11
(1,197)	1:A:5:LEU:HD23	1:A:9:TYR:HB2	20	0.11
(1,197)	1:A:5:LEU:HD23	1:A:9:TYR:HB3	20	0.11
(1,197)	1:A:5:LEU:HD11	1:A:9:TYR:HB2	24	0.11
(1,197)	1:A:5:LEU:HD11	1:A:9:TYR:HB3	24	0.11
(1,197)	1:A:5:LEU:HD12	1:A:9:TYR:HB2	24	0.11
(1,197)	1:A:5:LEU:HD12	1:A:9:TYR:HB3	24	0.11
(1,197)	1:A:5:LEU:HD13	1:A:9:TYR:HB2	24	0.11
(1,197)	1:A:5:LEU:HD13	1:A:9:TYR:HB3	24	0.11
(1,197)	1:A:5:LEU:HD21	1:A:9:TYR:HB2	24	0.11
(1,197)	1:A:5:LEU:HD21	1:A:9:TYR:HB3	24	0.11
(1,197)	1:A:5:LEU:HD22	1:A:9:TYR:HB2	24	0.11
(1,197)	1:A:5:LEU:HD22	1:A:9:TYR:HB3	24	0.11
(1,197)	1:A:5:LEU:HD23	1:A:9:TYR:HB2	24	0.11
(1,197)	1:A:5:LEU:HD23	1:A:9:TYR:HB3	24	0.11
(1,197)	1:A:5:LEU:HD11	1:A:9:TYR:HB2	32	0.11
(1,197)	1:A:5:LEU:HD11	1:A:9:TYR:HB3	32	0.11
(1,197)	1:A:5:LEU:HD12	1:A:9:TYR:HB2	32	0.11
(1,197)	1:A:5:LEU:HD12	1:A:9:TYR:HB3	32	0.11
(1,197)	1:A:5:LEU:HD13	1:A:9:TYR:HB2	32	0.11
(1,197)	1:A:5:LEU:HD13	1:A:9:TYR:HB3	32	0.11
(1,197)	1:A:5:LEU:HD21	1:A:9:TYR:HB2	32	0.11
(1,197)	1:A:5:LEU:HD21	1:A:9:TYR:HB3	32	0.11
(1,197)	1:A:5:LEU:HD22	1:A:9:TYR:HB2	32	0.11
(1,197)	1:A:5:LEU:HD22	1:A:9:TYR:HB3	32	0.11
(1,197)	1:A:5:LEU:HD23	1:A:9:TYR:HB2	32	0.11
(1,197)	1:A:5:LEU:HD23	1:A:9:TYR:HB3	32	0.11
(1,196)	1:A:5:LEU:HD11	1:A:8:GLU:H	21	0.11
(1,196)	1:A:5:LEU:HD12	1:A:8:GLU:H	21	0.11
(1,196)	1:A:5:LEU:HD13	1:A:8:GLU:H	21	0.11
(1,196)	1:A:5:LEU:HD21	1:A:8:GLU:H	21	0.11
(1,196)	1:A:5:LEU:HD22	1:A:8:GLU:H	21	0.11
(1,196)	1:A:5:LEU:HD23	1:A:8:GLU:H	21	0.11
(1,196)	1:A:5:LEU:HD11	1:A:8:GLU:H	23	0.11
(1,196)	1:A:5:LEU:HD12	1:A:8:GLU:H	23	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,196)	1:A:5:LEU:HD13	1:A:8:GLU:H	23	0.11
(1,196)	1:A:5:LEU:HD21	1:A:8:GLU:H	23	0.11
(1,196)	1:A:5:LEU:HD22	1:A:8:GLU:H	23	0.11
(1,196)	1:A:5:LEU:HD23	1:A:8:GLU:H	23	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE1	7	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE2	7	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE3	7	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE1	27	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE2	27	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE3	27	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE1	34	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE2	34	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE3	34	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE1	37	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE2	37	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE3	37	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE1	38	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE2	38	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE3	38	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE1	39	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE2	39	0.11
(1,180)	1:A:13:MET:H	1:A:13:MET:HE3	39	0.11
(1,174)	1:A:6:GLN:H	1:A:8:GLU:HB2	21	0.11
(1,174)	1:A:6:GLN:H	1:A:8:GLU:HB3	21	0.11
(1,16)	1:A:13:MET:HA	1:A:16:ILE:H	1	0.11
(1,16)	1:A:13:MET:HA	1:A:16:ILE:H	2	0.11
(1,16)	1:A:13:MET:HA	1:A:16:ILE:H	3	0.11
(1,16)	1:A:13:MET:HA	1:A:16:ILE:H	8	0.11
(1,16)	1:A:13:MET:HA	1:A:16:ILE:H	15	0.11
(1,16)	1:A:13:MET:HA	1:A:16:ILE:H	16	0.11
(1,16)	1:A:13:MET:HA	1:A:16:ILE:H	21	0.11
(1,16)	1:A:13:MET:HA	1:A:16:ILE:H	23	0.11
(1,16)	1:A:13:MET:HA	1:A:16:ILE:H	26	0.11
(1,16)	1:A:13:MET:HA	1:A:16:ILE:H	28	0.11
(1,16)	1:A:13:MET:HA	1:A:16:ILE:H	30	0.11
(1,16)	1:A:13:MET:HA	1:A:16:ILE:H	31	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found