



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:56 PM UTC

PDB ID : 6QXZ / pdb_00006qxz
BMRB ID : 34368
Title : Solution structure of the ASHH2 CW domain with the N-terminal histone H3 tail mimicking peptide monomethylated on lysine 4
Authors : Dobrovolska, O.; Madeleine, N.; Teigen, K.; Halskau, O.; Bril'kov, M.
Deposited on : 2019-03-08

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

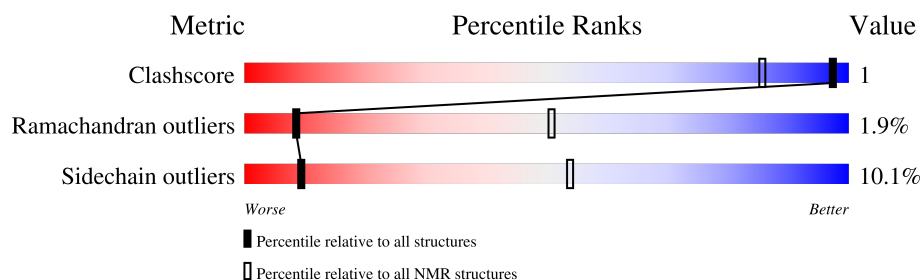
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	79	59% 10% 30%
2	B	9	22% 11% 67%

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:863-A:885, A:890-A:921, B:3-B:3, B:5-B:6 (58)	0.48	1

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

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

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

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1348 atoms, of which 650 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Histone-lysine N-methyltransferase ASHH2.

Mol	Chain	Residues	Atoms						Trace
1	A	79	Total	C	H	N	O	S	0
			1185	370	566	112	131	6	

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	850	GLY	-	expression tag	UNP Q2LAE1
A	851	SER	-	expression tag	UNP Q2LAE1
A	852	ARG	-	expression tag	UNP Q2LAE1
A	853	ARG	-	expression tag	UNP Q2LAE1
A	854	ALA	-	expression tag	UNP Q2LAE1
A	855	SER	-	expression tag	UNP Q2LAE1
A	856	VAL	-	expression tag	UNP Q2LAE1
A	857	GLY	-	expression tag	UNP Q2LAE1
A	858	SER	-	expression tag	UNP Q2LAE1
A	859	GLU	-	expression tag	UNP Q2LAE1
A	860	PHE	-	expression tag	UNP Q2LAE1

- Molecule 2 is a protein called ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR.

Mol	Chain	Residues	Atoms					Trace
2	B	9	Total	C	H	N	O	0
			162	47	84	17	14	

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

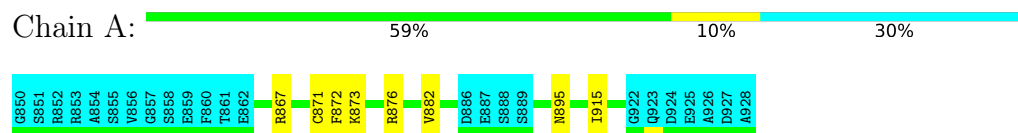
Mol	Chain	Residues	Atoms	
3	A	1	Total	Zn
			1	1

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: Histone-lysine N-methyltransferase ASHH2



- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR

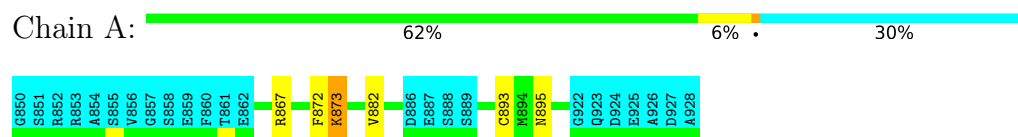


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

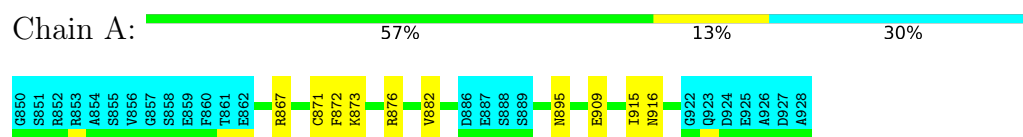


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.2 Score per residue for model 2

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

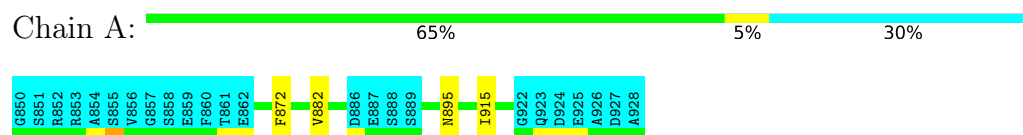


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.3 Score per residue for model 3

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

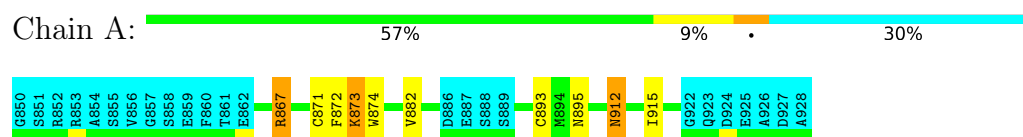


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.4 Score per residue for model 4

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

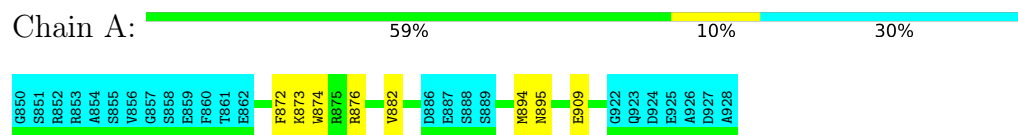


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.5 Score per residue for model 5

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

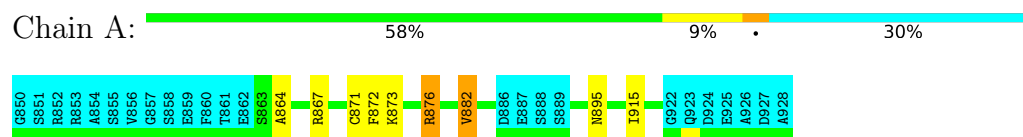


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.6 Score per residue for model 6

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

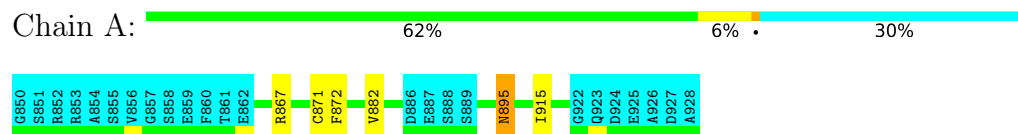


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.7 Score per residue for model 7

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

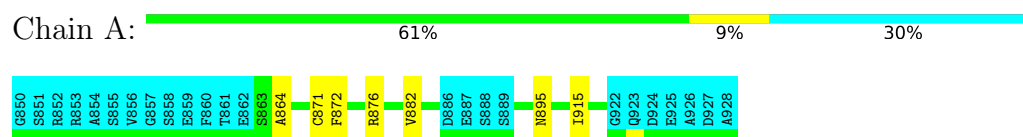


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.8 Score per residue for model 8

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

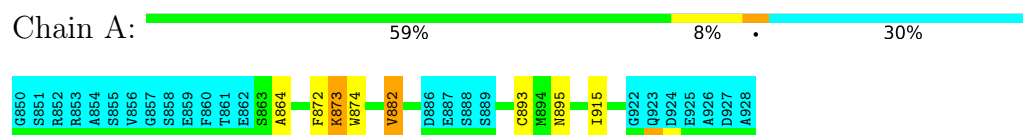


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.9 Score per residue for model 9

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

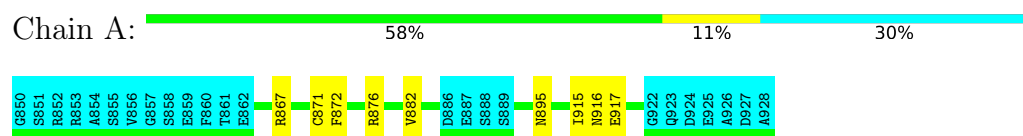


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.10 Score per residue for model 10

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

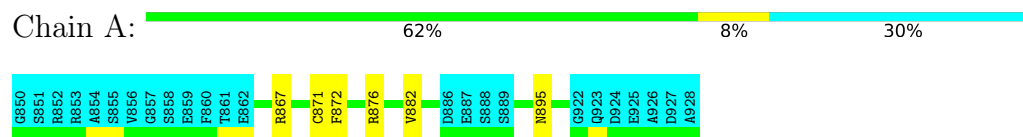


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.11 Score per residue for model 11

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

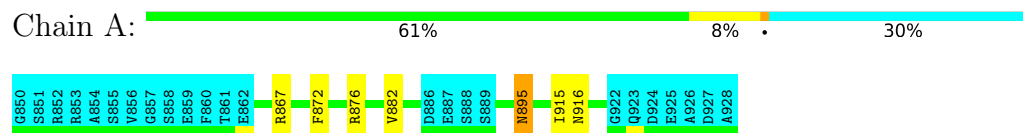


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.12 Score per residue for model 12

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

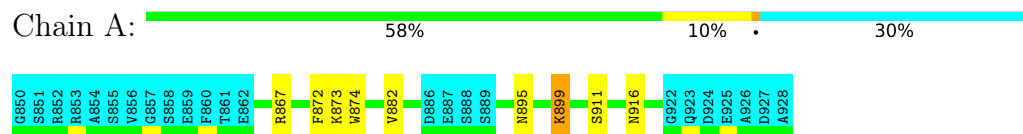


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.13 Score per residue for model 13

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

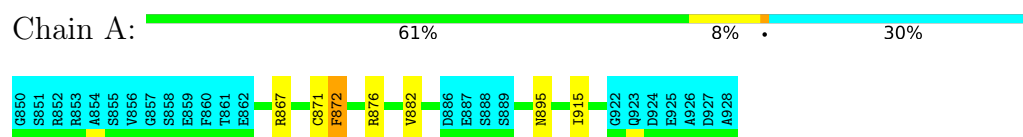


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.14 Score per residue for model 14

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

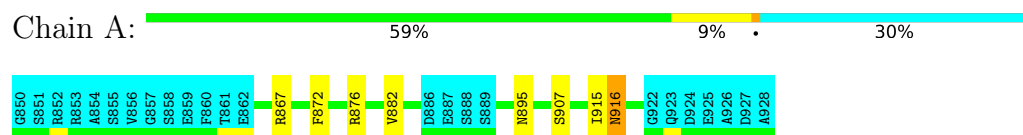


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.15 Score per residue for model 15

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

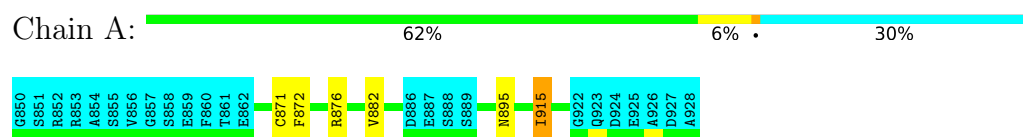


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.16 Score per residue for model 16

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

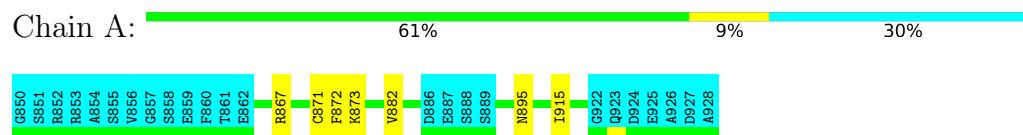


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.17 Score per residue for model 17

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

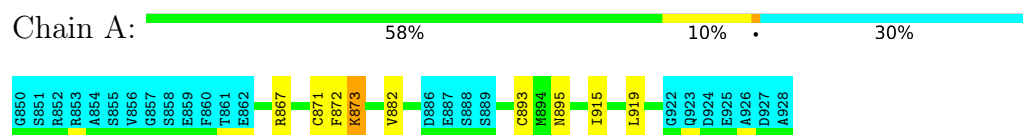


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.18 Score per residue for model 18

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

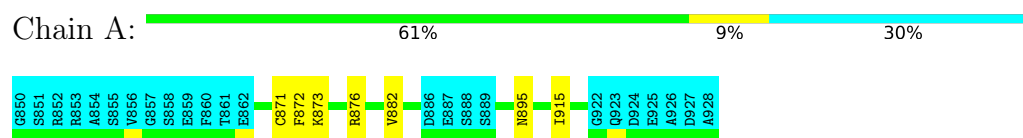


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.19 Score per residue for model 19

- Molecule 1: Histone-lysine N-methyltransferase ASHH2

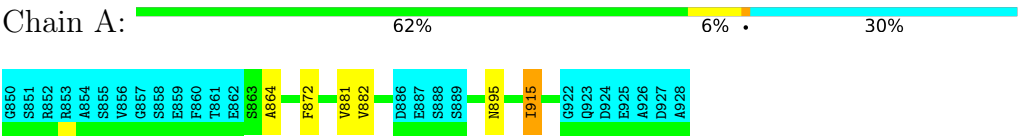


- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



4.2.20 Score per residue for model 20

- Molecule 1: Histone-lysine N-methyltransferase ASHH2



- Molecule 2: ALA-ARG-THR-MLZ-GLN-THR-ALA-ARG-TYR



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
Amber	refinement	
CYANA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	882
Number of shifts mapped to atoms	882
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MLZ, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.92±0.03	0±0/454 (0.1± 0.1%)	1.47±0.03	1±1/611 (0.2± 0.2%)
2	B	0.77±0.08	0±0/22 (0.0± 0.0%)	1.72±0.19	0±0/29 (0.0± 0.0%)
All	All	0.91	7/9520 (0.1%)	1.49	27/12800 (0.2%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.4±0.7
All	All	0	8

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	871	CYS	CA-C	8.06	1.56	1.52	10	7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	895	ASN	CA-CB-CG	7.71	120.31	112.60	12	2
1	A	907	SER	CA-C-N	7.24	134.14	120.97	15	1
1	A	907	SER	C-N-CA	7.24	134.14	120.97	15	1
1	A	871	CYS	CA-C-N	6.35	133.66	121.54	6	7
1	A	871	CYS	C-N-CA	6.35	133.66	121.54	6	7
1	A	916	ASN	CA-CB-CG	5.47	118.07	112.60	13	4
1	A	916	ASN	CA-C-N	5.16	127.19	120.28	2	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	916	ASN	C-N-CA	5.16	127.19	120.28	2	1
1	A	872	PHE	CA-C-N	5.14	128.38	120.82	14	1
1	A	872	PHE	C-N-CA	5.14	128.38	120.82	14	1
1	A	912	ASN	OD1-CG-ND2	-5.01	117.59	122.60	4	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	867	ARG	Sidechain	4
1	A	876	ARG	Sidechain	4

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	445	420	420	1±1
2	B	23	22	22	0±0
All	All	9380	8840	8840	11

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:864:ALA:HB3	1:A:882:VAL:HG11	0.58	1.76	20	4
1:A:873:LYS:HE2	1:A:893:CYS:SG	0.53	2.43	18	4
1:A:899:LYS:CA	1:A:899:LYS:HE3	0.44	2.42	13	1
1:A:919:LEU:CD2	2:B:5:GLN:H	0.41	2.29	18	1
1:A:867:ARG:HB2	1:A:874:TRP:CZ3	0.40	2.50	4	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	55/79 (70%)	50±1 (90±2%)	4±1 (8±2%)	1±0 (2±0%)	9	52
2	B	3/9 (33%)	2±1 (68±20%)	1±1 (28±19%)	0±0 (3±10%)	5	35
All	All	1160/1760 (66%)	1031 (89%)	107 (9%)	22 (2%)	8	51

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	872	PHE	20
2	B	3	THR	1
2	B	6	THR	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	50/68 (74%)	46±1 (91±2%)	4±1 (9±2%)	11	57
2	B	3/6 (50%)	2±1 (72±22%)	1±1 (28±22%)	1	19
All	All	1060/1480 (72%)	953 (90%)	107 (10%)	9	54

All 16 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	895	ASN	20
1	A	882	VAL	18
1	A	915	ILE	16
2	B	6	THR	11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	873	LYS	10
1	A	867	ARG	9
1	A	876	ARG	8
2	B	5	GLN	6
1	A	909	GLU	2
1	A	912	ASN	1
1	A	894	MET	1
1	A	917	GLU	1
1	A	899	LYS	1
1	A	911	SER	1
1	A	916	ASN	1
1	A	881	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	MLZ	B	4	2	8,9,10	0.83±0.06	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	MLZ	B	4	2	4,9,11	0.80±0.30	0±0 (2±7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLZ	B	4	2	-	0±0,7,8,10	-

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	4	MLZ	CM-NZ-CE	2.83	104.13	112.01	16	2

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	882
Number of shifts mapped to atoms	882
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	15

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	80	2.38 ± 0.16	Should be applied
$^{13}\text{C}_\beta$	76	2.74 ± 0.13	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	80	-0.95 ± 0.29	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 624 atoms were assigned a chemical shift out of a possible 783. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	224/290 (77%)	116/117 (99%)	54/116 (47%)	54/57 (95%)
Sidechain	352/437 (81%)	241/279 (86%)	103/134 (77%)	8/24 (33%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	48/56 (86%)	26/28 (93%)	19/25 (76%)	3/3 (100%)
Overall	624/783 (80%)	383/424 (90%)	176/275 (64%)	65/84 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 869 atoms were assigned a chemical shift out of a possible 1129. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	331/438 (76%)	171/178 (96%)	80/174 (46%)	80/86 (93%)
Sidechain	484/616 (79%)	332/391 (85%)	143/188 (76%)	9/37 (24%)
Aromatic	54/75 (72%)	30/37 (81%)	21/35 (60%)	3/3 (100%)
Overall	869/1129 (77%)	533/606 (88%)	244/397 (61%)	92/126 (73%)

7.1.4 Statistically unusual chemical shifts ⓘ

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

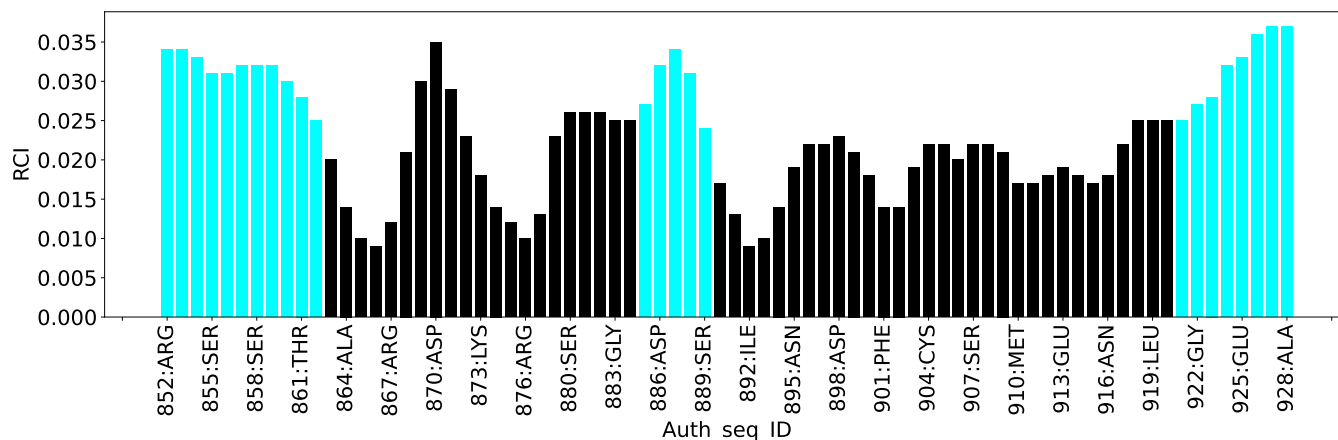
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	876	ARG	NE	132.31	76.53 – 92.65	29.6
1	B	6	THR	HG1	5.77	0.08 – 2.19	22.0
1	A	875	ARG	NE	119.31	76.53 – 92.65	21.5
1	A	867	ARG	NE	118.83	76.53 – 92.65	21.2
1	B	3	THR	HG1	5.61	0.08 – 2.19	21.2
1	A	915	ILE	HG12	-1.35	-0.69 – 3.24	-6.7
1	A	915	ILE	HD11	-0.95	-0.72 – 2.09	-5.8
1	A	915	ILE	HD12	-0.95	-0.72 – 2.09	-5.8
1	A	915	ILE	HD13	-0.95	-0.72 – 2.09	-5.8
1	A	866	VAL	HG21	-0.78	-0.58 – 2.19	-5.7
1	A	866	VAL	HG22	-0.78	-0.58 – 2.19	-5.7
1	A	866	VAL	HG23	-0.78	-0.58 – 2.19	-5.7
1	A	876	ARG	HB2	0.33	0.52 – 3.08	-5.7
1	A	867	ARG	HG2	0.12	0.26 – 2.87	-5.5
1	A	866	VAL	CG2	13.57	13.71 – 28.88	-5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

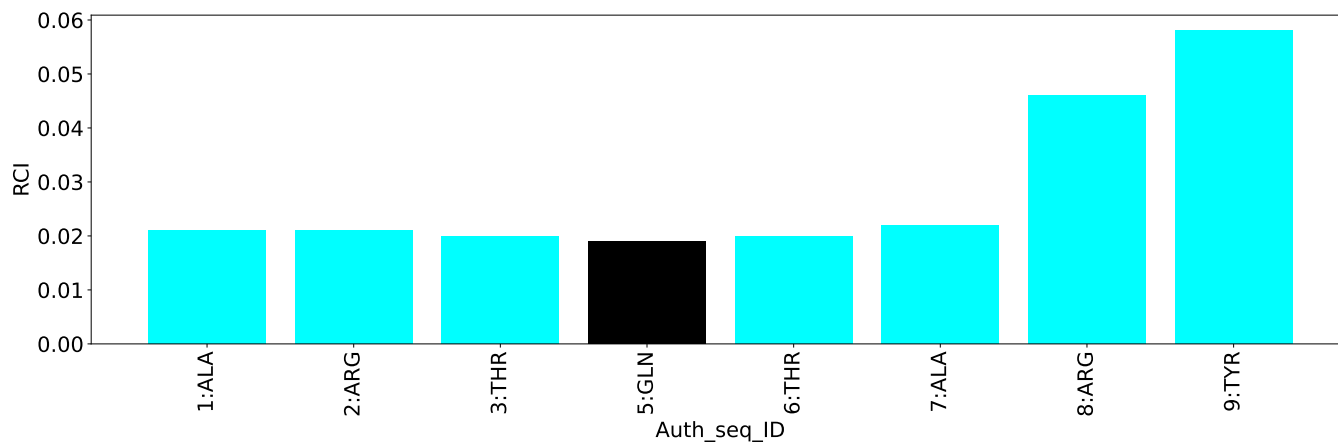
The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted 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:



Random coil index (RCI) for chain B:



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	947
Intra-residue ($ i-j =0$)	233
Sequential ($ i-j =1$)	302
Medium range ($ i-j >1$ and $ i-j <5$)	150
Long range ($ i-j \geq 5$)	183
Inter-chain	71
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	94
Number of unmapped restraints	0
Number of restraints per residue	11.7
Number of long range restraints per residue ¹	2.1

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	27.4	0.2
0.2-0.5 (Medium)	12.8	0.5
>0.5 (Large)	5.2	2.28

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	8.4	9.85
10.0-20.0 (Medium)	4.0	19.33
>20.0 (Large)	1.6	38.94

9 Distance violation analysis ⓘ

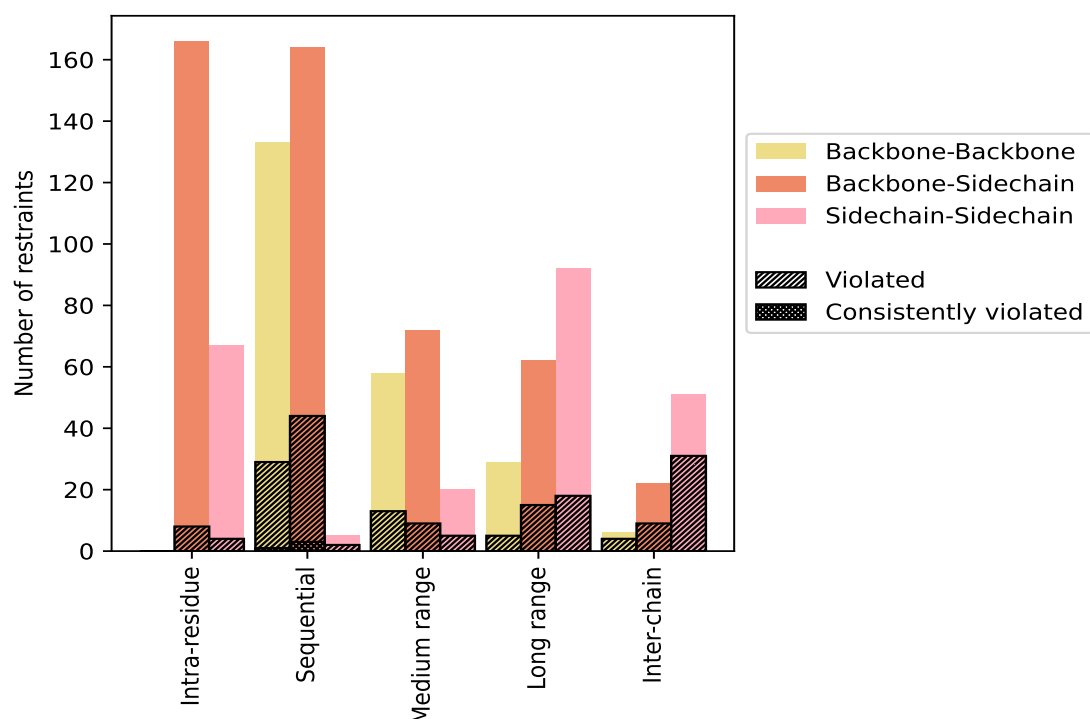
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	233	24.6	12	5.2	1.3	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	166	17.5	8	4.8	0.8	0	0.0	0.0
Sidechain-Sidechain	67	7.1	4	6.0	0.4	0	0.0	0.0
Sequential ($i-j =1$)	302	31.9	75	24.8	7.9	4	1.3	0.4
Backbone-Backbone	133	14.0	29	21.8	3.1	1	0.8	0.1
Backbone-Sidechain	164	17.3	44	26.8	4.6	3	1.8	0.3
Sidechain-Sidechain	5	0.5	2	40.0	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	150	15.8	27	18.0	2.9	0	0.0	0.0
Backbone-Backbone	58	6.1	13	22.4	1.4	0	0.0	0.0
Backbone-Sidechain	72	7.6	9	12.5	1.0	0	0.0	0.0
Sidechain-Sidechain	20	2.1	5	25.0	0.5	0	0.0	0.0
Long range ($i-j \geq 5$)	183	19.3	38	20.8	4.0	0	0.0	0.0
Backbone-Backbone	29	3.1	5	17.2	0.5	0	0.0	0.0
Backbone-Sidechain	62	6.5	15	24.2	1.6	0	0.0	0.0
Sidechain-Sidechain	92	9.7	18	19.6	1.9	0	0.0	0.0
Inter-chain	71	7.5	38	53.5	4.0	0	0.0	0.0
Backbone-Backbone	6	0.6	4	66.7	0.4	0	0.0	0.0
Backbone-Sidechain	22	2.3	9	40.9	1.0	0	0.0	0.0
Sidechain-Sidechain	43	4.5	25	58.1	2.6	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	947	100.0	196	20.7	20.7	4	0.4	0.4
Backbone-Backbone	226	23.9	51	22.6	5.4	1	0.4	0.1
Backbone-Sidechain	486	51.3	85	17.5	9.0	3	0.6	0.3
Sidechain-Sidechain	235	24.8	60	25.5	6.3	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	2	16	9	7	19	53	0.29	1.37	0.32	0.14
2	2	14	7	12	16	51	0.23	0.83	0.17	0.16
3	2	13	7	12	8	42	0.2	0.69	0.12	0.15
4	3	16	7	11	10	47	0.21	0.82	0.15	0.16
5	3	15	6	12	23	59	0.27	1.11	0.23	0.18
6	2	15	7	14	14	52	0.25	1.03	0.19	0.18
7	1	11	7	10	10	39	0.23	0.7	0.15	0.16
8	2	14	10	10	7	43	0.2	0.67	0.12	0.15
9	2	18	9	13	14	56	0.27	1.31	0.28	0.16
10	2	11	10	11	6	40	0.2	0.71	0.14	0.14

Continued on next page...

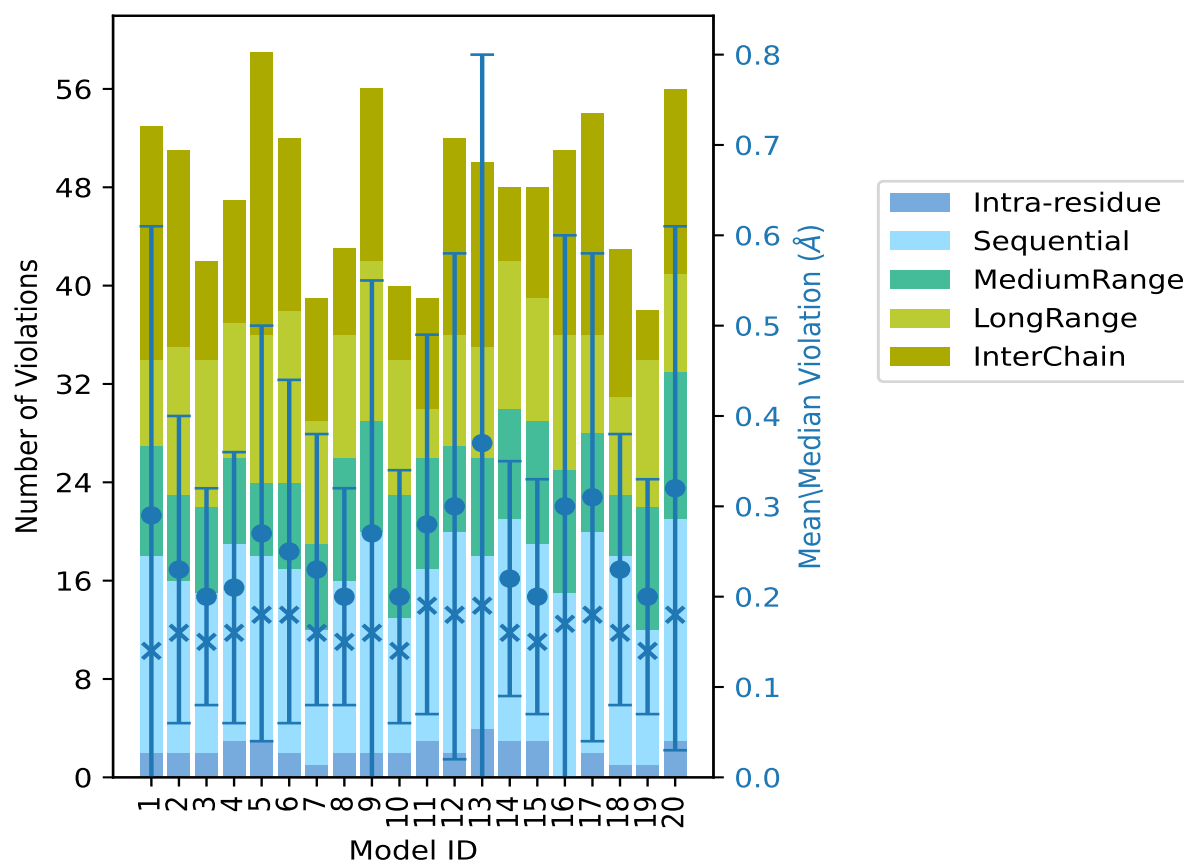
Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	3	14	9	4	9	39	0.28	1.06	0.21	0.19
12	2	18	7	9	16	52	0.3	1.54	0.28	0.18
13	4	14	8	9	15	50	0.37	2.28	0.43	0.19
14	3	18	9	12	6	48	0.22	0.7	0.13	0.16
15	3	16	10	10	9	48	0.2	0.63	0.13	0.15
16	0	15	10	11	15	51	0.3	1.29	0.3	0.17
17	2	18	8	8	18	54	0.31	1.17	0.27	0.18
18	1	17	5	8	12	43	0.23	0.62	0.15	0.16
19	1	11	10	12	4	38	0.2	0.65	0.13	0.14
20	3	18	12	8	15	56	0.32	1.17	0.29	0.18

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

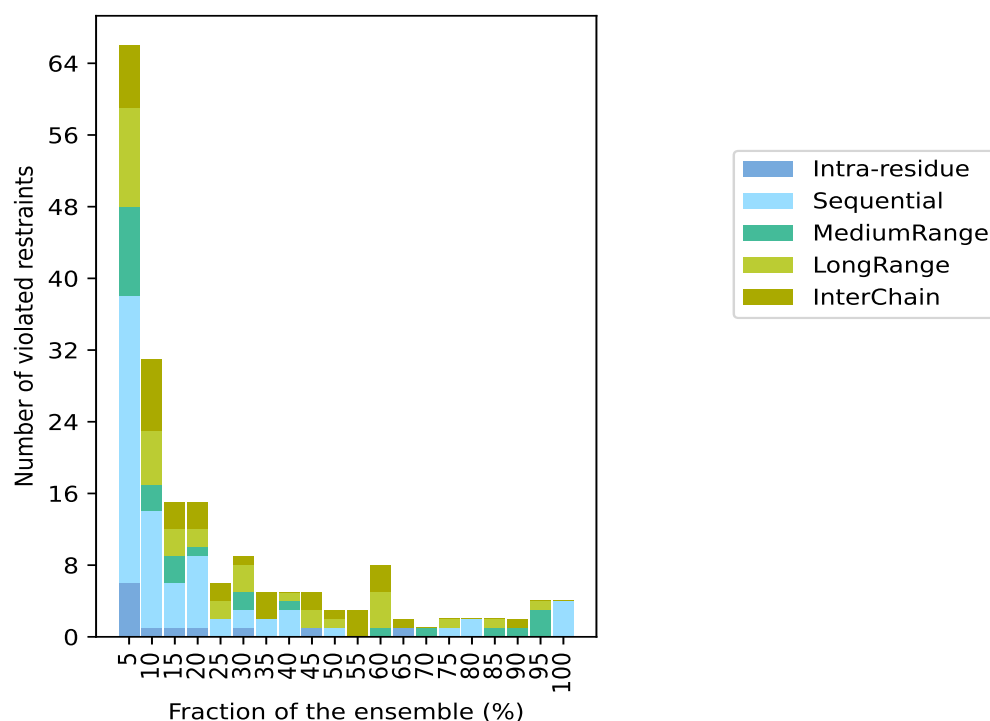
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 749(IR:221, SQ:227, MR:123, LR:145, IC:33) restraints are 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	%
6	32	10	11	7	66	1	5.0
1	13	3	6	8	31	2	10.0
1	5	3	3	3	15	3	15.0
1	8	1	2	3	15	4	20.0
0	2	0	2	2	6	5	25.0
1	2	2	3	1	9	6	30.0
0	2	0	0	3	5	7	35.0
0	3	1	1	0	5	8	40.0
1	0	0	2	2	5	9	45.0
0	1	0	1	1	3	10	50.0
0	0	0	0	3	3	11	55.0
0	0	1	4	3	8	12	60.0
1	0	0	0	1	2	13	65.0
0	0	1	0	0	1	14	70.0
0	1	0	1	0	2	15	75.0
0	2	0	0	0	2	16	80.0
0	0	1	1	0	2	17	85.0
0	0	1	0	1	2	18	90.0
0	0	3	1	0	4	19	95.0
0	4	0	0	0	4	20	100.0

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

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

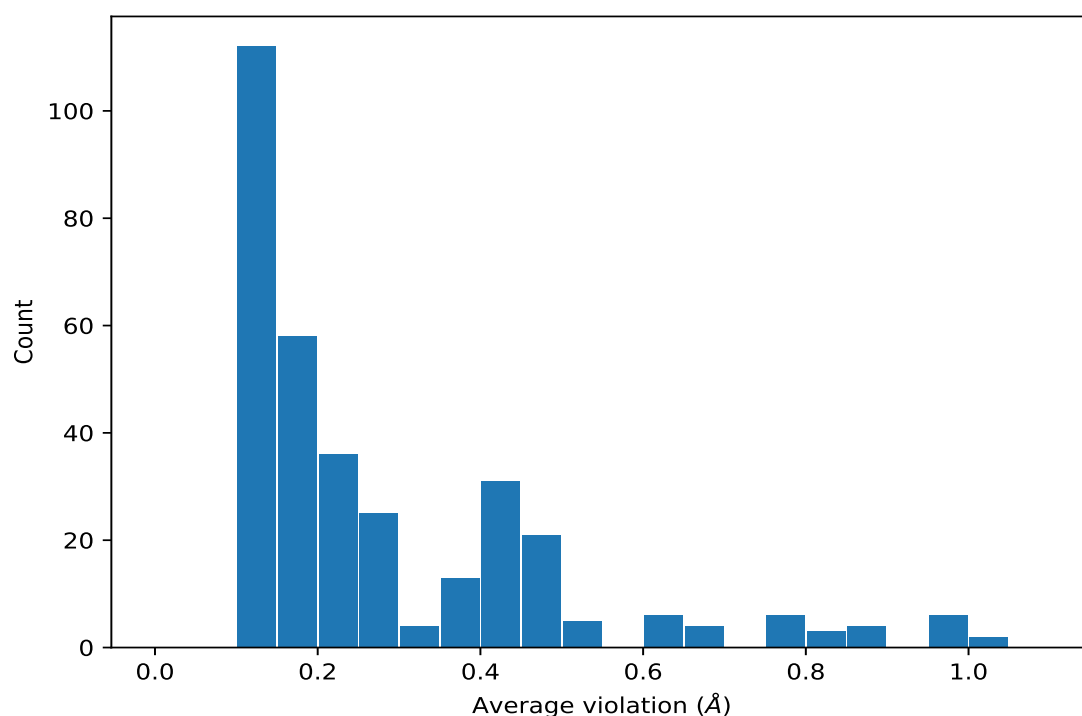
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	20	0.65	0.02	0.66
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	20	0.65	0.02	0.66
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	20	0.3	0.08	0.31
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	20	0.3	0.08	0.31
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	20	0.3	0.08	0.31
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	20	0.3	0.08	0.31
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	20	0.3	0.08	0.31
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	20	0.3	0.08	0.31
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	20	0.3	0.08	0.31
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	20	0.3	0.08	0.31
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	20	0.3	0.08	0.31
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	20	0.3	0.08	0.31
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	20	0.3	0.08	0.31
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	20	0.3	0.08	0.31
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	20	0.2	0.03	0.2
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	20	0.2	0.03	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	20	0.2	0.03	0.2
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	20	0.12	0.01	0.12
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	19	0.26	0.09	0.26
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	19	0.24	0.06	0.24
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	19	0.21	0.04	0.21
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	19	0.21	0.04	0.21
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	19	0.21	0.04	0.21
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	19	0.21	0.04	0.21
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	19	0.21	0.04	0.21
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	19	0.21	0.04	0.21
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	19	0.18	0.05	0.17
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	19	0.18	0.05	0.17
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	19	0.18	0.05	0.17
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	19	0.18	0.05	0.17
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	19	0.18	0.05	0.17
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	19	0.18	0.05	0.17
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	18	0.4	0.22	0.36
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	18	0.4	0.22	0.36
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	18	0.4	0.22	0.36
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	18	0.4	0.22	0.36
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	18	0.4	0.22	0.36
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	18	0.4	0.22	0.36
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	18	0.25	0.21	0.18
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	18	0.25	0.21	0.18
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	18	0.25	0.21	0.18
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	18	0.25	0.21	0.18
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	18	0.25	0.21	0.18
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	18	0.25	0.21	0.18
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	17	0.37	0.2	0.32
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	17	0.28	0.08	0.27
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	16	0.44	0.12	0.48
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	16	0.13	0.02	0.13
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	16	0.13	0.02	0.13
(1,623)	1:901:A:PHE:HA	1:902:A:ALA:H	15	0.14	0.02	0.14
(1,116)	1:865:A:TRP:HA	1:875:A:ARG:H	15	0.13	0.01	0.12
(1,389)	1:881:A:VAL:HA	1:883:A:GLY:H	14	0.12	0.02	0.12
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB2	13	0.65	0.26	0.67
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB3	13	0.65	0.26	0.67
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD2	13	0.19	0.08	0.17
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD3	13	0.19	0.08	0.17
(2,7)	1:904:A:CYS:CB	3:1001:A:ZN:ZN	13	0.14	0.03	0.13
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG2	12	0.86	0.28	0.87

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG3	12	0.86	0.28	0.87
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG2	12	0.86	0.28	0.87
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG3	12	0.86	0.28	0.87
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM1	12	0.47	0.32	0.38
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM2	12	0.47	0.32	0.38
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM3	12	0.47	0.32	0.38
(1,106)	1:865:A:TRP:H	2:4:B:MLZ:H	12	0.31	0.14	0.26
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG11	12	0.2	0.06	0.2
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG12	12	0.2	0.06	0.2
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG13	12	0.2	0.06	0.2
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG21	12	0.2	0.06	0.2
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG22	12	0.2	0.06	0.2
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG23	12	0.2	0.06	0.2
(1,648)	1:903:A:ASP:HA	1:906:A:LYS:H	12	0.16	0.04	0.14
(1,560)	1:896:A:ASN:HB2	1:902:A:ALA:H	12	0.14	0.02	0.14
(1,560)	1:896:A:ASN:HB3	1:902:A:ALA:H	12	0.14	0.02	0.14
(1,628)	1:901:A:PHE:HA	1:907:A:SER:H	12	0.13	0.02	0.13
(1,89)	1:864:A:ALA:H	1:879:A:ALA:H	12	0.13	0.02	0.13
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB2	11	0.96	0.36	1.11
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB3	11	0.96	0.36	1.11
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB2	11	0.96	0.36	1.11
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB3	11	0.96	0.36	1.11
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB2	11	0.96	0.36	1.11
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB3	11	0.96	0.36	1.11
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM1	11	0.36	0.12	0.42
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM2	11	0.36	0.12	0.42
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM3	11	0.36	0.12	0.42
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM1	11	0.36	0.12	0.42
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM2	11	0.36	0.12	0.42
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM3	11	0.36	0.12	0.42
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB2	11	0.35	0.13	0.35
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB3	11	0.35	0.13	0.35
(2,5)	1:893:A:CYS:CB	3:1001:A:ZN:ZN	11	0.12	0.02	0.11
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB2	10	0.77	0.32	0.88
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB3	10	0.77	0.32	0.88
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB2	10	0.77	0.32	0.88
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB3	10	0.77	0.32	0.88
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG11	10	0.19	0.06	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG12	10	0.19	0.06	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG13	10	0.19	0.06	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG21	10	0.19	0.06	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG22	10	0.19	0.06	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG23	10	0.19	0.06	0.16
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG11	10	0.14	0.03	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG12	10	0.14	0.03	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG13	10	0.14	0.03	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG21	10	0.14	0.03	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG22	10	0.14	0.03	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG23	10	0.14	0.03	0.14
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE2	9	1.02	0.62	1.04
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE3	9	1.02	0.62	1.04
(1,60)	1:861:A:THR:HA	1:861:A:THR:HB	9	0.17	0.01	0.18
(1,137)	1:865:A:TRP:HH2	1:909:A:GLU:H	9	0.14	0.02	0.14
(2,3)	1:871:A:CYS:CB	3:1001:A:ZN:ZN	9	0.13	0.04	0.12
(1,209)	1:867:A:ARG:HD2	2:3:B:THR:HA	9	0.13	0.02	0.11
(1,209)	1:867:A:ARG:HD3	2:3:B:THR:HA	9	0.13	0.02	0.11
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE21	9	0.12	0.01	0.12
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE22	9	0.12	0.01	0.12
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE21	9	0.12	0.01	0.12
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE22	9	0.12	0.01	0.12
(1,937)	2:8:B:ARG:H	2:9:B:TYR:H	8	0.22	0.13	0.16
(1,926)	2:2:B:ARG:HE	2:3:B:THR:HA	8	0.18	0.09	0.14
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB2	8	0.13	0.03	0.12
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB3	8	0.13	0.03	0.12
(1,918)	1:926:A:ALA:HA	1:928:A:ALA:H	8	0.13	0.01	0.13
(1,298)	1:874:A:TRP:HB2	1:875:A:ARG:H	8	0.12	0.01	0.11
(1,110)	1:865:A:TRP:H	2:5:B:GLN:HB2	7	0.75	0.23	0.82
(1,110)	1:865:A:TRP:H	2:5:B:GLN:HB3	7	0.75	0.23	0.82
(1,858)	1:919:A:LEU:HD11	1:920:A:GLY:H	7	0.4	0.07	0.39
(1,858)	1:919:A:LEU:HD12	1:920:A:GLY:H	7	0.4	0.07	0.39
(1,858)	1:919:A:LEU:HD13	1:920:A:GLY:H	7	0.4	0.07	0.39
(1,858)	1:919:A:LEU:HD21	1:920:A:GLY:H	7	0.4	0.07	0.39
(1,858)	1:919:A:LEU:HD22	1:920:A:GLY:H	7	0.4	0.07	0.39
(1,858)	1:919:A:LEU:HD23	1:920:A:GLY:H	7	0.4	0.07	0.39
(1,145)	1:865:A:TRP:HB2	2:4:B:MLZ:HB2	7	0.22	0.1	0.16
(1,145)	1:865:A:TRP:HB2	2:4:B:MLZ:HB3	7	0.22	0.1	0.16
(1,145)	1:865:A:TRP:HB3	2:4:B:MLZ:HB2	7	0.22	0.1	0.16
(1,145)	1:865:A:TRP:HB3	2:4:B:MLZ:HB3	7	0.22	0.1	0.16
(1,863)	1:919:A:LEU:HD11	2:6:B:THR:H	7	0.18	0.07	0.17
(1,863)	1:919:A:LEU:HD12	2:6:B:THR:H	7	0.18	0.07	0.17
(1,863)	1:919:A:LEU:HD13	2:6:B:THR:H	7	0.18	0.07	0.17
(1,863)	1:919:A:LEU:HD21	2:6:B:THR:H	7	0.18	0.07	0.17
(1,863)	1:919:A:LEU:HD22	2:6:B:THR:H	7	0.18	0.07	0.17
(1,863)	1:919:A:LEU:HD23	2:6:B:THR:H	7	0.18	0.07	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,39)	1:857:A:GLY:H	1:858:A:SER:H	7	0.14	0.04	0.13
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM1	6	0.81	0.45	0.76
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM2	6	0.81	0.45	0.76
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM3	6	0.81	0.45	0.76
(1,790)	1:915:A:ILE:HB	1:916:A:ASN:H	6	0.24	0.02	0.24
(1,679)	1:906:A:LYS:HB2	1:906:A:LYS:HD2	6	0.18	0.0	0.18
(1,679)	1:906:A:LYS:HB2	1:906:A:LYS:HD3	6	0.18	0.0	0.18
(1,679)	1:906:A:LYS:HB3	1:906:A:LYS:HD2	6	0.18	0.0	0.18
(1,679)	1:906:A:LYS:HB3	1:906:A:LYS:HD3	6	0.18	0.0	0.18
(1,755)	1:912:A:ASN:HA	1:916:A:ASN:H	6	0.16	0.02	0.16
(1,215)	1:867:A:ARG:HG2	1:874:A:TRP:HZ2	6	0.14	0.03	0.14
(1,215)	1:867:A:ARG:HG3	1:874:A:TRP:HZ2	6	0.14	0.03	0.14
(1,139)	1:865:A:TRP:HZ2	1:915:A:ILE:HA	6	0.13	0.02	0.14
(1,200)	1:867:A:ARG:HE	1:872:A:PHE:HB2	6	0.12	0.02	0.12
(1,200)	1:867:A:ARG:HE	1:872:A:PHE:HB3	6	0.12	0.02	0.12
(1,912)	1:925:A:GLU:HB2	1:926:A:ALA:H	6	0.12	0.02	0.12
(1,170)	1:866:A:VAL:HG11	1:868:A:CYS:H	6	0.12	0.02	0.11
(1,170)	1:866:A:VAL:HG12	1:868:A:CYS:H	6	0.12	0.02	0.11
(1,170)	1:866:A:VAL:HG13	1:868:A:CYS:H	6	0.12	0.02	0.11
(1,170)	1:866:A:VAL:HG21	1:868:A:CYS:H	6	0.12	0.02	0.11
(1,170)	1:866:A:VAL:HG22	1:868:A:CYS:H	6	0.12	0.02	0.11
(1,170)	1:866:A:VAL:HG23	1:868:A:CYS:H	6	0.12	0.02	0.11
(1,888)	1:922:A:GLY:H	1:923:A:GLN:H	5	0.24	0.11	0.21
(1,193)	1:867:A:ARG:H	2:4:B:MLZ:H	5	0.18	0.07	0.16
(1,265)	1:870:A:ASP:HB2	1:871:A:CYS:H	5	0.16	0.05	0.15
(1,265)	1:870:A:ASP:HB3	1:871:A:CYS:H	5	0.16	0.05	0.15
(1,895)	1:923:A:GLN:HE21	2:3:B:THR:HA	5	0.15	0.03	0.14
(1,305)	1:874:A:TRP:HE1	1:923:A:GLN:HG2	5	0.14	0.02	0.14
(1,305)	1:874:A:TRP:HE1	1:923:A:GLN:HG3	5	0.14	0.02	0.14
(1,631)	1:901:A:PHE:HD1	1:909:A:GLU:H	5	0.11	0.01	0.11
(1,631)	1:901:A:PHE:HD2	1:909:A:GLU:H	5	0.11	0.01	0.11
(1,313)	1:874:A:TRP:HH2	2:4:B:MLZ:HE2	4	0.53	0.31	0.36
(1,313)	1:874:A:TRP:HH2	2:4:B:MLZ:HE3	4	0.53	0.31	0.36
(1,147)	1:865:A:TRP:HB2	2:4:B:MLZ:HG2	4	0.38	0.1	0.34
(1,147)	1:865:A:TRP:HB2	2:4:B:MLZ:HG3	4	0.38	0.1	0.34
(1,147)	1:865:A:TRP:HB3	2:4:B:MLZ:HG2	4	0.38	0.1	0.34
(1,147)	1:865:A:TRP:HB3	2:4:B:MLZ:HG3	4	0.38	0.1	0.34
(1,371)	1:879:A:ALA:HA	1:882:A:VAL:HB	4	0.24	0.02	0.24
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG11	4	0.23	0.05	0.23
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG12	4	0.23	0.05	0.23
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG13	4	0.23	0.05	0.23
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG21	4	0.23	0.05	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG22	4	0.23	0.05	0.23
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG23	4	0.23	0.05	0.23
(1,539)	1:895:A:ASN:HB2	1:896:A:ASN:H	4	0.2	0.09	0.18
(1,539)	1:895:A:ASN:HB3	1:896:A:ASN:H	4	0.2	0.09	0.18
(1,407)	1:882:A:VAL:HB	1:883:A:GLY:H	4	0.16	0.01	0.16
(1,287)	1:873:A:LYS:HB2	1:874:A:TRP:HA	4	0.16	0.01	0.16
(1,287)	1:873:A:LYS:HB3	1:874:A:TRP:HA	4	0.16	0.01	0.16
(1,338)	1:876:A:ARG:HA	1:876:A:ARG:HD2	4	0.16	0.06	0.13
(1,338)	1:876:A:ARG:HA	1:876:A:ARG:HD3	4	0.16	0.06	0.13
(1,52)	1:859:A:GLU:HB2	1:860:A:PHE:H	4	0.14	0.03	0.13
(1,52)	1:859:A:GLU:HB3	1:860:A:PHE:H	4	0.14	0.03	0.13
(1,132)	1:865:A:TRP:HE1	2:6:B:THR:HA	4	0.13	0.01	0.14
(1,904)	1:924:A:ASP:H	1:925:A:GLU:H	4	0.13	0.02	0.12
(1,792)	1:915:A:ILE:HD11	1:916:A:ASN:HA	4	0.13	0.02	0.13
(1,792)	1:915:A:ILE:HD12	1:916:A:ASN:HA	4	0.13	0.02	0.13
(1,792)	1:915:A:ILE:HD13	1:916:A:ASN:HA	4	0.13	0.02	0.13
(1,430)	1:885:A:ILE:HG12	1:891:A:TRP:HA	4	0.12	0.02	0.11
(1,430)	1:885:A:ILE:HG13	1:891:A:TRP:HA	4	0.12	0.02	0.11
(1,42)	1:858:A:SER:H	1:859:A:GLU:H	4	0.11	0.01	0.12
(1,214)	1:867:A:ARG:HG2	1:874:A:TRP:HE1	4	0.11	0.01	0.11
(1,214)	1:867:A:ARG:HG3	1:874:A:TRP:HE1	4	0.11	0.01	0.11
(1,262)	1:870:A:ASP:HB3	1:871:A:CYS:H	3	0.33	0.09	0.37
(1,303)	1:874:A:TRP:HD1	2:4:B:MLZ:HCM1	3	0.27	0.07	0.26
(1,303)	1:874:A:TRP:HD1	2:4:B:MLZ:HCM2	3	0.27	0.07	0.26
(1,303)	1:874:A:TRP:HD1	2:4:B:MLZ:HCM3	3	0.27	0.07	0.26
(1,902)	1:923:A:GLN:HG2	1:924:A:ASP:H	3	0.27	0.08	0.32
(1,902)	1:923:A:GLN:HG3	1:924:A:ASP:H	3	0.27	0.08	0.32
(1,653)	1:903:A:ASP:HB2	1:904:A:CYS:H	3	0.2	0.03	0.2
(1,653)	1:903:A:ASP:HB3	1:904:A:CYS:H	3	0.2	0.03	0.2
(1,891)	1:923:A:GLN:H	1:923:A:GLN:HG2	3	0.2	0.04	0.21
(1,891)	1:923:A:GLN:H	1:923:A:GLN:HG3	3	0.2	0.04	0.21
(1,109)	1:865:A:TRP:H	2:5:B:GLN:HA	3	0.18	0.05	0.18
(1,649)	1:903:A:ASP:HB2	1:905:A:SER:H	3	0.17	0.0	0.17
(1,1)	1:851:A:SER:HA	1:852:A:ARG:H	3	0.15	0.03	0.14
(1,929)	2:5:B:GLN:H	2:6:B:THR:H	3	0.15	0.03	0.16
(1,315)	1:874:A:TRP:HZ2	1:923:A:GLN:HB2	3	0.14	0.03	0.15
(1,315)	1:874:A:TRP:HZ2	1:923:A:GLN:HB3	3	0.14	0.03	0.15
(1,446)	1:886:A:ASP:HB2	1:888:A:SER:H	3	0.13	0.02	0.12
(1,900)	1:923:A:GLN:HE21	2:3:B:THR:HA	3	0.13	0.01	0.12
(1,900)	1:923:A:GLN:HE22	2:3:B:THR:HA	3	0.13	0.01	0.12
(1,140)	1:865:A:TRP:HZ3	1:910:A:MET:H	3	0.12	0.01	0.13
(1,255)	1:870:A:ASP:H	1:872:A:PHE:H	3	0.12	0.01	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,289)	1:873:A:LYS:HE2	1:901:A:PHE:HB2	3	0.11	0.01	0.11
(1,289)	1:873:A:LYS:HE2	1:901:A:PHE:HB3	3	0.11	0.01	0.11
(1,289)	1:873:A:LYS:HE3	1:901:A:PHE:HB2	3	0.11	0.01	0.11
(1,289)	1:873:A:LYS:HE3	1:901:A:PHE:HB3	3	0.11	0.01	0.11
(1,883)	1:921:A:ILE:HD11	2:4:B:MLZ:HG2	2	0.62	0.46	0.62
(1,883)	1:921:A:ILE:HD11	2:4:B:MLZ:HG3	2	0.62	0.46	0.62
(1,883)	1:921:A:ILE:HD12	2:4:B:MLZ:HG2	2	0.62	0.46	0.62
(1,883)	1:921:A:ILE:HD12	2:4:B:MLZ:HG3	2	0.62	0.46	0.62
(1,883)	1:921:A:ILE:HD13	2:4:B:MLZ:HG2	2	0.62	0.46	0.62
(1,883)	1:921:A:ILE:HD13	2:4:B:MLZ:HG3	2	0.62	0.46	0.62
(1,307)	1:874:A:TRP:HE3	2:4:B:MLZ:HCM1	2	0.52	0.3	0.52
(1,307)	1:874:A:TRP:HE3	2:4:B:MLZ:HCM2	2	0.52	0.3	0.52
(1,307)	1:874:A:TRP:HE3	2:4:B:MLZ:HCM3	2	0.52	0.3	0.52
(1,859)	1:919:A:LEU:HD11	2:4:B:MLZ:HCM1	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD11	2:4:B:MLZ:HCM2	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD11	2:4:B:MLZ:HCM3	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD12	2:4:B:MLZ:HCM1	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD12	2:4:B:MLZ:HCM2	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD12	2:4:B:MLZ:HCM3	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD13	2:4:B:MLZ:HCM1	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD13	2:4:B:MLZ:HCM2	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD13	2:4:B:MLZ:HCM3	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD21	2:4:B:MLZ:HCM1	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD21	2:4:B:MLZ:HCM2	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD21	2:4:B:MLZ:HCM3	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD22	2:4:B:MLZ:HCM1	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD22	2:4:B:MLZ:HCM2	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD22	2:4:B:MLZ:HCM3	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD23	2:4:B:MLZ:HCM1	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD23	2:4:B:MLZ:HCM2	2	0.45	0.09	0.45
(1,859)	1:919:A:LEU:HD23	2:4:B:MLZ:HCM3	2	0.45	0.09	0.45
(1,882)	1:921:A:ILE:HD11	2:4:B:MLZ:HE2	2	0.4	0.16	0.4
(1,882)	1:921:A:ILE:HD11	2:4:B:MLZ:HE3	2	0.4	0.16	0.4
(1,882)	1:921:A:ILE:HD12	2:4:B:MLZ:HE2	2	0.4	0.16	0.4
(1,882)	1:921:A:ILE:HD12	2:4:B:MLZ:HE3	2	0.4	0.16	0.4
(1,882)	1:921:A:ILE:HD13	2:4:B:MLZ:HE2	2	0.4	0.16	0.4
(1,882)	1:921:A:ILE:HD13	2:4:B:MLZ:HE3	2	0.4	0.16	0.4
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG11	2	0.4	0.12	0.4
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG12	2	0.4	0.12	0.4
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG13	2	0.4	0.12	0.4
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG21	2	0.4	0.12	0.4
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG22	2	0.4	0.12	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG23	2	0.4	0.12	0.4
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG11	2	0.4	0.12	0.4
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG12	2	0.4	0.12	0.4
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG13	2	0.4	0.12	0.4
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG21	2	0.4	0.12	0.4
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG22	2	0.4	0.12	0.4
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG23	2	0.4	0.12	0.4
(1,54)	1:860:A:PHE:H	1:861:A:THR:H	2	0.39	0.1	0.39
(1,50)	1:859:A:GLU:HA	1:860:A:PHE:H	2	0.38	0.05	0.38
(1,63)	1:861:A:THR:HG21	1:862:A:GLU:H	2	0.18	0.08	0.18
(1,63)	1:861:A:THR:HG22	1:862:A:GLU:H	2	0.18	0.08	0.18
(1,63)	1:861:A:THR:HG23	1:862:A:GLU:H	2	0.18	0.08	0.18
(1,206)	1:867:A:ARG:HD2	1:872:A:PHE:HB2	2	0.18	0.04	0.18
(1,206)	1:867:A:ARG:HD2	1:872:A:PHE:HB3	2	0.18	0.04	0.18
(1,206)	1:867:A:ARG:HD3	1:872:A:PHE:HB2	2	0.18	0.04	0.18
(1,206)	1:867:A:ARG:HD3	1:872:A:PHE:HB3	2	0.18	0.04	0.18
(1,899)	1:923:A:GLN:HB2	1:924:A:ASP:H	2	0.18	0.01	0.18
(1,899)	1:923:A:GLN:HB3	1:924:A:ASP:H	2	0.18	0.01	0.18
(1,429)	1:885:A:ILE:HG12	1:891:A:TRP:H	2	0.18	0.06	0.18
(1,429)	1:885:A:ILE:HG13	1:891:A:TRP:H	2	0.18	0.06	0.18
(1,309)	1:874:A:TRP:HH2	2:3:B:THR:HA	2	0.17	0.04	0.17
(1,507)	1:892:A:ILE:HD11	1:895:A:ASN:HD21	2	0.16	0.02	0.16
(1,507)	1:892:A:ILE:HD11	1:895:A:ASN:HD22	2	0.16	0.02	0.16
(1,507)	1:892:A:ILE:HD12	1:895:A:ASN:HD21	2	0.16	0.02	0.16
(1,507)	1:892:A:ILE:HD12	1:895:A:ASN:HD22	2	0.16	0.02	0.16
(1,507)	1:892:A:ILE:HD13	1:895:A:ASN:HD21	2	0.16	0.02	0.16
(1,507)	1:892:A:ILE:HD13	1:895:A:ASN:HD22	2	0.16	0.02	0.16
(1,320)	1:874:A:TRP:HZ3	2:2:B:ARG:HG2	2	0.16	0.05	0.16
(1,320)	1:874:A:TRP:HZ3	2:2:B:ARG:HG3	2	0.16	0.05	0.16
(1,291)	1:873:A:LYS:HG2	1:873:A:LYS:HE2	2	0.15	0.0	0.15
(1,291)	1:873:A:LYS:HG2	1:873:A:LYS:HE3	2	0.15	0.0	0.15
(1,291)	1:873:A:LYS:HG3	1:873:A:LYS:HE2	2	0.15	0.0	0.15
(1,291)	1:873:A:LYS:HG3	1:873:A:LYS:HE3	2	0.15	0.0	0.15
(1,683)	1:906:A:LYS:HB2	1:907:A:SER:HB2	2	0.15	0.03	0.15
(1,683)	1:906:A:LYS:HB2	1:907:A:SER:HB3	2	0.15	0.03	0.15
(1,683)	1:906:A:LYS:HB3	1:907:A:SER:HB2	2	0.15	0.03	0.15
(1,683)	1:906:A:LYS:HB3	1:907:A:SER:HB3	2	0.15	0.03	0.15
(1,914)	1:925:A:GLU:HB3	1:926:A:ALA:H	2	0.15	0.0	0.15
(1,317)	1:874:A:TRP:HZ2	2:3:B:THR:HA	2	0.13	0.0	0.13
(1,917)	1:926:A:ALA:H	1:927:A:ASP:H	2	0.13	0.0	0.13
(1,325)	1:874:A:TRP:HB2	1:915:A:ILE:HG21	2	0.12	0.01	0.12
(1,325)	1:874:A:TRP:HB2	1:915:A:ILE:HG22	2	0.12	0.01	0.12

Continued on next page...

Continued from previous page...

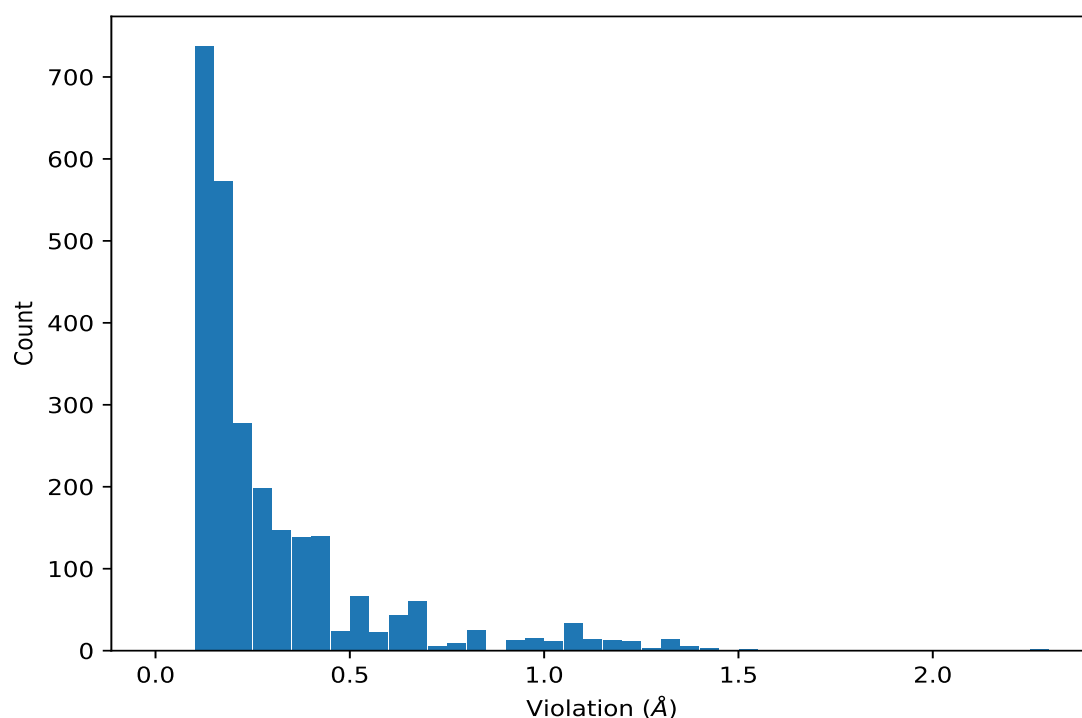
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,325)	1:874:A:TRP:HB2	1:915:A:ILE:HG23	2	0.12	0.01	0.12
(1,325)	1:874:A:TRP:HB3	1:915:A:ILE:HG21	2	0.12	0.01	0.12
(1,325)	1:874:A:TRP:HB3	1:915:A:ILE:HG22	2	0.12	0.01	0.12
(1,325)	1:874:A:TRP:HB3	1:915:A:ILE:HG23	2	0.12	0.01	0.12
(1,473)	1:890:A:ARG:HB2	1:891:A:TRP:H	2	0.12	0.01	0.12
(1,473)	1:890:A:ARG:HB3	1:891:A:TRP:H	2	0.12	0.01	0.12
(1,844)	1:918:A:GLU:HG2	2:8:B:ARG:HB2	2	0.12	0.02	0.12
(1,844)	1:918:A:GLU:HG2	2:8:B:ARG:HB3	2	0.12	0.02	0.12
(1,844)	1:918:A:GLU:HG3	2:8:B:ARG:HB2	2	0.12	0.02	0.12
(1,844)	1:918:A:GLU:HG3	2:8:B:ARG:HB3	2	0.12	0.02	0.12
(1,633)	1:902:A:ALA:H	1:903:A:ASP:H	2	0.12	0.0	0.12
(1,646)	1:903:A:ASP:HA	1:904:A:CYS:HA	2	0.12	0.0	0.12
(2,8)	1:904:A:CYS:SG	3:1001:A:ZN:ZN	2	0.12	0.0	0.12
(1,61)	1:861:A:THR:HA	1:862:A:GLU:H	2	0.11	0.01	0.11
(1,426)	1:885:A:ILE:HD11	1:891:A:TRP:HE1	2	0.11	0.0	0.11
(1,426)	1:885:A:ILE:HD12	1:891:A:TRP:HE1	2	0.11	0.0	0.11
(1,426)	1:885:A:ILE:HD13	1:891:A:TRP:HE1	2	0.11	0.0	0.11
(1,501)	1:892:A:ILE:HD11	1:894:A:MET:H	2	0.11	0.0	0.11
(1,501)	1:892:A:ILE:HD12	1:894:A:MET:H	2	0.11	0.0	0.11
(1,501)	1:892:A:ILE:HD13	1:894:A:MET:H	2	0.11	0.0	0.11
(1,385)	1:881:A:VAL:H	1:882:A:VAL:HA	2	0.11	0.0	0.11
(1,129)	1:865:A:TRP:HE1	1:918:A:GLU:HB2	2	0.1	0.0	0.1
(1,129)	1:865:A:TRP:HE1	1:918:A:GLU:HB3	2	0.1	0.0	0.1
(1,378)	1:880:A:SER:H	1:882:A:VAL:H	2	0.1	0.0	0.1
(1,565)	1:896:A:ASN:HD21	1:901:A:PHE:HA	2	0.1	0.0	0.1
(1,565)	1:896:A:ASN:HD22	1:901:A:PHE:HA	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE2	13	2.28
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE3	13	2.28
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE2	12	1.54
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE3	12	1.54
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM1	13	1.44
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM2	13	1.44
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM3	13	1.44
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB2	1	1.37
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB3	1	1.37
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB2	1	1.37
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB3	1	1.37
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB2	1	1.37
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB3	1	1.37
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB2	13	1.32
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB3	13	1.32
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB2	13	1.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB3	13	1.32
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB2	13	1.32
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB3	13	1.32
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB2	9	1.31
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB3	9	1.31
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB2	9	1.31
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB3	9	1.31
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB2	9	1.31
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB3	9	1.31
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE2	1	1.3
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE3	1	1.3
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM1	16	1.29
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM2	16	1.29
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM3	16	1.29
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG2	1	1.22
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG3	1	1.22
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG2	1	1.22
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG3	1	1.22
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG2	16	1.22
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG3	16	1.22
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG2	16	1.22
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG3	16	1.22
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB2	1	1.22
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB3	1	1.22
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB2	1	1.22
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB3	1	1.22
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB2	20	1.17
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB3	20	1.17
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB2	20	1.17
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB3	20	1.17
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB2	20	1.17
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB3	20	1.17
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM1	17	1.17
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM2	17	1.17
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM3	17	1.17
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG2	9	1.15
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG3	9	1.15
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG2	9	1.15
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG3	9	1.15
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB2	16	1.13
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB3	16	1.13
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB2	16	1.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB3	16	1.13
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB2	16	1.13
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB3	16	1.13
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE2	9	1.13
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE3	9	1.13
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB2	5	1.11
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB3	5	1.11
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB2	5	1.11
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB3	5	1.11
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB2	5	1.11
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB3	5	1.11
(1,883)	1:921:A:ILE:HD11	2:4:B:MLZ:HG2	17	1.09
(1,883)	1:921:A:ILE:HD11	2:4:B:MLZ:HG3	17	1.09
(1,883)	1:921:A:ILE:HD12	2:4:B:MLZ:HG2	17	1.09
(1,883)	1:921:A:ILE:HD12	2:4:B:MLZ:HG3	17	1.09
(1,883)	1:921:A:ILE:HD13	2:4:B:MLZ:HG2	17	1.09
(1,883)	1:921:A:ILE:HD13	2:4:B:MLZ:HG3	17	1.09
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB2	9	1.09
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB3	9	1.09
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB2	9	1.09
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB3	9	1.09
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	20	1.07
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	20	1.07
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	20	1.07
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	20	1.07
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	20	1.07
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	20	1.07
(1,313)	1:874:A:TRP:HH2	2:4:B:MLZ:HE2	13	1.07
(1,313)	1:874:A:TRP:HH2	2:4:B:MLZ:HE3	13	1.07
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	17	1.07
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	17	1.07
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	17	1.07
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	17	1.07
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	17	1.07
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	17	1.07
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG2	11	1.06
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG3	11	1.06
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG2	11	1.06
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG3	11	1.06
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB2	12	1.05
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB3	12	1.05
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB2	12	1.05

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB3	12	1.05
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB2	12	1.05
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB3	12	1.05
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG2	13	1.04
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG3	13	1.04
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG2	13	1.04
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG3	13	1.04
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE2	20	1.04
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE3	20	1.04
(1,110)	1:865:A:TRP:H	2:5:B:GLN:HB2	6	1.03
(1,110)	1:865:A:TRP:H	2:5:B:GLN:HB3	6	1.03
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB2	12	1.02
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB3	12	1.02
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB2	20	1.01
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB3	20	1.01
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB2	13	0.99
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB3	13	0.99
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB2	13	0.99
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB3	13	0.99
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM1	13	0.97
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM2	13	0.97
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM3	13	0.97
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB2	1	0.97
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB3	1	0.97
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB2	16	0.95
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB3	16	0.95
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB2	16	0.95
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB3	16	0.95
(1,110)	1:865:A:TRP:H	2:5:B:GLN:HB2	11	0.95
(1,110)	1:865:A:TRP:H	2:5:B:GLN:HB3	11	0.95
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG2	20	0.94
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG3	20	0.94
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG2	20	0.94
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG3	20	0.94
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB2	20	0.92
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB3	20	0.92
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB2	20	0.92
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB3	20	0.92
(1,110)	1:865:A:TRP:H	2:5:B:GLN:HB2	5	0.91
(1,110)	1:865:A:TRP:H	2:5:B:GLN:HB3	5	0.91
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM1	5	0.9
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM2	5	0.9

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM3	5	0.9
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB2	5	0.83
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB3	5	0.83
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB2	5	0.83
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB3	5	0.83
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE2	2	0.83
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE3	2	0.83
(1,307)	1:874:A:TRP:HE3	2:4:B:MLZ:HCM1	17	0.82
(1,307)	1:874:A:TRP:HE3	2:4:B:MLZ:HCM2	17	0.82
(1,307)	1:874:A:TRP:HE3	2:4:B:MLZ:HCM3	17	0.82
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB2	16	0.82
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB3	16	0.82
(1,110)	1:865:A:TRP:H	2:5:B:GLN:HB2	4	0.82
(1,110)	1:865:A:TRP:H	2:5:B:GLN:HB3	4	0.82
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG2	5	0.8
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG3	5	0.8
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG2	5	0.8
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG3	5	0.8
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG2	12	0.8
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG3	12	0.8
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG2	12	0.8
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG3	12	0.8
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB2	12	0.8
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB3	12	0.8
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB2	12	0.8
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB3	12	0.8
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB2	6	0.78
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB3	6	0.78
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB2	6	0.78
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB3	6	0.78
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB2	6	0.78
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB3	6	0.78
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB2	9	0.77
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB3	9	0.77
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	2	0.75
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE2	17	0.73
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE3	17	0.73
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	10	0.71
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	7	0.7
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	7	0.7
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	14	0.7
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	3	0.69

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	3	0.69
(1,396)	1:881:A:VAL:HG11	1:885:A:ILE:HG12	20	0.69
(1,396)	1:881:A:VAL:HG11	1:885:A:ILE:HG13	20	0.69
(1,396)	1:881:A:VAL:HG12	1:885:A:ILE:HG12	20	0.69
(1,396)	1:881:A:VAL:HG12	1:885:A:ILE:HG13	20	0.69
(1,396)	1:881:A:VAL:HG13	1:885:A:ILE:HG12	20	0.69
(1,396)	1:881:A:VAL:HG13	1:885:A:ILE:HG13	20	0.69
(1,396)	1:881:A:VAL:HG21	1:885:A:ILE:HG12	20	0.69
(1,396)	1:881:A:VAL:HG21	1:885:A:ILE:HG13	20	0.69
(1,396)	1:881:A:VAL:HG22	1:885:A:ILE:HG12	20	0.69
(1,396)	1:881:A:VAL:HG22	1:885:A:ILE:HG13	20	0.69
(1,396)	1:881:A:VAL:HG23	1:885:A:ILE:HG12	20	0.69
(1,396)	1:881:A:VAL:HG23	1:885:A:ILE:HG13	20	0.69
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB2	13	0.69
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB3	13	0.69
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	13	0.68
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	13	0.68
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	13	0.68
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	13	0.68
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	13	0.68
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	13	0.68
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	4	0.67
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	4	0.67
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	8	0.67
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	8	0.67
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	11	0.67
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	11	0.67
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	13	0.67
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	13	0.67
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	20	0.67
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	20	0.67
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM1	16	0.67
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM2	16	0.67
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM3	16	0.67
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB2	17	0.67
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB3	17	0.67
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG2	17	0.66
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG3	17	0.66
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG2	17	0.66
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG3	17	0.66
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	2	0.66
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	2	0.66

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	5	0.66
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	5	0.66
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	12	0.66
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	12	0.66
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	6	0.65
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	6	0.65
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	9	0.65
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	9	0.65
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	17	0.65
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	17	0.65
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	19	0.65
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	19	0.65
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	6	0.65
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	6	0.65
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	6	0.65
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	6	0.65
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	6	0.65
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	6	0.65
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	16	0.64
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	16	0.64
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	10	0.63
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	10	0.63
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	15	0.63
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	15	0.63
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM1	17	0.63
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM2	17	0.63
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM3	17	0.63
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	2	0.63
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB2	2	0.63
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB3	2	0.63
(1,110)	1:865:A:TRP:H	2:5:B:GLN:HB2	15	0.63
(1,110)	1:865:A:TRP:H	2:5:B:GLN:HB3	15	0.63
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	1	0.62
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	1	0.62
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	18	0.62
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	18	0.62
(1,397)	1:881:A:VAL:HG11	1:885:A:ILE:HG21	20	0.62
(1,397)	1:881:A:VAL:HG11	1:885:A:ILE:HG22	20	0.62
(1,397)	1:881:A:VAL:HG11	1:885:A:ILE:HG23	20	0.62
(1,397)	1:881:A:VAL:HG12	1:885:A:ILE:HG21	20	0.62
(1,397)	1:881:A:VAL:HG12	1:885:A:ILE:HG22	20	0.62
(1,397)	1:881:A:VAL:HG12	1:885:A:ILE:HG23	20	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:881:A:VAL:HG13	1:885:A:ILE:HG21	20	0.62
(1,397)	1:881:A:VAL:HG13	1:885:A:ILE:HG22	20	0.62
(1,397)	1:881:A:VAL:HG13	1:885:A:ILE:HG23	20	0.62
(1,397)	1:881:A:VAL:HG21	1:885:A:ILE:HG21	20	0.62
(1,397)	1:881:A:VAL:HG21	1:885:A:ILE:HG22	20	0.62
(1,397)	1:881:A:VAL:HG21	1:885:A:ILE:HG23	20	0.62
(1,397)	1:881:A:VAL:HG22	1:885:A:ILE:HG21	20	0.62
(1,397)	1:881:A:VAL:HG22	1:885:A:ILE:HG22	20	0.62
(1,397)	1:881:A:VAL:HG22	1:885:A:ILE:HG23	20	0.62
(1,397)	1:881:A:VAL:HG23	1:885:A:ILE:HG21	20	0.62
(1,397)	1:881:A:VAL:HG23	1:885:A:ILE:HG22	20	0.62
(1,397)	1:881:A:VAL:HG23	1:885:A:ILE:HG23	20	0.62
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	20	0.62
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB2	6	0.62
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB3	6	0.62
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB2	20	0.62
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB3	20	0.62
(1,508)	1:892:A:ILE:HG12	1:893:A:CYS:H	14	0.6
(1,508)	1:892:A:ILE:HG13	1:893:A:CYS:H	14	0.6
(1,110)	1:865:A:TRP:H	2:5:B:GLN:HB2	17	0.59
(1,110)	1:865:A:TRP:H	2:5:B:GLN:HB3	17	0.59
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB2	7	0.58
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB3	7	0.58
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB2	7	0.58
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB3	7	0.58
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB2	7	0.58
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB3	7	0.58
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM1	5	0.58
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM2	5	0.58
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM3	5	0.58
(1,882)	1:921:A:ILE:HD11	2:4:B:MLZ:HE2	9	0.56
(1,882)	1:921:A:ILE:HD11	2:4:B:MLZ:HE3	9	0.56
(1,882)	1:921:A:ILE:HD12	2:4:B:MLZ:HE2	9	0.56
(1,882)	1:921:A:ILE:HD12	2:4:B:MLZ:HE3	9	0.56
(1,882)	1:921:A:ILE:HD13	2:4:B:MLZ:HE2	9	0.56
(1,882)	1:921:A:ILE:HD13	2:4:B:MLZ:HE3	9	0.56
(1,147)	1:865:A:TRP:HB2	2:4:B:MLZ:HG2	18	0.55
(1,147)	1:865:A:TRP:HB2	2:4:B:MLZ:HG3	18	0.55
(1,147)	1:865:A:TRP:HB3	2:4:B:MLZ:HG2	18	0.55
(1,147)	1:865:A:TRP:HB3	2:4:B:MLZ:HG3	18	0.55
(1,106)	1:865:A:TRP:H	2:4:B:MLZ:H	16	0.55
(1,859)	1:919:A:LEU:HD11	2:4:B:MLZ:HCM1	18	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,859)	1:919:A:LEU:HD11	2:4:B:MLZ:HCM2	18	0.54
(1,859)	1:919:A:LEU:HD11	2:4:B:MLZ:HCM3	18	0.54
(1,859)	1:919:A:LEU:HD12	2:4:B:MLZ:HCM1	18	0.54
(1,859)	1:919:A:LEU:HD12	2:4:B:MLZ:HCM2	18	0.54
(1,859)	1:919:A:LEU:HD12	2:4:B:MLZ:HCM3	18	0.54
(1,859)	1:919:A:LEU:HD13	2:4:B:MLZ:HCM1	18	0.54
(1,859)	1:919:A:LEU:HD13	2:4:B:MLZ:HCM2	18	0.54
(1,859)	1:919:A:LEU:HD13	2:4:B:MLZ:HCM3	18	0.54
(1,859)	1:919:A:LEU:HD21	2:4:B:MLZ:HCM1	18	0.54
(1,859)	1:919:A:LEU:HD21	2:4:B:MLZ:HCM2	18	0.54
(1,859)	1:919:A:LEU:HD21	2:4:B:MLZ:HCM3	18	0.54
(1,859)	1:919:A:LEU:HD22	2:4:B:MLZ:HCM1	18	0.54
(1,859)	1:919:A:LEU:HD22	2:4:B:MLZ:HCM2	18	0.54
(1,859)	1:919:A:LEU:HD22	2:4:B:MLZ:HCM3	18	0.54
(1,859)	1:919:A:LEU:HD23	2:4:B:MLZ:HCM1	18	0.54
(1,859)	1:919:A:LEU:HD23	2:4:B:MLZ:HCM2	18	0.54
(1,859)	1:919:A:LEU:HD23	2:4:B:MLZ:HCM3	18	0.54
(1,858)	1:919:A:LEU:HD11	1:920:A:GLY:H	17	0.54
(1,858)	1:919:A:LEU:HD12	1:920:A:GLY:H	17	0.54
(1,858)	1:919:A:LEU:HD13	1:920:A:GLY:H	17	0.54
(1,858)	1:919:A:LEU:HD21	1:920:A:GLY:H	17	0.54
(1,858)	1:919:A:LEU:HD22	1:920:A:GLY:H	17	0.54
(1,858)	1:919:A:LEU:HD23	1:920:A:GLY:H	17	0.54
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM1	11	0.54
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM2	11	0.54
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM3	11	0.54
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG2	7	0.52
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG3	7	0.52
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG2	7	0.52
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG3	7	0.52
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	5	0.52
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	5	0.52
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	5	0.52
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	5	0.52
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	5	0.52
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	5	0.52
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG11	18	0.52
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG12	18	0.52
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG13	18	0.52
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG21	18	0.52
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG22	18	0.52
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG23	18	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG11	18	0.52
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG12	18	0.52
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG13	18	0.52
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG21	18	0.52
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG22	18	0.52
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG23	18	0.52
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	5	0.51
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	19	0.51
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	8	0.51
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	8	0.51
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	8	0.51
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	8	0.51
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	8	0.51
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	8	0.51
(1,106)	1:865:A:TRP:H	2:4:B:MLZ:H	10	0.51
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	8	0.5
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	9	0.5
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	16	0.5
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM1	11	0.5
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM2	11	0.5
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM3	11	0.5
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM1	11	0.5
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM2	11	0.5
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM3	11	0.5
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	18	0.49
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	7	0.49
(1,106)	1:865:A:TRP:H	2:4:B:MLZ:H	20	0.49
(1,54)	1:860:A:PHE:H	1:861:A:THR:H	7	0.49
(1,937)	2:8:B:ARG:H	2:9:B:TYR:H	14	0.48
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG2	2	0.47
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG3	2	0.47
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG2	2	0.47
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG3	2	0.47
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	4	0.47
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM1	4	0.47
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM2	4	0.47
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM3	4	0.47
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM1	4	0.47
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM2	4	0.47
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM3	4	0.47
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM1	14	0.46
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM2	14	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM3	14	0.46
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM1	14	0.46
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM2	14	0.46
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM3	14	0.46
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	12	0.45
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	5	0.45
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	17	0.44
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	11	0.44
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	19	0.44
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB2	12	0.44
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB3	12	0.44
(1,50)	1:859:A:GLU:HA	1:860:A:PHE:H	4	0.44
(1,888)	1:922:A:GLY:H	1:923:A:GLN:H	18	0.43
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB2	2	0.43
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB3	2	0.43
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB2	2	0.43
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB3	2	0.43
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB2	2	0.43
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB3	2	0.43
(1,448)	1:886:A:ASP:HB3	1:888:A:SER:H	3	0.43
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM1	12	0.43
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM2	12	0.43
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM3	12	0.43
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD2	12	0.43
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD3	12	0.43
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM1	8	0.43
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM2	8	0.43
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM3	8	0.43
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM1	8	0.43
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM2	8	0.43
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM3	8	0.43
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM1	19	0.43
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM2	19	0.43
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM3	19	0.43
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM1	19	0.43
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM2	19	0.43
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM3	19	0.43
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM1	12	0.42
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM2	12	0.42
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM3	12	0.42
(1,262)	1:870:A:ASP:HB3	1:871:A:CYS:H	14	0.42
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	6	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	11	0.42
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	11	0.42
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	11	0.42
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	11	0.42
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	11	0.42
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	11	0.42
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM1	3	0.42
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM2	3	0.42
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM3	3	0.42
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM1	3	0.42
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM2	3	0.42
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM3	3	0.42
(1,127)	1:865:A:TRP:HD1	2:4:B:MLZ:HG2	18	0.42
(1,127)	1:865:A:TRP:HD1	2:4:B:MLZ:HG3	18	0.42
(1,106)	1:865:A:TRP:H	2:4:B:MLZ:H	15	0.42
(1,858)	1:919:A:LEU:HD11	1:920:A:GLY:H	16	0.41
(1,858)	1:919:A:LEU:HD12	1:920:A:GLY:H	16	0.41
(1,858)	1:919:A:LEU:HD13	1:920:A:GLY:H	16	0.41
(1,858)	1:919:A:LEU:HD21	1:920:A:GLY:H	16	0.41
(1,858)	1:919:A:LEU:HD22	1:920:A:GLY:H	16	0.41
(1,858)	1:919:A:LEU:HD23	1:920:A:GLY:H	16	0.41
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	17	0.41
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	5	0.41
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	5	0.41
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	5	0.41
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	5	0.41
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	5	0.41
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	5	0.41
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	14	0.41
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	14	0.41
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	14	0.41
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	14	0.41
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	14	0.41
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	14	0.41
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	18	0.41
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	18	0.41
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	18	0.41
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	18	0.41
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	18	0.41
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	18	0.41
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM1	15	0.41
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM2	15	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM3	15	0.41
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM1	15	0.41
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM2	15	0.41
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM3	15	0.41
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB2	5	0.41
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB3	5	0.41
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB2	15	0.41
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB3	15	0.41
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB2	1	0.41
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB3	1	0.41
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB2	6	0.41
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB3	6	0.41
(1,858)	1:919:A:LEU:HD11	1:920:A:GLY:H	20	0.4
(1,858)	1:919:A:LEU:HD12	1:920:A:GLY:H	20	0.4
(1,858)	1:919:A:LEU:HD13	1:920:A:GLY:H	20	0.4
(1,858)	1:919:A:LEU:HD21	1:920:A:GLY:H	20	0.4
(1,858)	1:919:A:LEU:HD22	1:920:A:GLY:H	20	0.4
(1,858)	1:919:A:LEU:HD23	1:920:A:GLY:H	20	0.4
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG2	6	0.4
(1,801)	1:915:A:ILE:HG12	2:4:B:MLZ:HG3	6	0.4
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG2	6	0.4
(1,801)	1:915:A:ILE:HG13	2:4:B:MLZ:HG3	6	0.4
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	3	0.4
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	3	0.4
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	3	0.4
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	3	0.4
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	3	0.4
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	3	0.4
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	3	0.4
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	3	0.4
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	3	0.4
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	3	0.4
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	3	0.4
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	3	0.4
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	13	0.4
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	13	0.4
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	13	0.4
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	13	0.4
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	13	0.4
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	13	0.4
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	13	0.4
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	13	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	13	0.4
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	13	0.4
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	13	0.4
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	13	0.4
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	18	0.4
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	18	0.4
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	18	0.4
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	18	0.4
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	18	0.4
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	18	0.4
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	18	0.4
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	18	0.4
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	18	0.4
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	18	0.4
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	18	0.4
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	18	0.4
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	11	0.4
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	12	0.4
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB2	5	0.4
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB3	5	0.4
(1,858)	1:919:A:LEU:HD11	1:920:A:GLY:H	5	0.39
(1,858)	1:919:A:LEU:HD12	1:920:A:GLY:H	5	0.39
(1,858)	1:919:A:LEU:HD13	1:920:A:GLY:H	5	0.39
(1,858)	1:919:A:LEU:HD21	1:920:A:GLY:H	5	0.39
(1,858)	1:919:A:LEU:HD22	1:920:A:GLY:H	5	0.39
(1,858)	1:919:A:LEU:HD23	1:920:A:GLY:H	5	0.39
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	3	0.39
(1,145)	1:865:A:TRP:HB2	2:4:B:MLZ:HB2	1	0.39
(1,145)	1:865:A:TRP:HB2	2:4:B:MLZ:HB3	1	0.39
(1,145)	1:865:A:TRP:HB3	2:4:B:MLZ:HB2	1	0.39
(1,145)	1:865:A:TRP:HB3	2:4:B:MLZ:HB3	1	0.39
(1,937)	2:8:B:ARG:H	2:9:B:TYR:H	11	0.38
(1,858)	1:919:A:LEU:HD11	1:920:A:GLY:H	9	0.38
(1,858)	1:919:A:LEU:HD12	1:920:A:GLY:H	9	0.38
(1,858)	1:919:A:LEU:HD13	1:920:A:GLY:H	9	0.38
(1,858)	1:919:A:LEU:HD21	1:920:A:GLY:H	9	0.38
(1,858)	1:919:A:LEU:HD22	1:920:A:GLY:H	9	0.38
(1,858)	1:919:A:LEU:HD23	1:920:A:GLY:H	9	0.38
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	4	0.38
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	4	0.38
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	4	0.38
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	4	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	4	0.38
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	4	0.38
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	4	0.38
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	4	0.38
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	4	0.38
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	4	0.38
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	4	0.38
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	4	0.38
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	16	0.38
(1,145)	1:865:A:TRP:HB2	2:4:B:MLZ:HB2	20	0.38
(1,145)	1:865:A:TRP:HB2	2:4:B:MLZ:HB3	20	0.38
(1,145)	1:865:A:TRP:HB3	2:4:B:MLZ:HB2	20	0.38
(1,145)	1:865:A:TRP:HB3	2:4:B:MLZ:HB3	20	0.38
(1,893)	1:923:A:GLN:HA	1:924:A:ASP:H	9	0.37
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB2	7	0.37
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB3	7	0.37
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB2	7	0.37
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB3	7	0.37
(1,313)	1:874:A:TRP:HH2	2:4:B:MLZ:HE2	1	0.37
(1,313)	1:874:A:TRP:HH2	2:4:B:MLZ:HE3	1	0.37
(1,303)	1:874:A:TRP:HD1	2:4:B:MLZ:HCM1	6	0.37
(1,303)	1:874:A:TRP:HD1	2:4:B:MLZ:HCM2	6	0.37
(1,303)	1:874:A:TRP:HD1	2:4:B:MLZ:HCM3	6	0.37
(1,262)	1:870:A:ASP:HB3	1:871:A:CYS:H	10	0.37
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	15	0.37
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	4	0.37
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	20	0.37
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	15	0.37
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	15	0.37
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	15	0.37
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	15	0.37
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	15	0.37
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	15	0.37
(1,859)	1:919:A:LEU:HD11	2:4:B:MLZ:HCM1	11	0.36
(1,859)	1:919:A:LEU:HD11	2:4:B:MLZ:HCM2	11	0.36
(1,859)	1:919:A:LEU:HD11	2:4:B:MLZ:HCM3	11	0.36
(1,859)	1:919:A:LEU:HD12	2:4:B:MLZ:HCM1	11	0.36
(1,859)	1:919:A:LEU:HD12	2:4:B:MLZ:HCM2	11	0.36
(1,859)	1:919:A:LEU:HD12	2:4:B:MLZ:HCM3	11	0.36
(1,859)	1:919:A:LEU:HD13	2:4:B:MLZ:HCM1	11	0.36
(1,859)	1:919:A:LEU:HD13	2:4:B:MLZ:HCM2	11	0.36
(1,859)	1:919:A:LEU:HD13	2:4:B:MLZ:HCM3	11	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,859)	1:919:A:LEU:HD21	2:4:B:MLZ:HCM1	11	0.36
(1,859)	1:919:A:LEU:HD21	2:4:B:MLZ:HCM2	11	0.36
(1,859)	1:919:A:LEU:HD21	2:4:B:MLZ:HCM3	11	0.36
(1,859)	1:919:A:LEU:HD22	2:4:B:MLZ:HCM1	11	0.36
(1,859)	1:919:A:LEU:HD22	2:4:B:MLZ:HCM2	11	0.36
(1,859)	1:919:A:LEU:HD22	2:4:B:MLZ:HCM3	11	0.36
(1,859)	1:919:A:LEU:HD23	2:4:B:MLZ:HCM1	11	0.36
(1,859)	1:919:A:LEU:HD23	2:4:B:MLZ:HCM2	11	0.36
(1,859)	1:919:A:LEU:HD23	2:4:B:MLZ:HCM3	11	0.36
(1,858)	1:919:A:LEU:HD11	1:920:A:GLY:H	1	0.36
(1,858)	1:919:A:LEU:HD12	1:920:A:GLY:H	1	0.36
(1,858)	1:919:A:LEU:HD13	1:920:A:GLY:H	1	0.36
(1,858)	1:919:A:LEU:HD21	1:920:A:GLY:H	1	0.36
(1,858)	1:919:A:LEU:HD22	1:920:A:GLY:H	1	0.36
(1,858)	1:919:A:LEU:HD23	1:920:A:GLY:H	1	0.36
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	12	0.36
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	10	0.36
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	10	0.36
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	10	0.36
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	10	0.36
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	10	0.36
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	10	0.36
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	10	0.36
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	10	0.36
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	10	0.36
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	10	0.36
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	10	0.36
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	10	0.36
(1,398)	1:881:A:VAL:HG11	1:891:A:TRP:HD1	20	0.36
(1,398)	1:881:A:VAL:HG12	1:891:A:TRP:HD1	20	0.36
(1,398)	1:881:A:VAL:HG13	1:891:A:TRP:HD1	20	0.36
(1,398)	1:881:A:VAL:HG21	1:891:A:TRP:HD1	20	0.36
(1,398)	1:881:A:VAL:HG22	1:891:A:TRP:HD1	20	0.36
(1,398)	1:881:A:VAL:HG23	1:891:A:TRP:HD1	20	0.36
(1,313)	1:874:A:TRP:HH2	2:4:B:MLZ:HE2	17	0.36
(1,313)	1:874:A:TRP:HH2	2:4:B:MLZ:HE3	17	0.36
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	14	0.36
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	4	0.36
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	4	0.36
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	4	0.36
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	4	0.36
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	4	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	4	0.36
(1,926)	2:2:B:ARG:HE	2:3:B:THR:HA	10	0.35
(1,605)	1:899:A:LYS:HB2	1:899:A:LYS:HE2	13	0.35
(1,605)	1:899:A:LYS:HB2	1:899:A:LYS:HE3	13	0.35
(1,605)	1:899:A:LYS:HB3	1:899:A:LYS:HE2	13	0.35
(1,605)	1:899:A:LYS:HB3	1:899:A:LYS:HE3	13	0.35
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	1	0.35
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	1	0.35
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	1	0.35
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	1	0.35
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	1	0.35
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	1	0.35
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	1	0.35
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	1	0.35
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	1	0.35
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	1	0.35
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	1	0.35
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	1	0.35
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	14	0.35
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	14	0.35
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	14	0.35
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	14	0.35
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	14	0.35
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	14	0.35
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	1	0.35
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	17	0.35
(1,147)	1:865:A:TRP:HB2	2:4:B:MLZ:HG2	2	0.35
(1,147)	1:865:A:TRP:HB2	2:4:B:MLZ:HG3	2	0.35
(1,147)	1:865:A:TRP:HB3	2:4:B:MLZ:HG2	2	0.35
(1,147)	1:865:A:TRP:HB3	2:4:B:MLZ:HG3	2	0.35
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB2	2	0.35
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB3	2	0.35
(1,106)	1:865:A:TRP:H	2:4:B:MLZ:H	6	0.35
(1,902)	1:923:A:GLN:HG2	1:924:A:ASP:H	17	0.34
(1,902)	1:923:A:GLN:HG3	1:924:A:ASP:H	17	0.34
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	17	0.34
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	17	0.34
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	17	0.34
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	17	0.34
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	17	0.34
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	17	0.34
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	17	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	17	0.34
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	17	0.34
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	17	0.34
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	17	0.34
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	17	0.34
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM1	20	0.34
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM2	20	0.34
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM3	20	0.34
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	19	0.34
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	15	0.34
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	19	0.34
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	19	0.34
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	19	0.34
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	19	0.34
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	19	0.34
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	19	0.34
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB2	9	0.34
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB3	9	0.34
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG11	9	0.34
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG12	9	0.34
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG13	9	0.34
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG21	9	0.34
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG22	9	0.34
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG23	9	0.34
(1,863)	1:919:A:LEU:HD11	2:6:B:THR:H	7	0.33
(1,863)	1:919:A:LEU:HD12	2:6:B:THR:H	7	0.33
(1,863)	1:919:A:LEU:HD13	2:6:B:THR:H	7	0.33
(1,863)	1:919:A:LEU:HD21	2:6:B:THR:H	7	0.33
(1,863)	1:919:A:LEU:HD22	2:6:B:THR:H	7	0.33
(1,863)	1:919:A:LEU:HD23	2:6:B:THR:H	7	0.33
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	12	0.33
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	12	0.33
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	12	0.33
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	12	0.33
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	12	0.33
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	12	0.33
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	12	0.33
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	12	0.33
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	12	0.33
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	12	0.33
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	12	0.33
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	12	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	16	0.33
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	16	0.33
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	16	0.33
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	16	0.33
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	16	0.33
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	16	0.33
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	16	0.33
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	16	0.33
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	16	0.33
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	16	0.33
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	16	0.33
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	16	0.33
(1,50)	1:859:A:GLU:HA	1:860:A:PHE:H	6	0.33
(1,902)	1:923:A:GLN:HG2	1:924:A:ASP:H	20	0.32
(1,902)	1:923:A:GLN:HG3	1:924:A:ASP:H	20	0.32
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	8	0.32
(1,313)	1:874:A:TRP:HH2	2:4:B:MLZ:HE2	12	0.32
(1,313)	1:874:A:TRP:HH2	2:4:B:MLZ:HE3	12	0.32
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	12	0.32
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	15	0.32
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	10	0.32
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	10	0.32
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	10	0.32
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	10	0.32
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	10	0.32
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	10	0.32
(1,147)	1:865:A:TRP:HB2	2:4:B:MLZ:HG2	1	0.32
(1,147)	1:865:A:TRP:HB2	2:4:B:MLZ:HG3	1	0.32
(1,147)	1:865:A:TRP:HB3	2:4:B:MLZ:HG2	1	0.32
(1,147)	1:865:A:TRP:HB3	2:4:B:MLZ:HG3	1	0.32
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB2	7	0.32
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB3	7	0.32
(1,110)	1:865:A:TRP:H	2:5:B:GLN:HB2	18	0.32
(1,110)	1:865:A:TRP:H	2:5:B:GLN:HB3	18	0.32
(1,44)	1:858:A:SER:HA	1:859:A:GLU:H	14	0.32
(1,539)	1:895:A:ASN:HB2	1:896:A:ASN:H	7	0.31
(1,539)	1:895:A:ASN:HB3	1:896:A:ASN:H	7	0.31
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	14	0.31
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	14	0.31
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	14	0.31
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	14	0.31
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	14	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	14	0.31
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	14	0.31
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	14	0.31
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	14	0.31
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	14	0.31
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	14	0.31
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	14	0.31
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	19	0.31
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	19	0.31
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	19	0.31
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	19	0.31
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	19	0.31
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	19	0.31
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	19	0.31
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	19	0.31
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	19	0.31
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	19	0.31
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	19	0.31
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	19	0.31
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	3	0.31
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	3	0.31
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	3	0.31
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	3	0.31
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	3	0.31
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	3	0.31
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB2	16	0.31
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB3	16	0.31
(1,106)	1:865:A:TRP:H	2:4:B:MLZ:H	12	0.31
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG11	4	0.31
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG12	4	0.31
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG13	4	0.31
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG21	4	0.31
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG22	4	0.31
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG23	4	0.31
(1,926)	2:2:B:ARG:HE	2:3:B:THR:HA	5	0.3
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB2	2	0.3
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB3	2	0.3
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB2	2	0.3
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB3	2	0.3
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	18	0.3
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	14	0.3
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	14	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	14	0.3
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	14	0.3
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	14	0.3
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	14	0.3
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	6	0.3
(1,134)	1:865:A:TRP:HE3	1:866:A:VAL:H	17	0.3
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG11	19	0.3
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG12	19	0.3
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG13	19	0.3
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG21	19	0.3
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG22	19	0.3
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG23	19	0.3
(1,858)	1:919:A:LEU:HD11	1:920:A:GLY:H	12	0.29
(1,858)	1:919:A:LEU:HD12	1:920:A:GLY:H	12	0.29
(1,858)	1:919:A:LEU:HD13	1:920:A:GLY:H	12	0.29
(1,858)	1:919:A:LEU:HD21	1:920:A:GLY:H	12	0.29
(1,858)	1:919:A:LEU:HD22	1:920:A:GLY:H	12	0.29
(1,858)	1:919:A:LEU:HD23	1:920:A:GLY:H	12	0.29
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	2	0.29
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	2	0.29
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	2	0.29
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	2	0.29
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	2	0.29
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	2	0.29
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	2	0.29
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	2	0.29
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	2	0.29
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	2	0.29
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	2	0.29
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	2	0.29
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	5	0.29
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	5	0.29
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	5	0.29
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	5	0.29
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	5	0.29
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	5	0.29
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	5	0.29
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	5	0.29
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	5	0.29
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	5	0.29
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	5	0.29
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	5	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	7	0.29
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	7	0.29
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	7	0.29
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	7	0.29
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	7	0.29
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	7	0.29
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	7	0.29
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	7	0.29
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	7	0.29
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	7	0.29
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	7	0.29
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	7	0.29
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	16	0.29
(1,147)	1:865:A:TRP:HB2	2:4:B:MLZ:HG2	20	0.29
(1,147)	1:865:A:TRP:HB2	2:4:B:MLZ:HG3	20	0.29
(1,147)	1:865:A:TRP:HB3	2:4:B:MLZ:HG2	20	0.29
(1,147)	1:865:A:TRP:HB3	2:4:B:MLZ:HG3	20	0.29
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM1	7	0.29
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM2	7	0.29
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM3	7	0.29
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM1	7	0.29
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM2	7	0.29
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM3	7	0.29
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM1	17	0.29
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM2	17	0.29
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM3	17	0.29
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM1	17	0.29
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM2	17	0.29
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM3	17	0.29
(1,54)	1:860:A:PHE:H	1:861:A:THR:H	12	0.29
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB2	17	0.28
(1,795)	1:915:A:ILE:HD11	2:4:B:MLZ:HB3	17	0.28
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB2	17	0.28
(1,795)	1:915:A:ILE:HD12	2:4:B:MLZ:HB3	17	0.28
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB2	17	0.28
(1,795)	1:915:A:ILE:HD13	2:4:B:MLZ:HB3	17	0.28
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG11	6	0.28
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG12	6	0.28
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG13	6	0.28
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG21	6	0.28
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG22	6	0.28
(1,381)	1:880:A:SER:HB2	1:881:A:VAL:HG23	6	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG11	6	0.28
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG12	6	0.28
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG13	6	0.28
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG21	6	0.28
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG22	6	0.28
(1,381)	1:880:A:SER:HB3	1:881:A:VAL:HG23	6	0.28
(1,371)	1:879:A:ALA:HA	1:882:A:VAL:HB	8	0.28
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	18	0.28
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	18	0.28
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG11	16	0.28
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG12	16	0.28
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG13	16	0.28
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG21	16	0.28
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG22	16	0.28
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG23	16	0.28
(1,888)	1:922:A:GLY:H	1:923:A:GLN:H	13	0.27
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB2	6	0.27
(1,800)	1:915:A:ILE:HG12	2:4:B:MLZ:HB3	6	0.27
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB2	6	0.27
(1,800)	1:915:A:ILE:HG13	2:4:B:MLZ:HB3	6	0.27
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	4	0.27
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	14	0.27
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	11	0.27
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	11	0.27
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	11	0.27
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	11	0.27
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	11	0.27
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	11	0.27
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	11	0.27
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	11	0.27
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	11	0.27
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	11	0.27
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	11	0.27
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	11	0.27
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	20	0.27
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	20	0.27
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	20	0.27
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	20	0.27
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	20	0.27
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	20	0.27
(1,338)	1:876:A:ARG:HA	1:876:A:ARG:HD2	6	0.27
(1,338)	1:876:A:ARG:HA	1:876:A:ARG:HD3	6	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	1	0.27
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	13	0.27
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	13	0.27
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	8	0.27
(1,193)	1:867:A:ARG:H	2:4:B:MLZ:H	6	0.27
(1,827)	1:917:A:GLU:HB2	1:918:A:GLU:H	2	0.26
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	14	0.26
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	14	0.26
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	14	0.26
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	1	0.26
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	14	0.26
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	14	0.26
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	14	0.26
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	14	0.26
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	14	0.26
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	14	0.26
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	10	0.26
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	10	0.26
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	10	0.26
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	10	0.26
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	10	0.26
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	10	0.26
(1,303)	1:874:A:TRP:HD1	2:4:B:MLZ:HCM1	8	0.26
(1,303)	1:874:A:TRP:HD1	2:4:B:MLZ:HCM2	8	0.26
(1,303)	1:874:A:TRP:HD1	2:4:B:MLZ:HCM3	8	0.26
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	8	0.26
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	9	0.26
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	3	0.26
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	20	0.26
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	7	0.26
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	7	0.26
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	7	0.26
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	7	0.26
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	7	0.26
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	7	0.26
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB2	13	0.26
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB3	13	0.26
(1,63)	1:861:A:THR:HG21	1:862:A:GLU:H	17	0.26
(1,63)	1:861:A:THR:HG22	1:862:A:GLU:H	17	0.26
(1,63)	1:861:A:THR:HG23	1:862:A:GLU:H	17	0.26
(1,21)	1:853:A:ARG:HB3	1:854:A:ALA:H	16	0.26
(1,891)	1:923:A:GLN:H	1:923:A:GLN:HG2	14	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,891)	1:923:A:GLN:H	1:923:A:GLN:HG3	14	0.25
(1,882)	1:921:A:ILE:HD11	2:4:B:MLZ:HE2	18	0.25
(1,882)	1:921:A:ILE:HD11	2:4:B:MLZ:HE3	18	0.25
(1,882)	1:921:A:ILE:HD12	2:4:B:MLZ:HE2	18	0.25
(1,882)	1:921:A:ILE:HD12	2:4:B:MLZ:HE3	18	0.25
(1,882)	1:921:A:ILE:HD13	2:4:B:MLZ:HE2	18	0.25
(1,882)	1:921:A:ILE:HD13	2:4:B:MLZ:HE3	18	0.25
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	3	0.25
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	3	0.25
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	3	0.25
(1,790)	1:915:A:ILE:HB	1:916:A:ASN:H	4	0.25
(1,790)	1:915:A:ILE:HB	1:916:A:ASN:H	15	0.25
(1,790)	1:915:A:ILE:HB	1:916:A:ASN:H	19	0.25
(1,539)	1:895:A:ASN:HB2	1:896:A:ASN:H	12	0.25
(1,539)	1:895:A:ASN:HB3	1:896:A:ASN:H	12	0.25
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	13	0.25
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	20	0.25
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	17	0.25
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	17	0.25
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	17	0.25
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	17	0.25
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	17	0.25
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	17	0.25
(1,371)	1:879:A:ALA:HA	1:882:A:VAL:HB	20	0.25
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD2	10	0.25
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD3	10	0.25
(1,265)	1:870:A:ASP:HB2	1:871:A:CYS:H	14	0.25
(1,265)	1:870:A:ASP:HB3	1:871:A:CYS:H	14	0.25
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	9	0.25
(1,193)	1:867:A:ARG:H	2:4:B:MLZ:H	2	0.25
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG11	8	0.25
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG12	8	0.25
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG13	8	0.25
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG21	8	0.25
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG22	8	0.25
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG23	8	0.25
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG11	20	0.25
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG12	20	0.25
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG13	20	0.25
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG21	20	0.25
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG22	20	0.25
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG23	20	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:903:A:ASP:HB2	1:904:A:CYS:H	20	0.24
(1,653)	1:903:A:ASP:HB3	1:904:A:CYS:H	20	0.24
(1,648)	1:903:A:ASP:HA	1:906:A:LYS:H	12	0.24
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	2	0.24
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	3	0.24
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	16	0.24
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	17	0.24
(1,429)	1:885:A:ILE:HG12	1:891:A:TRP:H	3	0.24
(1,429)	1:885:A:ILE:HG13	1:891:A:TRP:H	3	0.24
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	15	0.24
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	15	0.24
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	15	0.24
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	15	0.24
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	15	0.24
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	15	0.24
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	15	0.24
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	15	0.24
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	15	0.24
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	15	0.24
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	15	0.24
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	15	0.24
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	7	0.24
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	7	0.24
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	7	0.24
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	7	0.24
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	7	0.24
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	7	0.24
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	15	0.24
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	15	0.24
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	15	0.24
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	15	0.24
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	15	0.24
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	15	0.24
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM1	18	0.24
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM2	18	0.24
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM3	18	0.24
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	7	0.24
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	6	0.24
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	20	0.24
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	20	0.24
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	20	0.24
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	20	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	20	0.24
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	20	0.24
(1,109)	1:865:A:TRP:H	2:5:B:GLN:HA	11	0.24
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG11	18	0.24
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG12	18	0.24
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG13	18	0.24
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG21	18	0.24
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG22	18	0.24
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG23	18	0.24
(1,31)	1:855:A:SER:HA	1:856:A:VAL:H	11	0.24
(2,3)	1:871:A:CYS:CB	3:1001:A:ZN:ZN	5	0.23
(1,937)	2:8:B:ARG:H	2:9:B:TYR:H	13	0.23
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	13	0.23
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	13	0.23
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	13	0.23
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	16	0.23
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	16	0.23
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	16	0.23
(1,790)	1:915:A:ILE:HB	1:916:A:ASN:H	8	0.23
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	11	0.23
(1,424)	1:885:A:ILE:HD11	1:886:A:ASP:H	5	0.23
(1,424)	1:885:A:ILE:HD12	1:886:A:ASP:H	5	0.23
(1,424)	1:885:A:ILE:HD13	1:886:A:ASP:H	5	0.23
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	16	0.23
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	16	0.23
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	16	0.23
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	16	0.23
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	16	0.23
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	16	0.23
(1,371)	1:879:A:ALA:HA	1:882:A:VAL:HB	6	0.23
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	3	0.23
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	16	0.23
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG11	6	0.23
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG12	6	0.23
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG13	6	0.23
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG21	6	0.23
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG22	6	0.23
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG23	6	0.23
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG11	14	0.23
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG12	14	0.23
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG13	14	0.23
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG21	14	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG22	14	0.23
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG23	14	0.23
(1,39)	1:857:A:GLY:H	1:858:A:SER:H	11	0.23
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	1	0.22
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	1	0.22
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	1	0.22
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	8	0.22
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	8	0.22
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	8	0.22
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	11	0.22
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	11	0.22
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	11	0.22
(1,790)	1:915:A:ILE:HB	1:916:A:ASN:H	14	0.22
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	10	0.22
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	10	0.22
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	10	0.22
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	10	0.22
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	10	0.22
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	10	0.22
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	8	0.22
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	8	0.22
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	8	0.22
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	8	0.22
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	8	0.22
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	8	0.22
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	12	0.22
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	12	0.22
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	12	0.22
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	12	0.22
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	12	0.22
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	12	0.22
(1,371)	1:879:A:ALA:HA	1:882:A:VAL:HB	9	0.22
(1,307)	1:874:A:TRP:HE3	2:4:B:MLZ:HCM1	4	0.22
(1,307)	1:874:A:TRP:HE3	2:4:B:MLZ:HCM2	4	0.22
(1,307)	1:874:A:TRP:HE3	2:4:B:MLZ:HCM3	4	0.22
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD2	8	0.22
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD3	8	0.22
(1,259)	1:870:A:ASP:HB2	1:871:A:CYS:H	15	0.22
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	2	0.22
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	5	0.22
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	12	0.22
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	12	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	12	0.22
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	12	0.22
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	12	0.22
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	12	0.22
(1,206)	1:867:A:ARG:HD2	1:872:A:PHE:HB2	6	0.22
(1,206)	1:867:A:ARG:HD2	1:872:A:PHE:HB3	6	0.22
(1,206)	1:867:A:ARG:HD3	1:872:A:PHE:HB2	6	0.22
(1,206)	1:867:A:ARG:HD3	1:872:A:PHE:HB3	6	0.22
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG11	5	0.22
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG12	5	0.22
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG13	5	0.22
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG21	5	0.22
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG22	5	0.22
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG23	5	0.22
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG11	2	0.22
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG12	2	0.22
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG13	2	0.22
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG21	2	0.22
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG22	2	0.22
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG23	2	0.22
(1,891)	1:923:A:GLN:H	1:923:A:GLN:HG2	5	0.21
(1,891)	1:923:A:GLN:H	1:923:A:GLN:HG3	5	0.21
(1,888)	1:922:A:GLY:H	1:923:A:GLN:H	5	0.21
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	6	0.21
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	6	0.21
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	6	0.21
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	12	0.21
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	12	0.21
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	12	0.21
(1,790)	1:915:A:ILE:HB	1:916:A:ASN:H	3	0.21
(1,648)	1:903:A:ASP:HA	1:906:A:LYS:H	13	0.21
(1,630)	1:901:A:PHE:HD1	1:908:A:GLN:H	15	0.21
(1,630)	1:901:A:PHE:HD2	1:908:A:GLN:H	15	0.21
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	7	0.21
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	9	0.21
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	8	0.21
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	8	0.21
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	8	0.21
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	8	0.21
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	8	0.21
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	8	0.21
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	15	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	15	0.21
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	15	0.21
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	15	0.21
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	15	0.21
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	15	0.21
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	6	0.21
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	6	0.21
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	6	0.21
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	6	0.21
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	6	0.21
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	6	0.21
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	13	0.21
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	13	0.21
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	13	0.21
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	13	0.21
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	13	0.21
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	13	0.21
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	2	0.21
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	2	0.21
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	2	0.21
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	2	0.21
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	2	0.21
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	2	0.21
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	13	0.21
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	13	0.21
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	13	0.21
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	13	0.21
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	13	0.21
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	13	0.21
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	19	0.21
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	19	0.21
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	19	0.21
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	19	0.21
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	19	0.21
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	19	0.21
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM1	1	0.21
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM2	1	0.21
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM3	1	0.21
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM1	10	0.21
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM2	10	0.21
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM3	10	0.21
(1,309)	1:874:A:TRP:HH2	2:3:B:THR:HA	5	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD2	7	0.21
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD3	7	0.21
(1,262)	1:870:A:ASP:HB3	1:871:A:CYS:H	6	0.21
(1,121)	1:865:A:TRP:HB2	1:866:A:VAL:H	17	0.21
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG11	13	0.21
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG12	13	0.21
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG13	13	0.21
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG21	13	0.21
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG22	13	0.21
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG23	13	0.21
(1,106)	1:865:A:TRP:H	2:4:B:MLZ:H	5	0.21
(1,106)	1:865:A:TRP:H	2:4:B:MLZ:H	8	0.21
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG11	12	0.21
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG12	12	0.21
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG13	12	0.21
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG21	12	0.21
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG22	12	0.21
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG23	12	0.21
(1,25)	1:853:A:ARG:HG2	1:867:A:ARG:HE	13	0.21
(1,25)	1:853:A:ARG:HG3	1:867:A:ARG:HE	13	0.21
(2,7)	1:904:A:CYS:CB	3:1001:A:ZN:ZN	15	0.2
(1,863)	1:919:A:LEU:HD11	2:6:B:THR:H	3	0.2
(1,863)	1:919:A:LEU:HD12	2:6:B:THR:H	3	0.2
(1,863)	1:919:A:LEU:HD13	2:6:B:THR:H	3	0.2
(1,863)	1:919:A:LEU:HD21	2:6:B:THR:H	3	0.2
(1,863)	1:919:A:LEU:HD22	2:6:B:THR:H	3	0.2
(1,863)	1:919:A:LEU:HD23	2:6:B:THR:H	3	0.2
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	5	0.2
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	5	0.2
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	5	0.2
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	15	0.2
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	15	0.2
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	15	0.2
(1,653)	1:903:A:ASP:HB2	1:904:A:CYS:H	11	0.2
(1,653)	1:903:A:ASP:HB3	1:904:A:CYS:H	11	0.2
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	4	0.2
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	4	0.2
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	4	0.2
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	4	0.2
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	4	0.2
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	4	0.2
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	10	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	10	0.2
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	10	0.2
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	10	0.2
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	10	0.2
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	10	0.2
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	1	0.2
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	1	0.2
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	1	0.2
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	1	0.2
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	1	0.2
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	1	0.2
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	3	0.2
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	3	0.2
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	3	0.2
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	3	0.2
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	3	0.2
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	3	0.2
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	18	0.2
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	18	0.2
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	18	0.2
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	18	0.2
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	18	0.2
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	18	0.2
(1,320)	1:874:A:TRP:HZ3	2:2:B:ARG:HG2	5	0.2
(1,320)	1:874:A:TRP:HZ3	2:2:B:ARG:HG3	5	0.2
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	11	0.2
(2,5)	1:893:A:CYS:CB	3:1001:A:ZN:ZN	5	0.19
(1,899)	1:923:A:GLN:HB2	1:924:A:ASP:H	4	0.19
(1,899)	1:923:A:GLN:HB3	1:924:A:ASP:H	4	0.19
(1,895)	1:923:A:GLN:HE21	2:3:B:THR:HA	4	0.19
(1,863)	1:919:A:LEU:HD11	2:6:B:THR:H	1	0.19
(1,863)	1:919:A:LEU:HD12	2:6:B:THR:H	1	0.19
(1,863)	1:919:A:LEU:HD13	2:6:B:THR:H	1	0.19
(1,863)	1:919:A:LEU:HD21	2:6:B:THR:H	1	0.19
(1,863)	1:919:A:LEU:HD22	2:6:B:THR:H	1	0.19
(1,863)	1:919:A:LEU:HD23	2:6:B:THR:H	1	0.19
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	4	0.19
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	4	0.19
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	4	0.19
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	17	0.19
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	17	0.19
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	17	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	19	0.19
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	19	0.19
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	19	0.19
(1,648)	1:903:A:ASP:HA	1:906:A:LYS:H	17	0.19
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	5	0.19
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	15	0.19
(1,507)	1:892:A:ILE:HD11	1:895:A:ASN:HD21	7	0.19
(1,507)	1:892:A:ILE:HD11	1:895:A:ASN:HD22	7	0.19
(1,507)	1:892:A:ILE:HD12	1:895:A:ASN:HD21	7	0.19
(1,507)	1:892:A:ILE:HD12	1:895:A:ASN:HD22	7	0.19
(1,507)	1:892:A:ILE:HD13	1:895:A:ASN:HD21	7	0.19
(1,507)	1:892:A:ILE:HD13	1:895:A:ASN:HD22	7	0.19
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	20	0.19
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	20	0.19
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	20	0.19
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	20	0.19
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	20	0.19
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	20	0.19
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	20	0.19
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	20	0.19
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	20	0.19
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	20	0.19
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	20	0.19
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	20	0.19
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	11	0.19
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	11	0.19
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	11	0.19
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	11	0.19
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	11	0.19
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	11	0.19
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	13	0.19
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	13	0.19
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	13	0.19
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	13	0.19
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	13	0.19
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	13	0.19
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	4	0.19
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	4	0.19
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	4	0.19
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	4	0.19
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	4	0.19
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	4	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	11	0.19
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	11	0.19
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	11	0.19
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	11	0.19
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	11	0.19
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	11	0.19
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM1	1	0.19
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM2	1	0.19
(1,318)	1:874:A:TRP:HZ2	2:4:B:MLZ:HCM3	1	0.19
(1,303)	1:874:A:TRP:HD1	2:4:B:MLZ:HCM1	14	0.19
(1,303)	1:874:A:TRP:HD1	2:4:B:MLZ:HCM2	14	0.19
(1,303)	1:874:A:TRP:HD1	2:4:B:MLZ:HCM3	14	0.19
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD2	3	0.19
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD3	3	0.19
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	12	0.19
(1,222)	1:868:A:CYS:H	1:891:A:TRP:HZ3	3	0.19
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	2	0.19
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	13	0.19
(1,106)	1:865:A:TRP:H	2:4:B:MLZ:H	2	0.19
(1,106)	1:865:A:TRP:H	2:4:B:MLZ:H	3	0.19
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG11	13	0.19
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG12	13	0.19
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG13	13	0.19
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG21	13	0.19
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG22	13	0.19
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG23	13	0.19
(1,52)	1:859:A:GLU:HB2	1:860:A:PHE:H	6	0.19
(1,52)	1:859:A:GLU:HB3	1:860:A:PHE:H	6	0.19
(1,1)	1:851:A:SER:HA	1:852:A:ARG:H	16	0.19
(2,7)	1:904:A:CYS:CB	3:1001:A:ZN:ZN	16	0.18
(1,926)	2:2:B:ARG:HE	2:3:B:THR:HA	2	0.18
(1,895)	1:923:A:GLN:HE21	2:3:B:THR:HA	17	0.18
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	20	0.18
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	20	0.18
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	20	0.18
(1,755)	1:912:A:ASN:HA	1:916:A:ASN:H	15	0.18
(1,683)	1:906:A:LYS:HB2	1:907:A:SER:HB2	15	0.18
(1,683)	1:906:A:LYS:HB2	1:907:A:SER:HB3	15	0.18
(1,683)	1:906:A:LYS:HB3	1:907:A:SER:HB2	15	0.18
(1,683)	1:906:A:LYS:HB3	1:907:A:SER:HB3	15	0.18
(1,679)	1:906:A:LYS:HB2	1:906:A:LYS:HD2	5	0.18
(1,679)	1:906:A:LYS:HB2	1:906:A:LYS:HD3	5	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,679)	1:906:A:LYS:HB3	1:906:A:LYS:HD2	5	0.18
(1,679)	1:906:A:LYS:HB3	1:906:A:LYS:HD3	5	0.18
(1,679)	1:906:A:LYS:HB2	1:906:A:LYS:HD2	6	0.18
(1,679)	1:906:A:LYS:HB2	1:906:A:LYS:HD3	6	0.18
(1,679)	1:906:A:LYS:HB3	1:906:A:LYS:HD2	6	0.18
(1,679)	1:906:A:LYS:HB3	1:906:A:LYS:HD3	6	0.18
(1,679)	1:906:A:LYS:HB2	1:906:A:LYS:HD2	8	0.18
(1,679)	1:906:A:LYS:HB2	1:906:A:LYS:HD3	8	0.18
(1,679)	1:906:A:LYS:HB3	1:906:A:LYS:HD2	8	0.18
(1,679)	1:906:A:LYS:HB3	1:906:A:LYS:HD3	8	0.18
(1,679)	1:906:A:LYS:HB2	1:906:A:LYS:HD2	11	0.18
(1,679)	1:906:A:LYS:HB2	1:906:A:LYS:HD3	11	0.18
(1,679)	1:906:A:LYS:HB3	1:906:A:LYS:HD2	11	0.18
(1,679)	1:906:A:LYS:HB3	1:906:A:LYS:HD3	11	0.18
(1,648)	1:903:A:ASP:HA	1:906:A:LYS:H	19	0.18
(1,595)	1:899:A:LYS:HA	1:899:A:LYS:HG2	13	0.18
(1,595)	1:899:A:LYS:HA	1:899:A:LYS:HG3	13	0.18
(1,407)	1:882:A:VAL:HB	1:883:A:GLY:H	9	0.18
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	2	0.18
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	2	0.18
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	2	0.18
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	2	0.18
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	2	0.18
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	2	0.18
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	6	0.18
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	6	0.18
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	6	0.18
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	6	0.18
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	6	0.18
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	6	0.18
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	9	0.18
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	9	0.18
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	9	0.18
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	9	0.18
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	9	0.18
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	9	0.18
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	18	0.18
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	18	0.18
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	18	0.18
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	18	0.18
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	18	0.18
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	18	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	2	0.18
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	2	0.18
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	2	0.18
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	2	0.18
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	2	0.18
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	2	0.18
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	7	0.18
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	7	0.18
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	7	0.18
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	7	0.18
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	7	0.18
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	7	0.18
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	9	0.18
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	9	0.18
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	9	0.18
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	9	0.18
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	9	0.18
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	9	0.18
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE2	6	0.18
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE3	6	0.18
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE2	16	0.18
(1,319)	1:874:A:TRP:HZ2	2:4:B:MLZ:HE3	16	0.18
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB2	10	0.18
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB3	10	0.18
(1,305)	1:874:A:TRP:HE1	1:923:A:GLN:HG2	6	0.18
(1,305)	1:874:A:TRP:HE1	1:923:A:GLN:HG3	6	0.18
(1,287)	1:873:A:LYS:HB2	1:874:A:TRP:HA	4	0.18
(1,287)	1:873:A:LYS:HB3	1:874:A:TRP:HA	4	0.18
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD2	14	0.18
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD3	14	0.18
(1,265)	1:870:A:ASP:HB2	1:871:A:CYS:H	10	0.18
(1,265)	1:870:A:ASP:HB3	1:871:A:CYS:H	10	0.18
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	3	0.18
(1,215)	1:867:A:ARG:HG2	1:874:A:TRP:HZ2	16	0.18
(1,215)	1:867:A:ARG:HG3	1:874:A:TRP:HZ2	16	0.18
(1,145)	1:865:A:TRP:HB2	2:4:B:MLZ:HB2	9	0.18
(1,145)	1:865:A:TRP:HB2	2:4:B:MLZ:HB3	9	0.18
(1,145)	1:865:A:TRP:HB3	2:4:B:MLZ:HB2	9	0.18
(1,145)	1:865:A:TRP:HB3	2:4:B:MLZ:HB3	9	0.18
(1,137)	1:865:A:TRP:HH2	1:909:A:GLU:H	15	0.18
(1,109)	1:865:A:TRP:H	2:5:B:GLN:HA	5	0.18
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG11	4	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG12	4	0.18
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG13	4	0.18
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG21	4	0.18
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG22	4	0.18
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG23	4	0.18
(1,60)	1:861:A:THR:HA	1:861:A:THR:HB	2	0.18
(1,60)	1:861:A:THR:HA	1:861:A:THR:HB	5	0.18
(1,60)	1:861:A:THR:HA	1:861:A:THR:HB	11	0.18
(1,60)	1:861:A:THR:HA	1:861:A:THR:HB	14	0.18
(1,60)	1:861:A:THR:HA	1:861:A:THR:HB	15	0.18
(1,929)	2:5:B:GLN:H	2:6:B:THR:H	1	0.17
(1,904)	1:924:A:ASP:H	1:925:A:GLU:H	11	0.17
(1,899)	1:923:A:GLN:HB2	1:924:A:ASP:H	14	0.17
(1,899)	1:923:A:GLN:HB3	1:924:A:ASP:H	14	0.17
(1,888)	1:922:A:GLY:H	1:923:A:GLN:H	11	0.17
(1,863)	1:919:A:LEU:HD11	2:6:B:THR:H	14	0.17
(1,863)	1:919:A:LEU:HD12	2:6:B:THR:H	14	0.17
(1,863)	1:919:A:LEU:HD13	2:6:B:THR:H	14	0.17
(1,863)	1:919:A:LEU:HD21	2:6:B:THR:H	14	0.17
(1,863)	1:919:A:LEU:HD22	2:6:B:THR:H	14	0.17
(1,863)	1:919:A:LEU:HD23	2:6:B:THR:H	14	0.17
(1,818)	1:916:A:ASN:HB2	1:923:A:GLN:HE21	17	0.17
(1,818)	1:916:A:ASN:HB2	1:923:A:GLN:HE22	17	0.17
(1,818)	1:916:A:ASN:HB3	1:923:A:GLN:HE21	17	0.17
(1,818)	1:916:A:ASN:HB3	1:923:A:GLN:HE22	17	0.17
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	10	0.17
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	10	0.17
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	10	0.17
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	18	0.17
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	18	0.17
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	18	0.17
(1,755)	1:912:A:ASN:HA	1:916:A:ASN:H	3	0.17
(1,755)	1:912:A:ASN:HA	1:916:A:ASN:H	14	0.17
(1,679)	1:906:A:LYS:HB2	1:906:A:LYS:HD2	4	0.17
(1,679)	1:906:A:LYS:HB2	1:906:A:LYS:HD3	4	0.17
(1,679)	1:906:A:LYS:HB3	1:906:A:LYS:HD2	4	0.17
(1,679)	1:906:A:LYS:HB3	1:906:A:LYS:HD3	4	0.17
(1,679)	1:906:A:LYS:HB2	1:906:A:LYS:HD2	20	0.17
(1,679)	1:906:A:LYS:HB2	1:906:A:LYS:HD3	20	0.17
(1,679)	1:906:A:LYS:HB3	1:906:A:LYS:HD2	20	0.17
(1,679)	1:906:A:LYS:HB3	1:906:A:LYS:HD3	20	0.17
(1,653)	1:903:A:ASP:HB2	1:904:A:CYS:H	9	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:903:A:ASP:HB3	1:904:A:CYS:H	9	0.17
(1,649)	1:903:A:ASP:HB2	1:905:A:SER:H	9	0.17
(1,649)	1:903:A:ASP:HB2	1:905:A:SER:H	20	0.17
(1,648)	1:903:A:ASP:HA	1:906:A:LYS:H	8	0.17
(1,628)	1:901:A:PHE:HA	1:907:A:SER:H	6	0.17
(1,623)	1:901:A:PHE:HA	1:902:A:ALA:H	1	0.17
(1,599)	1:899:A:LYS:HB2	1:899:A:LYS:HE2	13	0.17
(1,599)	1:899:A:LYS:HB2	1:899:A:LYS:HE3	13	0.17
(1,407)	1:882:A:VAL:HB	1:883:A:GLY:H	6	0.17
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	16	0.17
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	16	0.17
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	16	0.17
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	16	0.17
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	16	0.17
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	16	0.17
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	17	0.17
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	17	0.17
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	17	0.17
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	17	0.17
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	17	0.17
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	17	0.17
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	16	0.17
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	16	0.17
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	16	0.17
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	16	0.17
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	16	0.17
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	16	0.17
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	19	0.17
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	19	0.17
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	19	0.17
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	19	0.17
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	19	0.17
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	19	0.17
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	6	0.17
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	6	0.17
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	6	0.17
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	6	0.17
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	6	0.17
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	6	0.17
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	9	0.17
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	9	0.17
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	9	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	9	0.17
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	9	0.17
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	9	0.17
(1,315)	1:874:A:TRP:HZ2	1:923:A:GLN:HB2	1	0.17
(1,315)	1:874:A:TRP:HZ2	1:923:A:GLN:HB3	1	0.17
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB2	2	0.17
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB3	2	0.17
(1,287)	1:873:A:LYS:HB2	1:874:A:TRP:HA	1	0.17
(1,287)	1:873:A:LYS:HB3	1:874:A:TRP:HA	1	0.17
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD2	9	0.17
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD3	9	0.17
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	11	0.17
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	4	0.17
(1,215)	1:867:A:ARG:HG2	1:874:A:TRP:HZ2	2	0.17
(1,215)	1:867:A:ARG:HG3	1:874:A:TRP:HZ2	2	0.17
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM1	18	0.17
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM2	18	0.17
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM3	18	0.17
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM1	18	0.17
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM2	18	0.17
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM3	18	0.17
(1,137)	1:865:A:TRP:HH2	1:909:A:GLU:H	12	0.17
(1,111)	1:865:A:TRP:H	2:6:B:THR:H	5	0.17
(1,106)	1:865:A:TRP:H	2:4:B:MLZ:H	9	0.17
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG11	19	0.17
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG12	19	0.17
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG13	19	0.17
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG21	19	0.17
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG22	19	0.17
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG23	19	0.17
(1,60)	1:861:A:THR:HA	1:861:A:THR:HB	9	0.17
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG11	7	0.17
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG12	7	0.17
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG13	7	0.17
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG21	7	0.17
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG22	7	0.17
(1,32)	1:855:A:SER:HA	1:856:A:VAL:HG23	7	0.17
(1,27)	1:854:A:ALA:HA	1:855:A:SER:H	16	0.17
(2,7)	1:904:A:CYS:CB	3:1001:A:ZN:ZN	3	0.16
(2,7)	1:904:A:CYS:CB	3:1001:A:ZN:ZN	11	0.16
(2,7)	1:904:A:CYS:CB	3:1001:A:ZN:ZN	20	0.16
(1,937)	2:8:B:ARG:H	2:9:B:TYR:H	4	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,937)	2:8:B:ARG:H	2:9:B:TYR:H	19	0.16
(1,929)	2:5:B:GLN:H	2:6:B:THR:H	9	0.16
(1,912)	1:925:A:GLU:HB2	1:926:A:ALA:H	12	0.16
(1,902)	1:923:A:GLN:HG2	1:924:A:ASP:H	2	0.16
(1,902)	1:923:A:GLN:HG3	1:924:A:ASP:H	2	0.16
(1,889)	1:922:A:GLY:HA2	1:923:A:GLN:H	4	0.16
(1,889)	1:922:A:GLY:HA3	1:923:A:GLN:H	4	0.16
(1,883)	1:921:A:ILE:HD11	2:4:B:MLZ:HG2	16	0.16
(1,883)	1:921:A:ILE:HD11	2:4:B:MLZ:HG3	16	0.16
(1,883)	1:921:A:ILE:HD12	2:4:B:MLZ:HG2	16	0.16
(1,883)	1:921:A:ILE:HD12	2:4:B:MLZ:HG3	16	0.16
(1,883)	1:921:A:ILE:HD13	2:4:B:MLZ:HG2	16	0.16
(1,883)	1:921:A:ILE:HD13	2:4:B:MLZ:HG3	16	0.16
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	7	0.16
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	7	0.16
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	7	0.16
(1,755)	1:912:A:ASN:HA	1:916:A:ASN:H	4	0.16
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	4	0.16
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	4	0.16
(1,649)	1:903:A:ASP:HB2	1:905:A:SER:H	11	0.16
(1,623)	1:901:A:PHE:HA	1:902:A:ALA:H	18	0.16
(1,623)	1:901:A:PHE:HA	1:902:A:ALA:H	20	0.16
(1,560)	1:896:A:ASN:HB2	1:902:A:ALA:H	16	0.16
(1,560)	1:896:A:ASN:HB3	1:902:A:ALA:H	16	0.16
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	8	0.16
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	8	0.16
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	8	0.16
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	8	0.16
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	8	0.16
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	8	0.16
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	8	0.16
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	8	0.16
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	8	0.16
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	8	0.16
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	8	0.16
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	8	0.16
(1,407)	1:882:A:VAL:HB	1:883:A:GLY:H	8	0.16
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	7	0.16
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	7	0.16
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	7	0.16
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	7	0.16
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	7	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	7	0.16
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	12	0.16
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	12	0.16
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	12	0.16
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	12	0.16
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	12	0.16
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	12	0.16
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	20	0.16
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	20	0.16
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	20	0.16
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	20	0.16
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	20	0.16
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	20	0.16
(1,287)	1:873:A:LYS:HB2	1:874:A:TRP:HA	18	0.16
(1,287)	1:873:A:LYS:HB3	1:874:A:TRP:HA	18	0.16
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD2	20	0.16
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD3	20	0.16
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	4	0.16
(1,209)	1:867:A:ARG:HD2	2:3:B:THR:HA	5	0.16
(1,209)	1:867:A:ARG:HD3	2:3:B:THR:HA	5	0.16
(1,209)	1:867:A:ARG:HD2	2:3:B:THR:HA	9	0.16
(1,209)	1:867:A:ARG:HD3	2:3:B:THR:HA	9	0.16
(1,193)	1:867:A:ARG:H	2:4:B:MLZ:H	13	0.16
(1,145)	1:865:A:TRP:HB2	2:4:B:MLZ:HB2	13	0.16
(1,145)	1:865:A:TRP:HB2	2:4:B:MLZ:HB3	13	0.16
(1,145)	1:865:A:TRP:HB3	2:4:B:MLZ:HB2	13	0.16
(1,145)	1:865:A:TRP:HB3	2:4:B:MLZ:HB3	13	0.16
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB2	14	0.16
(1,126)	1:865:A:TRP:HD1	2:4:B:MLZ:HB3	14	0.16
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG11	1	0.16
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG12	1	0.16
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG13	1	0.16
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG21	1	0.16
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG22	1	0.16
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG23	1	0.16
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG11	20	0.16
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG12	20	0.16
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG13	20	0.16
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG21	20	0.16
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG22	20	0.16
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG23	20	0.16
(1,106)	1:865:A:TRP:H	2:4:B:MLZ:H	1	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG11	11	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG12	11	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG13	11	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG21	11	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG22	11	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG23	11	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG11	14	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG12	14	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG13	14	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG21	14	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG22	14	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG23	14	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG11	19	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG12	19	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG13	19	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG21	19	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG22	19	0.16
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG23	19	0.16
(1,89)	1:864:A:ALA:H	1:879:A:ALA:H	12	0.16
(1,60)	1:861:A:THR:HA	1:861:A:THR:HB	4	0.16
(1,918)	1:926:A:ALA:HA	1:928:A:ALA:H	14	0.15
(1,914)	1:925:A:GLU:HB3	1:926:A:ALA:H	13	0.15
(1,914)	1:925:A:GLU:HB3	1:926:A:ALA:H	17	0.15
(1,891)	1:923:A:GLN:H	1:923:A:GLN:HG2	18	0.15
(1,891)	1:923:A:GLN:H	1:923:A:GLN:HG3	18	0.15
(1,863)	1:919:A:LEU:HD11	2:6:B:THR:H	9	0.15
(1,863)	1:919:A:LEU:HD12	2:6:B:THR:H	9	0.15
(1,863)	1:919:A:LEU:HD13	2:6:B:THR:H	9	0.15
(1,863)	1:919:A:LEU:HD21	2:6:B:THR:H	9	0.15
(1,863)	1:919:A:LEU:HD22	2:6:B:THR:H	9	0.15
(1,863)	1:919:A:LEU:HD23	2:6:B:THR:H	9	0.15
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE21	20	0.15
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE22	20	0.15
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE21	20	0.15
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE22	20	0.15
(1,792)	1:915:A:ILE:HD11	1:916:A:ASN:HA	14	0.15
(1,792)	1:915:A:ILE:HD12	1:916:A:ASN:HA	14	0.15
(1,792)	1:915:A:ILE:HD13	1:916:A:ASN:HA	14	0.15
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	9	0.15
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	9	0.15
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	9	0.15
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	5	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	5	0.15
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	8	0.15
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	8	0.15
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	11	0.15
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	11	0.15
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	12	0.15
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	12	0.15
(1,628)	1:901:A:PHE:HA	1:907:A:SER:H	18	0.15
(1,623)	1:901:A:PHE:HA	1:902:A:ALA:H	4	0.15
(1,623)	1:901:A:PHE:HA	1:902:A:ALA:H	9	0.15
(1,623)	1:901:A:PHE:HA	1:902:A:ALA:H	15	0.15
(1,594)	1:899:A:LYS:HA	1:899:A:LYS:HD2	13	0.15
(1,594)	1:899:A:LYS:HA	1:899:A:LYS:HD3	13	0.15
(1,560)	1:896:A:ASN:HB2	1:902:A:ALA:H	5	0.15
(1,560)	1:896:A:ASN:HB3	1:902:A:ALA:H	5	0.15
(1,560)	1:896:A:ASN:HB2	1:902:A:ALA:H	6	0.15
(1,560)	1:896:A:ASN:HB3	1:902:A:ALA:H	6	0.15
(1,467)	1:890:A:ARG:H	1:891:A:TRP:H	3	0.15
(1,446)	1:886:A:ASP:HB2	1:888:A:SER:H	11	0.15
(1,430)	1:885:A:ILE:HG12	1:891:A:TRP:HA	5	0.15
(1,430)	1:885:A:ILE:HG13	1:891:A:TRP:HA	5	0.15
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	6	0.15
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	6	0.15
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	6	0.15
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	6	0.15
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	6	0.15
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	6	0.15
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	6	0.15
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	6	0.15
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	6	0.15
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	6	0.15
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	6	0.15
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	6	0.15
(1,407)	1:882:A:VAL:HB	1:883:A:GLY:H	20	0.15
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	19	0.15
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	19	0.15
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	19	0.15
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	19	0.15
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	19	0.15
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	19	0.15
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	17	0.15
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	17	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	17	0.15
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	17	0.15
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	17	0.15
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	17	0.15
(1,391)	1:881:A:VAL:HB	1:882:A:VAL:H	20	0.15
(1,389)	1:881:A:VAL:HA	1:883:A:GLY:H	10	0.15
(1,389)	1:881:A:VAL:HA	1:883:A:GLY:H	17	0.15
(1,370)	1:879:A:ALA:HA	1:882:A:VAL:HA	11	0.15
(1,315)	1:874:A:TRP:HZ2	1:923:A:GLN:HB2	9	0.15
(1,315)	1:874:A:TRP:HZ2	1:923:A:GLN:HB3	9	0.15
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM1	2	0.15
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM2	2	0.15
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM3	2	0.15
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM1	15	0.15
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM2	15	0.15
(1,312)	1:874:A:TRP:HH2	2:4:B:MLZ:HCM3	15	0.15
(1,305)	1:874:A:TRP:HE1	1:923:A:GLN:HG2	4	0.15
(1,305)	1:874:A:TRP:HE1	1:923:A:GLN:HG3	4	0.15
(1,302)	1:874:A:TRP:HD1	1:912:A:ASN:HD21	10	0.15
(1,302)	1:874:A:TRP:HD1	1:912:A:ASN:HD22	10	0.15
(1,298)	1:874:A:TRP:HB2	1:875:A:ARG:H	12	0.15
(1,291)	1:873:A:LYS:HG2	1:873:A:LYS:HE2	12	0.15
(1,291)	1:873:A:LYS:HG2	1:873:A:LYS:HE3	12	0.15
(1,291)	1:873:A:LYS:HG3	1:873:A:LYS:HE2	12	0.15
(1,291)	1:873:A:LYS:HG3	1:873:A:LYS:HE3	12	0.15
(1,291)	1:873:A:LYS:HG2	1:873:A:LYS:HE2	15	0.15
(1,291)	1:873:A:LYS:HG2	1:873:A:LYS:HE3	15	0.15
(1,291)	1:873:A:LYS:HG3	1:873:A:LYS:HE2	15	0.15
(1,291)	1:873:A:LYS:HG3	1:873:A:LYS:HE3	15	0.15
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD2	4	0.15
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD3	4	0.15
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD2	11	0.15
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD3	11	0.15
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD2	15	0.15
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD3	15	0.15
(1,265)	1:870:A:ASP:HB2	1:871:A:CYS:H	2	0.15
(1,265)	1:870:A:ASP:HB3	1:871:A:CYS:H	2	0.15
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	14	0.15
(1,206)	1:867:A:ARG:HD2	1:872:A:PHE:HB2	4	0.15
(1,206)	1:867:A:ARG:HD2	1:872:A:PHE:HB3	4	0.15
(1,206)	1:867:A:ARG:HD3	1:872:A:PHE:HB2	4	0.15
(1,206)	1:867:A:ARG:HD3	1:872:A:PHE:HB3	4	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,200)	1:867:A:ARG:HE	1:872:A:PHE:HB2	9	0.15
(1,200)	1:867:A:ARG:HE	1:872:A:PHE:HB3	9	0.15
(1,170)	1:866:A:VAL:HG11	1:868:A:CYS:H	16	0.15
(1,170)	1:866:A:VAL:HG12	1:868:A:CYS:H	16	0.15
(1,170)	1:866:A:VAL:HG13	1:868:A:CYS:H	16	0.15
(1,170)	1:866:A:VAL:HG21	1:868:A:CYS:H	16	0.15
(1,170)	1:866:A:VAL:HG22	1:868:A:CYS:H	16	0.15
(1,170)	1:866:A:VAL:HG23	1:868:A:CYS:H	16	0.15
(1,145)	1:865:A:TRP:HB2	2:4:B:MLZ:HB2	12	0.15
(1,145)	1:865:A:TRP:HB2	2:4:B:MLZ:HB3	12	0.15
(1,145)	1:865:A:TRP:HB3	2:4:B:MLZ:HB2	12	0.15
(1,145)	1:865:A:TRP:HB3	2:4:B:MLZ:HB3	12	0.15
(1,145)	1:865:A:TRP:HB2	2:4:B:MLZ:HB2	16	0.15
(1,145)	1:865:A:TRP:HB2	2:4:B:MLZ:HB3	16	0.15
(1,145)	1:865:A:TRP:HB3	2:4:B:MLZ:HB2	16	0.15
(1,145)	1:865:A:TRP:HB3	2:4:B:MLZ:HB3	16	0.15
(1,139)	1:865:A:TRP:HZ2	1:915:A:ILE:HA	3	0.15
(1,137)	1:865:A:TRP:HH2	1:909:A:GLU:H	8	0.15
(1,132)	1:865:A:TRP:HE1	2:6:B:THR:HA	17	0.15
(1,116)	1:865:A:TRP:HA	1:875:A:ARG:H	16	0.15
(1,116)	1:865:A:TRP:HA	1:875:A:ARG:H	18	0.15
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG11	15	0.15
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG12	15	0.15
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG13	15	0.15
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG21	15	0.15
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG22	15	0.15
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG23	15	0.15
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG11	2	0.15
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG12	2	0.15
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG13	2	0.15
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG21	2	0.15
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG22	2	0.15
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG23	2	0.15
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG11	16	0.15
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG12	16	0.15
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG13	16	0.15
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG21	16	0.15
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG22	16	0.15
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG23	16	0.15
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG11	2	0.15
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG12	2	0.15
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG13	2	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG21	2	0.15
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG22	2	0.15
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG23	2	0.15
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG11	7	0.15
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG12	7	0.15
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG13	7	0.15
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG21	7	0.15
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG22	7	0.15
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG23	7	0.15
(1,60)	1:861:A:THR:HA	1:861:A:THR:HB	10	0.15
(1,39)	1:857:A:GLY:H	1:858:A:SER:H	5	0.15
(2,4)	1:871:A:CYS:SG	3:1001:A:ZN:ZN	5	0.14
(2,3)	1:871:A:CYS:CB	3:1001:A:ZN:ZN	20	0.14
(1,938)	2:8:B:ARG:HA	2:9:B:TYR:H	2	0.14
(1,926)	2:2:B:ARG:HE	2:3:B:THR:HA	17	0.14
(1,921)	1:927:A:ASP:HA	1:928:A:ALA:H	13	0.14
(1,918)	1:926:A:ALA:HA	1:928:A:ALA:H	3	0.14
(1,912)	1:925:A:GLU:HB2	1:926:A:ALA:H	13	0.14
(1,900)	1:923:A:GLN:HE21	2:3:B:THR:HA	5	0.14
(1,900)	1:923:A:GLN:HE22	2:3:B:THR:HA	5	0.14
(1,895)	1:923:A:GLN:HE21	2:3:B:THR:HA	2	0.14
(1,792)	1:915:A:ILE:HD11	1:916:A:ASN:HA	3	0.14
(1,792)	1:915:A:ILE:HD12	1:916:A:ASN:HA	3	0.14
(1,792)	1:915:A:ILE:HD13	1:916:A:ASN:HA	3	0.14
(1,791)	1:915:A:ILE:HD11	1:916:A:ASN:H	2	0.14
(1,791)	1:915:A:ILE:HD12	1:916:A:ASN:H	2	0.14
(1,791)	1:915:A:ILE:HD13	1:916:A:ASN:H	2	0.14
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	15	0.14
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	15	0.14
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	17	0.14
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	17	0.14
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	20	0.14
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	20	0.14
(1,648)	1:903:A:ASP:HA	1:906:A:LYS:H	4	0.14
(1,648)	1:903:A:ASP:HA	1:906:A:LYS:H	6	0.14
(1,648)	1:903:A:ASP:HA	1:906:A:LYS:H	15	0.14
(1,628)	1:901:A:PHE:HA	1:907:A:SER:H	1	0.14
(1,628)	1:901:A:PHE:HA	1:907:A:SER:H	2	0.14
(1,623)	1:901:A:PHE:HA	1:902:A:ALA:H	2	0.14
(1,623)	1:901:A:PHE:HA	1:902:A:ALA:H	8	0.14
(1,623)	1:901:A:PHE:HA	1:902:A:ALA:H	13	0.14
(1,560)	1:896:A:ASN:HB2	1:902:A:ALA:H	3	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,560)	1:896:A:ASN:HB3	1:902:A:ALA:H	3	0.14
(1,560)	1:896:A:ASN:HB2	1:902:A:ALA:H	10	0.14
(1,560)	1:896:A:ASN:HB3	1:902:A:ALA:H	10	0.14
(1,560)	1:896:A:ASN:HB2	1:902:A:ALA:H	14	0.14
(1,560)	1:896:A:ASN:HB3	1:902:A:ALA:H	14	0.14
(1,560)	1:896:A:ASN:HB2	1:902:A:ALA:H	19	0.14
(1,560)	1:896:A:ASN:HB3	1:902:A:ALA:H	19	0.14
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	19	0.14
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	17	0.14
(1,507)	1:892:A:ILE:HD11	1:895:A:ASN:HD21	12	0.14
(1,507)	1:892:A:ILE:HD11	1:895:A:ASN:HD22	12	0.14
(1,507)	1:892:A:ILE:HD12	1:895:A:ASN:HD21	12	0.14
(1,507)	1:892:A:ILE:HD12	1:895:A:ASN:HD22	12	0.14
(1,507)	1:892:A:ILE:HD13	1:895:A:ASN:HD21	12	0.14
(1,507)	1:892:A:ILE:HD13	1:895:A:ASN:HD22	12	0.14
(1,464)	1:889:A:SER:HB2	1:890:A:ARG:H	18	0.14
(1,464)	1:889:A:SER:HB3	1:890:A:ARG:H	18	0.14
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	1	0.14
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	1	0.14
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	1	0.14
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	1	0.14
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	1	0.14
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	1	0.14
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	15	0.14
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	15	0.14
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	15	0.14
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	15	0.14
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	15	0.14
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	15	0.14
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	18	0.14
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	18	0.14
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	18	0.14
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	18	0.14
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	18	0.14
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	18	0.14
(1,392)	1:881:A:VAL:HG11	1:884:A:SER:H	8	0.14
(1,392)	1:881:A:VAL:HG12	1:884:A:SER:H	8	0.14
(1,392)	1:881:A:VAL:HG13	1:884:A:SER:H	8	0.14
(1,392)	1:881:A:VAL:HG21	1:884:A:SER:H	8	0.14
(1,392)	1:881:A:VAL:HG22	1:884:A:SER:H	8	0.14
(1,392)	1:881:A:VAL:HG23	1:884:A:SER:H	8	0.14
(1,389)	1:881:A:VAL:HA	1:883:A:GLY:H	6	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,389)	1:881:A:VAL:HA	1:883:A:GLY:H	8	0.14
(1,338)	1:876:A:ARG:HA	1:876:A:ARG:HD2	2	0.14
(1,338)	1:876:A:ARG:HA	1:876:A:ARG:HD3	2	0.14
(1,311)	1:874:A:TRP:HH2	2:3:B:THR:HG1	17	0.14
(1,305)	1:874:A:TRP:HE1	1:923:A:GLN:HG2	19	0.14
(1,305)	1:874:A:TRP:HE1	1:923:A:GLN:HG3	19	0.14
(1,287)	1:873:A:LYS:HB2	1:874:A:TRP:HA	9	0.14
(1,287)	1:873:A:LYS:HB3	1:874:A:TRP:HA	9	0.14
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD2	1	0.14
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD3	1	0.14
(1,265)	1:870:A:ASP:HB2	1:871:A:CYS:H	20	0.14
(1,265)	1:870:A:ASP:HB3	1:871:A:CYS:H	20	0.14
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	1	0.14
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	10	0.14
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	2	0.14
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	2	0.14
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	2	0.14
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	2	0.14
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	2	0.14
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	2	0.14
(1,215)	1:867:A:ARG:HG2	1:874:A:TRP:HZ2	6	0.14
(1,215)	1:867:A:ARG:HG3	1:874:A:TRP:HZ2	6	0.14
(1,215)	1:867:A:ARG:HG2	1:874:A:TRP:HZ2	15	0.14
(1,215)	1:867:A:ARG:HG3	1:874:A:TRP:HZ2	15	0.14
(1,209)	1:867:A:ARG:HD2	2:3:B:THR:HA	17	0.14
(1,209)	1:867:A:ARG:HD3	2:3:B:THR:HA	17	0.14
(1,200)	1:867:A:ARG:HE	1:872:A:PHE:HB2	1	0.14
(1,200)	1:867:A:ARG:HE	1:872:A:PHE:HB3	1	0.14
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM1	6	0.14
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM2	6	0.14
(1,146)	1:865:A:TRP:HB2	2:4:B:MLZ:HCM3	6	0.14
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM1	6	0.14
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM2	6	0.14
(1,146)	1:865:A:TRP:HB3	2:4:B:MLZ:HCM3	6	0.14
(1,145)	1:865:A:TRP:HB2	2:4:B:MLZ:HB2	5	0.14
(1,145)	1:865:A:TRP:HB2	2:4:B:MLZ:HB3	5	0.14
(1,145)	1:865:A:TRP:HB3	2:4:B:MLZ:HB2	5	0.14
(1,145)	1:865:A:TRP:HB3	2:4:B:MLZ:HB3	5	0.14
(1,139)	1:865:A:TRP:HZ2	1:915:A:ILE:HA	8	0.14
(1,139)	1:865:A:TRP:HZ2	1:915:A:ILE:HA	14	0.14
(1,137)	1:865:A:TRP:HH2	1:909:A:GLU:H	13	0.14
(1,137)	1:865:A:TRP:HH2	1:909:A:GLU:H	16	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,132)	1:865:A:TRP:HE1	2:6:B:THR:HA	13	0.14
(1,116)	1:865:A:TRP:HA	1:875:A:ARG:H	9	0.14
(1,116)	1:865:A:TRP:HA	1:875:A:ARG:H	13	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG11	7	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG12	7	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG13	7	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG21	7	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG22	7	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG23	7	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG11	11	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG12	11	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG13	11	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG21	11	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG22	11	0.14
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG23	11	0.14
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB2	8	0.14
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB3	8	0.14
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG11	18	0.14
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG12	18	0.14
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG13	18	0.14
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG21	18	0.14
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG22	18	0.14
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG23	18	0.14
(1,89)	1:864:A:ALA:H	1:879:A:ALA:H	17	0.14
(1,60)	1:861:A:THR:HA	1:861:A:THR:HB	1	0.14
(1,52)	1:859:A:GLU:HB2	1:860:A:PHE:H	14	0.14
(1,52)	1:859:A:GLU:HB3	1:860:A:PHE:H	14	0.14
(1,39)	1:857:A:GLY:H	1:858:A:SER:H	3	0.14
(1,1)	1:851:A:SER:HA	1:852:A:ARG:H	3	0.14
(2,7)	1:904:A:CYS:CB	3:1001:A:ZN:ZN	5	0.13
(2,7)	1:904:A:CYS:CB	3:1001:A:ZN:ZN	9	0.13
(2,5)	1:893:A:CYS:CB	3:1001:A:ZN:ZN	9	0.13
(2,3)	1:871:A:CYS:CB	3:1001:A:ZN:ZN	18	0.13
(1,926)	2:2:B:ARG:HE	2:3:B:THR:HA	18	0.13
(1,918)	1:926:A:ALA:HA	1:928:A:ALA:H	5	0.13
(1,918)	1:926:A:ALA:HA	1:928:A:ALA:H	12	0.13
(1,918)	1:926:A:ALA:HA	1:928:A:ALA:H	16	0.13
(1,918)	1:926:A:ALA:HA	1:928:A:ALA:H	19	0.13
(1,917)	1:926:A:ALA:H	1:927:A:ASP:H	2	0.13
(1,917)	1:926:A:ALA:H	1:927:A:ASP:H	8	0.13
(1,904)	1:924:A:ASP:H	1:925:A:GLU:H	13	0.13
(1,896)	1:923:A:GLN:HE21	2:4:B:MLZ:HG2	10	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,896)	1:923:A:GLN:HE21	2:4:B:MLZ:HG3	10	0.13
(1,895)	1:923:A:GLN:HE21	2:3:B:THR:HA	13	0.13
(1,863)	1:919:A:LEU:HD11	2:6:B:THR:H	19	0.13
(1,863)	1:919:A:LEU:HD12	2:6:B:THR:H	19	0.13
(1,863)	1:919:A:LEU:HD13	2:6:B:THR:H	19	0.13
(1,863)	1:919:A:LEU:HD21	2:6:B:THR:H	19	0.13
(1,863)	1:919:A:LEU:HD22	2:6:B:THR:H	19	0.13
(1,863)	1:919:A:LEU:HD23	2:6:B:THR:H	19	0.13
(1,844)	1:918:A:GLU:HG2	2:8:B:ARG:HB2	1	0.13
(1,844)	1:918:A:GLU:HG2	2:8:B:ARG:HB3	1	0.13
(1,844)	1:918:A:GLU:HG3	2:8:B:ARG:HB2	1	0.13
(1,844)	1:918:A:GLU:HG3	2:8:B:ARG:HB3	1	0.13
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE21	15	0.13
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE22	15	0.13
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE21	15	0.13
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE22	15	0.13
(1,755)	1:912:A:ASN:HA	1:916:A:ASN:H	8	0.13
(1,755)	1:912:A:ASN:HA	1:916:A:ASN:H	19	0.13
(1,634)	1:902:A:ALA:H	1:903:A:ASP:HB2	5	0.13
(1,634)	1:902:A:ALA:H	1:903:A:ASP:HB3	5	0.13
(1,631)	1:901:A:PHE:HD1	1:909:A:GLU:H	10	0.13
(1,631)	1:901:A:PHE:HD2	1:909:A:GLU:H	10	0.13
(1,628)	1:901:A:PHE:HA	1:907:A:SER:H	3	0.13
(1,628)	1:901:A:PHE:HA	1:907:A:SER:H	5	0.13
(1,628)	1:901:A:PHE:HA	1:907:A:SER:H	14	0.13
(1,623)	1:901:A:PHE:HA	1:902:A:ALA:H	7	0.13
(1,579)	1:898:A:ASP:HB2	1:899:A:LYS:H	3	0.13
(1,560)	1:896:A:ASN:HB2	1:902:A:ALA:H	2	0.13
(1,560)	1:896:A:ASN:HB3	1:902:A:ALA:H	2	0.13
(1,560)	1:896:A:ASN:HB2	1:902:A:ALA:H	18	0.13
(1,560)	1:896:A:ASN:HB3	1:902:A:ALA:H	18	0.13
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	3	0.13
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	11	0.13
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	12	0.13
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	13	0.13
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	14	0.13
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	15	0.13
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	16	0.13
(1,473)	1:890:A:ARG:HB2	1:891:A:TRP:H	12	0.13
(1,473)	1:890:A:ARG:HB3	1:891:A:TRP:H	12	0.13
(1,394)	1:881:A:VAL:HG11	1:885:A:ILE:HB	1	0.13
(1,394)	1:881:A:VAL:HG12	1:885:A:ILE:HB	1	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,394)	1:881:A:VAL:HG13	1:885:A:ILE:HB	1	0.13
(1,394)	1:881:A:VAL:HG21	1:885:A:ILE:HB	1	0.13
(1,394)	1:881:A:VAL:HG22	1:885:A:ILE:HB	1	0.13
(1,394)	1:881:A:VAL:HG23	1:885:A:ILE:HB	1	0.13
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	4	0.13
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	4	0.13
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	4	0.13
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	4	0.13
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	4	0.13
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	4	0.13
(1,325)	1:874:A:TRP:HB2	1:915:A:ILE:HG21	13	0.13
(1,325)	1:874:A:TRP:HB2	1:915:A:ILE:HG22	13	0.13
(1,325)	1:874:A:TRP:HB2	1:915:A:ILE:HG23	13	0.13
(1,325)	1:874:A:TRP:HB3	1:915:A:ILE:HG21	13	0.13
(1,325)	1:874:A:TRP:HB3	1:915:A:ILE:HG22	13	0.13
(1,325)	1:874:A:TRP:HB3	1:915:A:ILE:HG23	13	0.13
(1,317)	1:874:A:TRP:HZ2	2:3:B:THR:HA	5	0.13
(1,317)	1:874:A:TRP:HZ2	2:3:B:THR:HA	12	0.13
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB2	8	0.13
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB3	8	0.13
(1,309)	1:874:A:TRP:HH2	2:3:B:THR:HA	8	0.13
(1,298)	1:874:A:TRP:HB2	1:875:A:ARG:H	15	0.13
(1,255)	1:870:A:ASP:H	1:872:A:PHE:H	20	0.13
(1,225)	1:868:A:CYS:HA	1:891:A:TRP:HZ3	10	0.13
(1,221)	1:868:A:CYS:H	1:874:A:TRP:HA	7	0.13
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	5	0.13
(1,214)	1:867:A:ARG:HG2	1:874:A:TRP:HE1	3	0.13
(1,214)	1:867:A:ARG:HG3	1:874:A:TRP:HE1	3	0.13
(1,209)	1:867:A:ARG:HD2	2:3:B:THR:HA	1	0.13
(1,209)	1:867:A:ARG:HD3	2:3:B:THR:HA	1	0.13
(1,200)	1:867:A:ARG:HE	1:872:A:PHE:HB2	17	0.13
(1,200)	1:867:A:ARG:HE	1:872:A:PHE:HB3	17	0.13
(1,199)	1:867:A:ARG:HE	1:872:A:PHE:HA	6	0.13
(1,183)	1:866:A:VAL:HG11	2:3:B:THR:HG1	2	0.13
(1,183)	1:866:A:VAL:HG12	2:3:B:THR:HG1	2	0.13
(1,183)	1:866:A:VAL:HG13	2:3:B:THR:HG1	2	0.13
(1,183)	1:866:A:VAL:HG21	2:3:B:THR:HG1	2	0.13
(1,183)	1:866:A:VAL:HG22	2:3:B:THR:HG1	2	0.13
(1,183)	1:866:A:VAL:HG23	2:3:B:THR:HG1	2	0.13
(1,170)	1:866:A:VAL:HG11	1:868:A:CYS:H	14	0.13
(1,170)	1:866:A:VAL:HG12	1:868:A:CYS:H	14	0.13
(1,170)	1:866:A:VAL:HG13	1:868:A:CYS:H	14	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:866:A:VAL:HG21	1:868:A:CYS:H	14	0.13
(1,170)	1:866:A:VAL:HG22	1:868:A:CYS:H	14	0.13
(1,170)	1:866:A:VAL:HG23	1:868:A:CYS:H	14	0.13
(1,140)	1:865:A:TRP:HZ3	1:910:A:MET:H	12	0.13
(1,140)	1:865:A:TRP:HZ3	1:910:A:MET:H	13	0.13
(1,139)	1:865:A:TRP:HZ2	1:915:A:ILE:HA	15	0.13
(1,139)	1:865:A:TRP:HZ2	1:915:A:ILE:HA	19	0.13
(1,137)	1:865:A:TRP:HH2	1:909:A:GLU:H	14	0.13
(1,137)	1:865:A:TRP:HH2	1:909:A:GLU:H	17	0.13
(1,132)	1:865:A:TRP:HE1	2:6:B:THR:HA	6	0.13
(1,116)	1:865:A:TRP:HA	1:875:A:ARG:H	1	0.13
(1,116)	1:865:A:TRP:HA	1:875:A:ARG:H	4	0.13
(1,116)	1:865:A:TRP:HA	1:875:A:ARG:H	14	0.13
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG11	12	0.13
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG12	12	0.13
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG13	12	0.13
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG21	12	0.13
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG22	12	0.13
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG23	12	0.13
(1,89)	1:864:A:ALA:H	1:879:A:ALA:H	2	0.13
(1,89)	1:864:A:ALA:H	1:879:A:ALA:H	7	0.13
(1,89)	1:864:A:ALA:H	1:879:A:ALA:H	9	0.13
(1,89)	1:864:A:ALA:H	1:879:A:ALA:H	11	0.13
(1,89)	1:864:A:ALA:H	1:879:A:ALA:H	19	0.13
(1,80)	1:863:A:SER:HA	1:878:A:PRO:HA	9	0.13
(1,62)	1:861:A:THR:HB	1:862:A:GLU:H	18	0.13
(1,40)	1:857:A:GLY:HA2	1:858:A:SER:H	9	0.13
(1,40)	1:857:A:GLY:HA3	1:858:A:SER:H	9	0.13
(1,39)	1:857:A:GLY:H	1:858:A:SER:H	1	0.13
(1,39)	1:857:A:GLY:H	1:858:A:SER:H	8	0.13
(1,28)	1:854:A:ALA:HB1	1:855:A:SER:H	4	0.13
(1,28)	1:854:A:ALA:HB2	1:855:A:SER:H	4	0.13
(1,28)	1:854:A:ALA:HB3	1:855:A:SER:H	4	0.13
(2,8)	1:904:A:CYS:SG	3:1001:A:ZN:ZN	15	0.12
(2,7)	1:904:A:CYS:CB	3:1001:A:ZN:ZN	12	0.12
(2,7)	1:904:A:CYS:CB	3:1001:A:ZN:ZN	18	0.12
(2,5)	1:893:A:CYS:CB	3:1001:A:ZN:ZN	16	0.12
(2,5)	1:893:A:CYS:CB	3:1001:A:ZN:ZN	18	0.12
(2,5)	1:893:A:CYS:CB	3:1001:A:ZN:ZN	20	0.12
(2,3)	1:871:A:CYS:CB	3:1001:A:ZN:ZN	1	0.12
(2,3)	1:871:A:CYS:CB	3:1001:A:ZN:ZN	3	0.12
(2,3)	1:871:A:CYS:CB	3:1001:A:ZN:ZN	9	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,937)	2:8:B:ARG:H	2:9:B:TYR:H	16	0.12
(1,926)	2:2:B:ARG:HE	2:3:B:THR:HA	16	0.12
(1,918)	1:926:A:ALA:HA	1:928:A:ALA:H	1	0.12
(1,912)	1:925:A:GLU:HB2	1:926:A:ALA:H	6	0.12
(1,904)	1:924:A:ASP:H	1:925:A:GLU:H	1	0.12
(1,900)	1:923:A:GLN:HE21	2:3:B:THR:HA	10	0.12
(1,900)	1:923:A:GLN:HE22	2:3:B:THR:HA	10	0.12
(1,900)	1:923:A:GLN:HE21	2:3:B:THR:HA	12	0.12
(1,900)	1:923:A:GLN:HE22	2:3:B:THR:HA	12	0.12
(1,863)	1:919:A:LEU:HD11	2:6:B:THR:H	4	0.12
(1,863)	1:919:A:LEU:HD12	2:6:B:THR:H	4	0.12
(1,863)	1:919:A:LEU:HD13	2:6:B:THR:H	4	0.12
(1,863)	1:919:A:LEU:HD21	2:6:B:THR:H	4	0.12
(1,863)	1:919:A:LEU:HD22	2:6:B:THR:H	4	0.12
(1,863)	1:919:A:LEU:HD23	2:6:B:THR:H	4	0.12
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE21	4	0.12
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE22	4	0.12
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE21	4	0.12
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE22	4	0.12
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE21	10	0.12
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE22	10	0.12
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE21	10	0.12
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE22	10	0.12
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE21	14	0.12
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE22	14	0.12
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE21	14	0.12
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE22	14	0.12
(1,792)	1:915:A:ILE:HD11	1:916:A:ASN:HA	8	0.12
(1,792)	1:915:A:ILE:HD12	1:916:A:ASN:HA	8	0.12
(1,792)	1:915:A:ILE:HD13	1:916:A:ASN:HA	8	0.12
(1,683)	1:906:A:LYS:HB2	1:907:A:SER:HB2	2	0.12
(1,683)	1:906:A:LYS:HB2	1:907:A:SER:HB3	2	0.12
(1,683)	1:906:A:LYS:HB3	1:907:A:SER:HB2	2	0.12
(1,683)	1:906:A:LYS:HB3	1:907:A:SER:HB3	2	0.12
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	1	0.12
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	1	0.12
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	6	0.12
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	6	0.12
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	13	0.12
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	13	0.12
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	16	0.12
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	16	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	18	0.12
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	18	0.12
(1,648)	1:903:A:ASP:HA	1:906:A:LYS:H	1	0.12
(1,648)	1:903:A:ASP:HA	1:906:A:LYS:H	16	0.12
(1,646)	1:903:A:ASP:HA	1:904:A:CYS:HA	20	0.12
(1,633)	1:902:A:ALA:H	1:903:A:ASP:H	9	0.12
(1,631)	1:901:A:PHE:HD1	1:909:A:GLU:H	19	0.12
(1,631)	1:901:A:PHE:HD2	1:909:A:GLU:H	19	0.12
(1,628)	1:901:A:PHE:HA	1:907:A:SER:H	7	0.12
(1,628)	1:901:A:PHE:HA	1:907:A:SER:H	9	0.12
(1,623)	1:901:A:PHE:HA	1:902:A:ALA:H	5	0.12
(1,623)	1:901:A:PHE:HA	1:902:A:ALA:H	11	0.12
(1,623)	1:901:A:PHE:HA	1:902:A:ALA:H	17	0.12
(1,560)	1:896:A:ASN:HB2	1:902:A:ALA:H	7	0.12
(1,560)	1:896:A:ASN:HB3	1:902:A:ALA:H	7	0.12
(1,520)	1:893:A:CYS:HA	1:895:A:ASN:H	10	0.12
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	1	0.12
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	2	0.12
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	5	0.12
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	6	0.12
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	9	0.12
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	10	0.12
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	18	0.12
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	19	0.12
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	20	0.12
(1,473)	1:890:A:ARG:HB2	1:891:A:TRP:H	1	0.12
(1,473)	1:890:A:ARG:HB3	1:891:A:TRP:H	1	0.12
(1,446)	1:886:A:ASP:HB2	1:888:A:SER:H	2	0.12
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA2	9	0.12
(1,409)	1:882:A:VAL:HG11	1:883:A:GLY:HA3	9	0.12
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA2	9	0.12
(1,409)	1:882:A:VAL:HG12	1:883:A:GLY:HA3	9	0.12
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA2	9	0.12
(1,409)	1:882:A:VAL:HG13	1:883:A:GLY:HA3	9	0.12
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA2	9	0.12
(1,409)	1:882:A:VAL:HG21	1:883:A:GLY:HA3	9	0.12
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA2	9	0.12
(1,409)	1:882:A:VAL:HG22	1:883:A:GLY:HA3	9	0.12
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA2	9	0.12
(1,409)	1:882:A:VAL:HG23	1:883:A:GLY:HA3	9	0.12
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	3	0.12
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	3	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	3	0.12
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	3	0.12
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	3	0.12
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	3	0.12
(1,393)	1:881:A:VAL:HG11	1:885:A:ILE:H	11	0.12
(1,393)	1:881:A:VAL:HG12	1:885:A:ILE:H	11	0.12
(1,393)	1:881:A:VAL:HG13	1:885:A:ILE:H	11	0.12
(1,393)	1:881:A:VAL:HG21	1:885:A:ILE:H	11	0.12
(1,393)	1:881:A:VAL:HG22	1:885:A:ILE:H	11	0.12
(1,393)	1:881:A:VAL:HG23	1:885:A:ILE:H	11	0.12
(1,389)	1:881:A:VAL:HA	1:883:A:GLY:H	9	0.12
(1,389)	1:881:A:VAL:HA	1:883:A:GLY:H	14	0.12
(1,389)	1:881:A:VAL:HA	1:883:A:GLY:H	15	0.12
(1,350)	1:877:A:ILE:HD11	1:881:A:VAL:HG11	20	0.12
(1,350)	1:877:A:ILE:HD11	1:881:A:VAL:HG12	20	0.12
(1,350)	1:877:A:ILE:HD11	1:881:A:VAL:HG13	20	0.12
(1,350)	1:877:A:ILE:HD11	1:881:A:VAL:HG21	20	0.12
(1,350)	1:877:A:ILE:HD11	1:881:A:VAL:HG22	20	0.12
(1,350)	1:877:A:ILE:HD11	1:881:A:VAL:HG23	20	0.12
(1,350)	1:877:A:ILE:HD12	1:881:A:VAL:HG11	20	0.12
(1,350)	1:877:A:ILE:HD12	1:881:A:VAL:HG12	20	0.12
(1,350)	1:877:A:ILE:HD12	1:881:A:VAL:HG13	20	0.12
(1,350)	1:877:A:ILE:HD12	1:881:A:VAL:HG21	20	0.12
(1,350)	1:877:A:ILE:HD12	1:881:A:VAL:HG22	20	0.12
(1,350)	1:877:A:ILE:HD12	1:881:A:VAL:HG23	20	0.12
(1,350)	1:877:A:ILE:HD13	1:881:A:VAL:HG11	20	0.12
(1,350)	1:877:A:ILE:HD13	1:881:A:VAL:HG12	20	0.12
(1,350)	1:877:A:ILE:HD13	1:881:A:VAL:HG13	20	0.12
(1,350)	1:877:A:ILE:HD13	1:881:A:VAL:HG21	20	0.12
(1,350)	1:877:A:ILE:HD13	1:881:A:VAL:HG22	20	0.12
(1,350)	1:877:A:ILE:HD13	1:881:A:VAL:HG23	20	0.12
(1,338)	1:876:A:ARG:HA	1:876:A:ARG:HD2	17	0.12
(1,338)	1:876:A:ARG:HA	1:876:A:ARG:HD3	17	0.12
(1,325)	1:874:A:TRP:HB2	1:915:A:ILE:HG21	5	0.12
(1,325)	1:874:A:TRP:HB2	1:915:A:ILE:HG22	5	0.12
(1,325)	1:874:A:TRP:HB2	1:915:A:ILE:HG23	5	0.12
(1,325)	1:874:A:TRP:HB3	1:915:A:ILE:HG21	5	0.12
(1,325)	1:874:A:TRP:HB3	1:915:A:ILE:HG22	5	0.12
(1,325)	1:874:A:TRP:HB3	1:915:A:ILE:HG23	5	0.12
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB2	6	0.12
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB3	6	0.12
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB2	14	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB3	14	0.12
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB2	19	0.12
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB3	19	0.12
(1,305)	1:874:A:TRP:HE1	1:923:A:GLN:HG2	2	0.12
(1,305)	1:874:A:TRP:HE1	1:923:A:GLN:HG3	2	0.12
(1,289)	1:873:A:LYS:HE2	1:901:A:PHE:HB2	13	0.12
(1,289)	1:873:A:LYS:HE2	1:901:A:PHE:HB3	13	0.12
(1,289)	1:873:A:LYS:HE3	1:901:A:PHE:HB2	13	0.12
(1,289)	1:873:A:LYS:HE3	1:901:A:PHE:HB3	13	0.12
(1,269)	1:871:A:CYS:H	1:872:A:PHE:H	9	0.12
(1,255)	1:870:A:ASP:H	1:872:A:PHE:H	9	0.12
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM1	1	0.12
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM2	1	0.12
(1,216)	1:867:A:ARG:HG2	2:4:B:MLZ:HCM3	1	0.12
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM1	1	0.12
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM2	1	0.12
(1,216)	1:867:A:ARG:HG3	2:4:B:MLZ:HCM3	1	0.12
(1,200)	1:867:A:ARG:HE	1:872:A:PHE:HB2	20	0.12
(1,200)	1:867:A:ARG:HE	1:872:A:PHE:HB3	20	0.12
(1,193)	1:867:A:ARG:H	2:4:B:MLZ:H	7	0.12
(1,137)	1:865:A:TRP:HH2	1:909:A:GLU:H	10	0.12
(1,116)	1:865:A:TRP:HA	1:875:A:ARG:H	7	0.12
(1,116)	1:865:A:TRP:HA	1:875:A:ARG:H	12	0.12
(1,116)	1:865:A:TRP:HA	1:875:A:ARG:H	19	0.12
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG11	14	0.12
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG12	14	0.12
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG13	14	0.12
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG21	14	0.12
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG22	14	0.12
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG23	14	0.12
(1,109)	1:865:A:TRP:H	2:5:B:GLN:HA	17	0.12
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB2	7	0.12
(1,107)	1:865:A:TRP:H	2:4:B:MLZ:HB3	7	0.12
(1,89)	1:864:A:ALA:H	1:879:A:ALA:H	4	0.12
(1,67)	1:862:A:GLU:H	1:862:A:GLU:HG2	3	0.12
(1,67)	1:862:A:GLU:H	1:862:A:GLU:HG3	3	0.12
(1,61)	1:861:A:THR:HA	1:862:A:GLU:H	17	0.12
(1,52)	1:859:A:GLU:HB2	1:860:A:PHE:H	4	0.12
(1,52)	1:859:A:GLU:HB3	1:860:A:PHE:H	4	0.12
(1,45)	1:858:A:SER:HB2	1:859:A:GLU:H	14	0.12
(1,45)	1:858:A:SER:HB3	1:859:A:GLU:H	14	0.12
(1,42)	1:858:A:SER:H	1:859:A:GLU:H	9	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:858:A:SER:H	1:859:A:GLU:H	20	0.12
(1,7)	1:852:A:ARG:H	1:853:A:ARG:H	1	0.12
(2,8)	1:904:A:CYS:SG	3:1001:A:ZN:ZN	16	0.11
(2,6)	1:893:A:CYS:SG	3:1001:A:ZN:ZN	5	0.11
(2,5)	1:893:A:CYS:CB	3:1001:A:ZN:ZN	2	0.11
(2,5)	1:893:A:CYS:CB	3:1001:A:ZN:ZN	3	0.11
(2,5)	1:893:A:CYS:CB	3:1001:A:ZN:ZN	19	0.11
(1,937)	2:8:B:ARG:H	2:9:B:TYR:H	7	0.11
(1,937)	2:8:B:ARG:H	2:9:B:TYR:H	10	0.11
(1,929)	2:5:B:GLN:H	2:6:B:THR:H	12	0.11
(1,926)	2:2:B:ARG:HE	2:3:B:THR:HA	15	0.11
(1,918)	1:926:A:ALA:HA	1:928:A:ALA:H	10	0.11
(1,912)	1:925:A:GLU:HB2	1:926:A:ALA:H	9	0.11
(1,912)	1:925:A:GLU:HB2	1:926:A:ALA:H	17	0.11
(1,904)	1:924:A:ASP:H	1:925:A:GLU:H	4	0.11
(1,895)	1:923:A:GLN:HE21	2:3:B:THR:HA	1	0.11
(1,888)	1:922:A:GLY:H	1:923:A:GLN:H	12	0.11
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE21	8	0.11
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE22	8	0.11
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE21	8	0.11
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE22	8	0.11
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE21	9	0.11
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE22	9	0.11
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE21	9	0.11
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE22	9	0.11
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE21	12	0.11
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE22	12	0.11
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE21	12	0.11
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE22	12	0.11
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE21	19	0.11
(1,799)	1:915:A:ILE:HG12	1:923:A:GLN:HE22	19	0.11
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE21	19	0.11
(1,799)	1:915:A:ILE:HG13	1:923:A:GLN:HE22	19	0.11
(1,744)	1:911:A:SER:HA	1:913:A:GLU:H	5	0.11
(1,734)	1:910:A:MET:HB2	1:911:A:SER:H	20	0.11
(1,734)	1:910:A:MET:HB3	1:911:A:SER:H	20	0.11
(1,698)	1:908:A:GLN:HA	1:910:A:MET:H	19	0.11
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	3	0.11
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	3	0.11
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	10	0.11
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	10	0.11
(1,648)	1:903:A:ASP:HA	1:906:A:LYS:H	5	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,648)	1:903:A:ASP:HA	1:906:A:LYS:H	10	0.11
(1,646)	1:903:A:ASP:HA	1:904:A:CYS:HA	9	0.11
(1,633)	1:902:A:ALA:H	1:903:A:ASP:H	20	0.11
(1,631)	1:901:A:PHE:HD1	1:909:A:GLU:H	8	0.11
(1,631)	1:901:A:PHE:HD2	1:909:A:GLU:H	8	0.11
(1,623)	1:901:A:PHE:HA	1:902:A:ALA:H	12	0.11
(1,560)	1:896:A:ASN:HB2	1:902:A:ALA:H	12	0.11
(1,560)	1:896:A:ASN:HB3	1:902:A:ALA:H	12	0.11
(1,560)	1:896:A:ASN:HB2	1:902:A:ALA:H	20	0.11
(1,560)	1:896:A:ASN:HB3	1:902:A:ALA:H	20	0.11
(1,539)	1:895:A:ASN:HB2	1:896:A:ASN:H	6	0.11
(1,539)	1:895:A:ASN:HB3	1:896:A:ASN:H	6	0.11
(1,539)	1:895:A:ASN:HB2	1:896:A:ASN:H	8	0.11
(1,539)	1:895:A:ASN:HB3	1:896:A:ASN:H	8	0.11
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	4	0.11
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	8	0.11
(1,501)	1:892:A:ILE:HD11	1:894:A:MET:H	1	0.11
(1,501)	1:892:A:ILE:HD12	1:894:A:MET:H	1	0.11
(1,501)	1:892:A:ILE:HD13	1:894:A:MET:H	1	0.11
(1,501)	1:892:A:ILE:HD11	1:894:A:MET:H	18	0.11
(1,501)	1:892:A:ILE:HD12	1:894:A:MET:H	18	0.11
(1,501)	1:892:A:ILE:HD13	1:894:A:MET:H	18	0.11
(1,492)	1:892:A:ILE:H	1:893:A:CYS:H	12	0.11
(1,454)	1:887:A:GLU:HB2	1:888:A:SER:H	14	0.11
(1,454)	1:887:A:GLU:HB3	1:888:A:SER:H	14	0.11
(1,446)	1:886:A:ASP:HB2	1:888:A:SER:H	16	0.11
(1,430)	1:885:A:ILE:HG12	1:891:A:TRP:HA	6	0.11
(1,430)	1:885:A:ILE:HG13	1:891:A:TRP:HA	6	0.11
(1,430)	1:885:A:ILE:HG12	1:891:A:TRP:HA	8	0.11
(1,430)	1:885:A:ILE:HG13	1:891:A:TRP:HA	8	0.11
(1,430)	1:885:A:ILE:HG12	1:891:A:TRP:HA	9	0.11
(1,430)	1:885:A:ILE:HG13	1:891:A:TRP:HA	9	0.11
(1,429)	1:885:A:ILE:HG12	1:891:A:TRP:H	5	0.11
(1,429)	1:885:A:ILE:HG13	1:891:A:TRP:H	5	0.11
(1,426)	1:885:A:ILE:HD11	1:891:A:TRP:HE1	3	0.11
(1,426)	1:885:A:ILE:HD12	1:891:A:TRP:HE1	3	0.11
(1,426)	1:885:A:ILE:HD13	1:891:A:TRP:HE1	3	0.11
(1,426)	1:885:A:ILE:HD11	1:891:A:TRP:HE1	15	0.11
(1,426)	1:885:A:ILE:HD12	1:891:A:TRP:HE1	15	0.11
(1,426)	1:885:A:ILE:HD13	1:891:A:TRP:HE1	15	0.11
(1,389)	1:881:A:VAL:HA	1:883:A:GLY:H	7	0.11
(1,389)	1:881:A:VAL:HA	1:883:A:GLY:H	11	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,389)	1:881:A:VAL:HA	1:883:A:GLY:H	16	0.11
(1,389)	1:881:A:VAL:HA	1:883:A:GLY:H	19	0.11
(1,385)	1:881:A:VAL:H	1:882:A:VAL:HA	18	0.11
(1,338)	1:876:A:ARG:HA	1:876:A:ARG:HD2	19	0.11
(1,338)	1:876:A:ARG:HA	1:876:A:ARG:HD3	19	0.11
(1,320)	1:874:A:TRP:HZ3	2:2:B:ARG:HG2	2	0.11
(1,320)	1:874:A:TRP:HZ3	2:2:B:ARG:HG3	2	0.11
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB2	3	0.11
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB3	3	0.11
(1,308)	1:874:A:TRP:HH2	2:2:B:ARG:HG2	2	0.11
(1,308)	1:874:A:TRP:HH2	2:2:B:ARG:HG3	2	0.11
(1,305)	1:874:A:TRP:HE1	1:923:A:GLN:HG2	20	0.11
(1,305)	1:874:A:TRP:HE1	1:923:A:GLN:HG3	20	0.11
(1,298)	1:874:A:TRP:HB2	1:875:A:ARG:H	5	0.11
(1,298)	1:874:A:TRP:HB2	1:875:A:ARG:H	6	0.11
(1,298)	1:874:A:TRP:HB2	1:875:A:ARG:H	16	0.11
(1,298)	1:874:A:TRP:HB2	1:875:A:ARG:H	17	0.11
(1,298)	1:874:A:TRP:HB2	1:875:A:ARG:H	18	0.11
(1,292)	1:873:A:LYS:HG2	1:874:A:TRP:H	15	0.11
(1,292)	1:873:A:LYS:HG3	1:874:A:TRP:H	15	0.11
(1,289)	1:873:A:LYS:HE2	1:901:A:PHE:HB2	19	0.11
(1,289)	1:873:A:LYS:HE2	1:901:A:PHE:HB3	19	0.11
(1,289)	1:873:A:LYS:HE3	1:901:A:PHE:HB2	19	0.11
(1,289)	1:873:A:LYS:HE3	1:901:A:PHE:HB3	19	0.11
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD2	17	0.11
(1,278)	1:873:A:LYS:HA	1:873:A:LYS:HD3	17	0.11
(1,255)	1:870:A:ASP:H	1:872:A:PHE:H	17	0.11
(1,251)	1:869:A:ASP:HB2	1:891:A:TRP:H	3	0.11
(1,251)	1:869:A:ASP:HB3	1:891:A:TRP:H	3	0.11
(1,219)	1:868:A:CYS:H	1:872:A:PHE:HA	9	0.11
(1,215)	1:867:A:ARG:HG2	1:874:A:TRP:HZ2	1	0.11
(1,215)	1:867:A:ARG:HG3	1:874:A:TRP:HZ2	1	0.11
(1,215)	1:867:A:ARG:HG2	1:874:A:TRP:HZ2	10	0.11
(1,215)	1:867:A:ARG:HG3	1:874:A:TRP:HZ2	10	0.11
(1,214)	1:867:A:ARG:HG2	1:874:A:TRP:HE1	5	0.11
(1,214)	1:867:A:ARG:HG3	1:874:A:TRP:HE1	5	0.11
(1,214)	1:867:A:ARG:HG2	1:874:A:TRP:HE1	10	0.11
(1,214)	1:867:A:ARG:HG3	1:874:A:TRP:HE1	10	0.11
(1,209)	1:867:A:ARG:HD2	2:3:B:THR:HA	3	0.11
(1,209)	1:867:A:ARG:HD3	2:3:B:THR:HA	3	0.11
(1,209)	1:867:A:ARG:HD2	2:3:B:THR:HA	4	0.11
(1,209)	1:867:A:ARG:HD3	2:3:B:THR:HA	4	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:867:A:ARG:HD2	2:3:B:THR:HA	7	0.11
(1,209)	1:867:A:ARG:HD3	2:3:B:THR:HA	7	0.11
(1,209)	1:867:A:ARG:HD2	2:3:B:THR:HA	11	0.11
(1,209)	1:867:A:ARG:HD3	2:3:B:THR:HA	11	0.11
(1,209)	1:867:A:ARG:HD2	2:3:B:THR:HA	20	0.11
(1,209)	1:867:A:ARG:HD3	2:3:B:THR:HA	20	0.11
(1,208)	1:867:A:ARG:HD2	2:2:B:ARG:HG2	10	0.11
(1,208)	1:867:A:ARG:HD2	2:2:B:ARG:HG3	10	0.11
(1,208)	1:867:A:ARG:HD3	2:2:B:ARG:HG2	10	0.11
(1,208)	1:867:A:ARG:HD3	2:2:B:ARG:HG3	10	0.11
(1,193)	1:867:A:ARG:H	2:4:B:MLZ:H	4	0.11
(1,170)	1:866:A:VAL:HG11	1:868:A:CYS:H	1	0.11
(1,170)	1:866:A:VAL:HG12	1:868:A:CYS:H	1	0.11
(1,170)	1:866:A:VAL:HG13	1:868:A:CYS:H	1	0.11
(1,170)	1:866:A:VAL:HG21	1:868:A:CYS:H	1	0.11
(1,170)	1:866:A:VAL:HG22	1:868:A:CYS:H	1	0.11
(1,170)	1:866:A:VAL:HG23	1:868:A:CYS:H	1	0.11
(1,170)	1:866:A:VAL:HG11	1:868:A:CYS:H	15	0.11
(1,170)	1:866:A:VAL:HG12	1:868:A:CYS:H	15	0.11
(1,170)	1:866:A:VAL:HG13	1:868:A:CYS:H	15	0.11
(1,170)	1:866:A:VAL:HG21	1:868:A:CYS:H	15	0.11
(1,170)	1:866:A:VAL:HG22	1:868:A:CYS:H	15	0.11
(1,170)	1:866:A:VAL:HG23	1:868:A:CYS:H	15	0.11
(1,170)	1:866:A:VAL:HG11	1:868:A:CYS:H	17	0.11
(1,170)	1:866:A:VAL:HG12	1:868:A:CYS:H	17	0.11
(1,170)	1:866:A:VAL:HG13	1:868:A:CYS:H	17	0.11
(1,170)	1:866:A:VAL:HG21	1:868:A:CYS:H	17	0.11
(1,170)	1:866:A:VAL:HG22	1:868:A:CYS:H	17	0.11
(1,170)	1:866:A:VAL:HG23	1:868:A:CYS:H	17	0.11
(1,162)	1:866:A:VAL:HB	1:885:A:ILE:HG12	5	0.11
(1,162)	1:866:A:VAL:HB	1:885:A:ILE:HG13	5	0.11
(1,140)	1:865:A:TRP:HZ3	1:910:A:MET:H	16	0.11
(1,137)	1:865:A:TRP:HH2	1:909:A:GLU:H	9	0.11
(1,132)	1:865:A:TRP:HE1	2:6:B:THR:HA	15	0.11
(1,122)	1:865:A:TRP:HB2	1:874:A:TRP:HE3	2	0.11
(1,116)	1:865:A:TRP:HA	1:875:A:ARG:H	3	0.11
(1,116)	1:865:A:TRP:HA	1:875:A:ARG:H	6	0.11
(1,116)	1:865:A:TRP:HA	1:875:A:ARG:H	8	0.11
(1,116)	1:865:A:TRP:HA	1:875:A:ARG:H	10	0.11
(1,116)	1:865:A:TRP:HA	1:875:A:ARG:H	20	0.11
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG11	18	0.11
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG12	18	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG13	18	0.11
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG21	18	0.11
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG22	18	0.11
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG23	18	0.11
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG11	7	0.11
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG12	7	0.11
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG13	7	0.11
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG21	7	0.11
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG22	7	0.11
(1,104)	1:865:A:TRP:H	1:882:A:VAL:HG23	7	0.11
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG11	15	0.11
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG12	15	0.11
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG13	15	0.11
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG21	15	0.11
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG22	15	0.11
(1,93)	1:864:A:ALA:HA	1:882:A:VAL:HG23	15	0.11
(1,89)	1:864:A:ALA:H	1:879:A:ALA:H	6	0.11
(1,89)	1:864:A:ALA:H	1:879:A:ALA:H	16	0.11
(1,89)	1:864:A:ALA:H	1:879:A:ALA:H	18	0.11
(1,73)	1:862:A:GLU:HB2	1:863:A:SER:H	3	0.11
(1,73)	1:862:A:GLU:HB3	1:863:A:SER:H	3	0.11
(1,63)	1:861:A:THR:HG21	1:862:A:GLU:H	19	0.11
(1,63)	1:861:A:THR:HG22	1:862:A:GLU:H	19	0.11
(1,63)	1:861:A:THR:HG23	1:862:A:GLU:H	19	0.11
(1,52)	1:859:A:GLU:HB2	1:860:A:PHE:H	15	0.11
(1,52)	1:859:A:GLU:HB3	1:860:A:PHE:H	15	0.11
(1,42)	1:858:A:SER:H	1:859:A:GLU:H	12	0.11
(1,39)	1:857:A:GLY:H	1:858:A:SER:H	6	0.11
(1,39)	1:857:A:GLY:H	1:858:A:SER:H	17	0.11
(1,1)	1:851:A:SER:HA	1:852:A:ARG:H	1	0.11
(2,7)	1:904:A:CYS:CB	3:1001:A:ZN:ZN	6	0.1
(2,7)	1:904:A:CYS:CB	3:1001:A:ZN:ZN	13	0.1
(2,7)	1:904:A:CYS:CB	3:1001:A:ZN:ZN	14	0.1
(2,7)	1:904:A:CYS:CB	3:1001:A:ZN:ZN	17	0.1
(2,5)	1:893:A:CYS:CB	3:1001:A:ZN:ZN	1	0.1
(2,5)	1:893:A:CYS:CB	3:1001:A:ZN:ZN	4	0.1
(2,5)	1:893:A:CYS:CB	3:1001:A:ZN:ZN	8	0.1
(2,3)	1:871:A:CYS:CB	3:1001:A:ZN:ZN	4	0.1
(2,3)	1:871:A:CYS:CB	3:1001:A:ZN:ZN	12	0.1
(2,3)	1:871:A:CYS:CB	3:1001:A:ZN:ZN	16	0.1
(1,926)	2:2:B:ARG:HE	2:3:B:THR:HA	14	0.1
(1,912)	1:925:A:GLU:HB2	1:926:A:ALA:H	15	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,909)	1:925:A:GLU:H	1:926:A:ALA:H	19	0.1
(1,905)	1:924:A:ASP:HA	1:926:A:ALA:H	10	0.1
(1,852)	1:919:A:LEU:HG	1:920:A:GLY:H	5	0.1
(1,844)	1:918:A:GLU:HG2	2:8:B:ARG:HB2	18	0.1
(1,844)	1:918:A:GLU:HG2	2:8:B:ARG:HB3	18	0.1
(1,844)	1:918:A:GLU:HG3	2:8:B:ARG:HB2	18	0.1
(1,844)	1:918:A:GLU:HG3	2:8:B:ARG:HB3	18	0.1
(1,792)	1:915:A:ILE:HD11	1:916:A:ASN:HA	16	0.1
(1,792)	1:915:A:ILE:HD12	1:916:A:ASN:HA	16	0.1
(1,792)	1:915:A:ILE:HD13	1:916:A:ASN:HA	16	0.1
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB2	19	0.1
(1,663)	1:905:A:SER:H	1:906:A:LYS:HB3	19	0.1
(1,631)	1:901:A:PHE:HD1	1:909:A:GLU:H	5	0.1
(1,631)	1:901:A:PHE:HD2	1:909:A:GLU:H	5	0.1
(1,631)	1:901:A:PHE:HD1	1:909:A:GLU:H	7	0.1
(1,631)	1:901:A:PHE:HD2	1:909:A:GLU:H	7	0.1
(1,628)	1:901:A:PHE:HA	1:907:A:SER:H	4	0.1
(1,628)	1:901:A:PHE:HA	1:907:A:SER:H	8	0.1
(1,628)	1:901:A:PHE:HA	1:907:A:SER:H	16	0.1
(1,623)	1:901:A:PHE:HA	1:902:A:ALA:H	14	0.1
(1,565)	1:896:A:ASN:HD21	1:901:A:PHE:HA	2	0.1
(1,565)	1:896:A:ASN:HD22	1:901:A:PHE:HA	2	0.1
(1,565)	1:896:A:ASN:HD21	1:901:A:PHE:HA	4	0.1
(1,565)	1:896:A:ASN:HD22	1:901:A:PHE:HA	4	0.1
(1,519)	1:893:A:CYS:HA	1:894:A:MET:H	7	0.1
(1,456)	1:887:A:GLU:HG2	1:888:A:SER:H	15	0.1
(1,456)	1:887:A:GLU:HG3	1:888:A:SER:H	15	0.1
(1,444)	1:886:A:ASP:HA	1:889:A:SER:HB2	20	0.1
(1,444)	1:886:A:ASP:HA	1:889:A:SER:HB3	20	0.1
(1,405)	1:882:A:VAL:HA	1:885:A:ILE:H	8	0.1
(1,389)	1:881:A:VAL:HA	1:883:A:GLY:H	1	0.1
(1,389)	1:881:A:VAL:HA	1:883:A:GLY:H	2	0.1
(1,389)	1:881:A:VAL:HA	1:883:A:GLY:H	13	0.1
(1,385)	1:881:A:VAL:H	1:882:A:VAL:HA	14	0.1
(1,378)	1:880:A:SER:H	1:882:A:VAL:H	10	0.1
(1,378)	1:880:A:SER:H	1:882:A:VAL:H	15	0.1
(1,339)	1:876:A:ARG:HA	1:876:A:ARG:HG2	20	0.1
(1,339)	1:876:A:ARG:HA	1:876:A:ARG:HG3	20	0.1
(1,315)	1:874:A:TRP:HZ2	1:923:A:GLN:HB2	15	0.1
(1,315)	1:874:A:TRP:HZ2	1:923:A:GLN:HB3	15	0.1
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB2	17	0.1
(1,314)	1:874:A:TRP:HZ2	1:912:A:ASN:HB3	17	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:874:A:TRP:HB2	1:875:A:ARG:H	13	0.1
(1,289)	1:873:A:LYS:HE2	1:901:A:PHE:HB2	17	0.1
(1,289)	1:873:A:LYS:HE2	1:901:A:PHE:HB3	17	0.1
(1,289)	1:873:A:LYS:HE3	1:901:A:PHE:HB2	17	0.1
(1,289)	1:873:A:LYS:HE3	1:901:A:PHE:HB3	17	0.1
(1,265)	1:870:A:ASP:HB2	1:871:A:CYS:H	6	0.1
(1,265)	1:870:A:ASP:HB3	1:871:A:CYS:H	6	0.1
(1,245)	1:869:A:ASP:HB2	1:870:A:ASP:HA	10	0.1
(1,214)	1:867:A:ARG:HG2	1:874:A:TRP:HE1	14	0.1
(1,214)	1:867:A:ARG:HG3	1:874:A:TRP:HE1	14	0.1
(1,200)	1:867:A:ARG:HE	1:872:A:PHE:HB2	7	0.1
(1,200)	1:867:A:ARG:HE	1:872:A:PHE:HB3	7	0.1
(1,200)	1:867:A:ARG:HE	1:872:A:PHE:HB2	18	0.1
(1,200)	1:867:A:ARG:HE	1:872:A:PHE:HB3	18	0.1
(1,170)	1:866:A:VAL:HG11	1:868:A:CYS:H	13	0.1
(1,170)	1:866:A:VAL:HG12	1:868:A:CYS:H	13	0.1
(1,170)	1:866:A:VAL:HG13	1:868:A:CYS:H	13	0.1
(1,170)	1:866:A:VAL:HG21	1:868:A:CYS:H	13	0.1
(1,170)	1:866:A:VAL:HG22	1:868:A:CYS:H	13	0.1
(1,170)	1:866:A:VAL:HG23	1:868:A:CYS:H	13	0.1
(1,139)	1:865:A:TRP:HZ2	1:915:A:ILE:HA	9	0.1
(1,129)	1:865:A:TRP:HE1	1:918:A:GLU:HB2	6	0.1
(1,129)	1:865:A:TRP:HE1	1:918:A:GLU:HB3	6	0.1
(1,129)	1:865:A:TRP:HE1	1:918:A:GLU:HB2	7	0.1
(1,129)	1:865:A:TRP:HE1	1:918:A:GLU:HB3	7	0.1
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG11	8	0.1
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG12	8	0.1
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG13	8	0.1
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG21	8	0.1
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG22	8	0.1
(1,115)	1:865:A:TRP:HA	1:866:A:VAL:HG23	8	0.1
(1,89)	1:864:A:ALA:H	1:879:A:ALA:H	5	0.1
(1,61)	1:861:A:THR:HA	1:862:A:GLU:H	10	0.1
(1,42)	1:858:A:SER:H	1:859:A:GLU:H	16	0.1

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

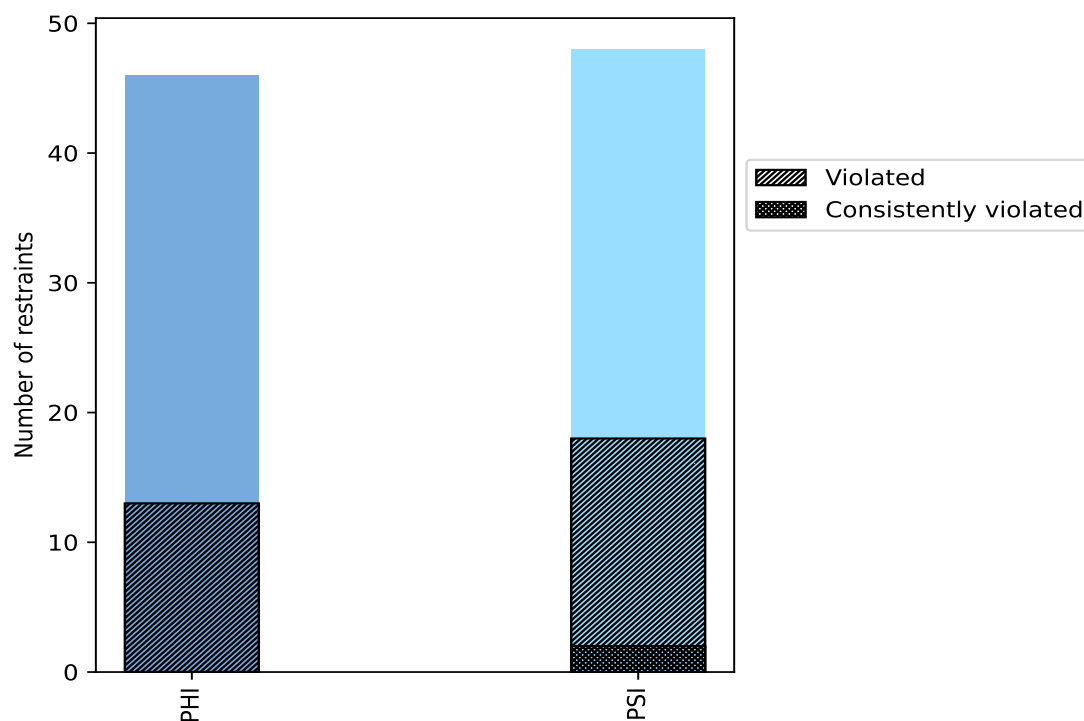
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	46	48.9	13	28.3	13.8	0	0.0	0.0
PSI	48	51.1	18	37.5	19.1	2	4.2	2.1
Total	94	100.0	31	33.0	33.0	2	2.1	2.1

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

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



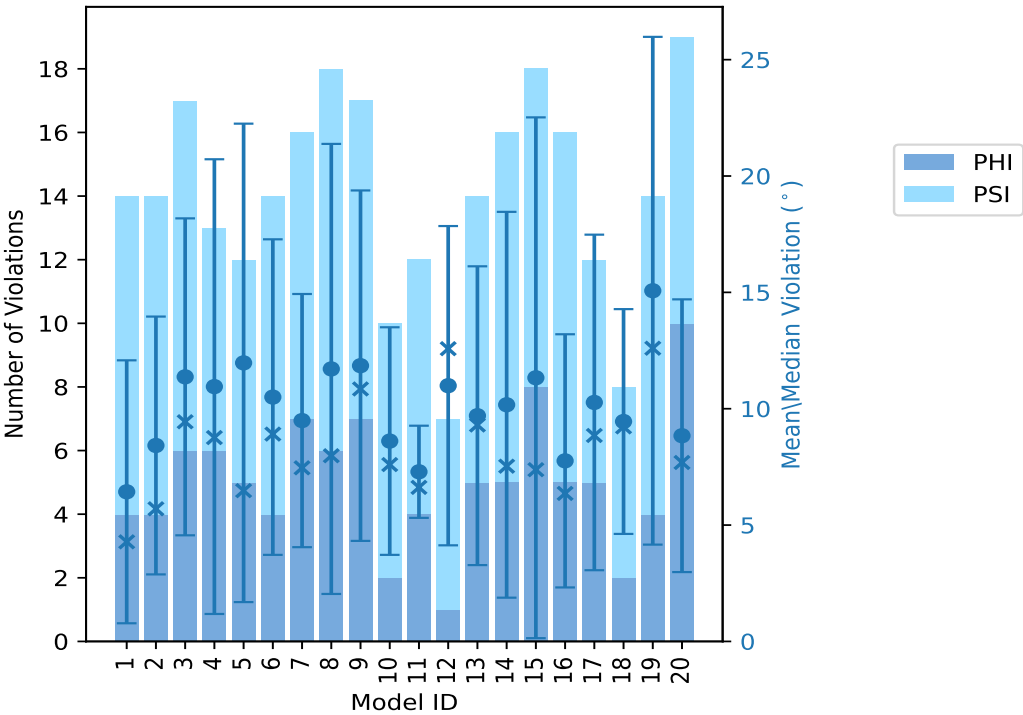
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	4	10	14	6.43	20.78	5.65	4.28
2	4	10	14	8.42	19.33	5.54	5.7
3	6	11	17	11.37	31.3	6.81	9.44
4	6	7	13	10.95	38.94	9.77	8.76
5	5	7	12	11.97	28.89	10.28	6.48
6	4	10	14	10.5	24.72	6.78	8.91
7	7	9	16	9.49	25.03	5.44	7.46
8	6	12	18	11.71	35.27	9.67	7.98
9	7	10	17	11.85	26.24	7.53	10.85
10	2	8	10	8.61	17.63	4.89	7.6
11	4	8	12	7.29	12.18	1.98	6.62
12	1	6	7	10.99	22.04	6.86	12.58
13	5	9	14	9.7	24.22	6.42	9.3
14	5	11	16	10.17	30.86	8.29	7.53
15	8	10	18	11.33	38.71	11.19	7.38
16	5	11	16	7.76	19.24	5.44	6.36
17	5	7	12	10.27	24.51	7.21	8.85
18	2	6	8	9.45	15.64	4.83	9.22
19	4	10	14	15.07	38.56	10.91	12.6
20	10	9	19	8.84	22.13	5.86	7.69

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



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

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

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

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

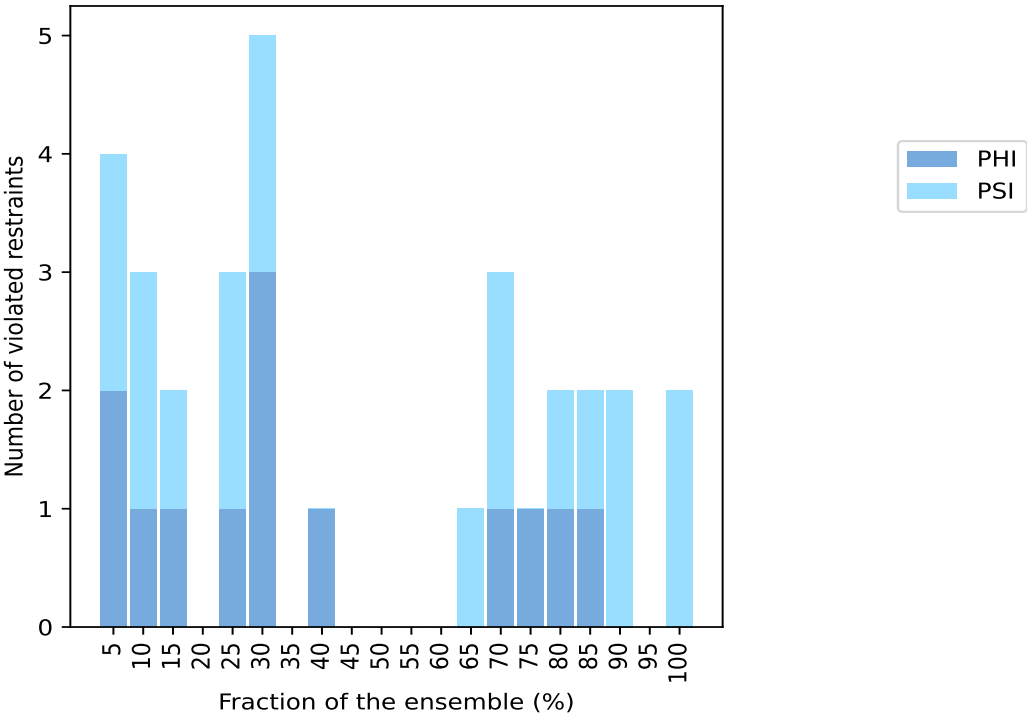
Continued on next page...

Continued from previous page...

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
0	1	1	13	65.0
1	2	3	14	70.0
1	0	1	15	75.0
1	1	2	16	80.0
1	1	2	17	85.0
0	2	2	18	90.0
0	0	0	19	95.0
0	2	2	20	100.0

¹ Number of models with violations

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

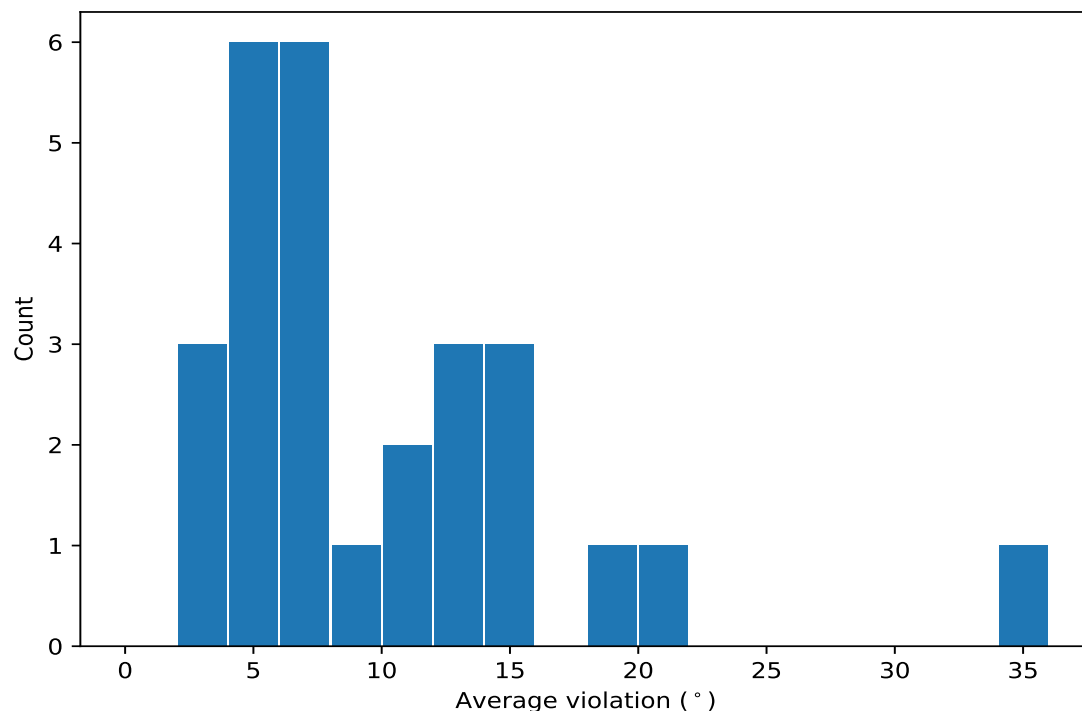


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	20	12.49	3.61	13.58
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	20	9.27	4.26	8.9
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	18	4.93	1.94	5.38
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	18	4.2	1.83	4.09
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	17	15.99	7.51	17.08
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	17	7.91	3.5	8.76
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	16	6.28	2.85	6.52
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	16	4.94	2.18	4.66
(1,69)	1:913:A:GLU:C	1:914:A:GLU:N	1:914:A:GLU:CA	1:914:A:GLU:C	15	15.92	7.52	15.47
(1,41)	1:889:A:SER:C	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	14	13.87	5.92	12.86
(1,40)	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	1:890:A:ARG:N	14	12.28	5.51	11.54
(1,68)	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	1:914:A:GLU:N	14	10.05	4.46	10.32
(1,42)	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	1:891:A:TRP:N	13	15.88	9.85	12.58
(1,33)	1:885:A:ILE:C	1:886:A:ASP:N	1:886:A:ASP:CA	1:886:A:ASP:C	8	10.49	8.72	6.79
(1,72)	1:915:A:ILE:N	1:915:A:ILE:CA	1:915:A:ILE:C	1:916:A:ASN:N	6	35.52	3.45	36.65
(1,73)	1:915:A:ILE:C	1:916:A:ASN:N	1:916:A:ASN:CA	1:916:A:ASN:C	6	19.84	5.81	20.73
(1,1)	1:862:A:GLU:C	1:863:A:SER:N	1:863:A:SER:CA	1:863:A:SER:C	6	5.86	4.9	4.26
(1,5)	1:864:A:ALA:C	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	6	5.07	2.25	5.36
(1,9)	1:867:A:ARG:N	1:867:A:ARG:CA	1:867:A:ARG:C	1:868:A:CYS:N	6	3.86	1.42	3.94
(1,37)	1:887:A:GLU:C	1:888:A:SER:N	1:888:A:SER:CA	1:888:A:SER:C	5	7.69	7.45	5.96

Continued on next page...

Continued from previous page...

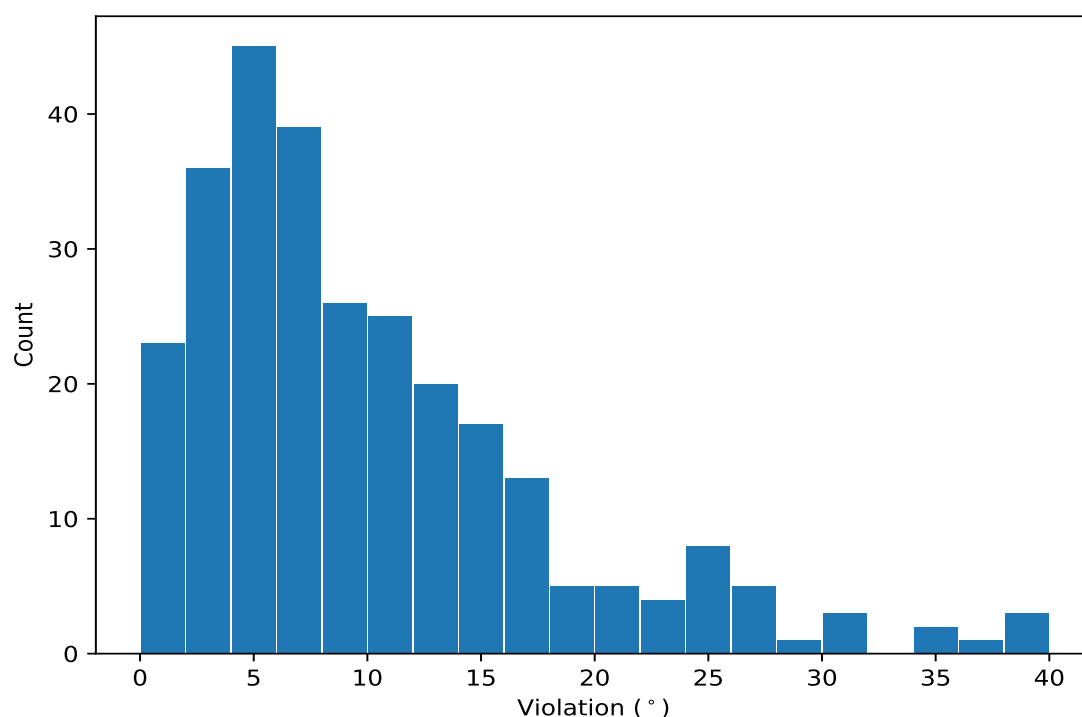
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,38)	1:888:A:SER:N	1:888:A:SER:CA	1:888:A:SER:C	1:889:A:SER:N	5	6.64	4.62	7.27
(1,82)	1:920:A:GLY:N	1:920:A:GLY:CA	1:920:A:GLY:C	1:921:A:ILE:N	5	3.68	3.07	1.77
(1,67)	1:912:A:ASN:C	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	3	6.25	4.25	3.39
(1,50)	1:897:A:SER:N	1:897:A:SER:CA	1:897:A:SER:C	1:898:A:ASP:N	3	2.78	1.2	2.22
(1,39)	1:888:A:SER:C	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	2	20.85	15.47	20.85
(1,17)	1:876:A:ARG:N	1:876:A:ARG:CA	1:876:A:ARG:C	1:877:A:ILE:N	2	7.42	1.6	7.42
(1,85)	1:870:A:ASP:N	1:870:A:ASP:CA	1:870:A:ASP:C	1:871:A:CYS:N	2	5.42	0.22	5.42

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

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,72)	1:915:A:ILE:N	1:915:A:ILE:CA	1:915:A:ILE:C	1:916:A:ASN:N	4	38.94

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,72)	1:915:A:ILE:N	1:915:A:ILE:CA	1:915:A:ILE:C	1:916:A:ASN:N	15	38.71
(1,72)	1:915:A:ILE:N	1:915:A:ILE:CA	1:915:A:ILE:C	1:916:A:ASN:N	19	38.56
(1,39)	1:888:A:SER:C	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	15	36.31
(1,42)	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	1:891:A:TRP:N	8	35.27
(1,72)	1:915:A:ILE:N	1:915:A:ILE:CA	1:915:A:ILE:C	1:916:A:ASN:N	8	34.74
(1,42)	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	1:891:A:TRP:N	19	31.75
(1,72)	1:915:A:ILE:N	1:915:A:ILE:CA	1:915:A:ILE:C	1:916:A:ASN:N	3	31.3
(1,72)	1:915:A:ILE:N	1:915:A:ILE:CA	1:915:A:ILE:C	1:916:A:ASN:N	14	30.86
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	5	28.89
(1,73)	1:915:A:ILE:C	1:916:A:ASN:N	1:916:A:ASN:CA	1:916:A:ASN:C	15	27.92
(1,33)	1:885:A:ILE:C	1:886:A:ASP:N	1:886:A:ASP:CA	1:886:A:ASP:C	5	27.67
(1,41)	1:889:A:SER:C	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	5	26.99
(1,69)	1:913:A:GLU:C	1:914:A:GLU:N	1:914:A:GLU:CA	1:914:A:GLU:C	9	26.24
(1,69)	1:913:A:GLU:C	1:914:A:GLU:N	1:914:A:GLU:CA	1:914:A:GLU:C	14	26.05
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	9	25.49
(1,69)	1:913:A:GLU:C	1:914:A:GLU:N	1:914:A:GLU:CA	1:914:A:GLU:C	7	25.03
(1,69)	1:913:A:GLU:C	1:914:A:GLU:N	1:914:A:GLU:CA	1:914:A:GLU:C	6	24.72
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	17	24.51
(1,41)	1:889:A:SER:C	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	13	24.22
(1,40)	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	1:890:A:ARG:N	19	24.15
(1,73)	1:915:A:ILE:C	1:916:A:ASN:N	1:916:A:ASN:CA	1:916:A:ASN:C	19	24.09
(1,42)	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	1:891:A:TRP:N	9	24.02
(1,42)	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	1:891:A:TRP:N	6	23.48
(1,73)	1:915:A:ILE:C	1:916:A:ASN:N	1:916:A:ASN:CA	1:916:A:ASN:C	4	23.23
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	20	22.13
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	12	22.04
(1,37)	1:887:A:GLU:C	1:888:A:SER:N	1:888:A:SER:CA	1:888:A:SER:C	3	21.76
(1,40)	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	1:890:A:ARG:N	5	20.96
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	1	20.78
(1,69)	1:913:A:GLU:C	1:914:A:GLU:N	1:914:A:GLU:CA	1:914:A:GLU:C	19	20.53
(1,69)	1:913:A:GLU:C	1:914:A:GLU:N	1:914:A:GLU:CA	1:914:A:GLU:C	17	20.45
(1,42)	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	1:891:A:TRP:N	2	19.33
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	16	19.24
(1,40)	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	1:890:A:ARG:N	8	19.07
(1,73)	1:915:A:ILE:C	1:916:A:ASN:N	1:916:A:ASN:CA	1:916:A:ASN:C	8	18.23
(1,33)	1:885:A:ILE:C	1:886:A:ASP:N	1:886:A:ASP:CA	1:886:A:ASP:C	9	18.08
(1,68)	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	1:914:A:GLU:N	6	17.91
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	10	17.63
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	14	17.44
(1,41)	1:889:A:SER:C	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	20	17.21
(1,41)	1:889:A:SER:C	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	8	17.15
(1,69)	1:913:A:GLU:C	1:914:A:GLU:N	1:914:A:GLU:CA	1:914:A:GLU:C	3	17.12
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	2	17.08
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	12	17.05
(1,33)	1:885:A:ILE:C	1:886:A:ASP:N	1:886:A:ASP:CA	1:886:A:ASP:C	15	16.68
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	10	16.55
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	7	16.46
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	17	16.13
(1,68)	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	1:914:A:GLU:N	14	16.03
(1,42)	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	1:891:A:TRP:N	18	15.64
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	18	15.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,69)	1:913:A:GLU:C	1:914:A:GLU:N	1:914:A:GLU:CA	1:914:A:GLU:C	20	15.47
(1,41)	1:889:A:SER:C	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	19	15.39
(1,68)	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	1:914:A:GLU:N	17	15.36
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	16	15.13
(1,1)	1:862:A:GLU:C	1:863:A:SER:N	1:863:A:SER:CA	1:863:A:SER:C	20	14.92
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	13	14.89
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	20	14.85
(1,41)	1:889:A:SER:C	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	2	14.82
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	13	14.7
(1,73)	1:915:A:ILE:C	1:916:A:ASN:N	1:916:A:ASN:CA	1:916:A:ASN:C	3	14.54
(1,69)	1:913:A:GLU:C	1:914:A:GLU:N	1:914:A:GLU:CA	1:914:A:GLU:C	8	14.39
(1,38)	1:888:A:SER:N	1:888:A:SER:CA	1:888:A:SER:C	1:889:A:SER:N	13	14.34
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	15	14.28
(1,41)	1:889:A:SER:C	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	16	14.25
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	19	14.01
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	12	13.91
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	13	13.91
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	1	13.9
(1,40)	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	1:890:A:ARG:N	13	13.78
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	7	13.61
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	4	13.56
(1,68)	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	1:914:A:GLU:N	9	13.54
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	2	13.47
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	1	13.38
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	16	13.29
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	18	13.26
(1,40)	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	1:890:A:ARG:N	3	12.9
(1,68)	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	1:914:A:GLU:N	20	12.89
(1,40)	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	1:890:A:ARG:N	9	12.89
(1,42)	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	1:891:A:TRP:N	12	12.58
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	3	12.4
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	4	12.32
(1,67)	1:912:A:ASN:C	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	9	12.26
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	11	12.18
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	14	12.04
(1,40)	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	1:890:A:ARG:N	17	11.87
(1,69)	1:913:A:GLU:C	1:914:A:GLU:N	1:914:A:GLU:CA	1:914:A:GLU:C	16	11.77
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	6	11.47
(1,41)	1:889:A:SER:C	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	9	11.46
(1,34)	1:886:A:ASP:N	1:886:A:ASP:CA	1:886:A:ASP:C	1:887:A:GLU:N	3	11.4
(1,68)	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	1:914:A:GLU:N	7	11.37
(1,69)	1:913:A:GLU:C	1:914:A:GLU:N	1:914:A:GLU:CA	1:914:A:GLU:C	2	11.35
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	18	11.32
(1,89)	1:890:A:ARG:C	1:891:A:TRP:N	1:891:A:TRP:CA	1:891:A:TRP:C	3	11.3
(1,40)	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	1:890:A:ARG:N	7	11.2
(1,68)	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	1:914:A:GLU:N	19	11.19
(1,73)	1:915:A:ILE:C	1:916:A:ASN:N	1:916:A:ASN:CA	1:916:A:ASN:C	14	11.05
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	20	11.03
(1,41)	1:889:A:SER:C	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	7	11.02
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	13	10.96
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	6	10.93

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	7	10.86
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	9	10.85
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	8	10.68
(1,41)	1:889:A:SER:C	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	17	10.43
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	6	10.41
(1,42)	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	1:891:A:TRP:N	10	10.4
(1,40)	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	1:890:A:ARG:N	20	10.17
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	15	10.09
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	1	10.05
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	9	9.85
(1,42)	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	1:891:A:TRP:N	16	9.61
(1,41)	1:889:A:SER:C	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	15	9.47
(1,68)	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	1:914:A:GLU:N	3	9.44
(1,82)	1:920:A:GLY:N	1:920:A:GLY:CA	1:920:A:GLY:C	1:921:A:ILE:N	10	9.42
(1,42)	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	1:891:A:TRP:N	4	9.39
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	19	9.38
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	6	9.22
(1,69)	1:913:A:GLU:C	1:914:A:GLU:N	1:914:A:GLU:CA	1:914:A:GLU:C	4	9.21
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	3	9.17
(1,1)	1:862:A:GLU:C	1:863:A:SER:N	1:863:A:SER:CA	1:863:A:SER:C	9	9.14
(1,69)	1:913:A:GLU:C	1:914:A:GLU:N	1:914:A:GLU:CA	1:914:A:GLU:C	11	9.12
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	11	9.07
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	3	9.02
(1,17)	1:876:A:ARG:N	1:876:A:ARG:CA	1:876:A:ARG:C	1:877:A:ILE:N	2	9.02
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	16	8.98
(1,40)	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	1:890:A:ARG:N	14	8.83
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	4	8.76
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	8	8.72
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	11	8.61
(1,41)	1:889:A:SER:C	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	6	8.59
(1,41)	1:889:A:SER:C	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	14	8.47
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	3	8.47
(1,40)	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	1:890:A:ARG:N	15	8.24
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	8	8.15
(1,40)	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	1:890:A:ARG:N	6	8.01
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	9	7.95
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	10	7.84
(1,38)	1:888:A:SER:N	1:888:A:SER:CA	1:888:A:SER:C	1:889:A:SER:N	20	7.83
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	8	7.8
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	6	7.75
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	19	7.72
(1,37)	1:887:A:GLU:C	1:888:A:SER:N	1:888:A:SER:CA	1:888:A:SER:C	20	7.69
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	9	7.66
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	13	7.63
(1,42)	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	1:891:A:TRP:N	7	7.61
(1,5)	1:864:A:ALA:C	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	5	7.6
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	15	7.55
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	20	7.46
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	4	7.37
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	10	7.37
(1,5)	1:864:A:ALA:C	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	7	7.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,38)	1:888:A:SER:N	1:888:A:SER:CA	1:888:A:SER:C	1:889:A:SER:N	17	7.27
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	15	7.22
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	4	7.17
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	7	7.16
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	5	7.15
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	18	7.11
(1,33)	1:885:A:ILE:C	1:886:A:ASP:N	1:886:A:ASP:CA	1:886:A:ASP:C	7	6.99
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	9	6.83
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	11	6.72
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	7	6.65
(1,5)	1:864:A:ALA:C	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	11	6.64
(1,68)	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	1:914:A:GLU:N	8	6.63
(1,33)	1:885:A:ILE:C	1:886:A:ASP:N	1:886:A:ASP:CA	1:886:A:ASP:C	11	6.59
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	14	6.59
(1,68)	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	1:914:A:GLU:N	16	6.55
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	10	6.49
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	11	6.33
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	3	6.28
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	13	6.21
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	8	6.21
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	8	6.2
(1,9)	1:867:A:ARG:N	1:867:A:ARG:CA	1:867:A:ARG:C	1:868:A:CYS:N	16	6.16
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	7	6.0
(1,37)	1:887:A:GLU:C	1:888:A:SER:N	1:888:A:SER:CA	1:888:A:SER:C	4	5.96
(1,42)	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	1:891:A:TRP:N	11	5.94
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	2	5.88
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	15	5.85
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	5	5.82
(1,17)	1:876:A:ARG:N	1:876:A:ARG:CA	1:876:A:ARG:C	1:877:A:ILE:N	11	5.82
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	7	5.8
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	18	5.8
(1,1)	1:862:A:GLU:C	1:863:A:SER:N	1:863:A:SER:CA	1:863:A:SER:C	13	5.76
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	17	5.7
(1,85)	1:870:A:ASP:N	1:870:A:ASP:CA	1:870:A:ASP:C	1:871:A:CYS:N	3	5.64
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	19	5.62
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	11	5.56
(1,68)	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	1:914:A:GLU:N	2	5.53
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	12	5.42
(1,39)	1:888:A:SER:C	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	20	5.38
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	14	5.32
(1,68)	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	1:914:A:GLU:N	1	5.2
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	6	5.2
(1,85)	1:870:A:ASP:N	1:870:A:ASP:CA	1:870:A:ASP:C	1:871:A:CYS:N	15	5.19
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	10	5.07
(1,40)	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	1:890:A:ARG:N	16	5.05
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	5	5.05
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	14	5.05
(1,68)	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	1:914:A:GLU:N	11	4.89
(1,40)	1:889:A:SER:N	1:889:A:SER:CA	1:889:A:SER:C	1:890:A:ARG:N	2	4.85
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	20	4.85
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	5	4.84

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,69)	1:913:A:GLU:C	1:914:A:GLU:N	1:914:A:GLU:CA	1:914:A:GLU:C	1	4.82
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	3	4.81
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	6	4.77
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	8	4.74
(1,41)	1:889:A:SER:C	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	3	4.73
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	1	4.73
(1,9)	1:867:A:ARG:N	1:867:A:ARG:CA	1:867:A:ARG:C	1:868:A:CYS:N	15	4.64
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	17	4.63
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	18	4.51
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	15	4.48
(1,50)	1:897:A:SER:N	1:897:A:SER:CA	1:897:A:SER:C	1:898:A:ASP:N	13	4.45
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	2	4.39
(1,82)	1:920:A:GLY:N	1:920:A:GLY:CA	1:920:A:GLY:C	1:921:A:ILE:N	16	4.32
(1,68)	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	1:914:A:GLU:N	5	4.2
(1,9)	1:867:A:ARG:N	1:867:A:ARG:CA	1:867:A:ARG:C	1:868:A:CYS:N	20	4.12
(1,5)	1:864:A:ALA:C	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	8	4.09
(1,33)	1:885:A:ILE:C	1:886:A:ASP:N	1:886:A:ASP:CA	1:886:A:ASP:C	2	4.01
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1	3.84
(1,9)	1:867:A:ARG:N	1:867:A:ARG:CA	1:867:A:ARG:C	1:868:A:CYS:N	14	3.75
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	8	3.56
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	1	3.53
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	17	3.51
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	14	3.49
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	10	3.44
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	19	3.44
(1,67)	1:912:A:ASN:C	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	20	3.39
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	4	3.34
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	15	3.18
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	20	3.17
(1,5)	1:864:A:ALA:C	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	14	3.14
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	12	3.1
(1,67)	1:912:A:ASN:C	1:913:A:GLU:N	1:913:A:GLU:CA	1:913:A:GLU:C	7	3.09
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	19	3.08
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	3	3.08
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	2	3.03
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	14	2.99
(1,9)	1:867:A:ARG:N	1:867:A:ARG:CA	1:867:A:ARG:C	1:868:A:CYS:N	8	2.98
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	2	2.94
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	6	2.9
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	12	2.83
(1,33)	1:885:A:ILE:C	1:886:A:ASP:N	1:886:A:ASP:CA	1:886:A:ASP:C	16	2.79
(1,1)	1:862:A:GLU:C	1:863:A:SER:N	1:863:A:SER:CA	1:863:A:SER:C	1	2.75
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	16	2.71
(1,69)	1:913:A:GLU:C	1:914:A:GLU:N	1:914:A:GLU:CA	1:914:A:GLU:C	5	2.53
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	13	2.5
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	18	2.39
(1,50)	1:897:A:SER:N	1:897:A:SER:CA	1:897:A:SER:C	1:898:A:ASP:N	8	2.22
(1,26)	1:881:A:VAL:N	1:881:A:VAL:CA	1:881:A:VAL:C	1:882:A:VAL:N	20	2.22
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	2	2.21
(1,84)	1:869:A:ASP:C	1:870:A:ASP:N	1:870:A:ASP:CA	1:870:A:ASP:C	20	2.13
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	16	2.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,18)	1:876:A:ARG:C	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	19	2.01
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	1	2.0
(1,38)	1:888:A:SER:N	1:888:A:SER:CA	1:888:A:SER:C	1:889:A:SER:N	5	1.94
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	10	1.9
(1,37)	1:887:A:GLU:C	1:888:A:SER:N	1:888:A:SER:CA	1:888:A:SER:C	17	1.86
(1,80)	1:919:A:LEU:N	1:919:A:LEU:CA	1:919:A:LEU:C	1:920:A:GLY:N	9	1.85
(1,38)	1:888:A:SER:N	1:888:A:SER:CA	1:888:A:SER:C	1:889:A:SER:N	1	1.8
(1,82)	1:920:A:GLY:N	1:920:A:GLY:CA	1:920:A:GLY:C	1:921:A:ILE:N	1	1.77
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	9	1.75
(1,50)	1:897:A:SER:N	1:897:A:SER:CA	1:897:A:SER:C	1:898:A:ASP:N	7	1.67
(1,82)	1:920:A:GLY:N	1:920:A:GLY:CA	1:920:A:GLY:C	1:921:A:ILE:N	6	1.65
(1,5)	1:864:A:ALA:C	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	15	1.63
(1,83)	1:920:A:GLY:C	1:921:A:ILE:N	1:921:A:ILE:CA	1:921:A:ILE:C	4	1.62
(1,30)	1:883:A:GLY:N	1:883:A:GLY:CA	1:883:A:GLY:C	1:884:A:SER:N	14	1.61
(1,19)	1:877:A:ILE:N	1:877:A:ILE:CA	1:877:A:ILE:C	1:878:A:PRO:N	17	1.55
(1,9)	1:867:A:ARG:N	1:867:A:ARG:CA	1:867:A:ARG:C	1:868:A:CYS:N	9	1.54
(1,1)	1:862:A:GLU:C	1:863:A:SER:N	1:863:A:SER:CA	1:863:A:SER:C	4	1.47
(1,42)	1:890:A:ARG:N	1:890:A:ARG:CA	1:890:A:ARG:C	1:891:A:TRP:N	1	1.46
(1,4)	1:864:A:ALA:N	1:864:A:ALA:CA	1:864:A:ALA:C	1:865:A:TRP:N	15	1.44
(1,82)	1:920:A:GLY:N	1:920:A:GLY:CA	1:920:A:GLY:C	1:921:A:ILE:N	13	1.22
(1,6)	1:865:A:TRP:N	1:865:A:TRP:CA	1:865:A:TRP:C	1:866:A:VAL:N	16	1.2
(1,37)	1:887:A:GLU:C	1:888:A:SER:N	1:888:A:SER:CA	1:888:A:SER:C	13	1.18
(1,1)	1:862:A:GLU:C	1:863:A:SER:N	1:863:A:SER:CA	1:863:A:SER:C	15	1.12
(1,33)	1:885:A:ILE:C	1:886:A:ASP:N	1:886:A:ASP:CA	1:886:A:ASP:C	20	1.11
(1,64)	1:910:A:MET:N	1:910:A:MET:CA	1:910:A:MET:C	1:911:A:SER:N	16	1.01