



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 12:48 AM UTC

PDB ID : 6FFU / pdb_00006ffu
BMRB ID : 34229
Title : Solution NMR structure of CBM64 from *S.thermophila* using 20% ¹³C, 100% ¹⁵N
Authors : Heikkinen, H.A.; Iwai, H.
Deposited on : 2018-01-09

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

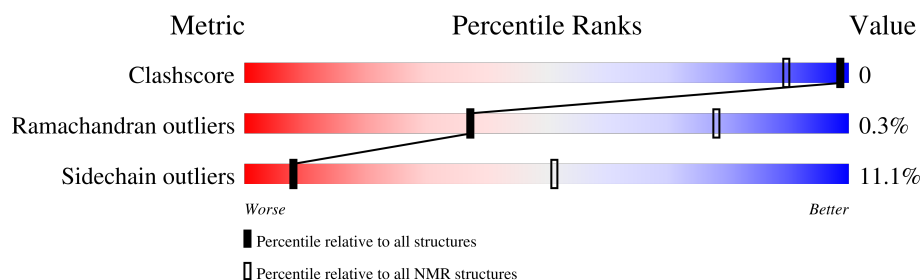
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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	86	

2 Ensemble composition and analysis

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:459-A:541 (83)	0.46	14

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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1347 atoms, of which 632 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Glycosyl hydrolase family 5 cellulase CBM64.

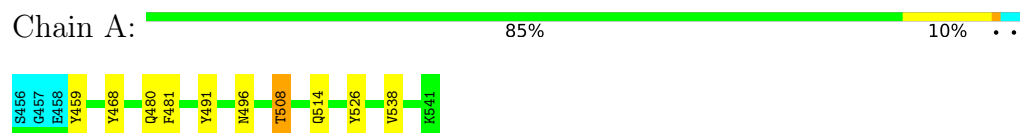
Mol	Chain	Residues	Atoms					Trace
1	A	86	Total	C	H	N	O	0
			1347	462	632	112	141	

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: Glycosyl hydrolase family 5 cellulase CBM64

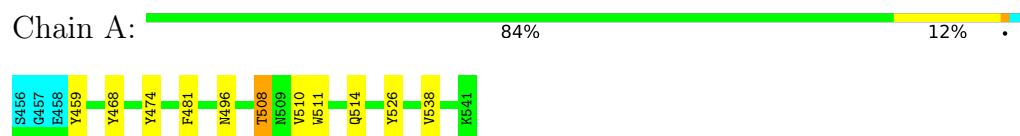


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

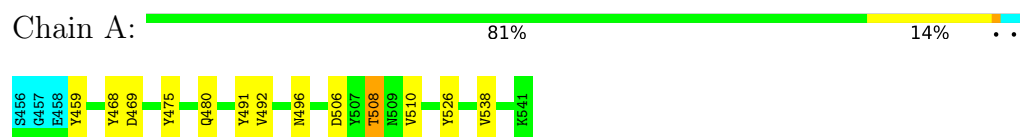
4.2.1 Score per residue for model 1

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



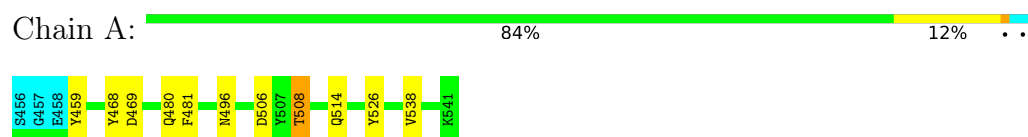
4.2.2 Score per residue for model 2

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



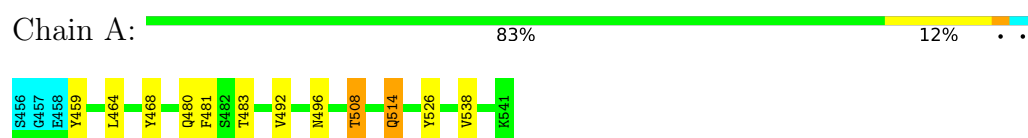
4.2.3 Score per residue for model 3

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



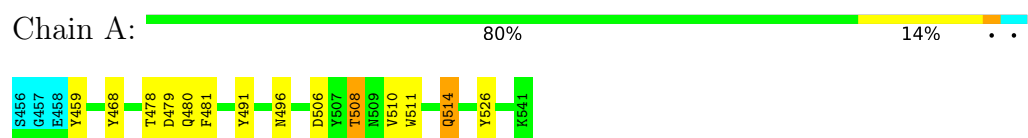
4.2.4 Score per residue for model 4

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



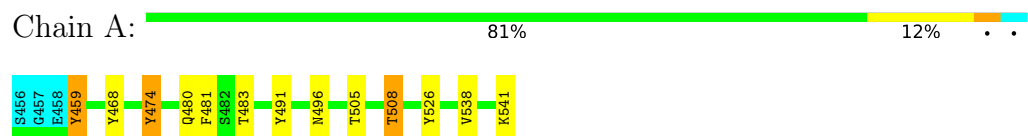
4.2.5 Score per residue for model 5

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



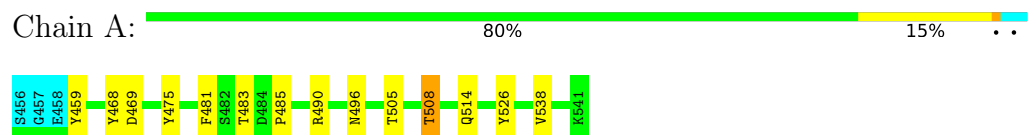
4.2.6 Score per residue for model 6

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



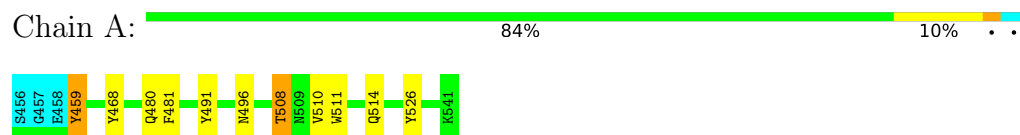
4.2.7 Score per residue for model 7

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



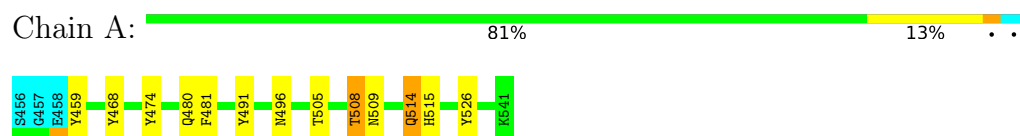
4.2.8 Score per residue for model 8

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



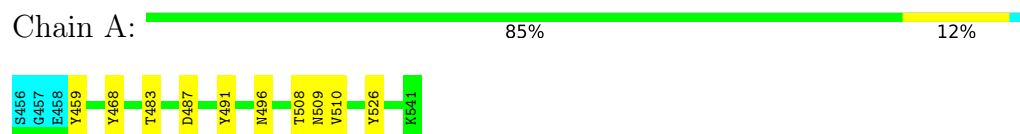
4.2.9 Score per residue for model 9

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



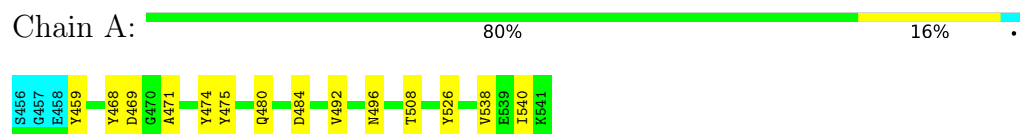
4.2.10 Score per residue for model 10

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



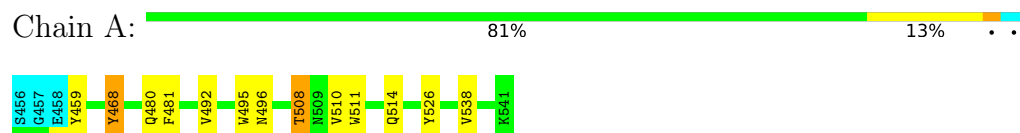
4.2.11 Score per residue for model 11

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



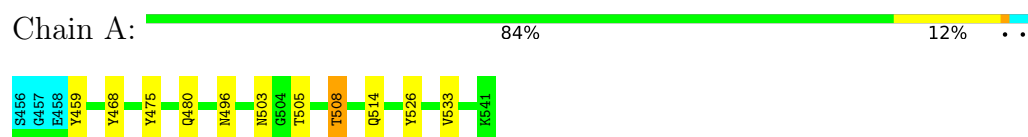
4.2.12 Score per residue for model 12

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



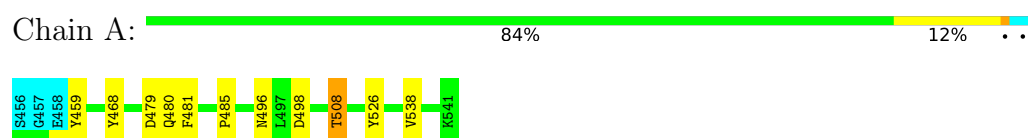
4.2.13 Score per residue for model 13

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



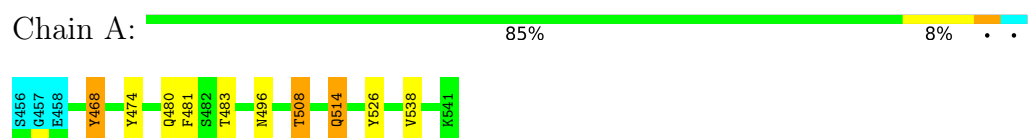
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



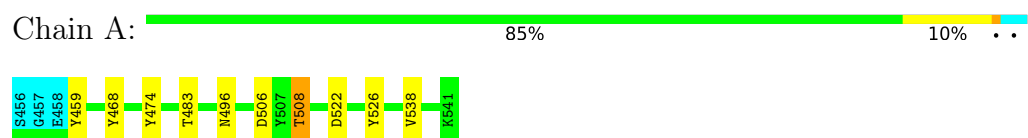
4.2.15 Score per residue for model 15

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



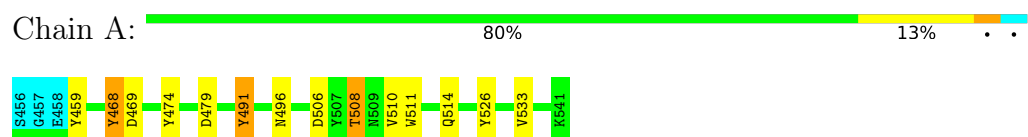
4.2.16 Score per residue for model 16

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



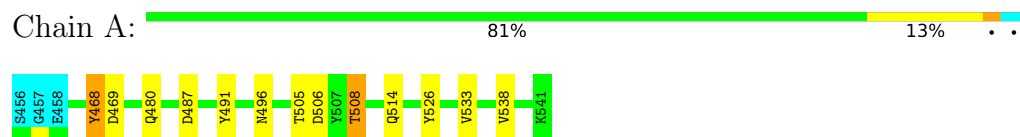
4.2.17 Score per residue for model 17

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



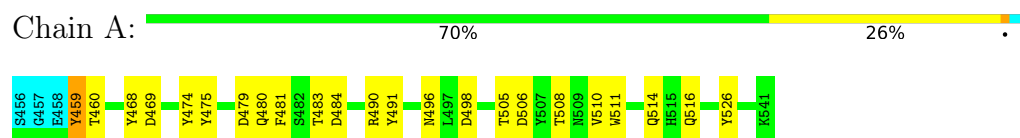
4.2.18 Score per residue for model 18

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



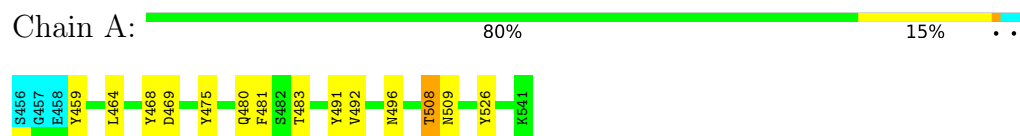
4.2.19 Score per residue for model 19

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



4.2.20 Score per residue for model 20

- Molecule 1: Glycosyl hydrolase family 5 cellulase CBM64



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
Amber	refinement	14
CYANA	structure calculation	3.97

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	1030
Number of shifts mapped to atoms	1030
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.88±0.01	0±0/724 (0.0± 0.0%)	1.51±0.03	5±2/993 (0.5± 0.2%)
All	All	0.88	0/14480 (0.0%)	1.51	96/19860 (0.5%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.8±0.7
All	All	0	16

There are no bond-length outliers.

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	459	TYR	N-CA-C	7.43	121.01	110.23	4	18
1	A	522	ASP	CA-CB-CG	6.87	119.47	112.60	16	1
1	A	508	THR	N-CA-C	6.75	118.64	111.28	3	17
1	A	515	HIS	CA-CB-CG	6.45	120.25	113.80	9	1
1	A	484	ASP	N-CA-C	6.24	117.52	109.65	19	1
1	A	481	PHE	CA-CB-CG	6.09	119.89	113.80	5	12
1	A	481	PHE	N-CA-C	6.00	118.04	110.24	19	5
1	A	474	TYR	N-CA-C	5.97	118.25	109.24	1	6
1	A	514	GLN	OE1-CD-NE2	-5.79	116.81	122.60	9	5
1	A	509	ASN	CA-CB-CG	5.66	118.26	112.60	10	1
1	A	469	ASP	N-CA-C	5.62	117.61	109.07	3	6
1	A	491	TYR	N-CA-C	5.60	117.31	108.96	5	4
1	A	469	ASP	CA-CB-CG	5.51	118.11	112.60	17	3
1	A	479	ASP	CA-CB-CG	5.51	118.11	112.60	19	4
1	A	510	VAL	N-CA-C	5.50	115.24	108.53	2	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	506	ASP	N-CA-C	5.41	118.43	109.46	5	2
1	A	506	ASP	CA-CB-CG	5.27	117.87	112.60	17	4
1	A	503	ASN	CA-CB-CG	5.22	117.82	112.60	13	1
1	A	498	ASP	CA-CB-CG	5.22	117.82	112.60	14	2
1	A	484	ASP	CA-CB-CG	5.18	117.78	112.60	11	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	491	TYR	Peptide,Sidechain	7
1	A	468	TYR	Sidechain	4
1	A	474	TYR	Peptide,Sidechain	3
1	A	475	TYR	Sidechain	1
1	A	490	ARG	Sidechain	1

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	696	616	616	0±0
All	All	13920	12320	12320	6

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:510:VAL:HG22	1:A:511:TRP:H	0.48	1.67	8	6

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	82/86 (95%)	77±1 (94±1%)	5±1 (6±1%)	0±0 (0±1%)	37	78
All	All	1640/1720 (95%)	1542 (94%)	93 (6%)	5 (0%)	37	78

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	485	PRO	2
1	A	487	ASP	2
1	A	471	ALA	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	72/74 (97%)	64±2 (89±2%)	8±2 (11±2%)	8	51
All	All	1440/1480 (97%)	1280 (89%)	160 (11%)	8	51

All 23 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	468	TYR	20
1	A	496	ASN	20
1	A	508	THR	20
1	A	526	TYR	20
1	A	480	GLN	15
1	A	514	GLN	12
1	A	538	VAL	12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	483	THR	8
1	A	505	THR	6
1	A	492	VAL	5
1	A	475	TYR	4
1	A	459	TYR	3
1	A	533	VAL	3
1	A	464	LEU	2
1	A	509	ASN	2
1	A	478	THR	1
1	A	541	LYS	1
1	A	490	ARG	1
1	A	540	ILE	1
1	A	495	TRP	1
1	A	506	ASP	1
1	A	460	THR	1
1	A	516	GLN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 91% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *TMB_31.bmrB*

7.1.1 Bookkeeping

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

Total number of shifts	1030
Number of shifts mapped to atoms	1030
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	85	0.08 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	78	-0.08 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	84	0.59 ± 0.22	Should be applied
^{15}N	81	-0.24 ± 0.28	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 1015 atoms were assigned a chemical shift out of a possible 1112. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	414/415 (100%)	169/169 (100%)	165/166 (99%)	80/80 (100%)
Sidechain	465/503 (92%)	313/326 (96%)	146/163 (90%)	6/14 (43%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	136/194 (70%)	79/94 (84%)	51/91 (56%)	6/9 (67%)
Overall	1015/1112 (91%)	561/589 (95%)	362/420 (86%)	92/103 (89%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1030 atoms were assigned a chemical shift out of a possible 1138. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	423/431 (98%)	173/176 (98%)	169/172 (98%)	81/83 (98%)
Sidechain	471/513 (92%)	317/332 (95%)	148/167 (89%)	6/14 (43%)
Aromatic	136/194 (70%)	79/94 (84%)	51/91 (56%)	6/9 (67%)
Overall	1030/1138 (91%)	569/602 (95%)	368/430 (86%)	93/106 (88%)

7.1.4 Statistically unusual chemical shifts ⓘ

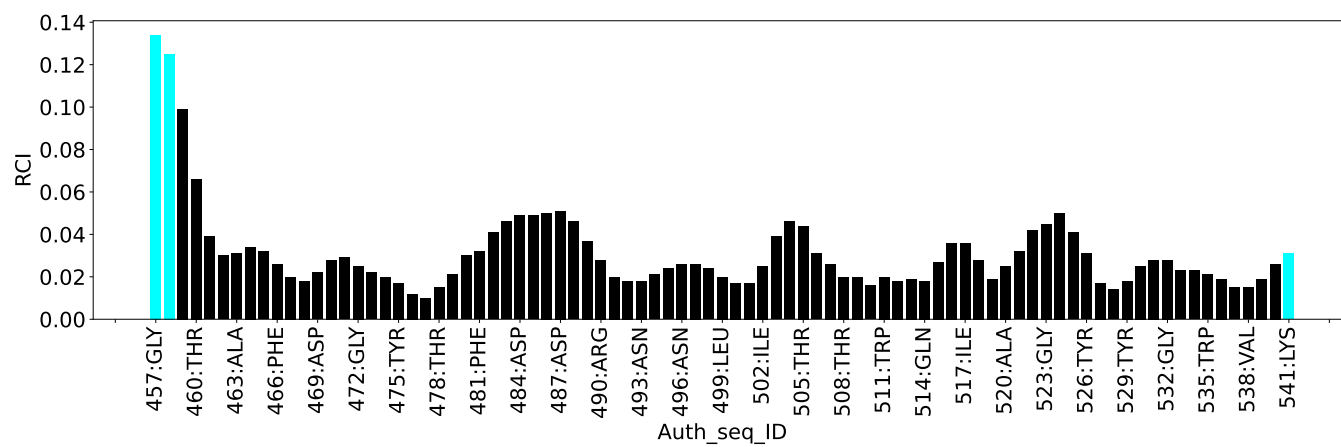
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	481	PHE	HB2	-0.46	1.20 – 4.80	-9.6
1	A	524	TYR	CE2	129.13	111.68 – 124.17	9.0
1	A	479	ASP	HB3	0.94	1.32 – 4.00	-6.4
1	A	514	GLN	HG3	0.59	0.91 – 3.68	-6.2
1	A	474	TYR	HB3	0.65	0.93 – 4.76	-5.7
1	A	519	ALA	HA	1.90	2.13 – 6.34	-5.5
1	A	476	TRP	HZ2	5.65	5.71 – 8.86	-5.2
1	A	537	HIS	HB3	1.12	1.18 – 4.91	-5.2
1	A	514	GLN	HG2	1.01	1.01 – 3.62	-5.0
1	A	524	TYR	HE1	5.58	5.59 – 7.82	-5.0

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:



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	1302
Intra-residue ($ i-j =0$)	281
Sequential ($ i-j =1$)	338
Medium range ($ i-j >1$ and $ i-j <5$)	168
Long range ($ i-j \geq 5$)	515
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	15.1
Number of long range restraints per residue ¹	6.0

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)	4.5	0.2
0.2-0.5 (Medium)	2.2	0.5
>0.5 (Large)	1.1	0.91

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

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

9 Distance violation analysis ⓘ

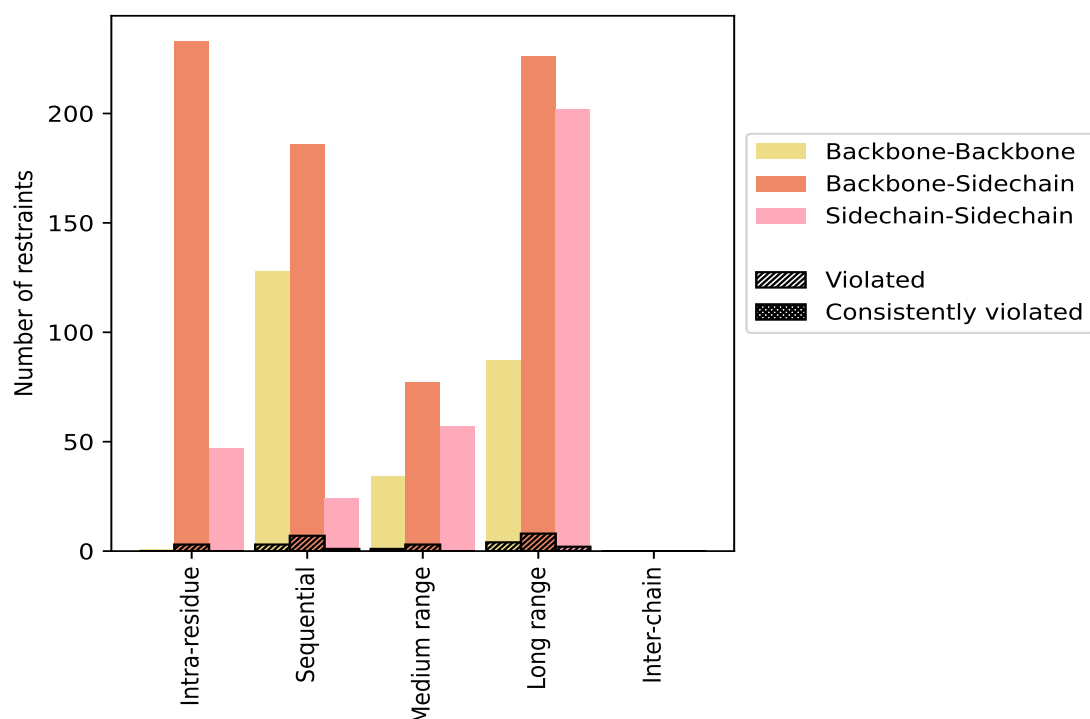
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	281	21.6	3	1.1	0.2	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	233	17.9	3	1.3	0.2	0	0.0	0.0
Sidechain-Sidechain	47	3.6	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	338	26.0	11	3.3	0.8	0	0.0	0.0
Backbone-Backbone	128	9.8	3	2.3	0.2	0	0.0	0.0
Backbone-Sidechain	186	14.3	7	3.8	0.5	0	0.0	0.0
Sidechain-Sidechain	24	1.8	1	4.2	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	168	12.9	4	2.4	0.3	0	0.0	0.0
Backbone-Backbone	34	2.6	1	2.9	0.1	0	0.0	0.0
Backbone-Sidechain	77	5.9	3	3.9	0.2	0	0.0	0.0
Sidechain-Sidechain	57	4.4	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	515	39.6	14	2.7	1.1	0	0.0	0.0
Backbone-Backbone	87	6.7	4	4.6	0.3	0	0.0	0.0
Backbone-Sidechain	226	17.4	8	3.5	0.6	0	0.0	0.0
Sidechain-Sidechain	202	15.5	2	1.0	0.2	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1302	100.0	32	2.5	2.5	0	0.0	0.0
Backbone-Backbone	250	19.2	8	3.2	0.6	0	0.0	0.0
Backbone-Sidechain	722	55.5	21	2.9	1.6	0	0.0	0.0
Sidechain-Sidechain	330	25.3	3	0.9	0.2	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 disulfied bonds are counted in their appropriate category on the x-axis

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	2	1	2	0	5	0.26	0.4	0.12	0.31
2	0	4	2	2	0	8	0.17	0.39	0.09	0.14
3	0	4	1	3	0	8	0.18	0.34	0.09	0.13
4	0	2	2	4	0	8	0.2	0.67	0.18	0.13
5	0	4	2	1	0	7	0.19	0.47	0.13	0.11
6	0	5	2	4	0	11	0.17	0.5	0.12	0.11
7	1	3	3	6	0	13	0.31	0.91	0.28	0.13
8	0	2	1	5	0	8	0.27	0.63	0.2	0.19
9	1	3	1	3	0	8	0.22	0.41	0.11	0.16
10	0	3	0	4	0	7	0.16	0.38	0.09	0.12

Continued on next page...

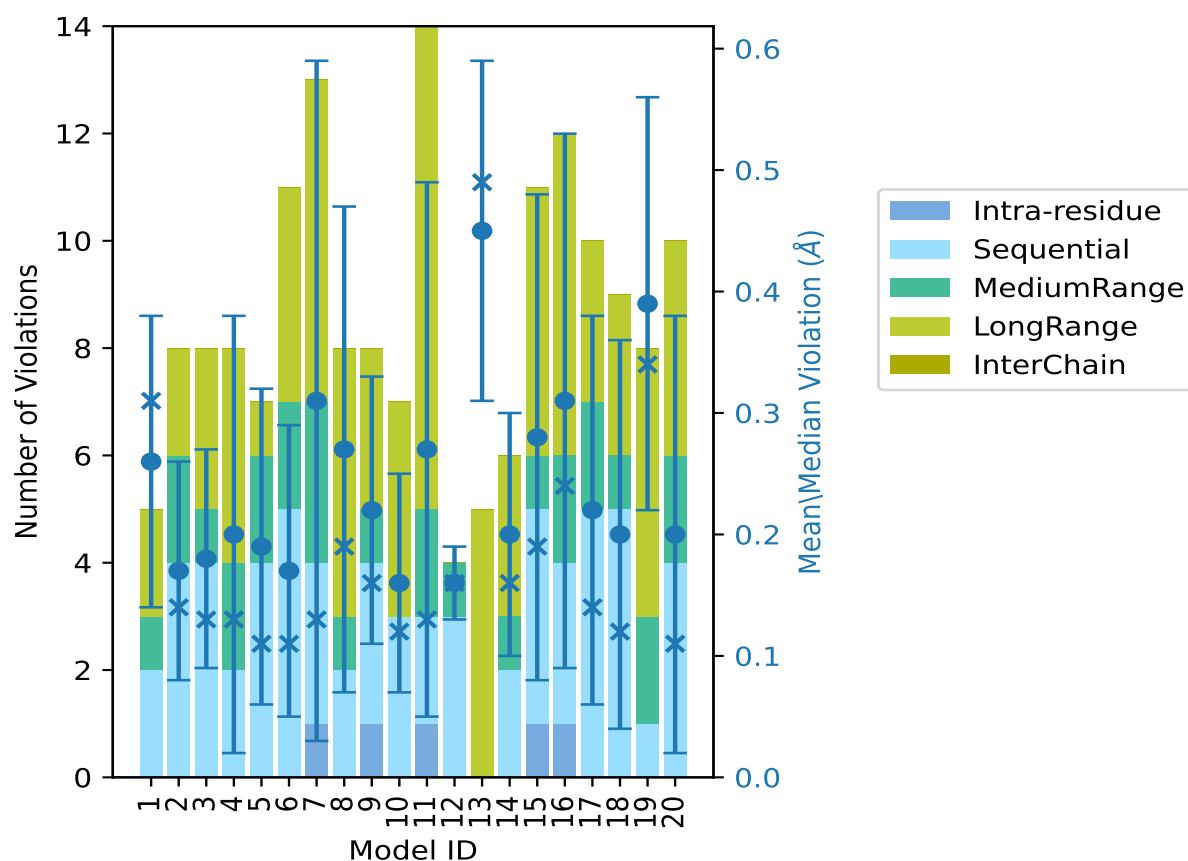
Continued from previous page...

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	1	2	2	9	0	14	0.27	0.77	0.22	0.13
12	0	3	1	0	0	4	0.16	0.21	0.03	0.16
13	0	0	0	5	0	5	0.45	0.61	0.14	0.49
14	0	2	1	3	0	6	0.2	0.35	0.1	0.16
15	1	4	1	5	0	11	0.28	0.72	0.2	0.19
16	1	3	2	6	0	12	0.31	0.78	0.22	0.24
17	0	5	2	3	0	10	0.22	0.54	0.16	0.14
18	0	5	1	3	0	9	0.2	0.58	0.16	0.12
19	0	1	2	5	0	8	0.39	0.65	0.17	0.34
20	0	4	2	4	0	10	0.2	0.62	0.18	0.11

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

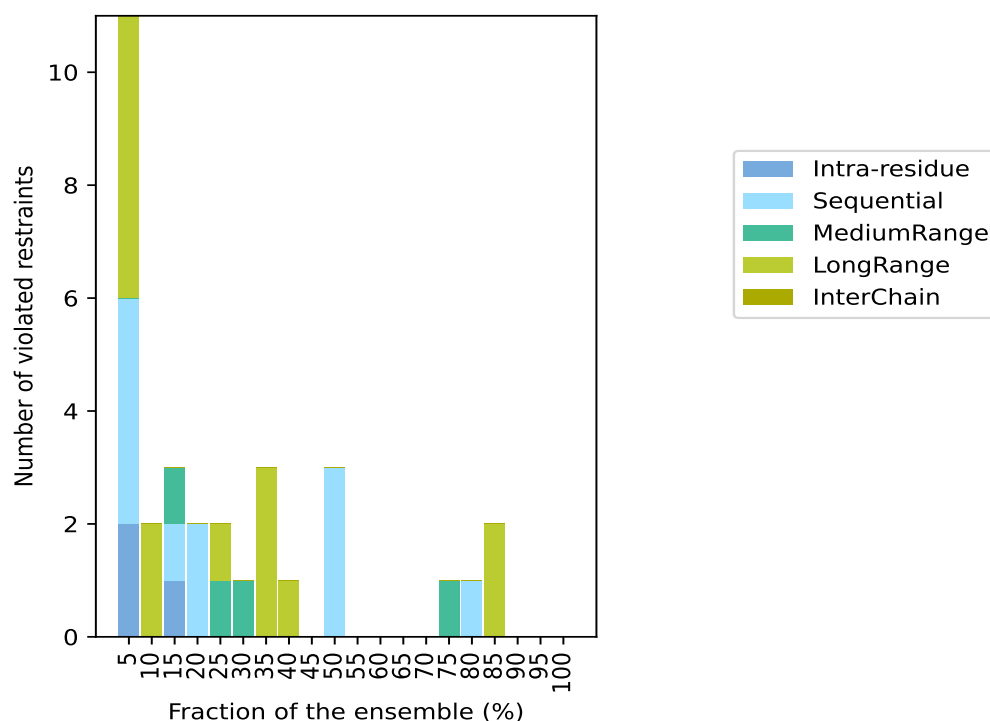
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1270(IR:278, SQ:327, MR:164, LR:501, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
2	4	0	5	0	11	1	5.0
0	0	0	2	0	2	2	10.0
1	1	1	0	0	3	3	15.0
0	2	0	0	0	2	4	20.0
0	0	1	1	0	2	5	25.0
0	0	1	0	0	1	6	30.0
0	0	0	3	0	3	7	35.0
0	0	0	1	0	1	8	40.0
0	0	0	0	0	0	9	45.0
0	3	0	0	0	3	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	1	0	0	1	15	75.0
0	1	0	0	0	1	16	80.0
0	0	0	2	0	2	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

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

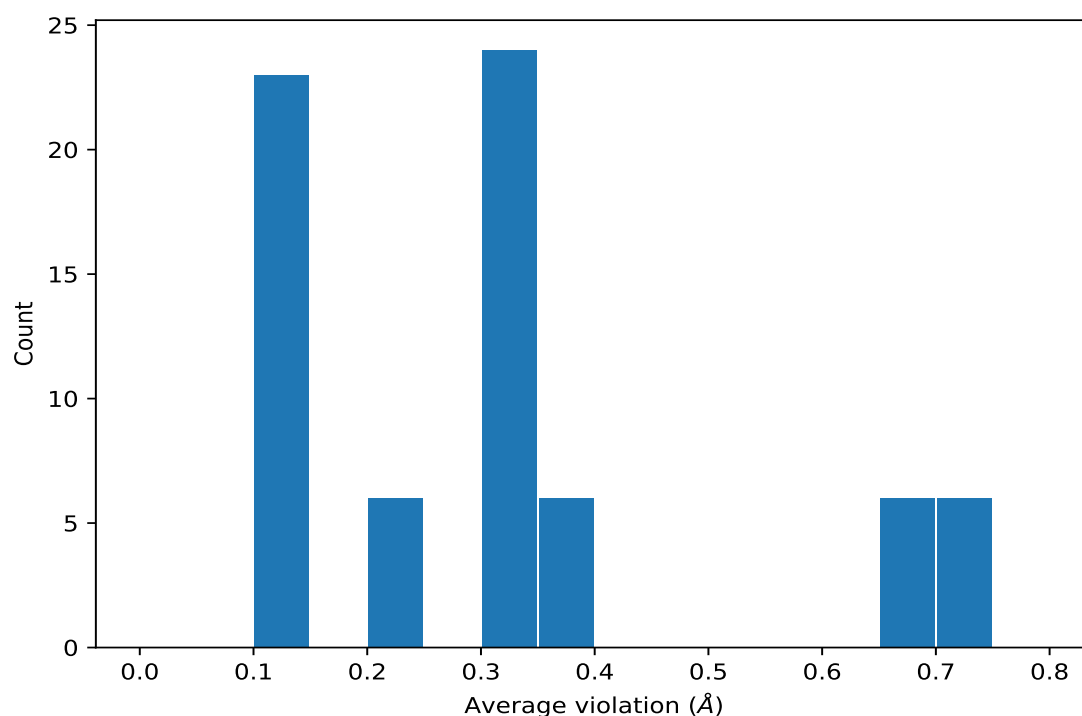
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	17	0.37	0.13	0.38
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	17	0.37	0.13	0.38
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	17	0.37	0.13	0.38
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	17	0.37	0.13	0.38
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	17	0.37	0.13	0.38
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	17	0.37	0.13	0.38
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	17	0.35	0.12	0.35
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	17	0.35	0.12	0.35
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	17	0.35	0.12	0.35
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	17	0.35	0.12	0.35
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	17	0.35	0.12	0.35
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	17	0.35	0.12	0.35
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	17	0.35	0.12	0.35
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	17	0.35	0.12	0.35
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	17	0.35	0.12	0.35
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	17	0.35	0.12	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	17	0.35	0.12	0.35
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	17	0.35	0.12	0.35
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	16	0.13	0.02	0.12
(1,1107)	1:464:A:LEU:HD11	1:466:A:PHE:H	15	0.32	0.16	0.3
(1,1107)	1:464:A:LEU:HD12	1:466:A:PHE:H	15	0.32	0.16	0.3
(1,1107)	1:464:A:LEU:HD13	1:466:A:PHE:H	15	0.32	0.16	0.3
(1,1107)	1:464:A:LEU:HD21	1:466:A:PHE:H	15	0.32	0.16	0.3
(1,1107)	1:464:A:LEU:HD22	1:466:A:PHE:H	15	0.32	0.16	0.3
(1,1107)	1:464:A:LEU:HD23	1:466:A:PHE:H	15	0.32	0.16	0.3
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD11	10	0.21	0.07	0.19
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD12	10	0.21	0.07	0.19
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD13	10	0.21	0.07	0.19
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD21	10	0.21	0.07	0.19
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD22	10	0.21	0.07	0.19
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD23	10	0.21	0.07	0.19
(1,250)	1:471:A:ALA:H	1:472:A:GLY:H	10	0.13	0.01	0.12
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB1	10	0.12	0.02	0.12
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB2	10	0.12	0.02	0.12
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB3	10	0.12	0.02	0.12
(1,263)	1:500:A:LEU:H	1:509:A:ASN:H	8	0.11	0.01	0.11
(1,1233)	1:499:A:LEU:HD11	1:508:A:THR:H	7	0.71	0.09	0.72
(1,1233)	1:499:A:LEU:HD12	1:508:A:THR:H	7	0.71	0.09	0.72
(1,1233)	1:499:A:LEU:HD13	1:508:A:THR:H	7	0.71	0.09	0.72
(1,1233)	1:499:A:LEU:HD21	1:508:A:THR:H	7	0.71	0.09	0.72
(1,1233)	1:499:A:LEU:HD22	1:508:A:THR:H	7	0.71	0.09	0.72
(1,1233)	1:499:A:LEU:HD23	1:508:A:THR:H	7	0.71	0.09	0.72
(1,1232)	1:499:A:LEU:HD11	1:507:A:TYR:H	7	0.65	0.11	0.64
(1,1232)	1:499:A:LEU:HD12	1:507:A:TYR:H	7	0.65	0.11	0.64
(1,1232)	1:499:A:LEU:HD13	1:507:A:TYR:H	7	0.65	0.11	0.64
(1,1232)	1:499:A:LEU:HD21	1:507:A:TYR:H	7	0.65	0.11	0.64
(1,1232)	1:499:A:LEU:HD22	1:507:A:TYR:H	7	0.65	0.11	0.64
(1,1232)	1:499:A:LEU:HD23	1:507:A:TYR:H	7	0.65	0.11	0.64
(1,1231)	1:499:A:LEU:HD11	1:506:A:ASP:HA	7	0.35	0.13	0.3
(1,1231)	1:499:A:LEU:HD12	1:506:A:ASP:HA	7	0.35	0.13	0.3
(1,1231)	1:499:A:LEU:HD13	1:506:A:ASP:HA	7	0.35	0.13	0.3
(1,1231)	1:499:A:LEU:HD21	1:506:A:ASP:HA	7	0.35	0.13	0.3
(1,1231)	1:499:A:LEU:HD22	1:506:A:ASP:HA	7	0.35	0.13	0.3
(1,1231)	1:499:A:LEU:HD23	1:506:A:ASP:HA	7	0.35	0.13	0.3
(1,361)	1:520:A:ALA:H	1:524:A:TYR:HB3	6	0.12	0.01	0.12
(1,889)	1:497:A:LEU:HG	1:538:A:VAL:HB	5	0.12	0.01	0.12
(1,1263)	1:514:A:GLN:HG2	1:516:A:GLN:H	5	0.12	0.01	0.12
(1,1263)	1:514:A:GLN:HG3	1:516:A:GLN:H	5	0.12	0.01	0.12

Continued on next page...

Continued from previous page...

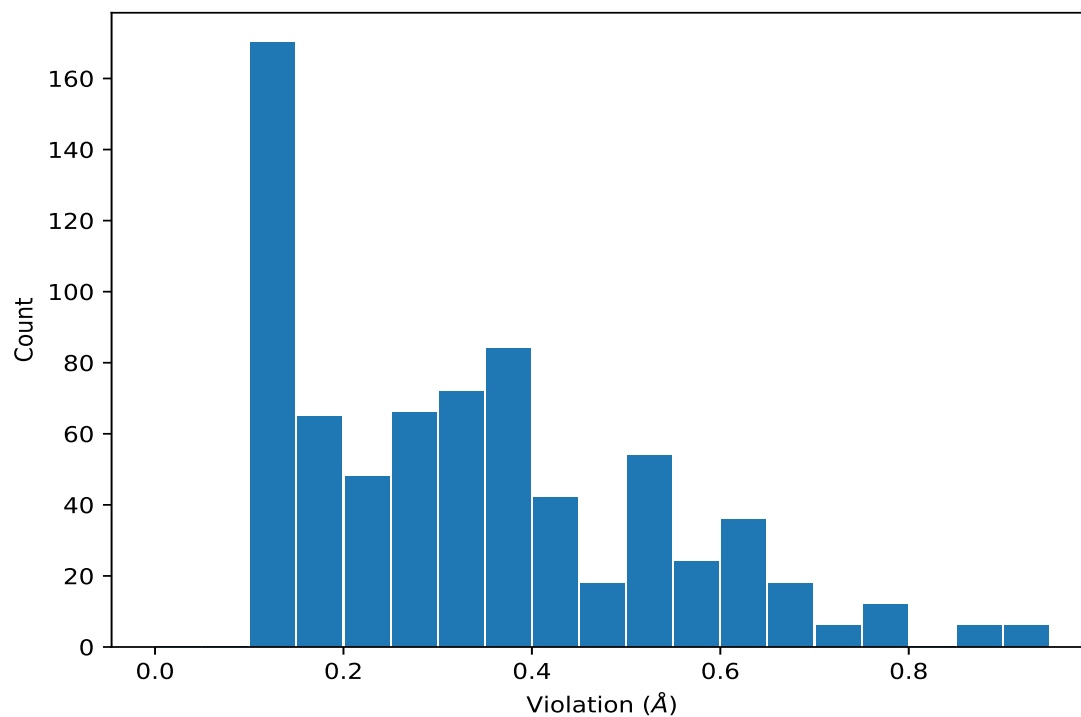
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,188)	1:505:A:THR:H	1:506:A:ASP:H	4	0.11	0.0	0.11
(1,542)	1:504:A:GLY:H	1:505:A:THR:HA	4	0.1	0.0	0.1
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD11	3	0.13	0.03	0.12
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD12	3	0.13	0.03	0.12
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD13	3	0.13	0.03	0.12
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD21	3	0.13	0.03	0.12
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD22	3	0.13	0.03	0.12
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD23	3	0.13	0.03	0.12
(1,1286)	1:535:A:TRP:HB2	1:536:A:GLY:HA3	3	0.13	0.02	0.13
(1,1286)	1:535:A:TRP:HB3	1:536:A:GLY:HA3	3	0.13	0.02	0.13
(1,299)	1:507:A:TYR:HA	1:510:A:VAL:H	3	0.11	0.0	0.11
(1,577)	1:493:A:ASN:H	1:540:A:ILE:HA	2	0.12	0.02	0.12
(1,380)	1:471:A:ALA:H	1:532:A:GLY:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1232)	1:499:A:LEU:HD11	1:507:A:TYR:H	7	0.91
(1,1232)	1:499:A:LEU:HD12	1:507:A:TYR:H	7	0.91
(1,1232)	1:499:A:LEU:HD13	1:507:A:TYR:H	7	0.91
(1,1232)	1:499:A:LEU:HD21	1:507:A:TYR:H	7	0.91
(1,1232)	1:499:A:LEU:HD22	1:507:A:TYR:H	7	0.91
(1,1232)	1:499:A:LEU:HD23	1:507:A:TYR:H	7	0.91
(1,1233)	1:499:A:LEU:HD11	1:508:A:THR:H	7	0.86
(1,1233)	1:499:A:LEU:HD12	1:508:A:THR:H	7	0.86
(1,1233)	1:499:A:LEU:HD13	1:508:A:THR:H	7	0.86
(1,1233)	1:499:A:LEU:HD21	1:508:A:THR:H	7	0.86
(1,1233)	1:499:A:LEU:HD22	1:508:A:THR:H	7	0.86
(1,1233)	1:499:A:LEU:HD23	1:508:A:THR:H	7	0.86
(1,1233)	1:499:A:LEU:HD11	1:508:A:THR:H	16	0.78
(1,1233)	1:499:A:LEU:HD12	1:508:A:THR:H	16	0.78
(1,1233)	1:499:A:LEU:HD13	1:508:A:THR:H	16	0.78
(1,1233)	1:499:A:LEU:HD21	1:508:A:THR:H	16	0.78
(1,1233)	1:499:A:LEU:HD22	1:508:A:THR:H	16	0.78
(1,1233)	1:499:A:LEU:HD23	1:508:A:THR:H	16	0.78
(1,1233)	1:499:A:LEU:HD11	1:508:A:THR:H	11	0.77
(1,1233)	1:499:A:LEU:HD12	1:508:A:THR:H	11	0.77
(1,1233)	1:499:A:LEU:HD13	1:508:A:THR:H	11	0.77
(1,1233)	1:499:A:LEU:HD21	1:508:A:THR:H	11	0.77
(1,1233)	1:499:A:LEU:HD22	1:508:A:THR:H	11	0.77
(1,1233)	1:499:A:LEU:HD23	1:508:A:THR:H	11	0.77
(1,1233)	1:499:A:LEU:HD11	1:508:A:THR:H	15	0.72
(1,1233)	1:499:A:LEU:HD12	1:508:A:THR:H	15	0.72
(1,1233)	1:499:A:LEU:HD13	1:508:A:THR:H	15	0.72
(1,1233)	1:499:A:LEU:HD21	1:508:A:THR:H	15	0.72
(1,1233)	1:499:A:LEU:HD22	1:508:A:THR:H	15	0.72
(1,1233)	1:499:A:LEU:HD23	1:508:A:THR:H	15	0.72
(1,1107)	1:464:A:LEU:HD11	1:466:A:PHE:H	4	0.67
(1,1107)	1:464:A:LEU:HD12	1:466:A:PHE:H	4	0.67
(1,1107)	1:464:A:LEU:HD13	1:466:A:PHE:H	4	0.67
(1,1107)	1:464:A:LEU:HD21	1:466:A:PHE:H	4	0.67
(1,1107)	1:464:A:LEU:HD22	1:466:A:PHE:H	4	0.67
(1,1107)	1:464:A:LEU:HD23	1:466:A:PHE:H	4	0.67
(1,1232)	1:499:A:LEU:HD11	1:507:A:TYR:H	11	0.66

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1232)	1:499:A:LEU:HD12	1:507:A:TYR:H	11	0.66
(1,1232)	1:499:A:LEU:HD13	1:507:A:TYR:H	11	0.66
(1,1232)	1:499:A:LEU:HD21	1:507:A:TYR:H	11	0.66
(1,1232)	1:499:A:LEU:HD22	1:507:A:TYR:H	11	0.66
(1,1232)	1:499:A:LEU:HD23	1:507:A:TYR:H	11	0.66
(1,1232)	1:499:A:LEU:HD11	1:507:A:TYR:H	19	0.65
(1,1232)	1:499:A:LEU:HD12	1:507:A:TYR:H	19	0.65
(1,1232)	1:499:A:LEU:HD13	1:507:A:TYR:H	19	0.65
(1,1232)	1:499:A:LEU:HD21	1:507:A:TYR:H	19	0.65
(1,1232)	1:499:A:LEU:HD22	1:507:A:TYR:H	19	0.65
(1,1232)	1:499:A:LEU:HD23	1:507:A:TYR:H	19	0.65
(1,1232)	1:499:A:LEU:HD11	1:507:A:TYR:H	15	0.64
(1,1232)	1:499:A:LEU:HD12	1:507:A:TYR:H	15	0.64
(1,1232)	1:499:A:LEU:HD13	1:507:A:TYR:H	15	0.64
(1,1232)	1:499:A:LEU:HD21	1:507:A:TYR:H	15	0.64
(1,1232)	1:499:A:LEU:HD22	1:507:A:TYR:H	15	0.64
(1,1232)	1:499:A:LEU:HD23	1:507:A:TYR:H	15	0.64
(1,1233)	1:499:A:LEU:HD11	1:508:A:THR:H	8	0.63
(1,1233)	1:499:A:LEU:HD12	1:508:A:THR:H	8	0.63
(1,1233)	1:499:A:LEU:HD13	1:508:A:THR:H	8	0.63
(1,1233)	1:499:A:LEU:HD21	1:508:A:THR:H	8	0.63
(1,1233)	1:499:A:LEU:HD22	1:508:A:THR:H	8	0.63
(1,1233)	1:499:A:LEU:HD23	1:508:A:THR:H	8	0.63
(1,1231)	1:499:A:LEU:HD11	1:506:A:ASP:HA	7	0.63
(1,1231)	1:499:A:LEU:HD12	1:506:A:ASP:HA	7	0.63
(1,1231)	1:499:A:LEU:HD13	1:506:A:ASP:HA	7	0.63
(1,1231)	1:499:A:LEU:HD21	1:506:A:ASP:HA	7	0.63
(1,1231)	1:499:A:LEU:HD22	1:506:A:ASP:HA	7	0.63
(1,1231)	1:499:A:LEU:HD23	1:506:A:ASP:HA	7	0.63
(1,1107)	1:464:A:LEU:HD11	1:466:A:PHE:H	20	0.62
(1,1107)	1:464:A:LEU:HD12	1:466:A:PHE:H	20	0.62
(1,1107)	1:464:A:LEU:HD13	1:466:A:PHE:H	20	0.62
(1,1107)	1:464:A:LEU:HD21	1:466:A:PHE:H	20	0.62
(1,1107)	1:464:A:LEU:HD22	1:466:A:PHE:H	20	0.62
(1,1107)	1:464:A:LEU:HD23	1:466:A:PHE:H	20	0.62
(1,1233)	1:499:A:LEU:HD11	1:508:A:THR:H	13	0.61
(1,1233)	1:499:A:LEU:HD12	1:508:A:THR:H	13	0.61
(1,1233)	1:499:A:LEU:HD13	1:508:A:THR:H	13	0.61
(1,1233)	1:499:A:LEU:HD21	1:508:A:THR:H	13	0.61
(1,1233)	1:499:A:LEU:HD22	1:508:A:THR:H	13	0.61
(1,1233)	1:499:A:LEU:HD23	1:508:A:THR:H	13	0.61
(1,1233)	1:499:A:LEU:HD11	1:508:A:THR:H	19	0.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1233)	1:499:A:LEU:HD12	1:508:A:THR:H	19	0.61
(1,1233)	1:499:A:LEU:HD13	1:508:A:THR:H	19	0.61
(1,1233)	1:499:A:LEU:HD21	1:508:A:THR:H	19	0.61
(1,1233)	1:499:A:LEU:HD22	1:508:A:THR:H	19	0.61
(1,1233)	1:499:A:LEU:HD23	1:508:A:THR:H	19	0.61
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	18	0.58
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	18	0.58
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	18	0.58
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	18	0.58
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	18	0.58
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	18	0.58
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	18	0.58
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	18	0.58
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	18	0.58
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	18	0.58
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	18	0.58
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	18	0.58
(1,1232)	1:499:A:LEU:HD11	1:507:A:TYR:H	8	0.58
(1,1232)	1:499:A:LEU:HD12	1:507:A:TYR:H	8	0.58
(1,1232)	1:499:A:LEU:HD13	1:507:A:TYR:H	8	0.58
(1,1232)	1:499:A:LEU:HD21	1:507:A:TYR:H	8	0.58
(1,1232)	1:499:A:LEU:HD22	1:507:A:TYR:H	8	0.58
(1,1232)	1:499:A:LEU:HD23	1:507:A:TYR:H	8	0.58
(1,1232)	1:499:A:LEU:HD11	1:507:A:TYR:H	16	0.58
(1,1232)	1:499:A:LEU:HD12	1:507:A:TYR:H	16	0.58
(1,1232)	1:499:A:LEU:HD13	1:507:A:TYR:H	16	0.58
(1,1232)	1:499:A:LEU:HD21	1:507:A:TYR:H	16	0.58
(1,1232)	1:499:A:LEU:HD22	1:507:A:TYR:H	16	0.58
(1,1232)	1:499:A:LEU:HD23	1:507:A:TYR:H	16	0.58
(1,1232)	1:499:A:LEU:HD11	1:507:A:TYR:H	13	0.54
(1,1232)	1:499:A:LEU:HD12	1:507:A:TYR:H	13	0.54
(1,1232)	1:499:A:LEU:HD13	1:507:A:TYR:H	13	0.54
(1,1232)	1:499:A:LEU:HD21	1:507:A:TYR:H	13	0.54
(1,1232)	1:499:A:LEU:HD22	1:507:A:TYR:H	13	0.54
(1,1232)	1:499:A:LEU:HD23	1:507:A:TYR:H	13	0.54
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	17	0.54
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	17	0.54
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	17	0.54
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	17	0.54
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	17	0.54
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	17	0.54
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	16	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	16	0.53
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	16	0.53
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	16	0.53
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	16	0.53
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	16	0.53
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	17	0.52
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	17	0.52
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	17	0.52
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	17	0.52
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	17	0.52
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	17	0.52
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	17	0.52
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	17	0.52
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	17	0.52
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	17	0.52
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	17	0.52
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	17	0.52
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	20	0.51
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	20	0.51
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	20	0.51
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	20	0.51
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	20	0.51
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	20	0.51
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	20	0.51
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	20	0.51
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	20	0.51
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	20	0.51
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	20	0.51
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	20	0.51
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	6	0.5
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	6	0.5
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	6	0.5
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	6	0.5
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	6	0.5
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	6	0.5
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	19	0.5
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	19	0.5
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	19	0.5
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	19	0.5
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	19	0.5
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	19	0.5
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	13	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	13	0.49
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	13	0.49
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	13	0.49
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	13	0.49
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	13	0.49
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	5	0.47
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	5	0.47
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	5	0.47
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	5	0.47
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	5	0.47
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	5	0.47
(1,1107)	1:464:A:LEU:HD11	1:466:A:PHE:H	11	0.47
(1,1107)	1:464:A:LEU:HD12	1:466:A:PHE:H	11	0.47
(1,1107)	1:464:A:LEU:HD13	1:466:A:PHE:H	11	0.47
(1,1107)	1:464:A:LEU:HD21	1:466:A:PHE:H	11	0.47
(1,1107)	1:464:A:LEU:HD22	1:466:A:PHE:H	11	0.47
(1,1107)	1:464:A:LEU:HD23	1:466:A:PHE:H	11	0.47
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	13	0.44
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	13	0.44
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	13	0.44
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	13	0.44
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	13	0.44
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	13	0.44
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	13	0.44
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	13	0.44
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	13	0.44
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	13	0.44
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	13	0.44
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	13	0.44
(1,1231)	1:499:A:LEU:HD11	1:506:A:ASP:HA	11	0.42
(1,1231)	1:499:A:LEU:HD12	1:506:A:ASP:HA	11	0.42
(1,1231)	1:499:A:LEU:HD13	1:506:A:ASP:HA	11	0.42
(1,1231)	1:499:A:LEU:HD21	1:506:A:ASP:HA	11	0.42
(1,1231)	1:499:A:LEU:HD22	1:506:A:ASP:HA	11	0.42
(1,1231)	1:499:A:LEU:HD23	1:506:A:ASP:HA	11	0.42
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	9	0.41
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	9	0.41
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	9	0.41
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	9	0.41
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	9	0.41
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	9	0.41
(1,1107)	1:464:A:LEU:HD11	1:466:A:PHE:H	16	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1107)	1:464:A:LEU:HD12	1:466:A:PHE:H	16	0.41
(1,1107)	1:464:A:LEU:HD13	1:466:A:PHE:H	16	0.41
(1,1107)	1:464:A:LEU:HD21	1:466:A:PHE:H	16	0.41
(1,1107)	1:464:A:LEU:HD22	1:466:A:PHE:H	16	0.41
(1,1107)	1:464:A:LEU:HD23	1:466:A:PHE:H	16	0.41
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	1	0.4
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	1	0.4
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	1	0.4
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	1	0.4
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	1	0.4
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	1	0.4
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	1	0.4
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	1	0.4
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	1	0.4
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	1	0.4
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	1	0.4
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	1	0.4
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	2	0.39
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	2	0.39
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	2	0.39
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	2	0.39
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	2	0.39
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	2	0.39
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	2	0.39
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	2	0.39
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	2	0.39
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	2	0.39
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	2	0.39
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	2	0.39
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	18	0.39
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	18	0.39
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	18	0.39
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	18	0.39
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	18	0.39
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	18	0.39
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	10	0.38
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	10	0.38
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	10	0.38
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	10	0.38
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	10	0.38
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	10	0.38
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	9	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	9	0.37
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	9	0.37
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	9	0.37
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	9	0.37
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	9	0.37
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	9	0.37
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	9	0.37
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	9	0.37
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	9	0.37
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	9	0.37
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	9	0.37
(1,1231)	1:499:A:LEU:HD11	1:506:A:ASP:HA	16	0.37
(1,1231)	1:499:A:LEU:HD12	1:506:A:ASP:HA	16	0.37
(1,1231)	1:499:A:LEU:HD13	1:506:A:ASP:HA	16	0.37
(1,1231)	1:499:A:LEU:HD21	1:506:A:ASP:HA	16	0.37
(1,1231)	1:499:A:LEU:HD22	1:506:A:ASP:HA	16	0.37
(1,1231)	1:499:A:LEU:HD23	1:506:A:ASP:HA	16	0.37
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	11	0.36
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	11	0.36
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	11	0.36
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	11	0.36
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	11	0.36
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	11	0.36
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	11	0.36
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	11	0.36
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	11	0.36
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	11	0.36
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	11	0.36
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	11	0.36
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	1	0.36
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	1	0.36
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	1	0.36
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	1	0.36
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	1	0.36
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	1	0.36
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	19	0.35
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	19	0.35
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	19	0.35
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	19	0.35
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	19	0.35
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	19	0.35
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	19	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	19	0.35
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	19	0.35
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	19	0.35
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	19	0.35
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	19	0.35
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	7	0.35
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	7	0.35
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	7	0.35
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	7	0.35
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	7	0.35
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	7	0.35
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	14	0.35
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	14	0.35
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	14	0.35
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	14	0.35
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	14	0.35
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	14	0.35
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	3	0.34
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	3	0.34
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	3	0.34
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	3	0.34
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	3	0.34
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	3	0.34
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	3	0.34
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	3	0.34
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	3	0.34
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	3	0.34
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	3	0.34
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	3	0.34
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	16	0.33
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	16	0.33
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	16	0.33
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	16	0.33
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	16	0.33
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	16	0.33
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	16	0.33
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	16	0.33
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	16	0.33
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	16	0.33
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	16	0.33
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	16	0.33
(1,1107)	1:464:A:LEU:HD11	1:466:A:PHE:H	5	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1107)	1:464:A:LEU:HD12	1:466:A:PHE:H	5	0.32
(1,1107)	1:464:A:LEU:HD13	1:466:A:PHE:H	5	0.32
(1,1107)	1:464:A:LEU:HD21	1:466:A:PHE:H	5	0.32
(1,1107)	1:464:A:LEU:HD22	1:466:A:PHE:H	5	0.32
(1,1107)	1:464:A:LEU:HD23	1:466:A:PHE:H	5	0.32
(1,1107)	1:464:A:LEU:HD11	1:466:A:PHE:H	14	0.32
(1,1107)	1:464:A:LEU:HD12	1:466:A:PHE:H	14	0.32
(1,1107)	1:464:A:LEU:HD13	1:466:A:PHE:H	14	0.32
(1,1107)	1:464:A:LEU:HD21	1:466:A:PHE:H	14	0.32
(1,1107)	1:464:A:LEU:HD22	1:466:A:PHE:H	14	0.32
(1,1107)	1:464:A:LEU:HD23	1:466:A:PHE:H	14	0.32
(1,1107)	1:464:A:LEU:HD11	1:466:A:PHE:H	19	0.32
(1,1107)	1:464:A:LEU:HD12	1:466:A:PHE:H	19	0.32
(1,1107)	1:464:A:LEU:HD13	1:466:A:PHE:H	19	0.32
(1,1107)	1:464:A:LEU:HD21	1:466:A:PHE:H	19	0.32
(1,1107)	1:464:A:LEU:HD22	1:466:A:PHE:H	19	0.32
(1,1107)	1:464:A:LEU:HD23	1:466:A:PHE:H	19	0.32
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	15	0.31
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	15	0.31
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	15	0.31
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	15	0.31
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	15	0.31
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	15	0.31
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD11	1	0.31
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD12	1	0.31
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD13	1	0.31
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD21	1	0.31
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD22	1	0.31
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD23	1	0.31
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD11	19	0.31
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD12	19	0.31
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD13	19	0.31
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD21	19	0.31
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD22	19	0.31
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD23	19	0.31
(1,1231)	1:499:A:LEU:HD11	1:506:A:ASP:HA	15	0.3
(1,1231)	1:499:A:LEU:HD12	1:506:A:ASP:HA	15	0.3
(1,1231)	1:499:A:LEU:HD13	1:506:A:ASP:HA	15	0.3
(1,1231)	1:499:A:LEU:HD21	1:506:A:ASP:HA	15	0.3
(1,1231)	1:499:A:LEU:HD22	1:506:A:ASP:HA	15	0.3
(1,1231)	1:499:A:LEU:HD23	1:506:A:ASP:HA	15	0.3
(1,1107)	1:464:A:LEU:HD11	1:466:A:PHE:H	9	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1107)	1:464:A:LEU:HD12	1:466:A:PHE:H	9	0.3
(1,1107)	1:464:A:LEU:HD13	1:466:A:PHE:H	9	0.3
(1,1107)	1:464:A:LEU:HD21	1:466:A:PHE:H	9	0.3
(1,1107)	1:464:A:LEU:HD22	1:466:A:PHE:H	9	0.3
(1,1107)	1:464:A:LEU:HD23	1:466:A:PHE:H	9	0.3
(1,1231)	1:499:A:LEU:HD11	1:506:A:ASP:HA	8	0.29
(1,1231)	1:499:A:LEU:HD12	1:506:A:ASP:HA	8	0.29
(1,1231)	1:499:A:LEU:HD13	1:506:A:ASP:HA	8	0.29
(1,1231)	1:499:A:LEU:HD21	1:506:A:ASP:HA	8	0.29
(1,1231)	1:499:A:LEU:HD22	1:506:A:ASP:HA	8	0.29
(1,1231)	1:499:A:LEU:HD23	1:506:A:ASP:HA	8	0.29
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD11	3	0.29
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD12	3	0.29
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD13	3	0.29
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD21	3	0.29
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD22	3	0.29
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD23	3	0.29
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	7	0.28
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	7	0.28
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	7	0.28
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	7	0.28
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	7	0.28
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	7	0.28
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	7	0.28
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	7	0.28
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	7	0.28
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	7	0.28
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	7	0.28
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	7	0.28
(1,1231)	1:499:A:LEU:HD11	1:506:A:ASP:HA	19	0.28
(1,1231)	1:499:A:LEU:HD12	1:506:A:ASP:HA	19	0.28
(1,1231)	1:499:A:LEU:HD13	1:506:A:ASP:HA	19	0.28
(1,1231)	1:499:A:LEU:HD21	1:506:A:ASP:HA	19	0.28
(1,1231)	1:499:A:LEU:HD22	1:506:A:ASP:HA	19	0.28
(1,1231)	1:499:A:LEU:HD23	1:506:A:ASP:HA	19	0.28
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	6	0.27
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	6	0.27
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	6	0.27
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	6	0.27
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	6	0.27
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	6	0.27
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	6	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	6	0.27
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	6	0.27
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	6	0.27
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	6	0.27
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	6	0.27
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	3	0.25
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	3	0.25
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	3	0.25
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	3	0.25
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	3	0.25
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	3	0.25
(1,1107)	1:464:A:LEU:HD11	1:466:A:PHE:H	8	0.25
(1,1107)	1:464:A:LEU:HD12	1:466:A:PHE:H	8	0.25
(1,1107)	1:464:A:LEU:HD13	1:466:A:PHE:H	8	0.25
(1,1107)	1:464:A:LEU:HD21	1:466:A:PHE:H	8	0.25
(1,1107)	1:464:A:LEU:HD22	1:466:A:PHE:H	8	0.25
(1,1107)	1:464:A:LEU:HD23	1:466:A:PHE:H	8	0.25
(1,1107)	1:464:A:LEU:HD11	1:466:A:PHE:H	17	0.25
(1,1107)	1:464:A:LEU:HD12	1:466:A:PHE:H	17	0.25
(1,1107)	1:464:A:LEU:HD13	1:466:A:PHE:H	17	0.25
(1,1107)	1:464:A:LEU:HD21	1:466:A:PHE:H	17	0.25
(1,1107)	1:464:A:LEU:HD22	1:466:A:PHE:H	17	0.25
(1,1107)	1:464:A:LEU:HD23	1:466:A:PHE:H	17	0.25
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD11	15	0.25
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD12	15	0.25
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD13	15	0.25
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD21	15	0.25
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD22	15	0.25
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD23	15	0.25
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	11	0.24
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	11	0.24
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	11	0.24
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	11	0.24
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	11	0.24
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	11	0.24
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	4	0.21
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	4	0.21
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	4	0.21
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	4	0.21
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	4	0.21
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	4	0.21
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	4	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	4	0.21
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	4	0.21
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	4	0.21
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	4	0.21
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	4	0.21
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	14	0.21
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	14	0.21
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	14	0.21
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	14	0.21
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	14	0.21
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	14	0.21
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	14	0.21
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	14	0.21
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	14	0.21
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	14	0.21
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	14	0.21
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	14	0.21
(1,1107)	1:464:A:LEU:HD11	1:466:A:PHE:H	6	0.21
(1,1107)	1:464:A:LEU:HD12	1:466:A:PHE:H	6	0.21
(1,1107)	1:464:A:LEU:HD13	1:466:A:PHE:H	6	0.21
(1,1107)	1:464:A:LEU:HD21	1:466:A:PHE:H	6	0.21
(1,1107)	1:464:A:LEU:HD22	1:466:A:PHE:H	6	0.21
(1,1107)	1:464:A:LEU:HD23	1:466:A:PHE:H	6	0.21
(1,1107)	1:464:A:LEU:HD11	1:466:A:PHE:H	12	0.21
(1,1107)	1:464:A:LEU:HD12	1:466:A:PHE:H	12	0.21
(1,1107)	1:464:A:LEU:HD13	1:466:A:PHE:H	12	0.21
(1,1107)	1:464:A:LEU:HD21	1:466:A:PHE:H	12	0.21
(1,1107)	1:464:A:LEU:HD22	1:466:A:PHE:H	12	0.21
(1,1107)	1:464:A:LEU:HD23	1:466:A:PHE:H	12	0.21
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD11	17	0.2
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD12	17	0.2
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD13	17	0.2
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD21	17	0.2
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD22	17	0.2
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD23	17	0.2
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	15	0.19
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	15	0.19
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	15	0.19
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	15	0.19
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	15	0.19
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	15	0.19
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	15	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	15	0.19
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	15	0.19
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	15	0.19
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	15	0.19
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	15	0.19
(1,1231)	1:499:A:LEU:HD11	1:506:A:ASP:HA	13	0.19
(1,1231)	1:499:A:LEU:HD12	1:506:A:ASP:HA	13	0.19
(1,1231)	1:499:A:LEU:HD13	1:506:A:ASP:HA	13	0.19
(1,1231)	1:499:A:LEU:HD21	1:506:A:ASP:HA	13	0.19
(1,1231)	1:499:A:LEU:HD22	1:506:A:ASP:HA	13	0.19
(1,1231)	1:499:A:LEU:HD23	1:506:A:ASP:HA	13	0.19
(1,1107)	1:464:A:LEU:HD11	1:466:A:PHE:H	2	0.18
(1,1107)	1:464:A:LEU:HD12	1:466:A:PHE:H	2	0.18
(1,1107)	1:464:A:LEU:HD13	1:466:A:PHE:H	2	0.18
(1,1107)	1:464:A:LEU:HD21	1:466:A:PHE:H	2	0.18
(1,1107)	1:464:A:LEU:HD22	1:466:A:PHE:H	2	0.18
(1,1107)	1:464:A:LEU:HD23	1:466:A:PHE:H	2	0.18
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD11	2	0.18
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD12	2	0.18
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD13	2	0.18
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD21	2	0.18
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD22	2	0.18
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD23	2	0.18
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD11	12	0.18
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD12	12	0.18
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD13	12	0.18
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD21	12	0.18
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD22	12	0.18
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD23	12	0.18
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD11	7	0.17
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD12	7	0.17
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD13	7	0.17
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD21	7	0.17
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD22	7	0.17
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD23	7	0.17
(1,287)	1:516:A:GLN:H	1:516:A:GLN:HG2	9	0.17
(1,287)	1:516:A:GLN:H	1:516:A:GLN:HG3	9	0.17
(1,1286)	1:535:A:TRP:HB2	1:536:A:GLY:HA3	2	0.16
(1,1286)	1:535:A:TRP:HB3	1:536:A:GLY:HA3	2	0.16
(1,1107)	1:464:A:LEU:HD11	1:466:A:PHE:H	15	0.16
(1,1107)	1:464:A:LEU:HD12	1:466:A:PHE:H	15	0.16
(1,1107)	1:464:A:LEU:HD13	1:466:A:PHE:H	15	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1107)	1:464:A:LEU:HD21	1:466:A:PHE:H	15	0.16
(1,1107)	1:464:A:LEU:HD22	1:466:A:PHE:H	15	0.16
(1,1107)	1:464:A:LEU:HD23	1:466:A:PHE:H	15	0.16
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	10	0.16
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD11	18	0.15
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD12	18	0.15
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD13	18	0.15
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD21	18	0.15
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD22	18	0.15
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD23	18	0.15
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB1	9	0.15
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB2	9	0.15
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB3	9	0.15
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	4	0.15
(1,361)	1:520:A:ALA:H	1:524:A:TYR:HB3	16	0.15
(1,250)	1:471:A:ALA:H	1:472:A:GLY:H	15	0.15
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB1	17	0.14
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB2	17	0.14
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB3	17	0.14
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	9	0.14
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	17	0.14
(1,250)	1:471:A:ALA:H	1:472:A:GLY:H	12	0.14
(1,250)	1:471:A:ALA:H	1:472:A:GLY:H	16	0.14
(1,1286)	1:535:A:TRP:HB2	1:536:A:GLY:HA3	7	0.13
(1,1286)	1:535:A:TRP:HB3	1:536:A:GLY:HA3	7	0.13
(1,1263)	1:514:A:GLN:HG2	1:516:A:GLN:H	5	0.13
(1,1263)	1:514:A:GLN:HG3	1:516:A:GLN:H	5	0.13
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD11	4	0.13
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD12	4	0.13
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD13	4	0.13
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD21	4	0.13
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD22	4	0.13
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD23	4	0.13
(1,889)	1:497:A:LEU:HG	1:538:A:VAL:HB	10	0.13
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB1	3	0.13
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB2	3	0.13
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB3	3	0.13
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB1	16	0.13
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB2	16	0.13
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB3	16	0.13
(1,577)	1:493:A:ASN:H	1:540:A:ILE:HA	4	0.13
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	7	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	8	0.13
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	11	0.13
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	12	0.13
(1,361)	1:520:A:ALA:H	1:524:A:TYR:HB3	7	0.13
(1,361)	1:520:A:ALA:H	1:524:A:TYR:HB3	11	0.13
(1,263)	1:500:A:LEU:H	1:509:A:ASN:H	17	0.13
(1,250)	1:471:A:ALA:H	1:472:A:GLY:H	3	0.13
(1,250)	1:471:A:ALA:H	1:472:A:GLY:H	6	0.13
(1,1263)	1:514:A:GLN:HG2	1:516:A:GLN:H	4	0.12
(1,1263)	1:514:A:GLN:HG3	1:516:A:GLN:H	4	0.12
(1,1263)	1:514:A:GLN:HG2	1:516:A:GLN:H	7	0.12
(1,1263)	1:514:A:GLN:HG3	1:516:A:GLN:H	7	0.12
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD2	10	0.12
(1,1235)	1:499:A:LEU:HD11	1:530:A:LYS:HD3	10	0.12
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD2	10	0.12
(1,1235)	1:499:A:LEU:HD12	1:530:A:LYS:HD3	10	0.12
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD2	10	0.12
(1,1235)	1:499:A:LEU:HD13	1:530:A:LYS:HD3	10	0.12
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD2	10	0.12
(1,1235)	1:499:A:LEU:HD21	1:530:A:LYS:HD3	10	0.12
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD2	10	0.12
(1,1235)	1:499:A:LEU:HD22	1:530:A:LYS:HD3	10	0.12
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD2	10	0.12
(1,1235)	1:499:A:LEU:HD23	1:530:A:LYS:HD3	10	0.12
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD11	11	0.12
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD12	11	0.12
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD13	11	0.12
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD21	11	0.12
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD22	11	0.12
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD23	11	0.12
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	20	0.12
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	20	0.12
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	20	0.12
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	20	0.12
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	20	0.12
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	20	0.12
(1,889)	1:497:A:LEU:HG	1:538:A:VAL:HB	3	0.12
(1,889)	1:497:A:LEU:HG	1:538:A:VAL:HB	16	0.12
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB1	6	0.12
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB2	6	0.12
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB3	6	0.12
(1,555)	1:495:A:TRP:HB3	1:496:A:ASN:H	14	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	2	0.12
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	18	0.12
(1,361)	1:520:A:ALA:H	1:524:A:TYR:HB3	20	0.12
(1,263)	1:500:A:LEU:H	1:509:A:ASN:H	7	0.12
(1,263)	1:500:A:LEU:H	1:509:A:ASN:H	11	0.12
(1,250)	1:471:A:ALA:H	1:472:A:GLY:H	18	0.12
(1,188)	1:505:A:THR:H	1:506:A:ASP:H	15	0.12
(1,1263)	1:514:A:GLN:HG2	1:516:A:GLN:H	1	0.11
(1,1263)	1:514:A:GLN:HG3	1:516:A:GLN:H	1	0.11
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD11	15	0.11
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD12	15	0.11
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD13	15	0.11
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD21	15	0.11
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD22	15	0.11
(1,1221)	1:499:A:LEU:HA	1:499:A:LEU:HD23	15	0.11
(1,1107)	1:464:A:LEU:HD11	1:466:A:PHE:H	3	0.11
(1,1107)	1:464:A:LEU:HD12	1:466:A:PHE:H	3	0.11
(1,1107)	1:464:A:LEU:HD13	1:466:A:PHE:H	3	0.11
(1,1107)	1:464:A:LEU:HD21	1:466:A:PHE:H	3	0.11
(1,1107)	1:464:A:LEU:HD22	1:466:A:PHE:H	3	0.11
(1,1107)	1:464:A:LEU:HD23	1:466:A:PHE:H	3	0.11
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD11	8	0.11
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD12	8	0.11
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD13	8	0.11
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD21	8	0.11
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD22	8	0.11
(1,1102)	1:463:A:ALA:H	1:464:A:LEU:HD23	8	0.11
(1,988)	1:477:A:LYS:HB2	1:524:A:TYR:HA	9	0.11
(1,889)	1:497:A:LEU:HG	1:538:A:VAL:HB	11	0.11
(1,825)	1:497:A:LEU:HD21	1:536:A:GLY:HA2	2	0.11
(1,825)	1:497:A:LEU:HD22	1:536:A:GLY:HA2	2	0.11
(1,825)	1:497:A:LEU:HD23	1:536:A:GLY:HA2	2	0.11
(1,593)	1:470:A:GLY:H	1:535:A:TRP:H	11	0.11
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB1	7	0.11
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB2	7	0.11
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB3	7	0.11
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB1	15	0.11
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB2	15	0.11
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB3	15	0.11
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB1	18	0.11
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB2	18	0.11
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB3	18	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:504:A:GLY:H	1:505:A:THR:HA	18	0.11
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	1	0.11
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	3	0.11
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	5	0.11
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	6	0.11
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	16	0.11
(1,424)	1:480:A:GLN:HE21	1:481:A:PHE:H	20	0.11
(1,380)	1:471:A:ALA:H	1:532:A:GLY:H	11	0.11
(1,361)	1:520:A:ALA:H	1:524:A:TYR:HB3	2	0.11
(1,361)	1:520:A:ALA:H	1:524:A:TYR:HB3	6	0.11
(1,299)	1:507:A:TYR:HA	1:510:A:VAL:H	7	0.11
(1,299)	1:507:A:TYR:HA	1:510:A:VAL:H	17	0.11
(1,299)	1:507:A:TYR:HA	1:510:A:VAL:H	18	0.11
(1,263)	1:500:A:LEU:H	1:509:A:ASN:H	4	0.11
(1,263)	1:500:A:LEU:H	1:509:A:ASN:H	6	0.11
(1,263)	1:500:A:LEU:H	1:509:A:ASN:H	10	0.11
(1,263)	1:500:A:LEU:H	1:509:A:ASN:H	20	0.11
(1,250)	1:471:A:ALA:H	1:472:A:GLY:H	5	0.11
(1,250)	1:471:A:ALA:H	1:472:A:GLY:H	9	0.11
(1,250)	1:471:A:ALA:H	1:472:A:GLY:H	17	0.11
(1,250)	1:471:A:ALA:H	1:472:A:GLY:H	20	0.11
(1,247)	1:458:A:GLU:H	1:459:A:TYR:HB3	6	0.11
(1,188)	1:505:A:THR:H	1:506:A:ASP:H	5	0.11
(1,188)	1:505:A:THR:H	1:506:A:ASP:H	6	0.11
(1,188)	1:505:A:THR:H	1:506:A:ASP:H	20	0.11
(1,1286)	1:535:A:TRP:HB2	1:536:A:GLY:HA3	5	0.1
(1,1286)	1:535:A:TRP:HB3	1:536:A:GLY:HA3	5	0.1
(1,1263)	1:514:A:GLN:HG2	1:516:A:GLN:H	19	0.1
(1,1263)	1:514:A:GLN:HG3	1:516:A:GLN:H	19	0.1
(1,1204)	1:492:A:VAL:HG11	1:513:A:ALA:HA	4	0.1
(1,1204)	1:492:A:VAL:HG12	1:513:A:ALA:HA	4	0.1
(1,1204)	1:492:A:VAL:HG13	1:513:A:ALA:HA	4	0.1
(1,1204)	1:492:A:VAL:HG21	1:513:A:ALA:HA	4	0.1
(1,1204)	1:492:A:VAL:HG22	1:513:A:ALA:HA	4	0.1
(1,1204)	1:492:A:VAL:HG23	1:513:A:ALA:HA	4	0.1
(1,1056)	1:517:A:ILE:HG21	1:518:A:PRO:HB3	17	0.1
(1,1056)	1:517:A:ILE:HG22	1:518:A:PRO:HB3	17	0.1
(1,1056)	1:517:A:ILE:HG23	1:518:A:PRO:HB3	17	0.1
(1,889)	1:497:A:LEU:HG	1:538:A:VAL:HB	18	0.1
(1,830)	1:471:A:ALA:HA	1:533:A:VAL:HG21	8	0.1
(1,830)	1:471:A:ALA:HA	1:533:A:VAL:HG22	8	0.1
(1,830)	1:471:A:ALA:HA	1:533:A:VAL:HG23	8	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,779)	1:496:A:ASN:HA	1:533:A:VAL:HG21	20	0.1
(1,779)	1:496:A:ASN:HA	1:533:A:VAL:HG22	20	0.1
(1,779)	1:496:A:ASN:HA	1:533:A:VAL:HG23	20	0.1
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB1	2	0.1
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB2	2	0.1
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB3	2	0.1
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB1	10	0.1
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB2	10	0.1
(1,591)	1:470:A:GLY:H	1:471:A:ALA:HB3	10	0.1
(1,577)	1:493:A:ASN:H	1:540:A:ILE:HA	8	0.1
(1,542)	1:504:A:GLY:H	1:505:A:THR:HA	10	0.1
(1,542)	1:504:A:GLY:H	1:505:A:THR:HA	14	0.1
(1,542)	1:504:A:GLY:H	1:505:A:THR:HA	20	0.1
(1,477)	1:486:A:ASN:HA	1:486:A:ASN:HD22	16	0.1
(1,380)	1:471:A:ALA:H	1:532:A:GLY:H	6	0.1
(1,263)	1:500:A:LEU:H	1:509:A:ASN:H	14	0.1
(1,8)	1:459:A:TYR:HD1	1:460:A:THR:H	11	0.1
(1,8)	1:459:A:TYR:HD2	1:460:A:THR:H	11	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found