



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 02:57 PM UTC

PDB ID : 9DE2 / pdb_00009de2
BMRB ID : 31200
Title : ETO2 MYND bound to MPPL peptide from GATAD2A
Authors : Williams, D.C.
Deposited on : 2024-08-28

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

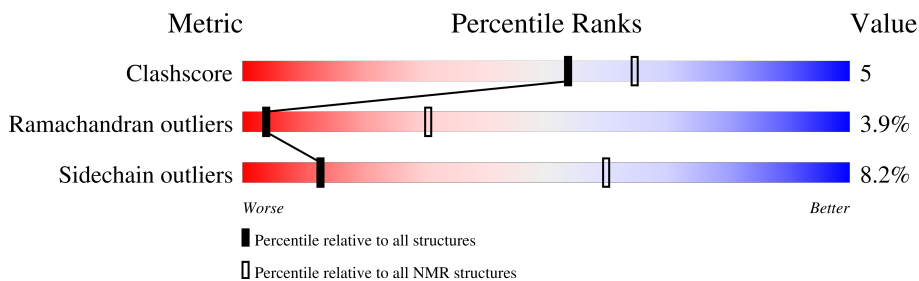
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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	71	

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 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:533-A:539, A:555-A:593 (46)	0.66	6

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1022 atoms, of which 487 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	71	1020	313	487	108	104	8	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	549	GLY	-	linker	PDB ?
A	550	SER	-	linker	PDB ?

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

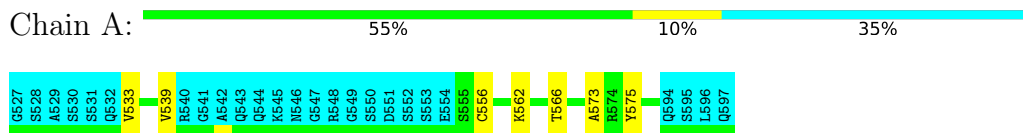
Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

4 Residue-property plots i

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: GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein

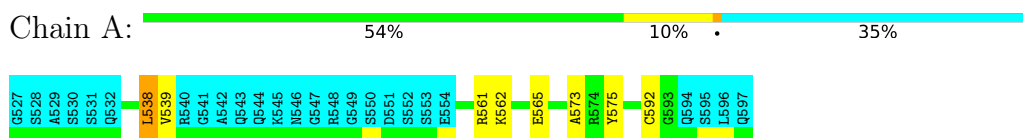


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

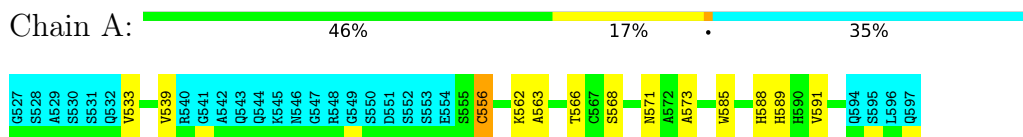
4.2.1 Score per residue for model 1

- Molecule 1: GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein



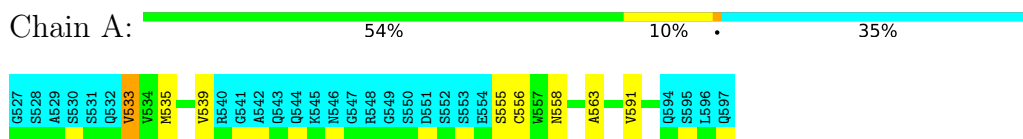
4.2.2 Score per residue for model 2

- Molecule 1: GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein



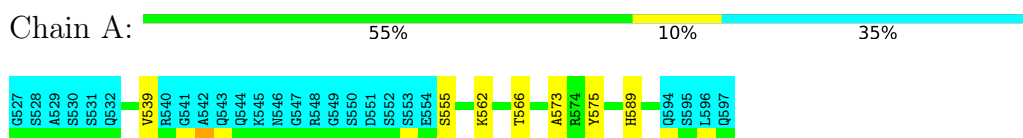
4.2.8 Score per residue for model 8

- Molecule 1: GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein



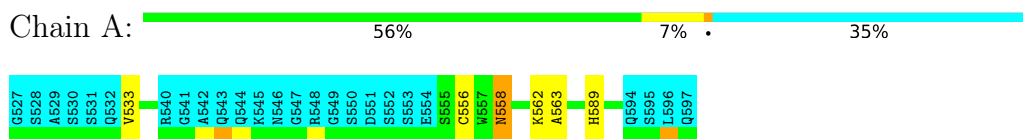
4.2.9 Score per residue for model 9

- Molecule 1: GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein



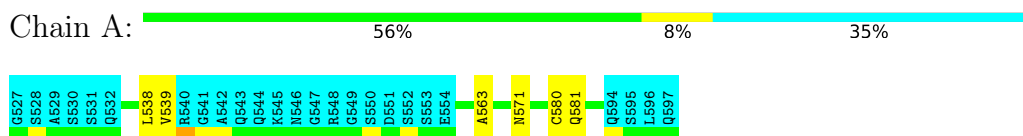
4.2.10 Score per residue for model 10

- Molecule 1: GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein



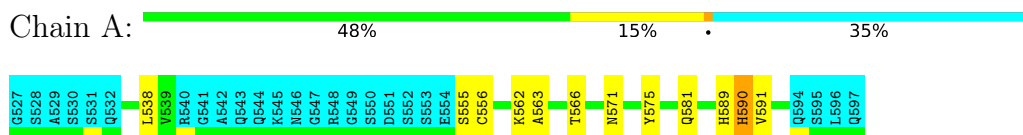
4.2.11 Score per residue for model 11

- Molecule 1: GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein



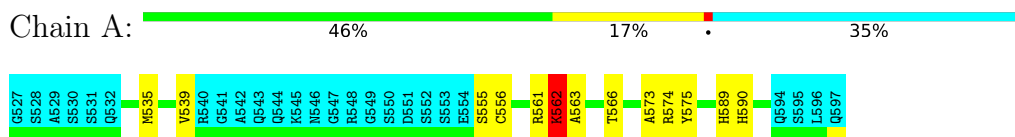
4.2.12 Score per residue for model 12

- Molecule 1: GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein



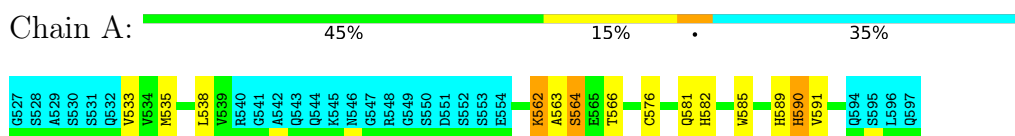
4.2.13 Score per residue for model 13

- Molecule 1: GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein



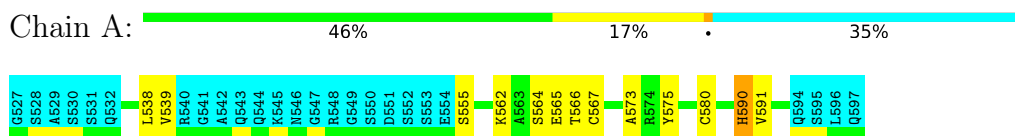
4.2.14 Score per residue for model 14

- Molecule 1: GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein



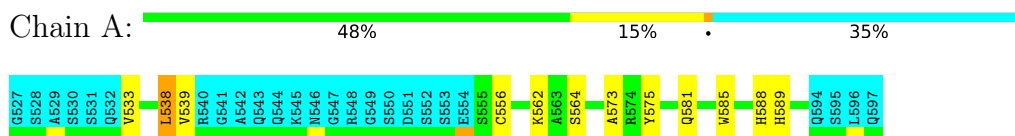
4.2.15 Score per residue for model 15

- Molecule 1: GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein



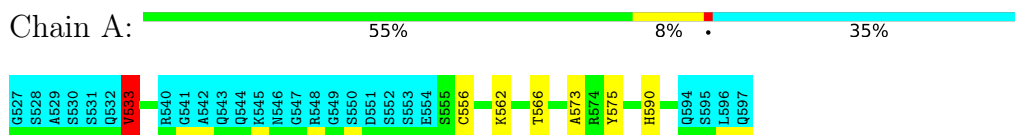
4.2.16 Score per residue for model 16

- Molecule 1: GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein



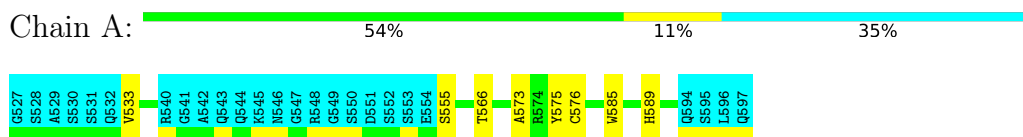
4.2.17 Score per residue for model 17

- Molecule 1: GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein



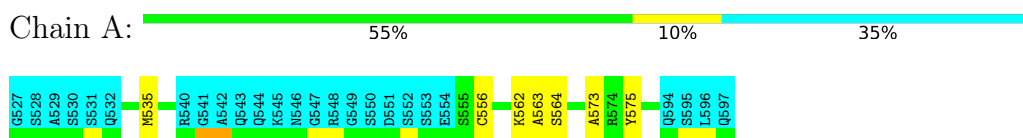
4.2.18 Score per residue for model 18

- Molecule 1: GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein



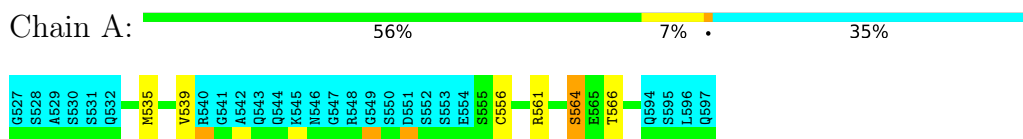
4.2.19 Score per residue for model 19

- Molecule 1: GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein



4.2.20 Score per residue for model 20

- Molecule 1: GATAD2A-MPPL motif and ETO2 NHR4 domain fusion protein



5 Refinement protocol and experimental data overview

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

Of the 100 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
X-PLOR NIH	structure calculation	3.8

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	702
Number of shifts mapped to atoms	702
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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:
ZN

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts 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	355	322	319	4±2
All	All	7140	6440	6380	70

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:573:ALA:HB1	1:A:575:TYR:CE2	0.70	2.22	4	8
1:A:538:LEU:HD13	1:A:565:GLU:CD	0.60	2.21	15	1
1:A:573:ALA:HB1	1:A:575:TYR:CE1	0.59	2.32	19	2
1:A:539:VAL:HG22	1:A:566:THR:O	0.58	1.98	6	5
1:A:538:LEU:HD21	1:A:581:GLN:OE1	0.58	1.99	11	2
1:A:566:THR:HG21	1:A:571:ASN:OD1	0.57	2.00	5	2
1:A:539:VAL:HG13	1:A:568:SER:OG	0.57	2.00	7	3
1:A:535:MET:HE1	1:A:582:HIS:CD2	0.57	2.34	14	1
1:A:563:ALA:HB1	1:A:575:TYR:C	0.56	2.25	3	4
1:A:538:LEU:HD11	1:A:581:GLN:CD	0.56	2.26	16	1
1:A:533:VAL:HG22	1:A:585:TRP:HE1	0.55	1.60	16	4
1:A:533:VAL:O	1:A:533:VAL:HG13	0.55	2.02	16	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:533:VAL:HG22	1:A:585:TRP:NE1	0.53	2.18	2	3
1:A:538:LEU:HD13	1:A:565:GLU:OE2	0.52	2.05	15	1
1:A:556:CYS:N	1:A:563:ALA:HB2	0.50	2.21	10	1
1:A:573:ALA:HB2	1:A:588:HIS:CE1	0.50	2.42	16	2
1:A:563:ALA:O	1:A:564:SER:CB	0.48	2.60	14	1
1:A:533:VAL:HG22	1:A:533:VAL:O	0.48	2.09	6	2
1:A:573:ALA:HB3	1:A:575:TYR:CE1	0.47	2.44	1	1
1:A:533:VAL:O	1:A:533:VAL:HG22	0.47	2.10	17	1
1:A:538:LEU:HD23	1:A:567:CYS:HA	0.47	1.87	15	1
1:A:556:CYS:CA	1:A:563:ALA:HB2	0.47	2.39	19	1
1:A:533:VAL:HG13	1:A:585:TRP:HE1	0.45	1.72	3	1
1:A:556:CYS:HB2	1:A:563:ALA:HB2	0.45	1.88	8	1
1:A:566:THR:HG22	1:A:571:ASN:HA	0.44	1.90	2	1
1:A:556:CYS:SG	1:A:563:ALA:HB2	0.44	2.52	12	1
1:A:590:HIS:CD2	1:A:591:VAL:HG23	0.44	2.47	14	3
1:A:538:LEU:HD11	1:A:581:GLN:OE1	0.43	2.13	14	1
1:A:538:LEU:HD13	1:A:581:GLN:NE2	0.43	2.28	3	1
1:A:538:LEU:HD12	1:A:565:GLU:CB	0.43	2.43	1	1
1:A:563:ALA:HB1	1:A:575:TYR:O	0.43	2.14	3	1
1:A:556:CYS:CB	1:A:563:ALA:HB2	0.42	2.43	2	1
1:A:563:ALA:HB3	1:A:574:ARG:HG2	0.42	1.91	5	1
1:A:561:ARG:O	1:A:562:LYS:C	0.42	2.63	5	2
1:A:591:VAL:O	1:A:591:VAL:HG12	0.40	2.15	2	1
1:A:570:CYS:O	1:A:571:ASN:CB	0.40	2.70	5	1
1:A:573:ALA:HB3	1:A:575:TYR:HE1	0.40	1.76	16	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	46/71 (65%)	41±2 (89±4%)	3±2 (7±3%)	2±1 (4±1%)	4	30
All	All	920/1420 (65%)	816 (89%)	68 (7%)	36 (4%)	4	30

All 7 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	562	LYS	15
1	A	555	SER	8
1	A	564	SER	7
1	A	561	ARG	2
1	A	558	ASN	2
1	A	563	ALA	1
1	A	533	VAL	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	39/58 (67%)	36±2 (92±4%)	3±2 (8±4%)	13	60
All	All	780/1160 (67%)	716 (92%)	64 (8%)	13	60

All 20 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	589	HIS	10
1	A	556	CYS	9
1	A	590	HIS	7
1	A	535	MET	5
1	A	539	VAL	4
1	A	533	VAL	4
1	A	566	THR	4
1	A	562	LYS	3
1	A	538	LEU	2
1	A	571	ASN	2
1	A	564	SER	2
1	A	574	ARG	2
1	A	580	CYS	2
1	A	576	CYS	2
1	A	561	ARG	1
1	A	592	CYS	1
1	A	555	SER	1
1	A	584	ASP	1
1	A	591	VAL	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	558	ASN	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](#)

Of 2 ligands modelled in this entry, 2 are 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 86% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *nef_chemical_shift_list_default*

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	702
Number of shifts mapped to atoms	702
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

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 C _α	69	-0.65 \pm 0.40	None needed (imprecise)
¹³ C _β	62	0.16 \pm 0.15	None needed (< 0.5 ppm)
¹³ C'	66	-0.34 \pm 0.22	None needed (< 0.5 ppm)
¹⁵ N	66	-0.51 \pm 0.34	None needed (imprecise)

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 86%, i.e. 498 atoms were assigned a chemical shift out of a possible 582. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	228/230 (99%)	94/94 (100%)	90/92 (98%)	44/44 (100%)
Sidechain	218/278 (78%)	143/180 (79%)	73/84 (87%)	2/14 (14%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	52/74 (70%)	26/37 (70%)	24/28 (86%)	2/9 (22%)
Overall	498/582 (86%)	263/311 (85%)	187/204 (92%)	48/67 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 702 atoms were assigned a chemical shift out of a possible 870. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	341/359 (95%)	140/148 (95%)	135/142 (95%)	66/69 (96%)
Sidechain	309/437 (71%)	200/279 (72%)	107/131 (82%)	2/27 (7%)
Aromatic	52/74 (70%)	26/37 (70%)	24/28 (86%)	2/9 (22%)
Overall	702/870 (81%)	366/464 (79%)	266/301 (88%)	70/105 (67%)

7.1.4 Statistically unusual chemical shifts [i](#)

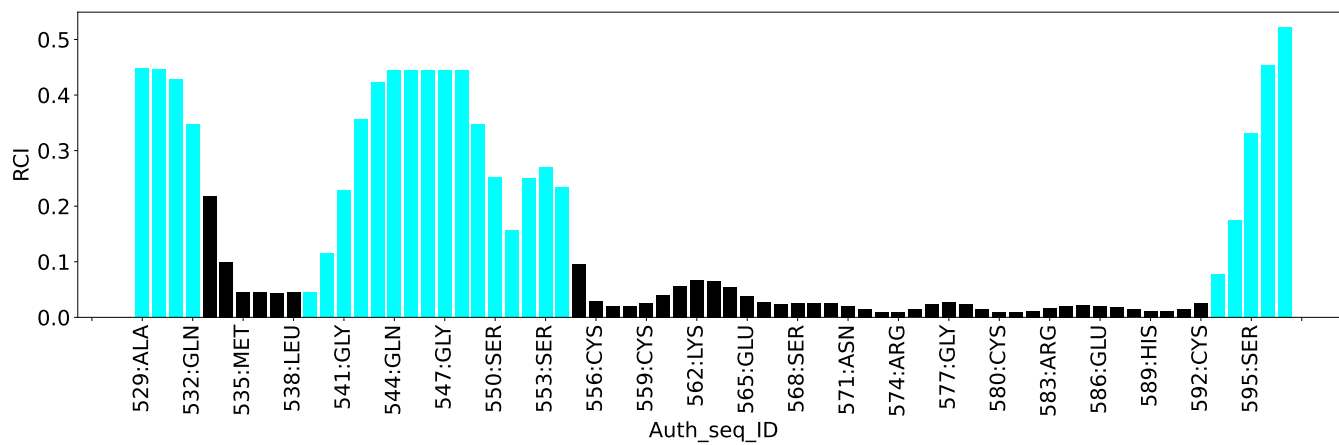
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	573	ALA	HA	0.96	2.13 – 6.34	-7.8
1	A	574	ARG	H	4.10	5.25 – 11.22	-6.9
1	A	589	HIS	HB2	0.79	1.36 – 4.85	-6.6
1	A	581	GLN	HA	1.90	2.17 – 6.35	-5.6
1	A	573	ALA	HB1	0.05	0.14 – 2.58	-5.3
1	A	573	ALA	HB2	0.05	0.14 – 2.58	-5.3
1	A	573	ALA	HB3	0.05	0.14 – 2.58	-5.3

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	837
Intra-residue ($ i-j =0$)	414
Sequential ($ i-j =1$)	168
Medium range ($ i-j >1$ and $ i-j <5$)	77
Long range ($ i-j \geq 5$)	178
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	11.5
Number of long range restraints per residue ¹	2.4

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)	3.0	0.2
0.2-0.5 (Medium)	6.8	0.5
>0.5 (Large)	11.4	3.66

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis [i](#)

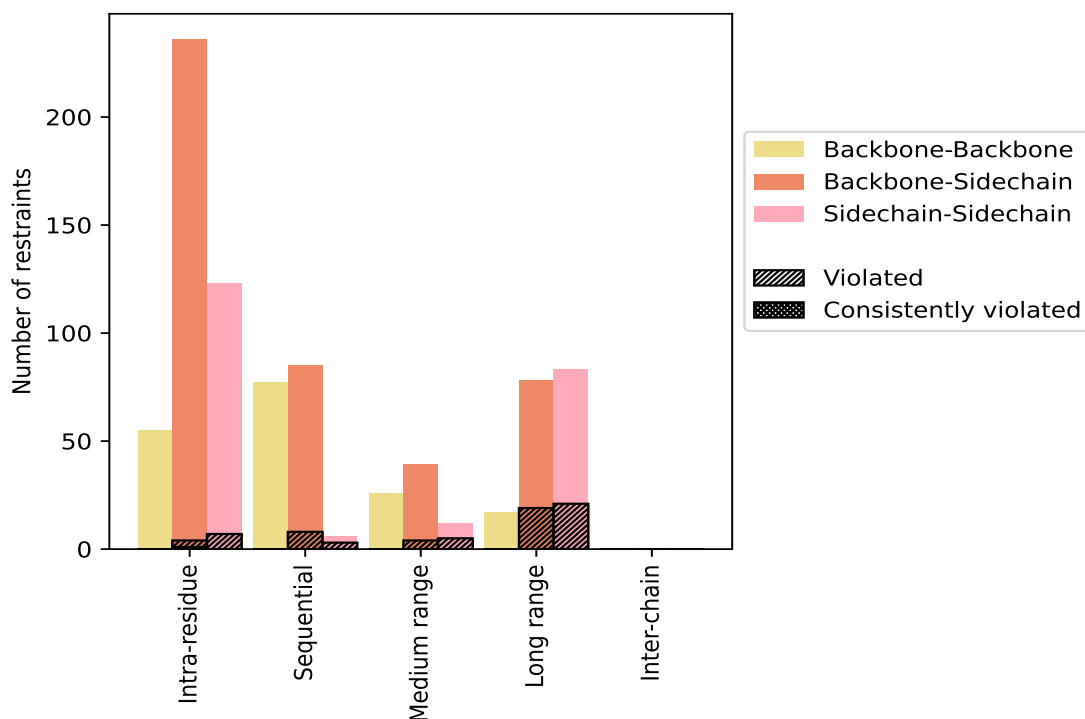
9.1 Summary of distance violations [i](#)

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	414	49.5	11	2.7	1.3	1	0.2	0.1
Backbone-Backbone	55	6.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	236	28.2	4	1.7	0.5	1	0.4	0.1
Sidechain-Sidechain	123	14.7	7	5.7	0.8	0	0.0	0.0
Sequential ($i-j =1$)	168	20.1	11	6.5	1.3	0	0.0	0.0
Backbone-Backbone	77	9.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	85	10.2	8	9.4	1.0	0	0.0	0.0
Sidechain-Sidechain	6	0.7	3	50.0	0.4	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	77	9.2	9	11.7	1.1	0	0.0	0.0
Backbone-Backbone	26	3.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	39	4.7	4	10.3	0.5	0	0.0	0.0
Sidechain-Sidechain	12	1.4	5	41.7	0.6	0	0.0	0.0
Long range ($i-j \geq 5$)	178	21.3	40	22.5	4.8	0	0.0	0.0
Backbone-Backbone	17	2.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	78	9.3	19	24.4	2.3	0	0.0	0.0
Sidechain-Sidechain	83	9.9	21	25.3	2.5	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	837	100.0	71	8.5	8.5	1	0.1	0.1
Backbone-Backbone	175	20.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	438	52.3	35	8.0	4.2	1	0.2	0.1
Sidechain-Sidechain	224	26.8	36	16.1	4.3	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 disulfid 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	5	3	6	5	0	19	0.69	1.58	0.39	0.64
2	6	4	4	12	0	26	0.49	1.28	0.29	0.46
3	4	4	5	10	0	23	0.7	3.41	0.72	0.53
4	4	2	4	10	0	20	0.7	3.37	0.74	0.5
5	6	3	6	16	0	31	0.64	3.5	0.63	0.52
6	4	4	4	11	0	23	0.8	3.46	0.88	0.52
7	5	3	4	16	0	28	0.61	3.32	0.64	0.44
8	4	3	3	6	0	16	0.54	1.7	0.35	0.46
9	7	3	4	12	0	26	0.78	3.52	0.74	0.55
10	4	5	3	7	0	19	0.56	1.85	0.42	0.44

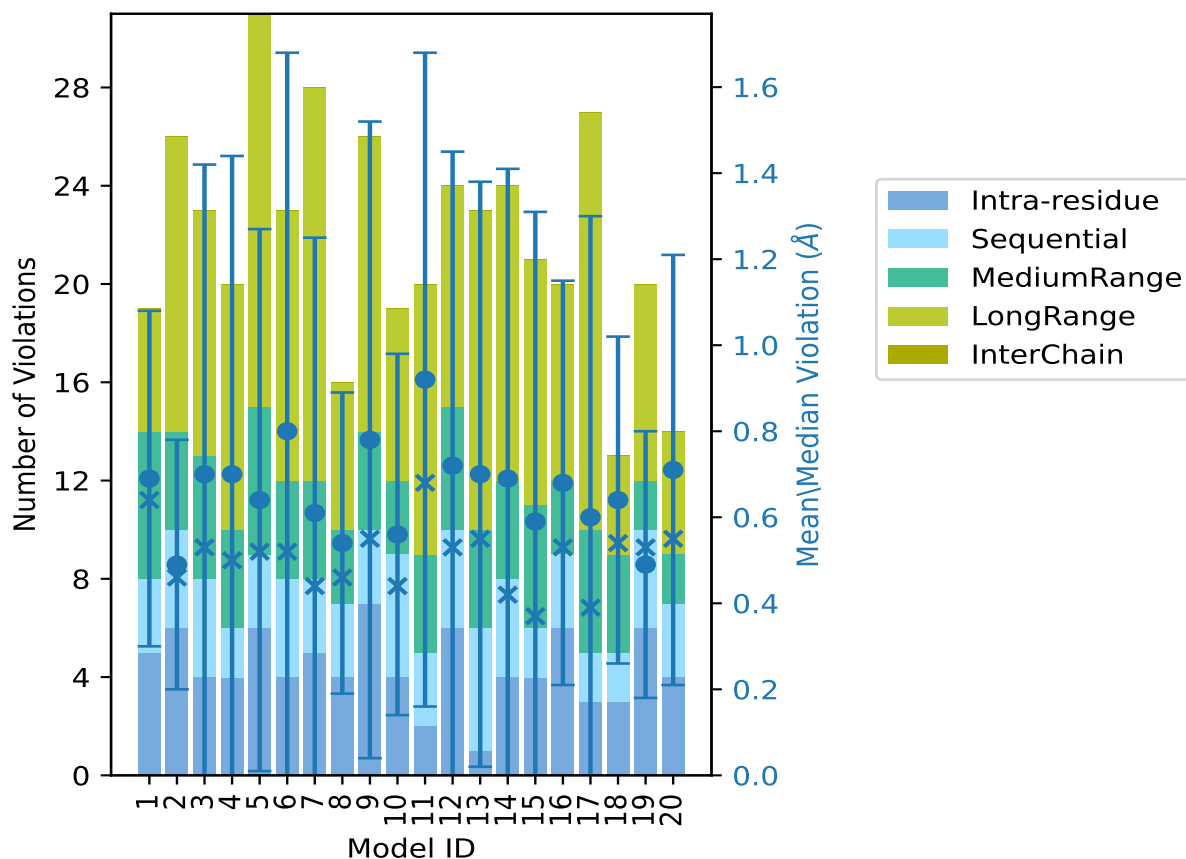
Continued on next page...

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	2	3	4	11	0	20	0.92	3.36	0.76	0.68
12	6	4	5	9	0	24	0.72	3.4	0.73	0.53
13	1	5	4	13	0	23	0.7	3.45	0.68	0.55
14	4	4	4	12	0	24	0.69	2.99	0.72	0.42
15	4	2	5	10	0	21	0.59	3.66	0.72	0.37
16	6	3	3	8	0	20	0.68	1.9	0.47	0.53
17	3	2	5	17	0	27	0.6	3.53	0.7	0.39
18	3	2	4	4	0	13	0.64	1.71	0.38	0.54
19	6	4	2	8	0	20	0.49	1.58	0.31	0.53
20	4	3	2	5	0	14	0.71	1.72	0.5	0.55

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

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



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

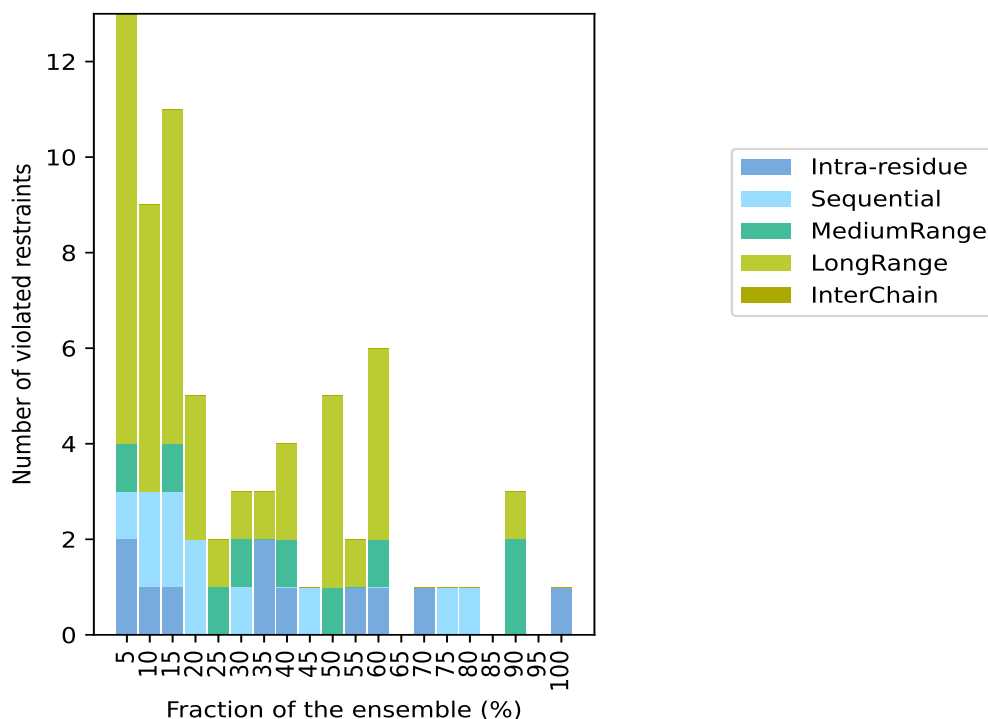
9.3 Distance violation statistics for the ensemble

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, 766(IR:403, SQ:157, MR:68, LR:138, 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	1	1	9	0	13	1	5.0
1	2	0	6	0	9	2	10.0
1	2	1	7	0	11	3	15.0
0	2	0	3	0	5	4	20.0
0	0	1	1	0	2	5	25.0
0	1	1	1	0	3	6	30.0
2	0	0	1	0	3	7	35.0
1	0	1	2	0	4	8	40.0
0	1	0	0	0	1	9	45.0
0	0	1	4	0	5	10	50.0
1	0	0	1	0	2	11	55.0
1	0	1	4	0	6	12	60.0
0	0	0	0	0	0	13	65.0
1	0	0	0	0	1	14	70.0
0	1	0	0	0	1	15	75.0
0	1	0	0	0	1	16	80.0
0	0	0	0	0	0	17	85.0
0	0	2	1	0	3	18	90.0
0	0	0	0	0	0	19	95.0
1	0	0	0	0	1	20	100.0

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

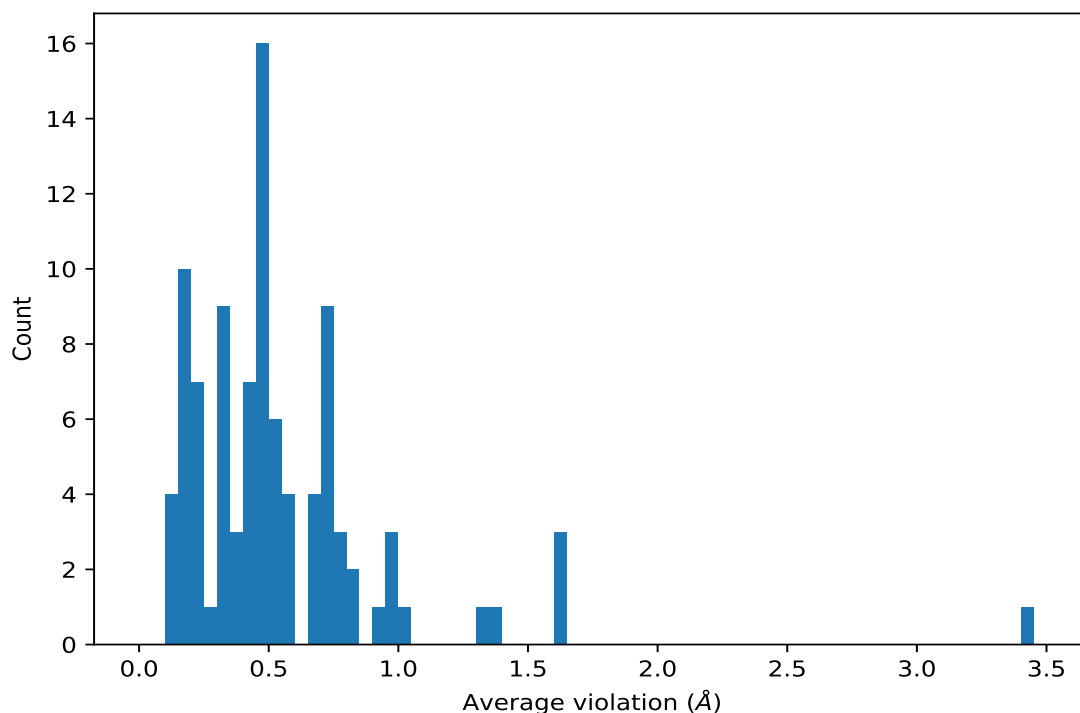
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	20	0.71	0.01	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	20	0.71	0.01	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	20	0.71	0.01	0.72
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	18	1.36	0.52	1.58
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	18	0.92	0.54	0.94
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	18	0.43	0.29	0.38
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	16	0.42	0.23	0.35
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	16	0.42	0.23	0.35
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	16	0.42	0.23	0.35
(1,810)	1:561:A:ARG:HB2	1:562:A:LYS:H	15	0.34	0.13	0.31
(1,456)	1:548:A:ARG:HD2	1:548:A:ARG:HG2	14	0.5	0.1	0.53
(1,605)	1:538:A:LEU:H	1:575:A:TYR:HD2	12	3.41	0.16	3.43
(1,520)	1:573:A:ALA:H	1:575:A:TYR:HE1	12	1.04	0.33	0.99
(1,526)	1:575:A:TYR:HD1	1:580:A:CYS:HB2	12	0.76	0.6	0.55
(1,626)	1:558:A:ASN:H	1:575:A:TYR:HD1	12	0.71	0.24	0.76
(1,143)	1:532:A:GLN:HB2	1:532:A:GLN:HG2	12	0.5	0.09	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,535)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	12	0.46	0.17	0.44
(1,535)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	12	0.46	0.17	0.44
(1,535)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	12	0.46	0.17	0.44
(1,535)	1:538:A:LEU:HD21	1:575:A:TYR:HD2	12	0.46	0.17	0.44
(1,535)	1:538:A:LEU:HD22	1:575:A:TYR:HD2	12	0.46	0.17	0.44
(1,535)	1:538:A:LEU:HD23	1:575:A:TYR:HD2	12	0.46	0.17	0.44
(1,316)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	11	0.68	0.53	0.57
(1,316)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	11	0.68	0.53	0.57
(1,316)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	11	0.68	0.53	0.57
(1,518)	1:585:A:TRP:HD1	1:585:A:TRP:HE1	11	0.1	0.0	0.1
(1,649)	1:558:A:ASN:HD21	1:580:A:CYS:HB2	10	0.7	0.31	0.76
(1,448)	1:538:A:LEU:HB3	1:540:A:ARG:HA	10	0.54	0.11	0.55
(1,470)	1:575:A:TYR:HE2	1:584:A:ASP:HB3	10	0.49	0.21	0.45
(1,470)	1:558:A:ASN:HB2	1:575:A:TYR:HE2	10	0.49	0.21	0.45
(1,494)	1:557:A:TRP:HD1	1:574:A:ARG:HB2	10	0.36	0.38	0.17
(1,550)	1:557:A:TRP:H	1:575:A:TYR:HD1	10	0.26	0.08	0.26
(1,266)	1:561:A:ARG:HD2	1:562:A:LYS:HD2	9	1.32	0.92	1.19
(1,532)	1:558:A:ASN:HB2	1:575:A:TYR:HD1	8	0.8	0.35	0.74
(1,532)	1:575:A:TYR:HD1	1:584:A:ASP:HB3	8	0.8	0.35	0.74
(1,83)	1:579:A:PHE:HD1	1:583:A:ARG:HD2	8	0.72	0.34	0.64
(1,83)	1:579:A:PHE:HD2	1:583:A:ARG:HD2	8	0.72	0.34	0.64
(1,122)	1:552:A:SER:HA	1:552:A:SER:HB3	8	0.49	0.12	0.54
(1,669)	1:538:A:LEU:H	1:581:A:GLN:HB2	8	0.31	0.15	0.27
(1,26)	1:562:A:LYS:HD2	1:562:A:LYS:HE2	7	0.53	0.0	0.53
(1,818)	1:570:A:CYS:HB2	1:595:A:SER:H	7	0.46	0.23	0.32
(1,43)	1:583:A:ARG:HA	1:583:A:ARG:HD2	7	0.31	0.18	0.21
(1,488)	1:586:A:GLU:HG2	1:589:A:HIS:HE1	6	0.77	0.37	0.7
(1,376)	1:561:A:ARG:HA	1:562:A:LYS:HD2	6	0.59	0.4	0.38
(1,638)	1:558:A:ASN:H	1:580:A:CYS:HB2	6	0.17	0.05	0.16
(1,522)	1:579:A:PHE:HD1	1:583:A:ARG:HG2	5	0.74	0.56	0.4
(1,522)	1:579:A:PHE:HD2	1:583:A:ARG:HG2	5	0.74	0.56	0.4
(1,127)	1:566:A:THR:HA	1:574:A:ARG:HD3	5	0.39	0.23	0.42
(1,468)	1:548:A:ARG:HG2	1:549:A:GLY:H	4	0.72	0.27	0.79
(1,481)	1:533:A:VAL:HG11	1:585:A:TRP:HH2	4	0.42	0.2	0.36
(1,481)	1:533:A:VAL:HG12	1:585:A:TRP:HH2	4	0.42	0.2	0.36
(1,481)	1:533:A:VAL:HG13	1:585:A:TRP:HH2	4	0.42	0.2	0.36
(1,313)	1:538:A:LEU:HD21	1:577:A:GLY:HA3	4	0.33	0.12	0.33
(1,313)	1:538:A:LEU:HD22	1:577:A:GLY:HA3	4	0.33	0.12	0.33
(1,313)	1:538:A:LEU:HD23	1:577:A:GLY:HA3	4	0.33	0.12	0.33
(1,685)	1:570:A:CYS:HB2	1:592:A:CYS:H	4	0.2	0.09	0.18
(1,85)	1:590:A:HIS:HB2	1:591:A:VAL:HG11	4	0.16	0.05	0.16
(1,85)	1:590:A:HIS:HB2	1:591:A:VAL:HG12	4	0.16	0.05	0.16

Continued on next page...

Continued from previous page...

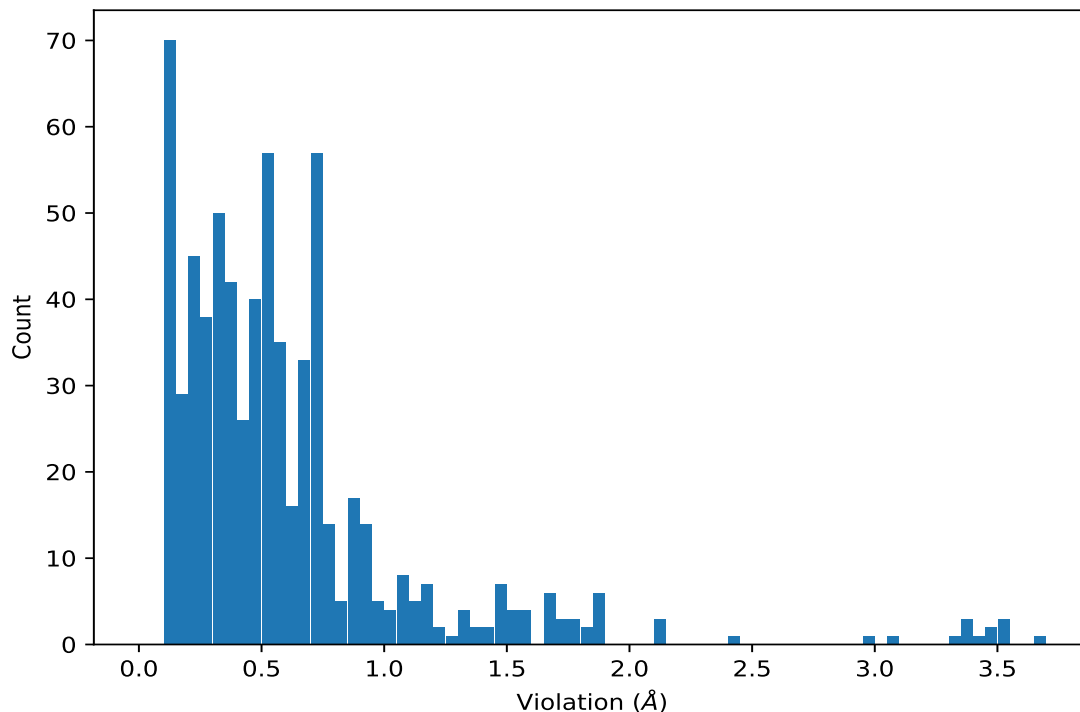
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,85)	1:590:A:HIS:HB2	1:591:A:VAL:HG13	4	0.16	0.05	0.16
(1,538)	1:533:A:VAL:HG11	1:589:A:HIS:HD2	3	1.65	0.13	1.7
(1,538)	1:533:A:VAL:HG12	1:589:A:HIS:HD2	3	1.65	0.13	1.7
(1,538)	1:533:A:VAL:HG13	1:589:A:HIS:HD2	3	1.65	0.13	1.7
(1,319)	1:539:A:VAL:HG11	1:568:A:SER:HB3	3	0.96	0.1	0.91
(1,319)	1:539:A:VAL:HG12	1:568:A:SER:HB3	3	0.96	0.1	0.91
(1,319)	1:539:A:VAL:HG13	1:568:A:SER:HB3	3	0.96	0.1	0.91
(1,118)	1:566:A:THR:HA	1:574:A:ARG:HD2	3	0.77	0.24	0.88
(1,355)	1:548:A:ARG:HB3	1:548:A:ARG:HG2	3	0.51	0.02	0.52
(1,202)	1:534:A:VAL:HA	1:535:A:MET:HB3	3	0.48	0.19	0.58
(1,273)	1:555:A:SER:HB2	1:562:A:LYS:HA	3	0.46	0.31	0.37
(1,91)	1:565:A:GLU:HB2	1:566:A:THR:HB	3	0.37	0.02	0.37
(1,734)	1:536:A:PRO:HG3	1:569:A:GLY:H	3	0.33	0.16	0.34
(1,594)	1:585:A:TRP:H	1:586:A:GLU:HB2	3	0.23	0.04	0.25
(1,293)	1:537:A:PRO:HB2	1:539:A:VAL:HG21	3	0.23	0.05	0.2
(1,293)	1:537:A:PRO:HB2	1:539:A:VAL:HG22	3	0.23	0.05	0.2
(1,293)	1:537:A:PRO:HB2	1:539:A:VAL:HG23	3	0.23	0.05	0.2
(1,490)	1:533:A:VAL:HG11	1:589:A:HIS:HE1	3	0.19	0.11	0.13
(1,490)	1:533:A:VAL:HG12	1:589:A:HIS:HE1	3	0.19	0.11	0.13
(1,490)	1:533:A:VAL:HG13	1:589:A:HIS:HE1	3	0.19	0.11	0.13
(1,430)	1:535:A:MET:HE1	1:582:A:HIS:HB2	2	0.57	0.02	0.57
(1,430)	1:535:A:MET:HE2	1:582:A:HIS:HB2	2	0.57	0.02	0.57
(1,430)	1:535:A:MET:HE3	1:582:A:HIS:HB2	2	0.57	0.02	0.57
(1,439)	1:532:A:GLN:HB3	1:532:A:GLN:HG2	2	0.52	0.01	0.52
(1,257)	1:566:A:THR:HG21	1:571:A:ASN:HB3	2	0.49	0.04	0.49
(1,257)	1:566:A:THR:HG22	1:571:A:ASN:HB3	2	0.49	0.04	0.49
(1,257)	1:566:A:THR:HG23	1:571:A:ASN:HB3	2	0.49	0.04	0.49
(1,300)	1:536:A:PRO:HB3	1:569:A:GLY:H	2	0.49	0.21	0.49
(1,837)	1:534:A:VAL:H	1:534:A:VAL:HG11	2	0.35	0.02	0.35
(1,837)	1:534:A:VAL:H	1:534:A:VAL:HG13	2	0.35	0.02	0.35
(1,816)	1:574:A:ARG:HD3	1:575:A:TYR:H	2	0.22	0.02	0.22
(1,729)	1:567:A:CYS:H	1:575:A:TYR:HE1	2	0.2	0.05	0.2
(1,133)	1:566:A:THR:HG21	1:574:A:ARG:HD2	2	0.17	0.02	0.17
(1,133)	1:566:A:THR:HG22	1:574:A:ARG:HD2	2	0.17	0.02	0.17
(1,133)	1:566:A:THR:HG23	1:574:A:ARG:HD2	2	0.17	0.02	0.17
(1,299)	1:539:A:VAL:HG11	1:568:A:SER:HB2	2	0.13	0.02	0.13
(1,299)	1:539:A:VAL:HG12	1:568:A:SER:HB2	2	0.13	0.02	0.13
(1,299)	1:539:A:VAL:HG13	1:568:A:SER:HB2	2	0.13	0.02	0.13

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)
(1,605)	1:538:A:LEU:H	1:575:A:TYR:HD2	15	3.66
(1,605)	1:538:A:LEU:H	1:575:A:TYR:HD2	17	3.53
(1,605)	1:538:A:LEU:H	1:575:A:TYR:HD2	9	3.52
(1,605)	1:538:A:LEU:H	1:575:A:TYR:HD2	5	3.5
(1,605)	1:538:A:LEU:H	1:575:A:TYR:HD2	6	3.46
(1,605)	1:538:A:LEU:H	1:575:A:TYR:HD2	13	3.45
(1,605)	1:538:A:LEU:H	1:575:A:TYR:HD2	3	3.41
(1,605)	1:538:A:LEU:H	1:575:A:TYR:HD2	12	3.4
(1,605)	1:538:A:LEU:H	1:575:A:TYR:HD2	4	3.37
(1,605)	1:538:A:LEU:H	1:575:A:TYR:HD2	11	3.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,605)	1:538:A:LEU:H	1:575:A:TYR:HD2	7	3.32
(1,266)	1:561:A:ARG:HD2	1:562:A:LYS:HD2	6	3.08
(1,605)	1:538:A:LEU:H	1:575:A:TYR:HD2	14	2.99
(1,266)	1:561:A:ARG:HD2	1:562:A:LYS:HD2	11	2.41
(1,316)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	9	2.14
(1,316)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	9	2.14
(1,316)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	9	2.14
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	14	1.9
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	16	1.9
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	3	1.89
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	12	1.88
(1,520)	1:573:A:ALA:H	1:575:A:TYR:HE1	14	1.87
(1,526)	1:575:A:TYR:HD1	1:580:A:CYS:HB2	10	1.85
(1,526)	1:575:A:TYR:HD1	1:580:A:CYS:HB2	16	1.84
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	4	1.8
(1,538)	1:533:A:VAL:HG11	1:589:A:HIS:HD2	6	1.78
(1,538)	1:533:A:VAL:HG12	1:589:A:HIS:HD2	6	1.78
(1,538)	1:533:A:VAL:HG13	1:589:A:HIS:HD2	6	1.78
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	20	1.72
(1,266)	1:561:A:ARG:HD2	1:562:A:LYS:HD2	12	1.71
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	18	1.71
(1,538)	1:533:A:VAL:HG11	1:589:A:HIS:HD2	8	1.7
(1,538)	1:533:A:VAL:HG12	1:589:A:HIS:HD2	8	1.7
(1,538)	1:533:A:VAL:HG13	1:589:A:HIS:HD2	8	1.7
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	9	1.7
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	5	1.69
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	14	1.66
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	17	1.59
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	19	1.58
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	1	1.58
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	7	1.57
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	13	1.52
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	6	1.51
(1,522)	1:579:A:PHE:HD1	1:583:A:ARG:HG2	7	1.5
(1,522)	1:579:A:PHE:HD2	1:583:A:ARG:HG2	7	1.5
(1,266)	1:561:A:ARG:HD2	1:562:A:LYS:HD2	9	1.49
(1,538)	1:533:A:VAL:HG11	1:589:A:HIS:HD2	17	1.48
(1,538)	1:533:A:VAL:HG12	1:589:A:HIS:HD2	17	1.48
(1,538)	1:533:A:VAL:HG13	1:589:A:HIS:HD2	17	1.48
(1,526)	1:575:A:TYR:HD1	1:580:A:CYS:HB2	20	1.48
(1,488)	1:586:A:GLU:HG2	1:589:A:HIS:HE1	3	1.46
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	1	1.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	1:561:A:ARG:HA	1:562:A:LYS:HD2	11	1.45
(1,520)	1:573:A:ALA:H	1:575:A:TYR:HE1	12	1.41
(1,83)	1:579:A:PHE:HD1	1:583:A:ARG:HD2	11	1.37
(1,83)	1:579:A:PHE:HD2	1:583:A:ARG:HD2	11	1.37
(1,532)	1:558:A:ASN:HB2	1:575:A:TYR:HD1	20	1.34
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	10	1.32
(1,522)	1:579:A:PHE:HD1	1:583:A:ARG:HG2	4	1.31
(1,522)	1:579:A:PHE:HD2	1:583:A:ARG:HG2	4	1.31
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	2	1.28
(1,520)	1:573:A:ALA:H	1:575:A:TYR:HE1	6	1.24
(1,649)	1:558:A:ASN:HD21	1:580:A:CYS:HB2	9	1.21
(1,266)	1:561:A:ARG:HD2	1:562:A:LYS:HD2	20	1.19
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	11	1.17
(1,532)	1:558:A:ASN:HB2	1:575:A:TYR:HD1	16	1.17
(1,494)	1:557:A:TRP:HD1	1:574:A:ARG:HB2	9	1.17
(1,316)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	5	1.16
(1,316)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	5	1.16
(1,316)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	5	1.16
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	13	1.13
(1,682)	1:538:A:LEU:HB3	1:540:A:ARG:H	1	1.12
(1,319)	1:539:A:VAL:HG11	1:568:A:SER:HB3	12	1.1
(1,319)	1:539:A:VAL:HG12	1:568:A:SER:HB3	12	1.1
(1,319)	1:539:A:VAL:HG13	1:568:A:SER:HB3	12	1.1
(1,520)	1:573:A:ALA:H	1:575:A:TYR:HE1	11	1.09
(1,520)	1:573:A:ALA:H	1:575:A:TYR:HE1	3	1.07
(1,494)	1:557:A:TRP:HD1	1:574:A:ARG:HB2	5	1.07
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	4	1.06
(1,532)	1:575:A:TYR:HD1	1:584:A:ASP:HB3	10	1.06
(1,520)	1:573:A:ALA:H	1:575:A:TYR:HE1	7	1.06
(1,83)	1:579:A:PHE:HD1	1:583:A:ARG:HD2	1	1.06
(1,83)	1:579:A:PHE:HD2	1:583:A:ARG:HD2	1	1.06
(1,266)	1:561:A:ARG:HD2	1:562:A:LYS:HD2	13	1.04
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	17	1.02
(1,468)	1:548:A:ARG:HG2	1:549:A:GLY:H	2	1.01
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	5	1.0
(1,118)	1:566:A:THR:HA	1:574:A:ARG:HD2	16	0.99
(1,576)	1:555:A:SER:HB2	1:563:A:ALA:H	11	0.98
(1,116)	1:538:A:LEU:HD11	1:565:A:GLU:HB2	9	0.97
(1,116)	1:538:A:LEU:HD12	1:565:A:GLU:HB2	9	0.97
(1,116)	1:538:A:LEU:HD13	1:565:A:GLU:HB2	9	0.97
(1,626)	1:558:A:ASN:H	1:575:A:TYR:HD1	12	0.95
(1,626)	1:558:A:ASN:H	1:575:A:TYR:HD1	15	0.95

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:575:A:TYR:HE2	1:584:A:ASP:HB3	11	0.95
(1,649)	1:558:A:ASN:HD21	1:580:A:CYS:HB2	17	0.94
(1,488)	1:586:A:GLU:HG2	1:589:A:HIS:HE1	14	0.94
(1,626)	1:558:A:ASN:H	1:575:A:TYR:HD1	3	0.92
(1,520)	1:573:A:ALA:H	1:575:A:TYR:HE1	5	0.91
(1,319)	1:539:A:VAL:HG11	1:568:A:SER:HB3	14	0.91
(1,319)	1:539:A:VAL:HG12	1:568:A:SER:HB3	14	0.91
(1,319)	1:539:A:VAL:HG13	1:568:A:SER:HB3	14	0.91
(1,468)	1:548:A:ARG:HG2	1:549:A:GLY:H	6	0.9
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	16	0.9
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	16	0.9
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	16	0.9
(1,649)	1:558:A:ASN:HD21	1:580:A:CYS:HB2	6	0.89
(1,520)	1:573:A:ALA:H	1:575:A:TYR:HE1	13	0.89
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	14	0.89
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	14	0.89
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	14	0.89
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	1	0.88
(1,626)	1:558:A:ASN:H	1:575:A:TYR:HD1	13	0.88
(1,118)	1:566:A:THR:HA	1:574:A:ARG:HD2	2	0.88
(1,83)	1:579:A:PHE:HD1	1:583:A:ARG:HD2	18	0.88
(1,83)	1:579:A:PHE:HD2	1:583:A:ARG:HD2	18	0.88
(1,626)	1:558:A:ASN:H	1:575:A:TYR:HD1	5	0.87
(1,273)	1:555:A:SER:HB2	1:562:A:LYS:HA	2	0.87
(1,649)	1:558:A:ASN:HD21	1:580:A:CYS:HB2	3	0.86
(1,526)	1:575:A:TYR:HD1	1:580:A:CYS:HB2	1	0.86
(1,319)	1:539:A:VAL:HG11	1:568:A:SER:HB3	18	0.86
(1,319)	1:539:A:VAL:HG12	1:568:A:SER:HB3	18	0.86
(1,319)	1:539:A:VAL:HG13	1:568:A:SER:HB3	18	0.86
(1,649)	1:558:A:ASN:HD21	1:580:A:CYS:HB2	7	0.85
(1,488)	1:586:A:GLU:HG2	1:589:A:HIS:HE1	8	0.82
(1,626)	1:558:A:ASN:H	1:575:A:TYR:HD1	7	0.81
(1,520)	1:573:A:ALA:H	1:575:A:TYR:HE1	17	0.81
(1,532)	1:575:A:TYR:HD1	1:584:A:ASP:HB3	13	0.8
(1,520)	1:573:A:ALA:H	1:575:A:TYR:HE1	15	0.79
(1,818)	1:570:A:CYS:HB2	1:595:A:SER:H	5	0.77
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	18	0.76
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	18	0.76
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	18	0.76
(1,818)	1:570:A:CYS:HB2	1:595:A:SER:H	15	0.75
(1,535)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	9	0.75
(1,535)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	9	0.75

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,535)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	9	0.75
(1,535)	1:538:A:LEU:HD21	1:575:A:TYR:HD2	9	0.75
(1,535)	1:538:A:LEU:HD22	1:575:A:TYR:HD2	9	0.75
(1,535)	1:538:A:LEU:HD23	1:575:A:TYR:HD2	9	0.75
(1,448)	1:538:A:LEU:HB3	1:540:A:ARG:HA	1	0.75
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	11	0.75
(1,535)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	3	0.73
(1,535)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	3	0.73
(1,535)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	3	0.73
(1,535)	1:538:A:LEU:HD21	1:575:A:TYR:HD2	3	0.73
(1,535)	1:538:A:LEU:HD22	1:575:A:TYR:HD2	3	0.73
(1,535)	1:538:A:LEU:HD23	1:575:A:TYR:HD2	3	0.73
(1,481)	1:533:A:VAL:HG11	1:585:A:TRP:HH2	17	0.73
(1,481)	1:533:A:VAL:HG12	1:585:A:TRP:HH2	17	0.73
(1,481)	1:533:A:VAL:HG13	1:585:A:TRP:HH2	17	0.73
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	3	0.73
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	3	0.73
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	3	0.73
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	14	0.73
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	14	0.73
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	14	0.73
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	15	0.73
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	15	0.73
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	15	0.73
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	16	0.73
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	16	0.73
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	16	0.73
(1,83)	1:579:A:PHE:HD1	1:583:A:ARG:HD2	5	0.73
(1,83)	1:579:A:PHE:HD2	1:583:A:ARG:HD2	5	0.73
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	2	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	2	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	2	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	4	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	4	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	4	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	9	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	9	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	9	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	10	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	10	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	10	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	12	0.72

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	12	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	12	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	13	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	13	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	13	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	18	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	18	0.72
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	18	0.72
(1,626)	1:558:A:ASN:H	1:575:A:TYR:HD1	4	0.71
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	1	0.71
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	1	0.71
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	1	0.71
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	5	0.71
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	5	0.71
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	5	0.71
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	11	0.71
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	11	0.71
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	11	0.71
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	19	0.71
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	19	0.71
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	19	0.71
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	20	0.7
(1,626)	1:558:A:ASN:H	1:575:A:TYR:HD1	6	0.7
(1,300)	1:536:A:PRO:HB3	1:569:A:GLY:H	2	0.7
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	17	0.7
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	17	0.7
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	17	0.7
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	20	0.7
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	20	0.7
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	20	0.7
(1,626)	1:558:A:ASN:H	1:575:A:TYR:HD1	17	0.69
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	6	0.69
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	6	0.69
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	6	0.69
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	8	0.69
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	8	0.69
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	8	0.69
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	19	0.69
(1,468)	1:548:A:ARG:HG2	1:549:A:GLY:H	3	0.68
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG11	7	0.68
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG12	7	0.68
(1,262)	1:533:A:VAL:HA	1:533:A:VAL:HG13	7	0.68

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,649)	1:558:A:ASN:HD21	1:580:A:CYS:HB2	5	0.67
(1,649)	1:558:A:ASN:HD21	1:580:A:CYS:HB2	13	0.67
(1,532)	1:558:A:ASN:HB2	1:575:A:TYR:HD1	1	0.67
(1,470)	1:575:A:TYR:HE2	1:584:A:ASP:HB3	4	0.67
(1,470)	1:575:A:TYR:HE2	1:584:A:ASP:HB3	9	0.67
(1,316)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	7	0.67
(1,316)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	7	0.67
(1,316)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	7	0.67
(1,520)	1:573:A:ALA:H	1:575:A:TYR:HE1	4	0.66
(1,127)	1:566:A:THR:HA	1:574:A:ARG:HD3	10	0.66
(1,818)	1:570:A:CYS:HB2	1:595:A:SER:H	7	0.65
(1,202)	1:534:A:VAL:HA	1:535:A:MET:HB3	14	0.65
(1,810)	1:561:A:ARG:HB2	1:562:A:LYS:H	1	0.64
(1,532)	1:575:A:TYR:HD1	1:584:A:ASP:HB3	11	0.64
(1,520)	1:573:A:ALA:H	1:575:A:TYR:HE1	9	0.64
(1,649)	1:558:A:ASN:HD21	1:580:A:CYS:HB2	16	0.63
(1,448)	1:538:A:LEU:HB3	1:540:A:ARG:HA	9	0.63
(1,236)	1:538:A:LEU:HD21	1:565:A:GLU:HB2	2	0.63
(1,236)	1:538:A:LEU:HD22	1:565:A:GLU:HB2	2	0.63
(1,236)	1:538:A:LEU:HD23	1:565:A:GLU:HB2	2	0.63
(1,526)	1:575:A:TYR:HD1	1:580:A:CYS:HB2	2	0.62
(1,266)	1:561:A:ARG:HD2	1:562:A:LYS:HD2	8	0.62
(1,316)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	4	0.61
(1,316)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	4	0.61
(1,316)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	4	0.61
(1,316)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	14	0.61
(1,316)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	14	0.61
(1,316)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	14	0.61
(1,532)	1:558:A:ASN:HB2	1:575:A:TYR:HD1	19	0.6
(1,376)	1:561:A:ARG:HA	1:562:A:LYS:HD2	8	0.6
(1,127)	1:566:A:THR:HA	1:574:A:ARG:HD3	16	0.6
(1,535)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	5	0.59
(1,535)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	5	0.59
(1,535)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	5	0.59
(1,535)	1:538:A:LEU:HD21	1:575:A:TYR:HD2	5	0.59
(1,535)	1:538:A:LEU:HD22	1:575:A:TYR:HD2	5	0.59
(1,535)	1:538:A:LEU:HD23	1:575:A:TYR:HD2	5	0.59
(1,488)	1:586:A:GLU:HG2	1:589:A:HIS:HE1	2	0.59
(1,430)	1:535:A:MET:HE1	1:582:A:HIS:HB2	3	0.59
(1,430)	1:535:A:MET:HE2	1:582:A:HIS:HB2	3	0.59
(1,430)	1:535:A:MET:HE3	1:582:A:HIS:HB2	3	0.59
(1,202)	1:534:A:VAL:HA	1:535:A:MET:HB3	19	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:583:A:ARG:HA	1:583:A:ARG:HD2	6	0.58
(1,43)	1:583:A:ARG:HA	1:583:A:ARG:HD2	20	0.58
(1,626)	1:558:A:ASN:H	1:575:A:TYR:HD1	9	0.57
(1,448)	1:538:A:LEU:HB3	1:540:A:ARG:HA	13	0.57
(1,316)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	13	0.57
(1,316)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	13	0.57
(1,316)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	13	0.57
(1,810)	1:561:A:ARG:HB2	1:562:A:LYS:H	19	0.56
(1,316)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	12	0.56
(1,316)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	12	0.56
(1,316)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	12	0.56
(1,83)	1:579:A:PHE:HD1	1:583:A:ARG:HD2	2	0.56
(1,83)	1:579:A:PHE:HD2	1:583:A:ARG:HD2	2	0.56
(1,669)	1:538:A:LEU:H	1:581:A:GLN:HB2	11	0.55
(1,526)	1:575:A:TYR:HD1	1:580:A:CYS:HB2	13	0.55
(1,448)	1:538:A:LEU:HB3	1:540:A:ARG:HA	12	0.55
(1,448)	1:538:A:LEU:HB3	1:540:A:ARG:HA	18	0.55
(1,430)	1:535:A:MET:HE1	1:582:A:HIS:HB2	19	0.55
(1,430)	1:535:A:MET:HE2	1:582:A:HIS:HB2	19	0.55
(1,430)	1:535:A:MET:HE3	1:582:A:HIS:HB2	19	0.55
(1,122)	1:552:A:SER:HA	1:552:A:SER:HB3	16	0.55
(1,526)	1:575:A:TYR:HD1	1:580:A:CYS:HB2	18	0.54
(1,470)	1:575:A:TYR:HE2	1:584:A:ASP:HB3	19	0.54
(1,448)	1:538:A:LEU:HB3	1:540:A:ARG:HA	7	0.54
(1,122)	1:552:A:SER:HA	1:552:A:SER:HB3	9	0.54
(1,122)	1:552:A:SER:HA	1:552:A:SER:HB3	10	0.54
(1,122)	1:552:A:SER:HA	1:552:A:SER:HB3	18	0.54
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	16	0.53
(1,810)	1:561:A:ARG:HB2	1:562:A:LYS:H	10	0.53
(1,734)	1:536:A:PRO:HG3	1:569:A:GLY:H	2	0.53
(1,456)	1:548:A:ARG:HD2	1:548:A:ARG:HG2	1	0.53
(1,456)	1:548:A:ARG:HD2	1:548:A:ARG:HG2	2	0.53
(1,456)	1:548:A:ARG:HD2	1:548:A:ARG:HG2	3	0.53
(1,456)	1:548:A:ARG:HD2	1:548:A:ARG:HG2	5	0.53
(1,456)	1:548:A:ARG:HD2	1:548:A:ARG:HG2	8	0.53
(1,456)	1:548:A:ARG:HD2	1:548:A:ARG:HG2	9	0.53
(1,456)	1:548:A:ARG:HD2	1:548:A:ARG:HG2	12	0.53
(1,456)	1:548:A:ARG:HD2	1:548:A:ARG:HG2	15	0.53
(1,456)	1:548:A:ARG:HD2	1:548:A:ARG:HG2	16	0.53
(1,456)	1:548:A:ARG:HD2	1:548:A:ARG:HG2	17	0.53
(1,456)	1:548:A:ARG:HD2	1:548:A:ARG:HG2	19	0.53
(1,439)	1:532:A:GLN:HB3	1:532:A:GLN:HG2	15	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,355)	1:548:A:ARG:HB3	1:548:A:ARG:HG2	16	0.53
(1,257)	1:566:A:THR:HG21	1:571:A:ASN:HB3	10	0.53
(1,257)	1:566:A:THR:HG22	1:571:A:ASN:HB3	10	0.53
(1,257)	1:566:A:THR:HG23	1:571:A:ASN:HB3	10	0.53
(1,143)	1:532:A:GLN:HB2	1:532:A:GLN:HG2	1	0.53
(1,143)	1:532:A:GLN:HB2	1:532:A:GLN:HG2	2	0.53
(1,143)	1:532:A:GLN:HB2	1:532:A:GLN:HG2	3	0.53
(1,143)	1:532:A:GLN:HB2	1:532:A:GLN:HG2	8	0.53
(1,143)	1:532:A:GLN:HB2	1:532:A:GLN:HG2	9	0.53
(1,143)	1:532:A:GLN:HB2	1:532:A:GLN:HG2	11	0.53
(1,143)	1:532:A:GLN:HB2	1:532:A:GLN:HG2	12	0.53
(1,122)	1:552:A:SER:HA	1:552:A:SER:HB3	5	0.53
(1,122)	1:552:A:SER:HA	1:552:A:SER:HB3	12	0.53
(1,122)	1:552:A:SER:HA	1:552:A:SER:HB3	19	0.53
(1,26)	1:562:A:LYS:HD2	1:562:A:LYS:HE2	1	0.53
(1,26)	1:562:A:LYS:HD2	1:562:A:LYS:HE2	5	0.53
(1,26)	1:562:A:LYS:HD2	1:562:A:LYS:HE2	9	0.53
(1,26)	1:562:A:LYS:HD2	1:562:A:LYS:HE2	12	0.53
(1,26)	1:562:A:LYS:HD2	1:562:A:LYS:HE2	16	0.53
(1,26)	1:562:A:LYS:HD2	1:562:A:LYS:HE2	19	0.53
(1,26)	1:562:A:LYS:HD2	1:562:A:LYS:HE2	20	0.53
(1,456)	1:548:A:ARG:HD2	1:548:A:ARG:HG2	6	0.52
(1,456)	1:548:A:ARG:HD2	1:548:A:ARG:HG2	18	0.52
(1,448)	1:538:A:LEU:HB3	1:540:A:ARG:HA	11	0.52
(1,439)	1:532:A:GLN:HB3	1:532:A:GLN:HG2	7	0.52
(1,355)	1:548:A:ARG:HB3	1:548:A:ARG:HG2	7	0.52
(1,143)	1:532:A:GLN:HB2	1:532:A:GLN:HG2	4	0.52
(1,143)	1:532:A:GLN:HB2	1:532:A:GLN:HG2	5	0.52
(1,143)	1:532:A:GLN:HB2	1:532:A:GLN:HG2	6	0.52
(1,143)	1:532:A:GLN:HB2	1:532:A:GLN:HG2	19	0.52
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	9	0.51
(1,470)	1:575:A:TYR:HE2	1:584:A:ASP:HB3	13	0.5
(1,448)	1:538:A:LEU:HB3	1:540:A:ARG:HA	5	0.5
(1,316)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	15	0.5
(1,316)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	15	0.5
(1,316)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	15	0.5
(1,535)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	13	0.49
(1,535)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	13	0.49
(1,535)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	13	0.49
(1,535)	1:538:A:LEU:HD21	1:575:A:TYR:HD2	13	0.49
(1,535)	1:538:A:LEU:HD22	1:575:A:TYR:HD2	13	0.49
(1,535)	1:538:A:LEU:HD23	1:575:A:TYR:HD2	13	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,488)	1:586:A:GLU:HG2	1:589:A:HIS:HE1	12	0.49
(1,313)	1:538:A:LEU:HD21	1:577:A:GLY:HA3	11	0.49
(1,313)	1:538:A:LEU:HD22	1:577:A:GLY:HA3	11	0.49
(1,313)	1:538:A:LEU:HD23	1:577:A:GLY:HA3	11	0.49
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	3	0.49
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	3	0.49
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	3	0.49
(1,535)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	4	0.48
(1,535)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	4	0.48
(1,535)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	4	0.48
(1,535)	1:538:A:LEU:HD21	1:575:A:TYR:HD2	4	0.48
(1,535)	1:538:A:LEU:HD22	1:575:A:TYR:HD2	4	0.48
(1,535)	1:538:A:LEU:HD23	1:575:A:TYR:HD2	4	0.48
(1,526)	1:575:A:TYR:HD1	1:580:A:CYS:HB2	5	0.48
(1,355)	1:548:A:ARG:HB3	1:548:A:ARG:HG2	8	0.48
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	14	0.47
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	1	0.47
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	1	0.47
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	1	0.47
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	19	0.47
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	19	0.47
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	19	0.47
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	7	0.46
(1,669)	1:538:A:LEU:H	1:581:A:GLN:HB2	14	0.46
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	18	0.45
(1,535)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	7	0.45
(1,535)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	7	0.45
(1,535)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	7	0.45
(1,535)	1:538:A:LEU:HD21	1:575:A:TYR:HD2	7	0.45
(1,535)	1:538:A:LEU:HD22	1:575:A:TYR:HD2	7	0.45
(1,535)	1:538:A:LEU:HD23	1:575:A:TYR:HD2	7	0.45
(1,257)	1:566:A:THR:HG21	1:571:A:ASN:HB3	8	0.45
(1,257)	1:566:A:THR:HG22	1:571:A:ASN:HB3	8	0.45
(1,257)	1:566:A:THR:HG23	1:571:A:ASN:HB3	8	0.45
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	10	0.44
(1,535)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	12	0.44
(1,535)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	12	0.44
(1,535)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	12	0.44
(1,535)	1:538:A:LEU:HD21	1:575:A:TYR:HD2	12	0.44
(1,535)	1:538:A:LEU:HD22	1:575:A:TYR:HD2	12	0.44
(1,535)	1:538:A:LEU:HD23	1:575:A:TYR:HD2	12	0.44
(1,481)	1:533:A:VAL:HG11	1:585:A:TRP:HH2	8	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,481)	1:533:A:VAL:HG12	1:585:A:TRP:HH2	8	0.44
(1,481)	1:533:A:VAL:HG13	1:585:A:TRP:HH2	8	0.44
(1,448)	1:538:A:LEU:HB3	1:540:A:ARG:HA	15	0.44
(1,205)	1:558:A:ASN:HD21	1:559:A:CYS:HA	10	0.44
(1,118)	1:566:A:THR:HA	1:574:A:ARG:HD2	10	0.44
(1,83)	1:579:A:PHE:HD1	1:583:A:ARG:HD2	8	0.43
(1,83)	1:579:A:PHE:HD2	1:583:A:ARG:HD2	8	0.43
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	17	0.42
(1,669)	1:538:A:LEU:H	1:581:A:GLN:HB2	7	0.42
(1,316)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	3	0.42
(1,316)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	3	0.42
(1,316)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	3	0.42
(1,127)	1:566:A:THR:HA	1:574:A:ARG:HD3	18	0.42
(1,470)	1:575:A:TYR:HE2	1:584:A:ASP:HB3	17	0.41
(1,810)	1:561:A:ARG:HB2	1:562:A:LYS:H	17	0.4
(1,522)	1:579:A:PHE:HD1	1:583:A:ARG:HG2	5	0.4
(1,522)	1:579:A:PHE:HD2	1:583:A:ARG:HG2	5	0.4
(1,91)	1:565:A:GLU:HB2	1:566:A:THR:HB	16	0.4
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	19	0.39
(1,550)	1:557:A:TRP:H	1:575:A:TYR:HD1	5	0.39
(1,535)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	17	0.39
(1,535)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	17	0.39
(1,535)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	17	0.39
(1,535)	1:538:A:LEU:HD21	1:575:A:TYR:HD2	17	0.39
(1,535)	1:538:A:LEU:HD22	1:575:A:TYR:HD2	17	0.39
(1,535)	1:538:A:LEU:HD23	1:575:A:TYR:HD2	17	0.39
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	10	0.39
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	10	0.39
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	10	0.39
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	2	0.38
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	16	0.38
(1,522)	1:579:A:PHE:HD1	1:583:A:ARG:HG2	17	0.38
(1,522)	1:579:A:PHE:HD2	1:583:A:ARG:HG2	17	0.38
(1,470)	1:575:A:TYR:HE2	1:584:A:ASP:HB3	5	0.38
(1,376)	1:561:A:ARG:HA	1:562:A:LYS:HD2	7	0.38
(1,83)	1:579:A:PHE:HD1	1:583:A:ARG:HD2	15	0.38
(1,83)	1:579:A:PHE:HD2	1:583:A:ARG:HD2	15	0.38
(1,837)	1:534:A:VAL:H	1:534:A:VAL:HG13	14	0.37
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	15	0.37
(1,810)	1:561:A:ARG:HB2	1:562:A:LYS:H	15	0.37
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	15	0.37
(1,550)	1:557:A:TRP:H	1:575:A:TYR:HD1	7	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,535)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	14	0.37
(1,535)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	14	0.37
(1,535)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	14	0.37
(1,535)	1:538:A:LEU:HD21	1:575:A:TYR:HD2	14	0.37
(1,535)	1:538:A:LEU:HD22	1:575:A:TYR:HD2	14	0.37
(1,535)	1:538:A:LEU:HD23	1:575:A:TYR:HD2	14	0.37
(1,376)	1:561:A:ARG:HA	1:562:A:LYS:HD2	4	0.37
(1,376)	1:561:A:ARG:HA	1:562:A:LYS:HD2	6	0.37
(1,273)	1:555:A:SER:HB2	1:562:A:LYS:HA	8	0.37
(1,91)	1:565:A:GLU:HB2	1:566:A:THR:HB	1	0.37
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	4	0.36
(1,313)	1:538:A:LEU:HD21	1:577:A:GLY:HA3	17	0.36
(1,313)	1:538:A:LEU:HD22	1:577:A:GLY:HA3	17	0.36
(1,313)	1:538:A:LEU:HD23	1:577:A:GLY:HA3	17	0.36
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	11	0.36
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	11	0.36
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	11	0.36
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	6	0.36
(1,535)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	11	0.35
(1,535)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	11	0.35
(1,535)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	11	0.35
(1,535)	1:538:A:LEU:HD21	1:575:A:TYR:HD2	11	0.35
(1,535)	1:538:A:LEU:HD22	1:575:A:TYR:HD2	11	0.35
(1,535)	1:538:A:LEU:HD23	1:575:A:TYR:HD2	11	0.35
(1,490)	1:533:A:VAL:HG11	1:589:A:HIS:HE1	16	0.35
(1,490)	1:533:A:VAL:HG12	1:589:A:HIS:HE1	16	0.35
(1,490)	1:533:A:VAL:HG13	1:589:A:HIS:HE1	16	0.35
(1,376)	1:561:A:ARG:HA	1:562:A:LYS:HD2	20	0.35
(1,28)	1:539:A:VAL:HG11	1:566:A:THR:H	2	0.35
(1,28)	1:539:A:VAL:HG12	1:566:A:THR:H	2	0.35
(1,28)	1:539:A:VAL:HG13	1:566:A:THR:H	2	0.35
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	10	0.34
(1,810)	1:561:A:ARG:HB2	1:562:A:LYS:H	12	0.34
(1,734)	1:536:A:PRO:HG3	1:569:A:GLY:H	15	0.34
(1,669)	1:538:A:LEU:H	1:581:A:GLN:HB2	13	0.34
(1,550)	1:557:A:TRP:H	1:575:A:TYR:HD1	13	0.34
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	9	0.34
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	9	0.34
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	9	0.34
(1,267)	1:538:A:LEU:HD11	1:567:A:CYS:HB2	1	0.34
(1,267)	1:538:A:LEU:HD12	1:567:A:CYS:HB2	1	0.34
(1,267)	1:538:A:LEU:HD13	1:567:A:CYS:HB2	1	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	1:532:A:GLN:HB2	1:534:A:VAL:HB	15	0.34
(1,91)	1:565:A:GLU:HB2	1:566:A:THR:HB	8	0.34
(1,83)	1:579:A:PHE:HD1	1:583:A:ARG:HD2	10	0.34
(1,83)	1:579:A:PHE:HD2	1:583:A:ARG:HD2	10	0.34
(1,837)	1:534:A:VAL:H	1:534:A:VAL:HG11	16	0.33
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	2	0.33
(1,810)	1:561:A:ARG:HB2	1:562:A:LYS:H	16	0.33
(1,535)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	15	0.33
(1,535)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	15	0.33
(1,535)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	15	0.33
(1,535)	1:538:A:LEU:HD21	1:575:A:TYR:HD2	15	0.33
(1,535)	1:538:A:LEU:HD22	1:575:A:TYR:HD2	15	0.33
(1,535)	1:538:A:LEU:HD23	1:575:A:TYR:HD2	15	0.33
(1,818)	1:570:A:CYS:HB2	1:595:A:SER:H	20	0.32
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	5	0.32
(1,685)	1:570:A:CYS:HB2	1:592:A:CYS:H	4	0.32
(1,526)	1:575:A:TYR:HD1	1:580:A:CYS:HB2	7	0.32
(1,470)	1:575:A:TYR:HE2	1:584:A:ASP:HB3	7	0.32
(1,448)	1:538:A:LEU:HB3	1:540:A:ARG:HA	20	0.32
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	15	0.32
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	15	0.32
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	15	0.32
(1,43)	1:583:A:ARG:HA	1:583:A:ARG:HD2	7	0.32
(1,810)	1:561:A:ARG:HB2	1:562:A:LYS:H	2	0.31
(1,488)	1:586:A:GLU:HG2	1:589:A:HIS:HE1	17	0.31
(1,468)	1:548:A:ARG:HG2	1:549:A:GLY:H	19	0.31
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	12	0.3
(1,626)	1:558:A:ASN:H	1:575:A:TYR:HD1	11	0.3
(1,470)	1:558:A:ASN:HB2	1:575:A:TYR:HE2	20	0.3
(1,313)	1:538:A:LEU:HD21	1:577:A:GLY:HA3	6	0.3
(1,313)	1:538:A:LEU:HD22	1:577:A:GLY:HA3	6	0.3
(1,313)	1:538:A:LEU:HD23	1:577:A:GLY:HA3	6	0.3
(1,293)	1:537:A:PRO:HB2	1:539:A:VAL:HG21	1	0.3
(1,293)	1:537:A:PRO:HB2	1:539:A:VAL:HG22	1	0.3
(1,293)	1:537:A:PRO:HB2	1:539:A:VAL:HG23	1	0.3
(1,818)	1:570:A:CYS:HB2	1:595:A:SER:H	10	0.29
(1,810)	1:561:A:ARG:HB2	1:562:A:LYS:H	7	0.29
(1,481)	1:533:A:VAL:HG11	1:585:A:TRP:HH2	7	0.29
(1,481)	1:533:A:VAL:HG12	1:585:A:TRP:HH2	7	0.29
(1,481)	1:533:A:VAL:HG13	1:585:A:TRP:HH2	7	0.29
(1,300)	1:536:A:PRO:HB3	1:569:A:GLY:H	15	0.28
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	8	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:585:A:TRP:H	1:586:A:GLU:HB2	2	0.27
(1,550)	1:557:A:TRP:H	1:575:A:TYR:HD1	3	0.27
(1,550)	1:557:A:TRP:H	1:575:A:TYR:HD1	12	0.27
(1,526)	1:575:A:TYR:HD1	1:580:A:CYS:HB2	3	0.27
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	13	0.26
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	2	0.26
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	2	0.26
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	2	0.26
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	20	0.26
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	20	0.26
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	20	0.26
(1,729)	1:567:A:CYS:H	1:575:A:TYR:HE1	14	0.25
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	3	0.25
(1,638)	1:558:A:ASN:H	1:580:A:CYS:HB2	13	0.25
(1,594)	1:585:A:TRP:H	1:586:A:GLU:HB2	3	0.25
(1,433)	1:538:A:LEU:HD11	1:565:A:GLU:HB3	9	0.25
(1,433)	1:538:A:LEU:HD12	1:565:A:GLU:HB3	9	0.25
(1,433)	1:538:A:LEU:HD13	1:565:A:GLU:HB3	9	0.25
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	4	0.25
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	4	0.25
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	4	0.25
(1,102)	1:586:A:GLU:HA	1:586:A:GLU:HG2	2	0.25
(1,818)	1:570:A:CYS:HB2	1:595:A:SER:H	2	0.24
(1,816)	1:574:A:ARG:HD3	1:575:A:TYR:H	10	0.24
(1,810)	1:561:A:ARG:HB2	1:562:A:LYS:H	5	0.24
(1,810)	1:561:A:ARG:HB2	1:562:A:LYS:H	14	0.24
(1,685)	1:570:A:CYS:HB2	1:592:A:CYS:H	5	0.24
(1,550)	1:557:A:TRP:H	1:575:A:TYR:HD1	4	0.24
(1,513)	1:533:A:VAL:HG11	1:585:A:TRP:HZ2	17	0.24
(1,513)	1:533:A:VAL:HG12	1:585:A:TRP:HZ2	17	0.24
(1,513)	1:533:A:VAL:HG13	1:585:A:TRP:HZ2	17	0.24
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	12	0.24
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	12	0.24
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	12	0.24
(1,818)	1:570:A:CYS:HB2	1:595:A:SER:H	11	0.23
(1,810)	1:561:A:ARG:HB2	1:562:A:LYS:H	3	0.23
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	6	0.23
(1,686)	1:538:A:LEU:HB3	1:541:A:GLY:H	12	0.23
(1,649)	1:558:A:ASN:HD21	1:580:A:CYS:HB2	19	0.23
(1,494)	1:557:A:TRP:HD1	1:574:A:ARG:HB2	13	0.23
(1,85)	1:590:A:HIS:HB2	1:591:A:VAL:HG11	5	0.23
(1,85)	1:590:A:HIS:HB2	1:591:A:VAL:HG12	5	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	1:590:A:HIS:HB2	1:591:A:VAL:HG13	5	0.23
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	8	0.22
(1,810)	1:561:A:ARG:HB2	1:562:A:LYS:H	9	0.22
(1,810)	1:561:A:ARG:HB2	1:562:A:LYS:H	13	0.22
(1,550)	1:557:A:TRP:H	1:575:A:TYR:HD1	17	0.22
(1,481)	1:533:A:VAL:HG11	1:585:A:TRP:HH2	6	0.22
(1,481)	1:533:A:VAL:HG12	1:585:A:TRP:HH2	6	0.22
(1,481)	1:533:A:VAL:HG13	1:585:A:TRP:HH2	6	0.22
(1,202)	1:534:A:VAL:HA	1:535:A:MET:HB3	13	0.22
(1,810)	1:561:A:ARG:HB2	1:562:A:LYS:H	6	0.21
(1,638)	1:558:A:ASN:H	1:580:A:CYS:HB2	9	0.21
(1,470)	1:575:A:TYR:HE2	1:584:A:ASP:HB3	14	0.21
(1,43)	1:583:A:ARG:HA	1:583:A:ARG:HD2	2	0.21
(1,816)	1:574:A:ARG:HD3	1:575:A:TYR:H	7	0.2
(1,669)	1:538:A:LEU:H	1:581:A:GLN:HB2	5	0.2
(1,550)	1:557:A:TRP:H	1:575:A:TYR:HD1	15	0.2
(1,494)	1:557:A:TRP:HD1	1:574:A:ARG:HB2	15	0.2
(1,293)	1:537:A:PRO:HB2	1:539:A:VAL:HG21	3	0.2
(1,293)	1:537:A:PRO:HB2	1:539:A:VAL:HG22	3	0.2
(1,293)	1:537:A:PRO:HB2	1:539:A:VAL:HG23	3	0.2
(1,266)	1:561:A:ARG:HD2	1:562:A:LYS:HD2	18	0.2
(1,85)	1:590:A:HIS:HB2	1:591:A:VAL:HG11	13	0.2
(1,85)	1:590:A:HIS:HB2	1:591:A:VAL:HG12	13	0.2
(1,85)	1:590:A:HIS:HB2	1:591:A:VAL:HG13	13	0.2
(1,43)	1:583:A:ARG:HA	1:583:A:ARG:HD2	4	0.2
(1,669)	1:538:A:LEU:H	1:581:A:GLN:HB2	6	0.19
(1,619)	1:557:A:TRP:H	1:574:A:ARG:HB2	5	0.19
(1,550)	1:557:A:TRP:H	1:575:A:TYR:HD1	9	0.19
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	13	0.19
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	13	0.19
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	13	0.19
(1,143)	1:532:A:GLN:HB2	1:532:A:GLN:HG2	10	0.19
(1,133)	1:566:A:THR:HG21	1:574:A:ARG:HD2	17	0.19
(1,133)	1:566:A:THR:HG22	1:574:A:ARG:HD2	17	0.19
(1,133)	1:566:A:THR:HG23	1:574:A:ARG:HD2	17	0.19
(1,638)	1:558:A:ASN:H	1:580:A:CYS:HB2	4	0.18
(1,293)	1:537:A:PRO:HB2	1:539:A:VAL:HG21	16	0.18
(1,293)	1:537:A:PRO:HB2	1:539:A:VAL:HG22	16	0.18
(1,293)	1:537:A:PRO:HB2	1:539:A:VAL:HG23	16	0.18
(1,122)	1:552:A:SER:HA	1:552:A:SER:HB3	2	0.18
(1,833)	1:538:A:LEU:H	1:565:A:GLU:HG3	3	0.17
(1,594)	1:585:A:TRP:H	1:586:A:GLU:HB2	12	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,494)	1:557:A:TRP:HD1	1:574:A:ARG:HB2	12	0.17
(1,494)	1:557:A:TRP:HD1	1:574:A:ARG:HB2	17	0.17
(1,313)	1:538:A:LEU:HD21	1:577:A:GLY:HA3	14	0.17
(1,313)	1:538:A:LEU:HD22	1:577:A:GLY:HA3	14	0.17
(1,313)	1:538:A:LEU:HD23	1:577:A:GLY:HA3	14	0.17
(1,669)	1:538:A:LEU:H	1:581:A:GLN:HB2	17	0.16
(1,626)	1:558:A:ASN:H	1:575:A:TYR:HD1	14	0.16
(1,526)	1:575:A:TYR:HD1	1:580:A:CYS:HB2	19	0.16
(1,494)	1:557:A:TRP:HD1	1:574:A:ARG:HB2	4	0.16
(1,494)	1:557:A:TRP:HD1	1:574:A:ARG:HB2	6	0.16
(1,494)	1:557:A:TRP:HD1	1:574:A:ARG:HB2	7	0.16
(1,266)	1:561:A:ARG:HD2	1:562:A:LYS:HD2	10	0.16
(1,756)	1:538:A:LEU:HB3	1:565:A:GLU:H	2	0.15
(1,729)	1:567:A:CYS:H	1:575:A:TYR:HE1	12	0.15
(1,550)	1:557:A:TRP:H	1:575:A:TYR:HD1	6	0.15
(1,532)	1:558:A:ASN:HB2	1:575:A:TYR:HD1	2	0.15
(1,494)	1:557:A:TRP:HD1	1:574:A:ARG:HB2	3	0.15
(1,456)	1:548:A:ARG:HD2	1:548:A:ARG:HG2	7	0.15
(1,308)	1:533:A:VAL:HG11	1:534:A:VAL:HB	5	0.15
(1,308)	1:533:A:VAL:HG12	1:534:A:VAL:HB	5	0.15
(1,308)	1:533:A:VAL:HG13	1:534:A:VAL:HB	5	0.15
(1,299)	1:539:A:VAL:HG11	1:568:A:SER:HB2	5	0.15
(1,299)	1:539:A:VAL:HG12	1:568:A:SER:HB2	5	0.15
(1,299)	1:539:A:VAL:HG13	1:568:A:SER:HB2	5	0.15
(1,133)	1:566:A:THR:HG21	1:574:A:ARG:HD2	14	0.15
(1,133)	1:566:A:THR:HG22	1:574:A:ARG:HD2	14	0.15
(1,133)	1:566:A:THR:HG23	1:574:A:ARG:HD2	14	0.15
(1,43)	1:583:A:ARG:HA	1:583:A:ARG:HD2	14	0.15
(1,669)	1:538:A:LEU:H	1:581:A:GLN:HB2	19	0.14
(1,638)	1:558:A:ASN:H	1:580:A:CYS:HB2	7	0.14
(1,316)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	11	0.14
(1,316)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	11	0.14
(1,316)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	11	0.14
(1,127)	1:566:A:THR:HA	1:574:A:ARG:HD3	1	0.14
(1,43)	1:583:A:ARG:HA	1:583:A:ARG:HD2	9	0.14
(1,734)	1:536:A:PRO:HG3	1:569:A:GLY:H	9	0.13
(1,685)	1:570:A:CYS:HB2	1:592:A:CYS:H	18	0.13
(1,638)	1:558:A:ASN:H	1:580:A:CYS:HB2	5	0.13
(1,490)	1:533:A:VAL:HG11	1:589:A:HIS:HE1	14	0.13
(1,490)	1:533:A:VAL:HG12	1:589:A:HIS:HE1	14	0.13
(1,490)	1:533:A:VAL:HG13	1:589:A:HIS:HE1	14	0.13
(1,434)	1:540:A:ARG:HB2	1:540:A:ARG:HD2	14	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,316)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	17	0.13
(1,316)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	17	0.13
(1,316)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	17	0.13
(1,273)	1:555:A:SER:HB2	1:562:A:LYS:HA	16	0.13
(1,638)	1:558:A:ASN:H	1:580:A:CYS:HB2	17	0.12
(1,535)	1:538:A:LEU:HD11	1:575:A:TYR:HD2	6	0.12
(1,535)	1:538:A:LEU:HD12	1:575:A:TYR:HD2	6	0.12
(1,535)	1:538:A:LEU:HD13	1:575:A:TYR:HD2	6	0.12
(1,535)	1:538:A:LEU:HD21	1:575:A:TYR:HD2	6	0.12
(1,535)	1:538:A:LEU:HD22	1:575:A:TYR:HD2	6	0.12
(1,535)	1:538:A:LEU:HD23	1:575:A:TYR:HD2	6	0.12
(1,127)	1:566:A:THR:HA	1:574:A:ARG:HD3	2	0.12
(1,685)	1:570:A:CYS:HB2	1:592:A:CYS:H	7	0.11
(1,522)	1:579:A:PHE:HD1	1:583:A:ARG:HG2	6	0.11
(1,522)	1:579:A:PHE:HD2	1:583:A:ARG:HG2	6	0.11
(1,518)	1:585:A:TRP:HD1	1:585:A:TRP:HE1	1	0.11
(1,518)	1:585:A:TRP:HD1	1:585:A:TRP:HE1	17	0.11
(1,299)	1:539:A:VAL:HG11	1:568:A:SER:HB2	19	0.11
(1,299)	1:539:A:VAL:HG12	1:568:A:SER:HB2	19	0.11
(1,299)	1:539:A:VAL:HG13	1:568:A:SER:HB2	19	0.11
(1,85)	1:590:A:HIS:HB2	1:591:A:VAL:HG11	14	0.11
(1,85)	1:590:A:HIS:HB2	1:591:A:VAL:HG12	14	0.11
(1,85)	1:590:A:HIS:HB2	1:591:A:VAL:HG13	14	0.11
(1,85)	1:590:A:HIS:HB2	1:591:A:VAL:HG11	17	0.11
(1,85)	1:590:A:HIS:HB2	1:591:A:VAL:HG12	17	0.11
(1,85)	1:590:A:HIS:HB2	1:591:A:VAL:HG13	17	0.11
(1,649)	1:558:A:ASN:HD21	1:580:A:CYS:HB2	8	0.1
(1,526)	1:575:A:TYR:HD1	1:580:A:CYS:HB2	17	0.1
(1,518)	1:585:A:TRP:HD1	1:585:A:TRP:HE1	3	0.1
(1,518)	1:585:A:TRP:HD1	1:585:A:TRP:HE1	4	0.1
(1,518)	1:585:A:TRP:HD1	1:585:A:TRP:HE1	5	0.1
(1,518)	1:585:A:TRP:HD1	1:585:A:TRP:HE1	9	0.1
(1,518)	1:585:A:TRP:HD1	1:585:A:TRP:HE1	10	0.1
(1,518)	1:585:A:TRP:HD1	1:585:A:TRP:HE1	12	0.1
(1,518)	1:585:A:TRP:HD1	1:585:A:TRP:HE1	15	0.1
(1,518)	1:585:A:TRP:HD1	1:585:A:TRP:HE1	19	0.1
(1,518)	1:585:A:TRP:HD1	1:585:A:TRP:HE1	20	0.1
(1,490)	1:533:A:VAL:HG11	1:589:A:HIS:HE1	7	0.1
(1,490)	1:533:A:VAL:HG12	1:589:A:HIS:HE1	7	0.1
(1,490)	1:533:A:VAL:HG13	1:589:A:HIS:HE1	7	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found