



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 3, 2023 – 05:24 PM EDT

PDB ID : 2MOQ  
BMRB ID : 19056  
Title : Solution Structure and Molecular determinants of Hemoglobin Binding of the first NEAT Domain of IsdB in Staphylococcus aureus  
Authors : Fonner, B.A.; Tripet, B.P.; Eilers, B.J.; Stanisich, J.; Sullivan-Springhetti, R.K.; Moore, R.; Lui, M.; Lei, B.; Copie, V.  
Deposited on : 2014-04-29

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.33

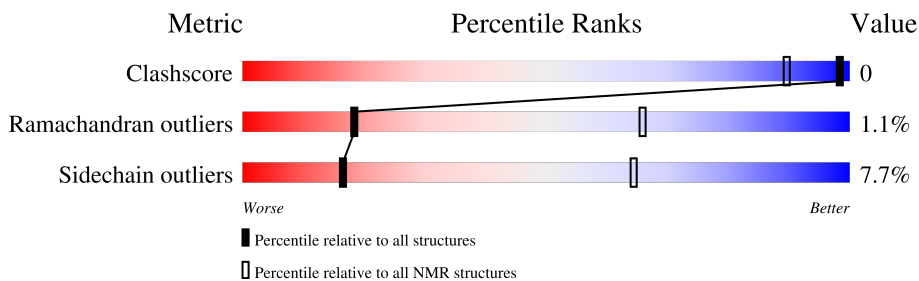
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 61%.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	163	

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 2 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:127-A:262 (136)	1.41	2

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

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

The models can be grouped into 4 clusters and 5 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2414 atoms, of which 1195 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Iron-regulated surface determinant protein B.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	148	2414	779	1195	202	236	2	0

There are 15 discrepancies between the modelled and reference sequences:


Chain	Residue	Modelled	Actual	Comment	Reference
A	110	MET	-	expression tag	UNP Q8NX66
A	111	ALA	-	expression tag	UNP Q8NX66
A	112	HIS	-	expression tag	UNP Q8NX66
A	113	HIS	-	expression tag	UNP Q8NX66
A	114	HIS	-	expression tag	UNP Q8NX66
A	115	HIS	-	expression tag	UNP Q8NX66
A	116	HIS	-	expression tag	UNP Q8NX66
A	117	HIS	-	expression tag	UNP Q8NX66
A	118	VAL	-	expression tag	UNP Q8NX66
A	119	ASP	-	expression tag	UNP Q8NX66
A	120	ASP	-	expression tag	UNP Q8NX66
A	121	ASP	-	expression tag	UNP Q8NX66
A	122	ASP	-	expression tag	UNP Q8NX66
A	123	LYS	-	expression tag	UNP Q8NX66
A	124	MET	-	expression tag	UNP Q8NX66

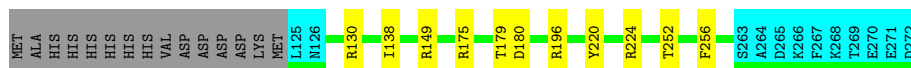
## 4 Residue-property plots

### 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: Iron-regulated surface determinant protein B

Chain A: 



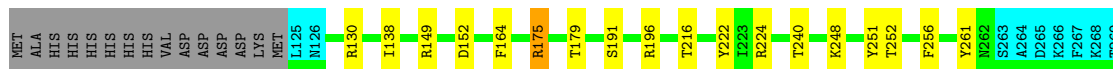
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Iron-regulated surface determinant protein B


Chain A: 





#### 4.2.2 Score per residue for model 2 (medoid)

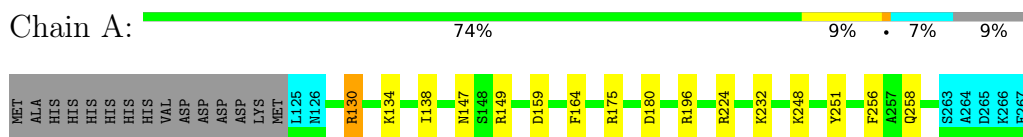
- Molecule 1: Iron-regulated surface determinant protein B

Chain A: 



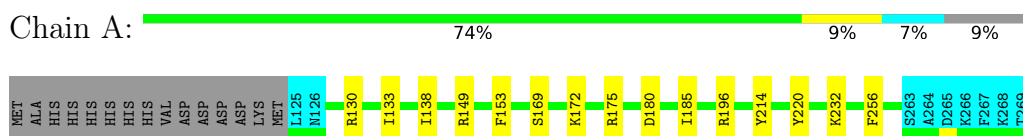
### 4.2.3 Score per residue for model 3

- Molecule 1: Iron-regulated surface determinant protein B



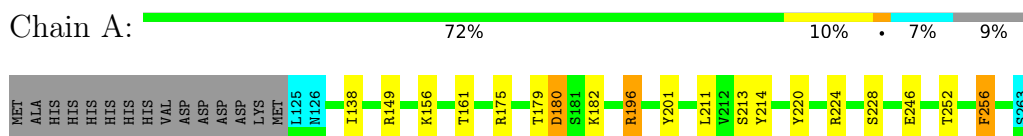
### 4.2.4 Score per residue for model 4

- Molecule 1: Iron-regulated surface determinant protein B



### 4.2.5 Score per residue for model 5

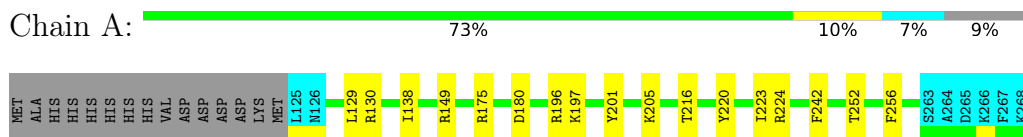
- Molecule 1: Iron-regulated surface determinant protein B



T269  
E270  
E271  
D272

### 4.2.6 Score per residue for model 6

- Molecule 1: Iron-regulated surface determinant protein B



### 4.2.7 Score per residue for model 7

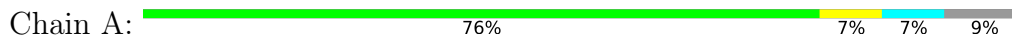
- Molecule 1: Iron-regulated surface determinant protein B





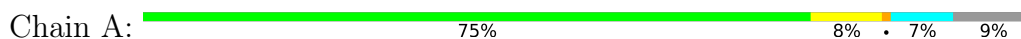
#### 4.2.8 Score per residue for model 8

- Molecule 1: Iron-regulated surface determinant protein B



#### 4.2.9 Score per residue for model 9

- Molecule 1: Iron-regulated surface determinant protein B



#### 4.2.10 Score per residue for model 10

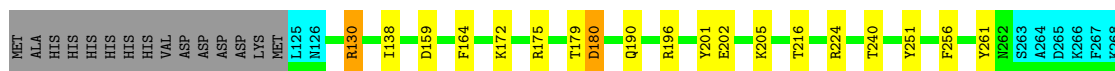
- Molecule 1: Iron-regulated surface determinant protein B



D272

#### 4.2.11 Score per residue for model 11

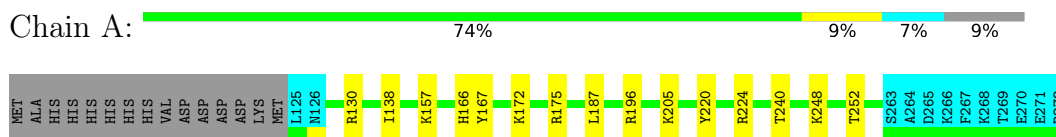
- Molecule 1: Iron-regulated surface determinant protein B



T269  
E270  
E271  
D272

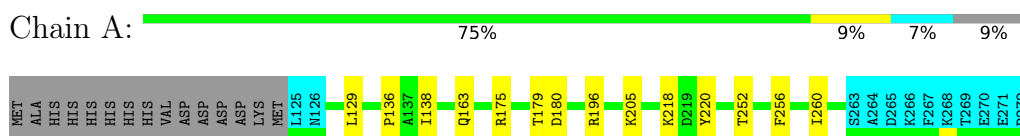
#### 4.2.12 Score per residue for model 12

- Molecule 1: Iron-regulated surface determinant protein B



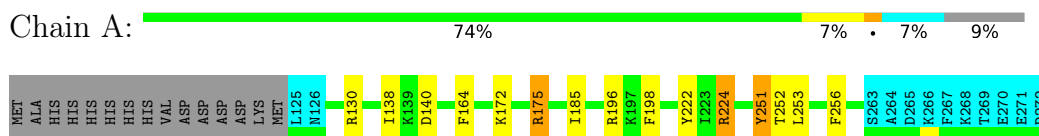
#### 4.2.13 Score per residue for model 13

- Molecule 1: Iron-regulated surface determinant protein B



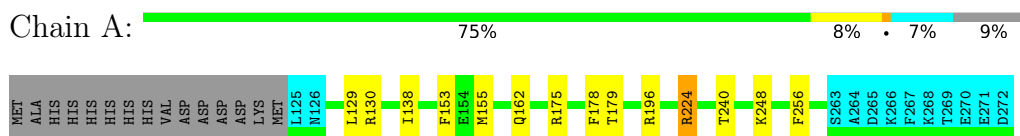
#### 4.2.14 Score per residue for model 14

- Molecule 1: Iron-regulated surface determinant protein B



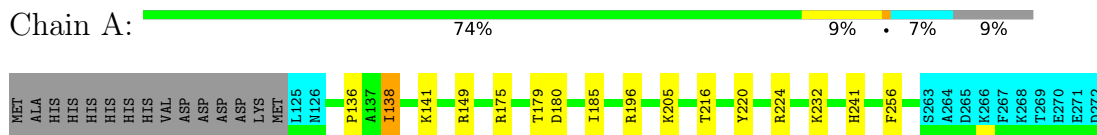
#### 4.2.15 Score per residue for model 15

- Molecule 1: Iron-regulated surface determinant protein B



#### 4.2.16 Score per residue for model 16

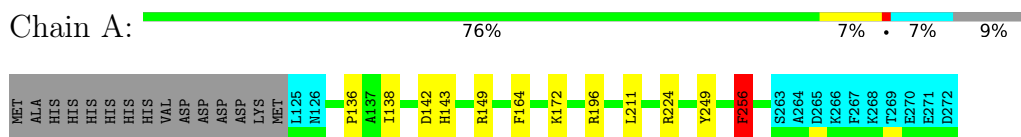
- Molecule 1: Iron-regulated surface determinant protein B





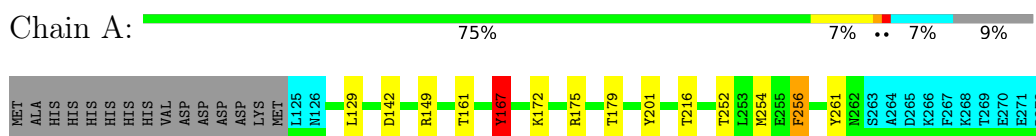
#### 4.2.17 Score per residue for model 17

- Molecule 1: Iron-regulated surface determinant protein B



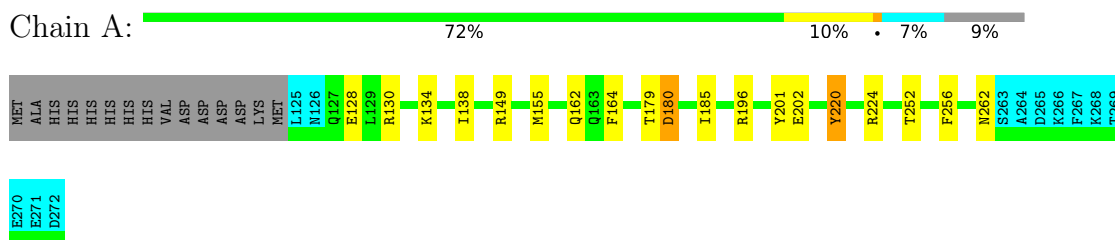
#### 4.2.18 Score per residue for model 18

- Molecule 1: Iron-regulated surface determinant protein B



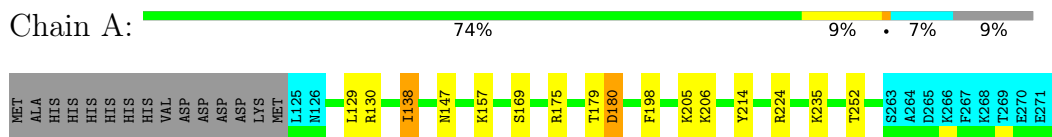
#### 4.2.19 Score per residue for model 19

- Molecule 1: Iron-regulated surface determinant protein B



#### 4.2.20 Score per residue for model 20

- Molecule 1: Iron-regulated surface determinant protein B



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, molecular dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	refinement	
Amber	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1280
Number of shifts mapped to atoms	1280
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	61%

## 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	0.75±0.01	0±0/1150 ( 0.0± 0.0%)	1.05±0.03	5±2/1550 ( 0.3± 0.1%)
All	All	0.75	0/23000 ( 0.0%)	1.05	95/31000 ( 0.3%)

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±0.9
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	196	ARG	NE-CZ-NH1	9.47	125.03	120.30	9	15
1	A	149	ARG	NE-CZ-NH1	9.13	124.87	120.30	3	11
1	A	224	ARG	NE-CZ-NH1	8.99	124.79	120.30	8	16
1	A	175	ARG	NE-CZ-NH1	8.32	124.46	120.30	8	15
1	A	130	ARG	NE-CZ-NH1	7.72	124.16	120.30	11	13
1	A	224	ARG	NE-CZ-NH2	-7.21	116.70	120.30	12	6
1	A	130	ARG	NE-CZ-NH2	-6.84	116.88	120.30	1	3
1	A	249	TYR	CB-CG-CD2	-6.53	117.08	121.00	17	1
1	A	196	ARG	NE-CZ-NH2	-6.14	117.23	120.30	3	2
1	A	149	ARG	NE-CZ-NH2	-5.99	117.31	120.30	4	3
1	A	214	TYR	CB-CG-CD2	-5.45	117.73	121.00	9	2
1	A	175	ARG	NE-CZ-NH2	-5.36	117.62	120.30	16	2
1	A	167	TYR	CB-CG-CD2	-5.27	117.84	121.00	18	1
1	A	220	TYR	CB-CG-CD2	-5.17	117.90	121.00	19	1
1	A	256	PHE	CB-CG-CD2	-5.16	117.19	120.80	18	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	256	PHE	CB-CG-CD1	5.13	124.39	120.80	17	2

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	175	ARG	Sidechain	2
1	A	211	LEU	Peptide	2
1	A	256	PHE	Peptide	2
1	A	168	ALA	Peptide	1
1	A	179	THR	Peptide	1
1	A	242	PHE	Peptide	1
1	A	227	VAL	Peptide	1
1	A	170	SER	Peptide	1
1	A	142	ASP	Peptide	1
1	A	167	TYR	Peptide	1
1	A	222	TYR	Sidechain	1
1	A	178	PHE	Peptide	1
1	A	143	HIS	Peptide	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	1121	1106	1106	0±1
All	All	22420	22120	22120	10

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:133:ILE:HG22	1:A:214:TYR:CE1	0.59	2.33	4	1
1:A:138:ILE:HD12	1:A:138:ILE:H	0.56	1.61	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:THR:HG22	1:A:180:ASP:H	0.52	1.62	19	6
1:A:138:ILE:HD13	1:A:138:ILE:H	0.46	1.71	16	1
1:A:246:GLU:CD	1:A:246:GLU:H	0.45	2.15	5	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	136/163 (83%)	124±2 (91±2%)	10±2 (7±2%)	2±1 (1±1%)	18	66
All	All	2720/3260 (83%)	2488 (91%)	201 (7%)	31 (1%)	18	66

All 9 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	180	ASP	11
1	A	164	PHE	7
1	A	251	TYR	4
1	A	136	PRO	3
1	A	147	ASN	2
1	A	127	GLN	1
1	A	196	ARG	1
1	A	140	ASP	1
1	A	167	TYR	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	123/148 (83%)	114±2 (92±2%)	9±2 (8±2%)	16	64
All	All	2460/2960 (83%)	2271 (92%)	189 (8%)	16	64

All 61 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	138	ILE	19
1	A	256	PHE	15
1	A	252	THR	13
1	A	220	TYR	10
1	A	205	LYS	8
1	A	172	LYS	7
1	A	129	LEU	7
1	A	201	TYR	6
1	A	216	THR	5
1	A	248	LYS	5
1	A	185	ILE	5
1	A	179	THR	4
1	A	240	THR	4
1	A	261	TYR	4
1	A	202	GLU	4
1	A	232	LYS	4
1	A	198	PHE	4
1	A	130	ARG	3
1	A	134	LYS	3
1	A	162	GLN	3
1	A	157	LYS	3
1	A	222	TYR	2
1	A	251	TYR	2
1	A	235	LYS	2
1	A	159	ASP	2
1	A	258	GLN	2
1	A	153	PHE	2
1	A	169	SER	2
1	A	161	THR	2
1	A	182	LYS	2
1	A	214	TYR	2
1	A	224	ARG	2
1	A	155	MET	2
1	A	142	ASP	2
1	A	152	ASP	1
1	A	191	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	156	LYS	1
1	A	213	SER	1
1	A	228	SER	1
1	A	197	LYS	1
1	A	223	ILE	1
1	A	144	SER	1
1	A	196	ARG	1
1	A	244	ASN	1
1	A	247	GLU	1
1	A	190	GLN	1
1	A	166	HIS	1
1	A	187	LEU	1
1	A	163	GLN	1
1	A	218	LYS	1
1	A	260	ILE	1
1	A	164	PHE	1
1	A	175	ARG	1
1	A	253	LEU	1
1	A	141	LYS	1
1	A	241	HIS	1
1	A	167	TYR	1
1	A	254	MET	1
1	A	128	GLU	1
1	A	262	ASN	1
1	A	206	LYS	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 monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 61% for the well-defined parts and 62% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping [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	1280
Number of shifts mapped to atoms	1280
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	143	$-0.41 \pm 0.20$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	138	$-0.38 \pm 0.16$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	131	$-0.03 \pm 0.26$	None needed ( $< 0.5$ ppm)

#### 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 61%, i.e. 1169 atoms were assigned a chemical shift out of a possible 1906. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	500/671 (75%)	250/270 (93%)	131/272 (48%)	119/129 (92%)
Sidechain	652/1041 (63%)	399/668 (60%)	253/329 (77%)	0/44 (0%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	17/194 (9%)	16/94 (17%)	0/96 (0%)	1/4 (25%)
Overall	1169/1906 (61%)	665/1032 (64%)	384/697 (55%)	120/177 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 62%, i.e. 1280 atoms were assigned a chemical shift out of a possible 2060. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	547/731 (75%)	273/294 (93%)	143/296 (48%)	131/141 (93%)
Sidechain	715/1125 (64%)	439/720 (61%)	276/358 (77%)	0/47 (0%)
Aromatic	18/204 (9%)	17/99 (17%)	0/101 (0%)	1/4 (25%)
Overall	1280/2060 (62%)	729/1113 (65%)	419/755 (55%)	132/192 (69%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

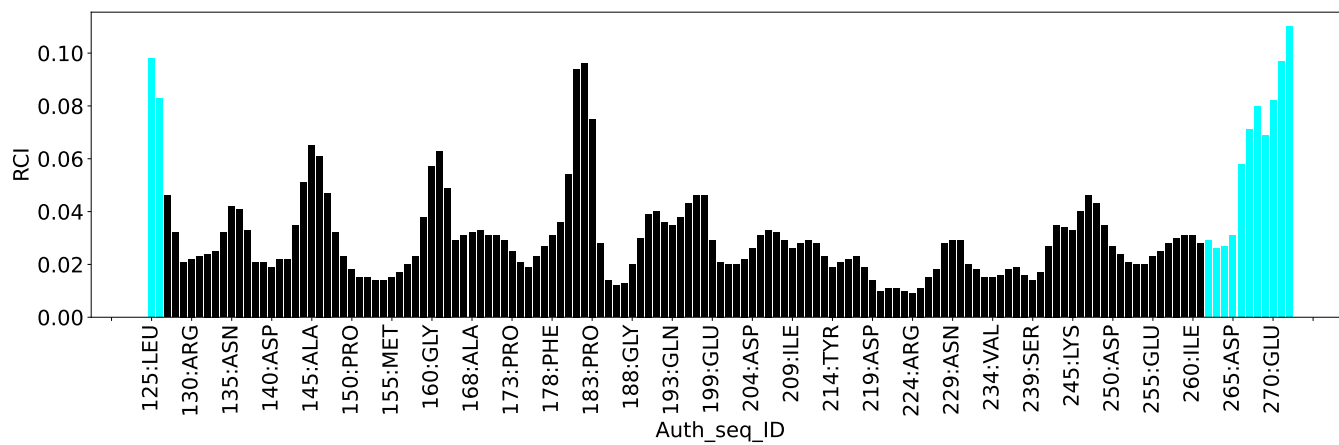
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	218	LYS	HB2	0.50	0.58 – 2.97	-5.4

#### 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	878
Intra-residue ( $ i-j =0$ )	121
Sequential ( $ i-j =1$ )	288
Medium range ( $ i-j >1$ and $ i-j <5$ )	97
Long range ( $ i-j \geq 5$ )	280
Inter-chain	0
Hydrogen bond restraints	92
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	5.4
Number of long range restraints per residue <sup>1</sup>	2.2

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

### 8.2 Residual restraint violations

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

#### 8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	1.1	0.18
0.2-0.5 (Medium)	0.7	0.49
>0.5 (Large)	None	None

### 8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis [i](#)

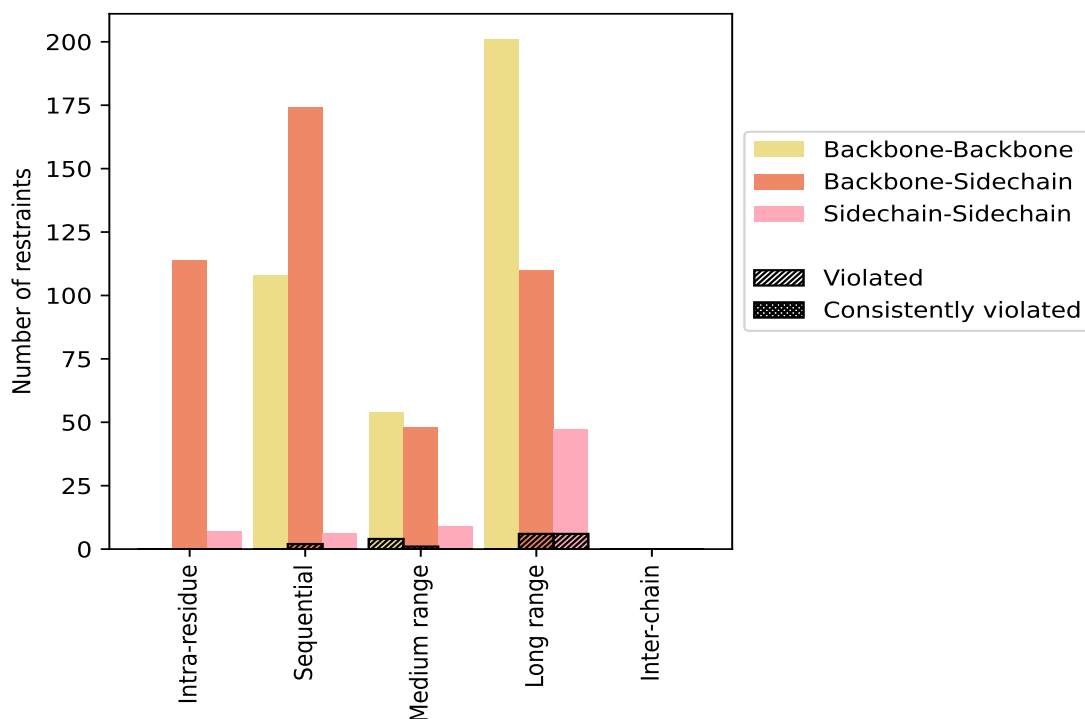
### 9.1 Summary of distance violations [i](#)

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	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>121</b>	<b>13.8</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	114	13.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	7	0.8	0	0.0	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>288</b>	<b>32.8</b>	<b>2</b>	<b>0.7</b>	<b>0.2</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	108	12.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	174	19.8	2	1.1	0.2	0	0.0	0.0
Sidechain-Sidechain	6	0.7	0	0.0	0.0	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>97</b>	<b>11.0</b>	<b>4</b>	<b>4.1</b>	<b>0.5</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	40	4.6	3	7.5	0.3	0	0.0	0.0
Backbone-Sidechain	48	5.5	1	2.1	0.1	0	0.0	0.0
Sidechain-Sidechain	9	1.0	0	0.0	0.0	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>280</b>	<b>31.9</b>	<b>12</b>	<b>4.3</b>	<b>1.4</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	123	14.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	110	12.5	6	5.5	0.7	0	0.0	0.0
Sidechain-Sidechain	47	5.4	6	12.8	0.7	0	0.0	0.0
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
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
<b>Hydrogen bond</b>	<b>92</b>	<b>10.5</b>	<b>1</b>	<b>1.1</b>	<b>0.1</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>878</b>	<b>100.0</b>	<b>19</b>	<b>2.2</b>	<b>2.2</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	363	41.3	4	1.1	0.5	0	0.0	0.0
Backbone-Sidechain	446	50.8	9	2.0	1.0	0	0.0	0.0
Sidechain-Sidechain	69	7.9	6	8.7	0.7	0	0.0	0.0

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> 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 <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	0	0	2	1	0	3	0.15	0.17	0.01	0.15
2	0	0	0	1	0	1	0.12	0.12	0.0	0.12
3	0	0	1	2	0	3	0.29	0.49	0.15	0.27
4	0	1	0	0	0	1	0.12	0.12	0.0	0.12
5	0	1	3	0	0	4	0.15	0.27	0.07	0.11
6	0	0	0	1	0	1	0.24	0.24	0.0	0.24
7	0	0	1	1	0	2	0.3	0.48	0.18	0.3
8	0	0	0	1	0	1	0.18	0.18	0.0	0.18
9	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	0	1	1	1	0	3	0.28	0.46	0.14	0.26
11	0	0	0	1	0	1	0.28	0.28	0.0	0.28

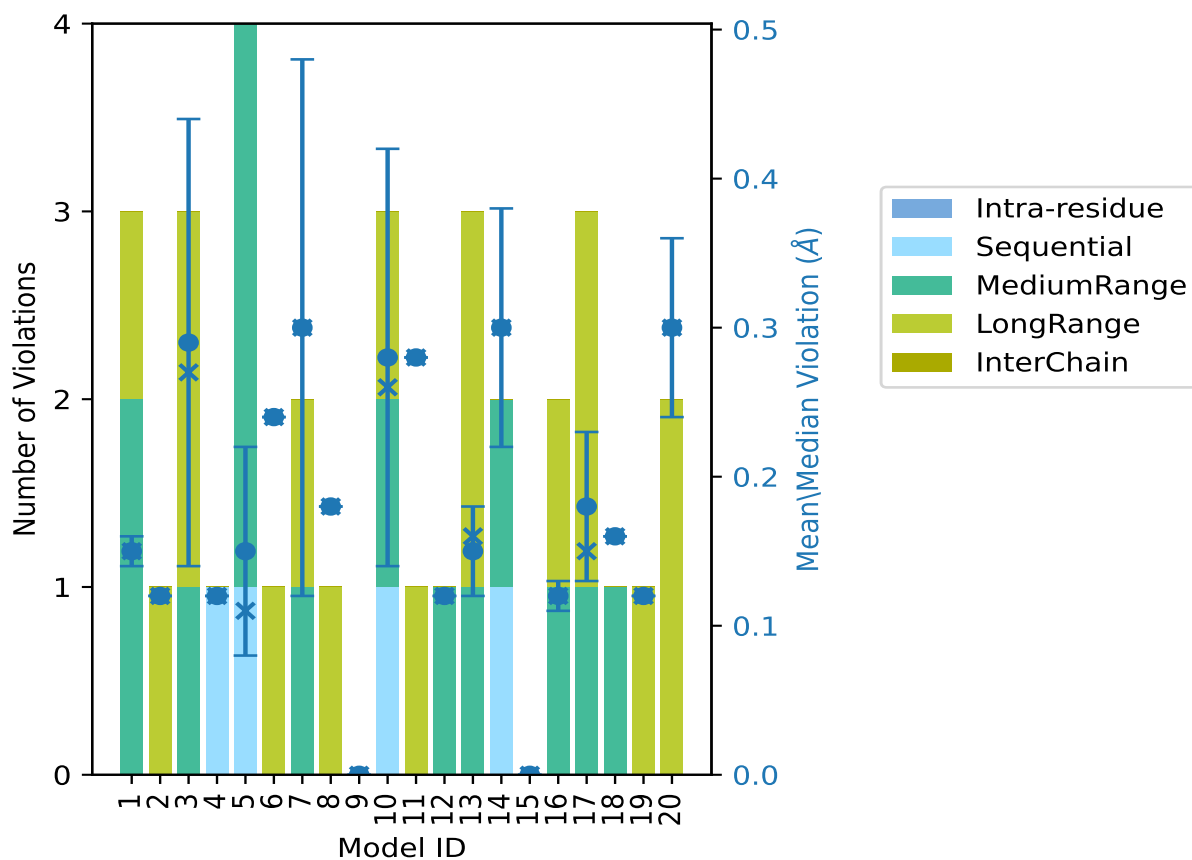
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
12	0	0	1	0	0	1	0.12	0.12	0.0	0.12
13	0	0	1	2	0	3	0.15	0.17	0.03	0.16
14	0	1	1	0	0	2	0.3	0.39	0.08	0.3
15	0	0	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	1	1	0	2	0.12	0.13	0.01	0.12
17	0	0	1	2	0	3	0.18	0.25	0.05	0.15
18	0	0	1	0	0	1	0.16	0.16	0.0	0.16
19	0	0	0	1	0	1	0.12	0.12	0.0	0.12
20	0	0	0	2	0	2	0.3	0.36	0.06	0.3

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard 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



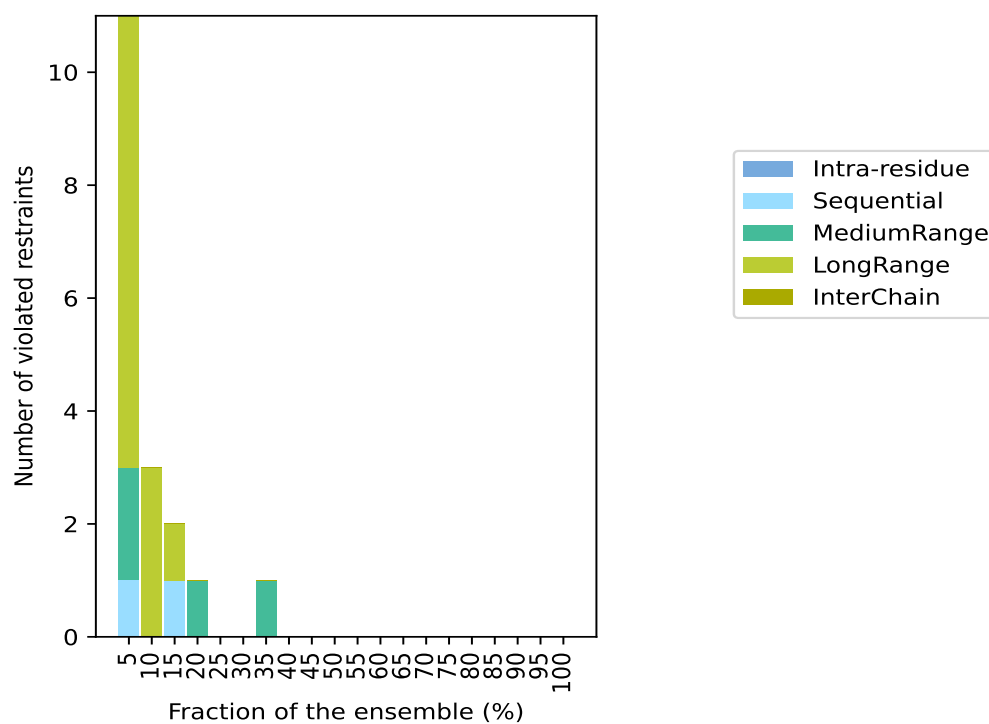
### 9.3 Distance violation statistics for the ensemble

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, 768(IR:121, SQ:286, MR:93, LR:268, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	1	2	8	0	11	1	5.0
0	0	0	3	0	3	2	10.0
0	1	0	1	0	2	3	15.0
0	0	1	0	0	1	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	1	0	0	1	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	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	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	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

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

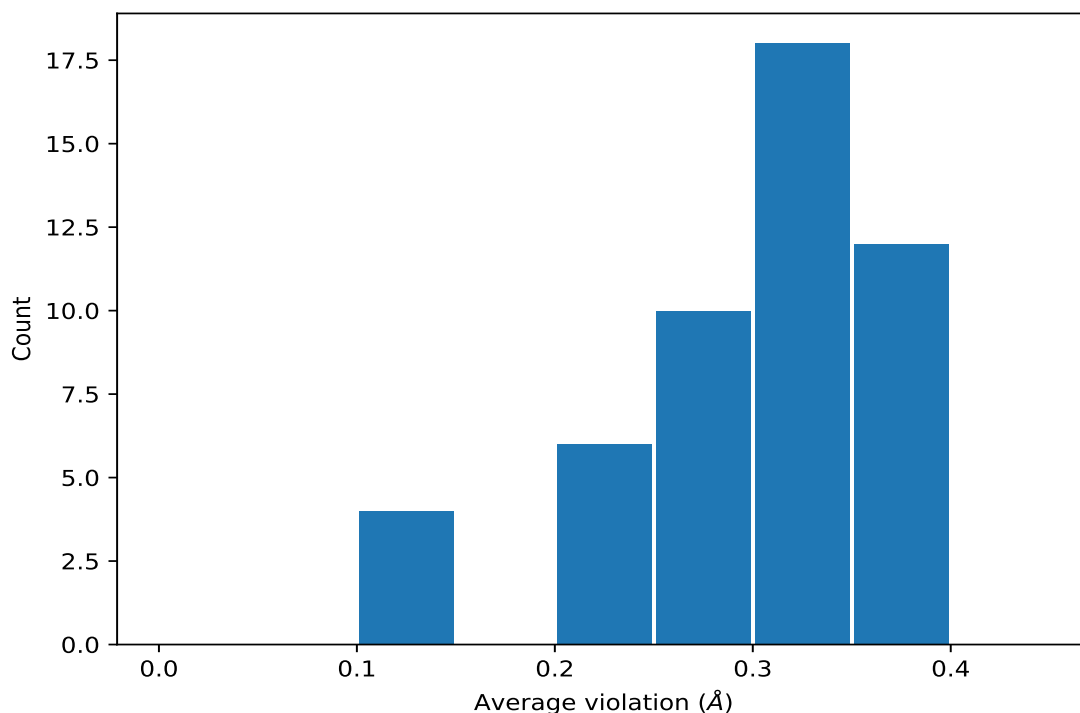
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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 <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,523)	1:A:212:VAL:HG11	1:A:214:TYR:H	7	0.21	0.05	0.22
(1,523)	1:A:212:VAL:HG12	1:A:214:TYR:H	7	0.21	0.05	0.22
(1,523)	1:A:212:VAL:HG13	1:A:214:TYR:H	7	0.21	0.05	0.22
(1,523)	1:A:212:VAL:HG21	1:A:214:TYR:H	7	0.21	0.05	0.22
(1,523)	1:A:212:VAL:HG22	1:A:214:TYR:H	7	0.21	0.05	0.22
(1,523)	1:A:212:VAL:HG23	1:A:214:TYR:H	7	0.21	0.05	0.22
(1,254)	1:A:175:ARG:HA	1:A:177:ILE:H	4	0.12	0.01	0.12
(2,2)	1:A:151:ILE:HG12	1:A:256:PHE:HD1	3	0.27	0.16	0.16
(2,2)	1:A:151:ILE:HG12	1:A:256:PHE:HD2	3	0.27	0.16	0.16
(2,2)	1:A:151:ILE:HG13	1:A:256:PHE:HD1	3	0.27	0.16	0.16
(2,2)	1:A:151:ILE:HG13	1:A:256:PHE:HD2	3	0.27	0.16	0.16
(1,727)	1:A:253:LEU:HD11	1:A:254:MET:H	3	0.26	0.11	0.26
(1,727)	1:A:253:LEU:HD12	1:A:254:MET:H	3	0.26	0.11	0.26
(1,727)	1:A:253:LEU:HD13	1:A:254:MET:H	3	0.26	0.11	0.26
(1,727)	1:A:253:LEU:HD21	1:A:254:MET:H	3	0.26	0.11	0.26
(1,727)	1:A:253:LEU:HD22	1:A:254:MET:H	3	0.26	0.11	0.26

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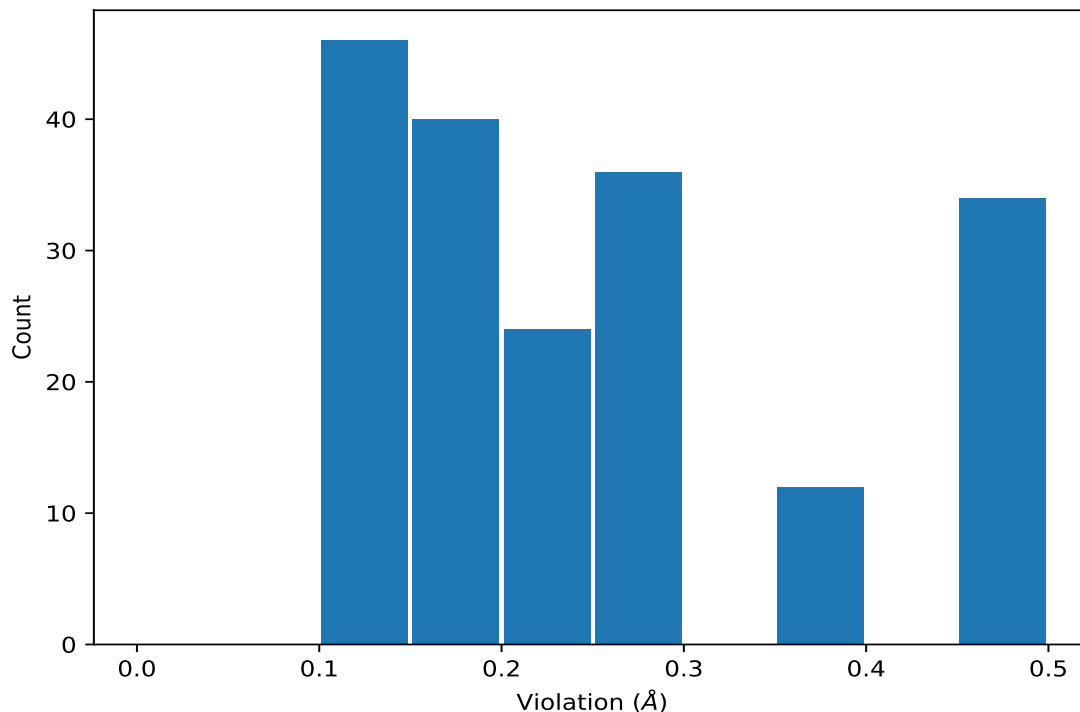
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,727)	1:A:253:LEU:HD23	1:A:254:MET:H	3	0.26	0.11	0.26
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG11	2	0.38	0.1	0.38
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG12	2	0.38	0.1	0.38
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG13	2	0.38	0.1	0.38
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG21	2	0.38	0.1	0.38
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG22	2	0.38	0.1	0.38
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG23	2	0.38	0.1	0.38
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG11	2	0.38	0.1	0.38
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG12	2	0.38	0.1	0.38
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG13	2	0.38	0.1	0.38
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG21	2	0.38	0.1	0.38
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG22	2	0.38	0.1	0.38
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG23	2	0.38	0.1	0.38
(1,358)	1:A:187:LEU:HD11	1:A:223:ILE:HD11	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD11	1:A:223:ILE:HD12	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD11	1:A:223:ILE:HD13	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD12	1:A:223:ILE:HD11	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD12	1:A:223:ILE:HD12	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD12	1:A:223:ILE:HD13	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD13	1:A:223:ILE:HD11	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD13	1:A:223:ILE:HD12	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD13	1:A:223:ILE:HD13	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD21	1:A:223:ILE:HD11	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD21	1:A:223:ILE:HD12	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD21	1:A:223:ILE:HD13	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD22	1:A:223:ILE:HD11	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD22	1:A:223:ILE:HD12	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD22	1:A:223:ILE:HD13	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD23	1:A:223:ILE:HD11	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD23	1:A:223:ILE:HD12	2	0.32	0.15	0.32
(1,358)	1:A:187:LEU:HD23	1:A:223:ILE:HD13	2	0.32	0.15	0.32
(1,235)	1:A:161:THR:HB	1:A:252:THR:HG21	2	0.12	0.0	0.12
(1,235)	1:A:161:THR:HB	1:A:252:THR:HG22	2	0.12	0.0	0.12
(1,235)	1:A:161:THR:HB	1:A:252:THR:HG23	2	0.12	0.0	0.12

<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:A:151:ILE:HG12	1:A:256:PHE:HD1	3	0.49
(2,2)	1:A:151:ILE:HG12	1:A:256:PHE:HD2	3	0.49
(2,2)	1:A:151:ILE:HG13	1:A:256:PHE:HD1	3	0.49
(2,2)	1:A:151:ILE:HG13	1:A:256:PHE:HD2	3	0.49
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG11	7	0.48
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG12	7	0.48
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG13	7	0.48
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG21	7	0.48
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG22	7	0.48
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG23	7	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG11	7	0.48
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG12	7	0.48
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG13	7	0.48
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG21	7	0.48
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG22	7	0.48
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG23	7	0.48
(1,358)	1:A:187:LEU:HD11	1:A:223:ILE:HD11	10	0.46
(1,358)	1:A:187:LEU:HD11	1:A:223:ILE:HD12	10	0.46
(1,358)	1:A:187:LEU:HD11	1:A:223:ILE:HD13	10	0.46
(1,358)	1:A:187:LEU:HD12	1:A:223:ILE:HD11	10	0.46
(1,358)	1:A:187:LEU:HD12	1:A:223:ILE:HD12	10	0.46
(1,358)	1:A:187:LEU:HD12	1:A:223:ILE:HD13	10	0.46
(1,358)	1:A:187:LEU:HD13	1:A:223:ILE:HD11	10	0.46
(1,358)	1:A:187:LEU:HD13	1:A:223:ILE:HD12	10	0.46
(1,358)	1:A:187:LEU:HD13	1:A:223:ILE:HD13	10	0.46
(1,358)	1:A:187:LEU:HD21	1:A:223:ILE:HD11	10	0.46
(1,358)	1:A:187:LEU:HD21	1:A:223:ILE:HD12	10	0.46
(1,358)	1:A:187:LEU:HD21	1:A:223:ILE:HD13	10	0.46
(1,358)	1:A:187:LEU:HD22	1:A:223:ILE:HD11	10	0.46
(1,358)	1:A:187:LEU:HD22	1:A:223:ILE:HD12	10	0.46
(1,358)	1:A:187:LEU:HD22	1:A:223:ILE:HD13	10	0.46
(1,358)	1:A:187:LEU:HD23	1:A:223:ILE:HD11	10	0.46
(1,358)	1:A:187:LEU:HD23	1:A:223:ILE:HD12	10	0.46
(1,358)	1:A:187:LEU:HD23	1:A:223:ILE:HD13	10	0.46
(1,727)	1:A:253:LEU:HD11	1:A:254:MET:H	14	0.39
(1,727)	1:A:253:LEU:HD12	1:A:254:MET:H	14	0.39
(1,727)	1:A:253:LEU:HD13	1:A:254:MET:H	14	0.39
(1,727)	1:A:253:LEU:HD21	1:A:254:MET:H	14	0.39
(1,727)	1:A:253:LEU:HD22	1:A:254:MET:H	14	0.39
(1,727)	1:A:253:LEU:HD23	1:A:254:MET:H	14	0.39
(2,1)	1:A:129:LEU:HD11	1:A:221:ALA:H	20	0.36
(2,1)	1:A:129:LEU:HD12	1:A:221:ALA:H	20	0.36
(2,1)	1:A:129:LEU:HD13	1:A:221:ALA:H	20	0.36
(2,1)	1:A:129:LEU:HD21	1:A:221:ALA:H	20	0.36
(2,1)	1:A:129:LEU:HD22	1:A:221:ALA:H	20	0.36
(2,1)	1:A:129:LEU:HD23	1:A:221:ALA:H	20	0.36
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG11	11	0.28
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG12	11	0.28
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG13	11	0.28
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG21	11	0.28
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG22	11	0.28
(1,317)	1:A:183:PRO:HB2	1:A:227:VAL:HG23	11	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG11	11	0.28
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG12	11	0.28
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG13	11	0.28
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG21	11	0.28
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG22	11	0.28
(1,317)	1:A:183:PRO:HB3	1:A:227:VAL:HG23	11	0.28
(1,523)	1:A:212:VAL:HG11	1:A:214:TYR:H	3	0.27
(1,523)	1:A:212:VAL:HG12	1:A:214:TYR:H	3	0.27
(1,523)	1:A:212:VAL:HG13	1:A:214:TYR:H	3	0.27
(1,523)	1:A:212:VAL:HG21	1:A:214:TYR:H	3	0.27
(1,523)	1:A:212:VAL:HG22	1:A:214:TYR:H	3	0.27
(1,523)	1:A:212:VAL:HG23	1:A:214:TYR:H	3	0.27
(1,523)	1:A:212:VAL:HG11	1:A:214:TYR:H	5	0.27
(1,523)	1:A:212:VAL:HG12	1:A:214:TYR:H	5	0.27
(1,523)	1:A:212:VAL:HG13	1:A:214:TYR:H	5	0.27
(1,523)	1:A:212:VAL:HG21	1:A:214:TYR:H	5	0.27
(1,523)	1:A:212:VAL:HG22	1:A:214:TYR:H	5	0.27
(1,523)	1:A:212:VAL:HG23	1:A:214:TYR:H	5	0.27
(1,727)	1:A:253:LEU:HD11	1:A:254:MET:H	10	0.26
(1,727)	1:A:253:LEU:HD12	1:A:254:MET:H	10	0.26
(1,727)	1:A:253:LEU:HD13	1:A:254:MET:H	10	0.26
(1,727)	1:A:253:LEU:HD21	1:A:254:MET:H	10	0.26
(1,727)	1:A:253:LEU:HD22	1:A:254:MET:H	10	0.26
(1,727)	1:A:253:LEU:HD23	1:A:254:MET:H	10	0.26
(1,523)	1:A:212:VAL:HG11	1:A:214:TYR:H	17	0.25
(1,523)	1:A:212:VAL:HG12	1:A:214:TYR:H	17	0.25
(1,523)	1:A:212:VAL:HG13	1:A:214:TYR:H	17	0.25
(1,523)	1:A:212:VAL:HG21	1:A:214:TYR:H	17	0.25
(1,523)	1:A:212:VAL:HG22	1:A:214:TYR:H	17	0.25
(1,523)	1:A:212:VAL:HG23	1:A:214:TYR:H	17	0.25
(1,5)	1:A:127:GLN:HG2	1:A:132:ALA:HB1	6	0.24
(1,5)	1:A:127:GLN:HG2	1:A:132:ALA:HB2	6	0.24
(1,5)	1:A:127:GLN:HG2	1:A:132:ALA:HB3	6	0.24
(1,5)	1:A:127:GLN:HG3	1:A:132:ALA:HB1	6	0.24
(1,5)	1:A:127:GLN:HG3	1:A:132:ALA:HB2	6	0.24
(1,5)	1:A:127:GLN:HG3	1:A:132:ALA:HB3	6	0.24
(1,524)	1:A:212:VAL:HG11	1:A:224:ARG:HB2	20	0.23
(1,524)	1:A:212:VAL:HG11	1:A:224:ARG:HB3	20	0.23
(1,524)	1:A:212:VAL:HG12	1:A:224:ARG:HB2	20	0.23
(1,524)	1:A:212:VAL:HG12	1:A:224:ARG:HB3	20	0.23
(1,524)	1:A:212:VAL:HG13	1:A:224:ARG:HB2	20	0.23
(1,524)	1:A:212:VAL:HG13	1:A:224:ARG:HB3	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,524)	1:A:212:VAL:HG21	1:A:224:ARG:HB2	20	0.23
(1,524)	1:A:212:VAL:HG21	1:A:224:ARG:HB3	20	0.23
(1,524)	1:A:212:VAL:HG22	1:A:224:ARG:HB2	20	0.23
(1,524)	1:A:212:VAL:HG22	1:A:224:ARG:HB3	20	0.23
(1,524)	1:A:212:VAL:HG23	1:A:224:ARG:HB2	20	0.23
(1,524)	1:A:212:VAL:HG23	1:A:224:ARG:HB3	20	0.23
(1,523)	1:A:212:VAL:HG11	1:A:214:TYR:H	14	0.22
(1,523)	1:A:212:VAL:HG12	1:A:214:TYR:H	14	0.22
(1,523)	1:A:212:VAL:HG13	1:A:214:TYR:H	14	0.22
(1,523)	1:A:212:VAL:HG21	1:A:214:TYR:H	14	0.22
(1,523)	1:A:212:VAL:HG22	1:A:214:TYR:H	14	0.22
(1,523)	1:A:212:VAL:HG23	1:A:214:TYR:H	14	0.22
(1,194)	1:A:156:LYS:H	1:A:253:LEU:HD11	8	0.18
(1,194)	1:A:156:LYS:H	1:A:253:LEU:HD12	8	0.18
(1,194)	1:A:156:LYS:H	1:A:253:LEU:HD13	8	0.18
(1,194)	1:A:156:LYS:H	1:A:253:LEU:HD21	8	0.18
(1,194)	1:A:156:LYS:H	1:A:253:LEU:HD22	8	0.18
(1,194)	1:A:156:LYS:H	1:A:253:LEU:HD23	8	0.18
(1,523)	1:A:212:VAL:HG11	1:A:214:TYR:H	13	0.17
(1,523)	1:A:212:VAL:HG12	1:A:214:TYR:H	13	0.17
(1,523)	1:A:212:VAL:HG13	1:A:214:TYR:H	13	0.17
(1,523)	1:A:212:VAL:HG21	1:A:214:TYR:H	13	0.17
(1,523)	1:A:212:VAL:HG22	1:A:214:TYR:H	13	0.17
(1,523)	1:A:212:VAL:HG23	1:A:214:TYR:H	13	0.17
(1,358)	1:A:187:LEU:HD11	1:A:223:ILE:HD11	1	0.17
(1,358)	1:A:187:LEU:HD11	1:A:223:ILE:HD12	1	0.17
(1,358)	1:A:187:LEU:HD11	1:A:223:ILE:HD13	1	0.17
(1,358)	1:A:187:LEU:HD12	1:A:223:ILE:HD11	1	0.17
(1,358)	1:A:187:LEU:HD12	1:A:223:ILE:HD12	1	0.17
(1,358)	1:A:187:LEU:HD12	1:A:223:ILE:HD13	1	0.17
(1,358)	1:A:187:LEU:HD13	1:A:223:ILE:HD11	1	0.17
(1,358)	1:A:187:LEU:HD13	1:A:223:ILE:HD12	1	0.17
(1,358)	1:A:187:LEU:HD13	1:A:223:ILE:HD13	1	0.17
(1,358)	1:A:187:LEU:HD21	1:A:223:ILE:HD11	1	0.17
(1,358)	1:A:187:LEU:HD21	1:A:223:ILE:HD12	1	0.17
(1,358)	1:A:187:LEU:HD21	1:A:223:ILE:HD13	1	0.17
(1,358)	1:A:187:LEU:HD22	1:A:223:ILE:HD11	1	0.17
(1,358)	1:A:187:LEU:HD22	1:A:223:ILE:HD12	1	0.17
(1,358)	1:A:187:LEU:HD22	1:A:223:ILE:HD13	1	0.17
(1,358)	1:A:187:LEU:HD23	1:A:223:ILE:HD11	1	0.17
(1,358)	1:A:187:LEU:HD23	1:A:223:ILE:HD12	1	0.17
(1,358)	1:A:187:LEU:HD23	1:A:223:ILE:HD13	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:A:151:ILE:HG12	1:A:256:PHE:HD1	13	0.16
(2,2)	1:A:151:ILE:HG12	1:A:256:PHE:HD2	13	0.16
(2,2)	1:A:151:ILE:HG13	1:A:256:PHE:HD1	13	0.16
(2,2)	1:A:151:ILE:HG13	1:A:256:PHE:HD2	13	0.16
(1,523)	1:A:212:VAL:HG11	1:A:214:TYR:H	18	0.16
(1,523)	1:A:212:VAL:HG12	1:A:214:TYR:H	18	0.16
(1,523)	1:A:212:VAL:HG13	1:A:214:TYR:H	18	0.16
(1,523)	1:A:212:VAL:HG21	1:A:214:TYR:H	18	0.16
(1,523)	1:A:212:VAL:HG22	1:A:214:TYR:H	18	0.16
(1,523)	1:A:212:VAL:HG23	1:A:214:TYR:H	18	0.16
(2,2)	1:A:151:ILE:HG12	1:A:256:PHE:HD1	17	0.15
(2,2)	1:A:151:ILE:HG12	1:A:256:PHE:HD2	17	0.15
(2,2)	1:A:151:ILE:HG13	1:A:256:PHE:HD1	17	0.15
(2,2)	1:A:151:ILE:HG13	1:A:256:PHE:HD2	17	0.15
(1,523)	1:A:212:VAL:HG11	1:A:214:TYR:H	1	0.15
(1,523)	1:A:212:VAL:HG12	1:A:214:TYR:H	1	0.15
(1,523)	1:A:212:VAL:HG13	1:A:214:TYR:H	1	0.15
(1,523)	1:A:212:VAL:HG21	1:A:214:TYR:H	1	0.15
(1,523)	1:A:212:VAL:HG22	1:A:214:TYR:H	1	0.15
(1,523)	1:A:212:VAL:HG23	1:A:214:TYR:H	1	0.15
(1,436)	1:A:201:TYR:H	1:A:237:VAL:HG11	17	0.15
(1,436)	1:A:201:TYR:H	1:A:237:VAL:HG12	17	0.15
(1,436)	1:A:201:TYR:H	1:A:237:VAL:HG13	17	0.15
(1,436)	1:A:201:TYR:H	1:A:237:VAL:HG21	17	0.15
(1,436)	1:A:201:TYR:H	1:A:237:VAL:HG22	17	0.15
(1,436)	1:A:201:TYR:H	1:A:237:VAL:HG23	17	0.15
(1,254)	1:A:175:ARG:HA	1:A:177:ILE:H	1	0.14
(1,254)	1:A:175:ARG:HA	1:A:177:ILE:H	16	0.13
(1,727)	1:A:253:LEU:HD11	1:A:254:MET:H	4	0.12
(1,727)	1:A:253:LEU:HD12	1:A:254:MET:H	4	0.12
(1,727)	1:A:253:LEU:HD13	1:A:254:MET:H	4	0.12
(1,727)	1:A:253:LEU:HD21	1:A:254:MET:H	4	0.12
(1,727)	1:A:253:LEU:HD22	1:A:254:MET:H	4	0.12
(1,727)	1:A:253:LEU:HD23	1:A:254:MET:H	4	0.12
(1,653)	1:A:234:VAL:HG11	1:A:256:PHE:H	19	0.12
(1,653)	1:A:234:VAL:HG12	1:A:256:PHE:H	19	0.12
(1,653)	1:A:234:VAL:HG13	1:A:256:PHE:H	19	0.12
(1,653)	1:A:234:VAL:HG21	1:A:256:PHE:H	19	0.12
(1,653)	1:A:234:VAL:HG22	1:A:256:PHE:H	19	0.12
(1,653)	1:A:234:VAL:HG23	1:A:256:PHE:H	19	0.12
(1,311)	1:A:180:ASP:HA	1:A:182:LYS:H	12	0.12
(1,254)	1:A:175:ARG:HA	1:A:177:ILE:H	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,235)	1:A:161:THR:HB	1:A:252:THR:HG21	2	0.12
(1,235)	1:A:161:THR:HB	1:A:252:THR:HG22	2	0.12
(1,235)	1:A:161:THR:HB	1:A:252:THR:HG23	2	0.12
(1,235)	1:A:161:THR:HB	1:A:252:THR:HG21	3	0.12
(1,235)	1:A:161:THR:HB	1:A:252:THR:HG22	3	0.12
(1,235)	1:A:161:THR:HB	1:A:252:THR:HG23	3	0.12
(3,85)	1:A:130:ARG:O	1:A:133:ILE:H	5	0.11
(1,682)	1:A:237:VAL:H	1:A:252:THR:HB	16	0.11
(1,536)	1:A:214:TYR:HA	1:A:216:THR:H	5	0.11
(1,526)	1:A:213:SER:H	1:A:214:TYR:HB2	5	0.11
(1,526)	1:A:213:SER:H	1:A:214:TYR:HB3	5	0.11
(1,340)	1:A:185:ILE:HG12	1:A:225:PHE:H	13	0.11
(1,340)	1:A:185:ILE:HG13	1:A:225:PHE:H	13	0.11
(1,254)	1:A:175:ARG:HA	1:A:177:ILE:H	7	0.11

## 10 Dihedral-angle violation analysis

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value