



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 6, 2023 – 01:24 pm BST

PDB ID : 5MGQ  
BMRB ID : 34069  
Title : Solution structure of oxidized and amidated human IAPP (1-37), the diabetes II peptide.  
Authors : Rodriguez Camargo, D.C.; Tripsianes, K.; Reif, B.  
Deposited on : 2016-11-21

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<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  
Mogul : 1.8.4, CSD as541be (2020)  
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

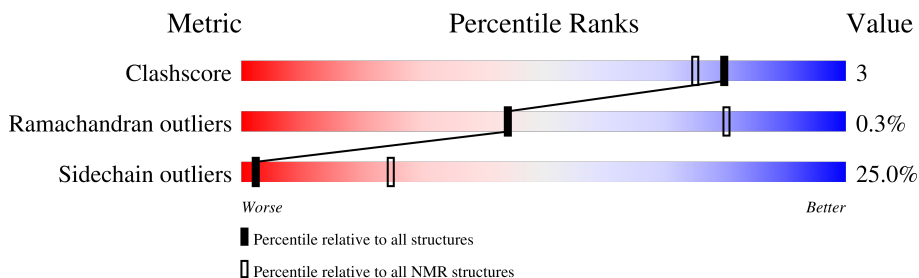
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 76%.

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	37	

## 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: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:17 (15)	0.20	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 2 clusters and 3 single-model clusters were found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 538 atoms, of which 265 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Islet amyloid polypeptide.

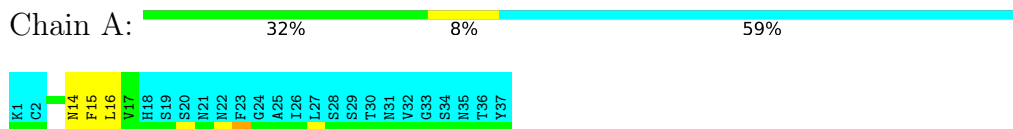
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	37	538	165	265	51	55	2	0

## 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: Islet amyloid polypeptide

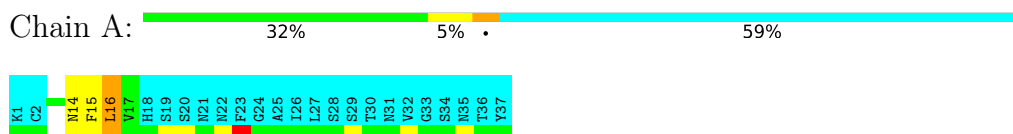


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

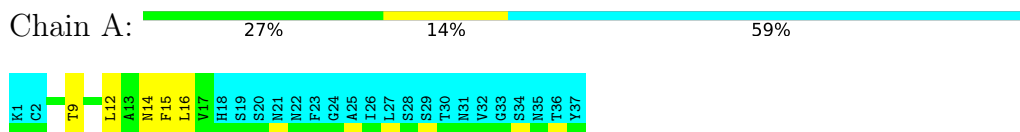
#### 4.2.1 Score per residue for model 1

- Molecule 1: Islet amyloid polypeptide



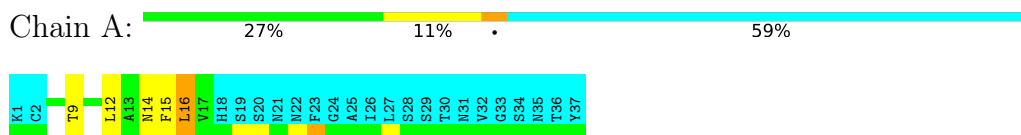
#### 4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Islet amyloid polypeptide



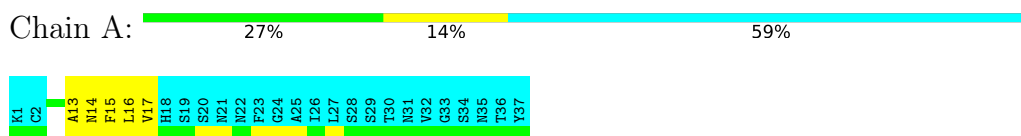
### 4.2.3 Score per residue for model 3

- Molecule 1: Islet amyloid polypeptide



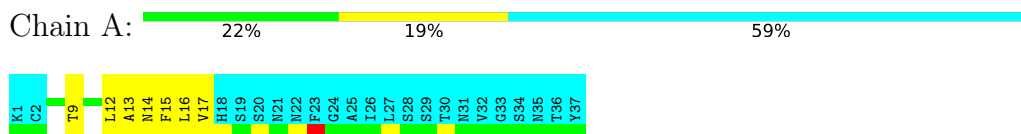
### 4.2.4 Score per residue for model 4

- Molecule 1: Islet amyloid polypeptide



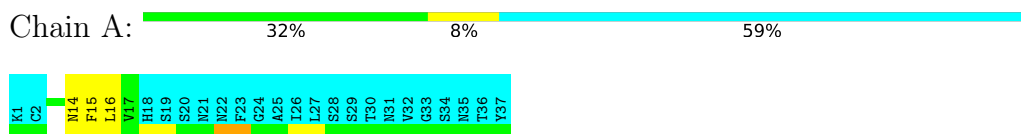
### 4.2.5 Score per residue for model 5

- Molecule 1: Islet amyloid polypeptide



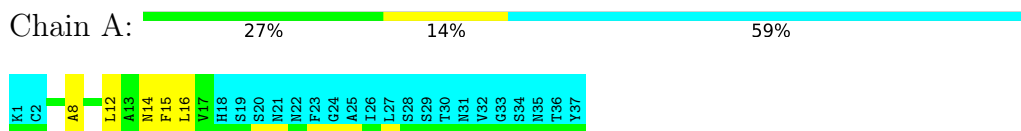
### 4.2.6 Score per residue for model 6

- Molecule 1: Islet amyloid polypeptide



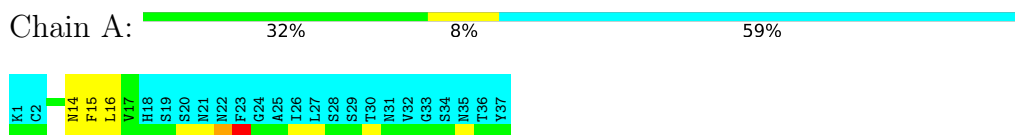
### 4.2.7 Score per residue for model 7

- Molecule 1: Islet amyloid polypeptide



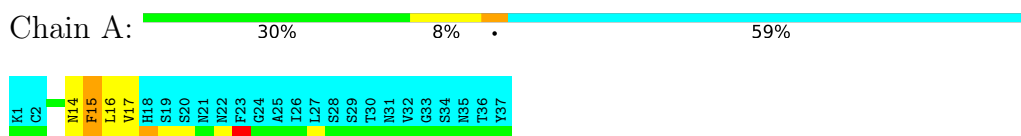
#### 4.2.8 Score per residue for model 8

- Molecule 1: Islet amyloid polypeptide



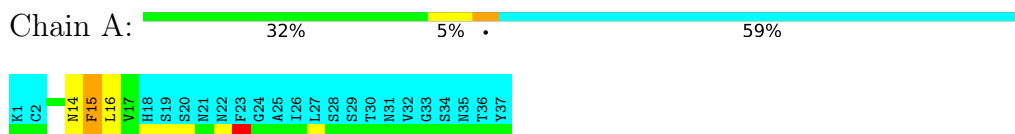
#### 4.2.9 Score per residue for model 9

- Molecule 1: Islet amyloid polypeptide



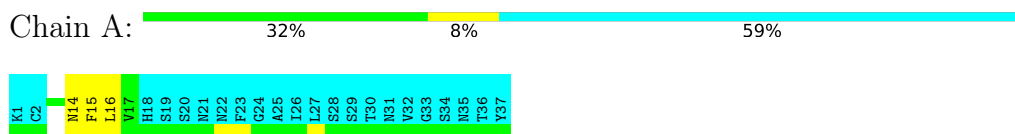
#### 4.2.10 Score per residue for model 10

- Molecule 1: Islet amyloid polypeptide



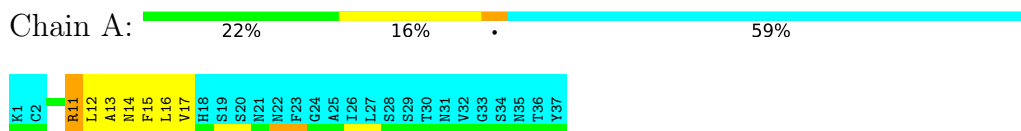
#### 4.2.11 Score per residue for model 11

- Molecule 1: Islet amyloid polypeptide



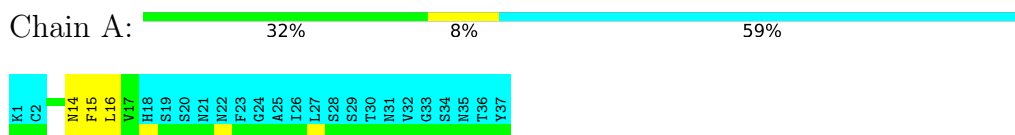
#### 4.2.12 Score per residue for model 12

- Molecule 1: Islet amyloid polypeptide



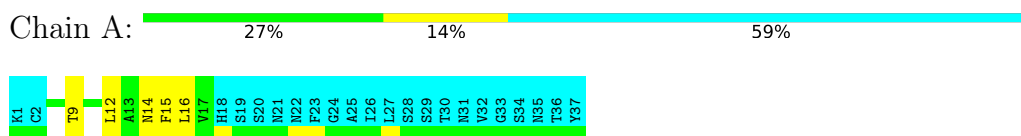
#### 4.2.13 Score per residue for model 13

- Molecule 1: Islet amyloid polypeptide



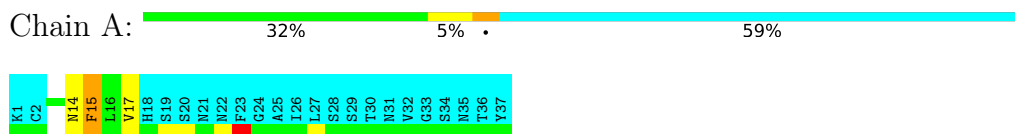
#### 4.2.14 Score per residue for model 14

- Molecule 1: Islet amyloid polypeptide



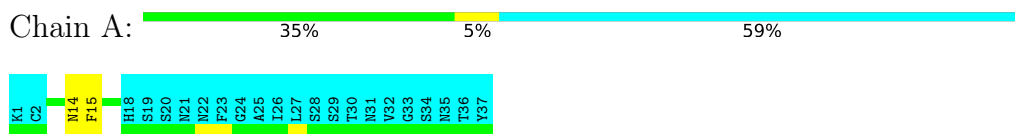
#### 4.2.15 Score per residue for model 15

- Molecule 1: Islet amyloid polypeptide



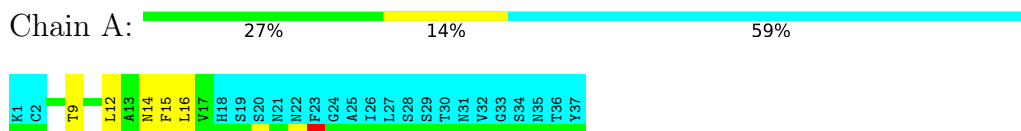
#### 4.2.16 Score per residue for model 16

- Molecule 1: Islet amyloid polypeptide



#### 4.2.17 Score per residue for model 17

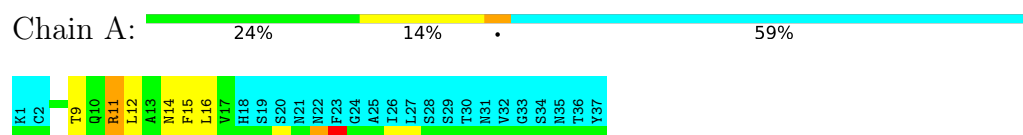
- Molecule 1: Islet amyloid polypeptide





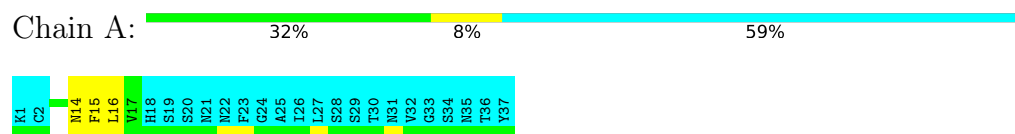
#### 4.2.18 Score per residue for model 18

- Molecule 1: Islet amyloid polypeptide



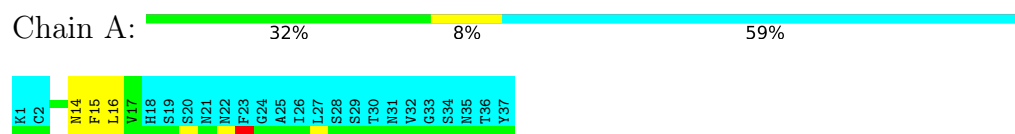
#### 4.2.19 Score per residue for model 19

- Molecule 1: Islet amyloid polypeptide



#### 4.2.20 Score per residue for model 20

- Molecule 1: Islet amyloid polypeptide



## 5 Refinement protocol and experimental data overview

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

Of the 200 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
CNS	refinement	
CYANA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	336
Number of shifts mapped to atoms	336
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

## 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: TYC

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	112	113	113	1±1
All	All	2240	2260	2260	12

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ALA:O	1:A:17:VAL:HB	0.52	2.03	4	3
1:A:9:THR:O	1:A:12:LEU:HB2	0.45	2.12	5	6
1:A:11:ARG:HD3	1:A:12:LEU:N	0.42	2.29	12	2
1:A:8:ALA:O	1:A:12:LEU:HG	0.41	2.16	7	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	15/37 (41%)	13±1 (89±4%)	2±1 (11±4%)	0±0 (0±1%)	44	80
All	All	300/740 (41%)	266 (89%)	33 (11%)	1 (0%)	44	80

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	17	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	12/30 (40%)	9±0 (75±4%)	3±0 (25±4%)	2	25
All	All	240/600 (40%)	180 (75%)	60 (25%)	2	25

All 4 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	14	ASN	20
1	A	15	PHE	20
1	A	16	LEU	18
1	A	11	ARG	2

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	TYC	A	37	1	13,13,13	0.46±0.03	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	TYC	A	37	1	17,17,17	0.33±0.07	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TYC	A	37	1	-	0±0,8,8,8	0±0,1,1,1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 76% for the well-defined parts and 73% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 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	336
Number of shifts mapped to atoms	336
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	22	—	None (insufficient data)
$^{13}\text{C}_\beta$	22	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	35	$-0.83 \pm 0.28$	Should be applied

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 76%, i.e. 152 atoms were assigned a chemical shift out of a possible 199. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	58/75 (77%)	30/30 (100%)	13/30 (43%)	15/15 (100%)
Sidechain	90/114 (79%)	69/75 (92%)	17/33 (52%)	4/6 (67%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	4/10 (40%)	4/5 (80%)	0/5 (0%)	0/0 (—%)
Overall	152/199 (76%)	103/110 (94%)	30/68 (44%)	19/21 (90%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 323 atoms were assigned a chemical shift out of a possible 441. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	130/182 (71%)	73/74 (99%)	22/72 (31%)	35/36 (97%)
Sidechain	183/231 (79%)	145/151 (96%)	32/69 (46%)	6/11 (55%)
Aromatic	10/28 (36%)	10/14 (71%)	0/12 (0%)	0/2 (0%)
Overall	323/441 (73%)	228/239 (95%)	54/153 (35%)	41/49 (84%)

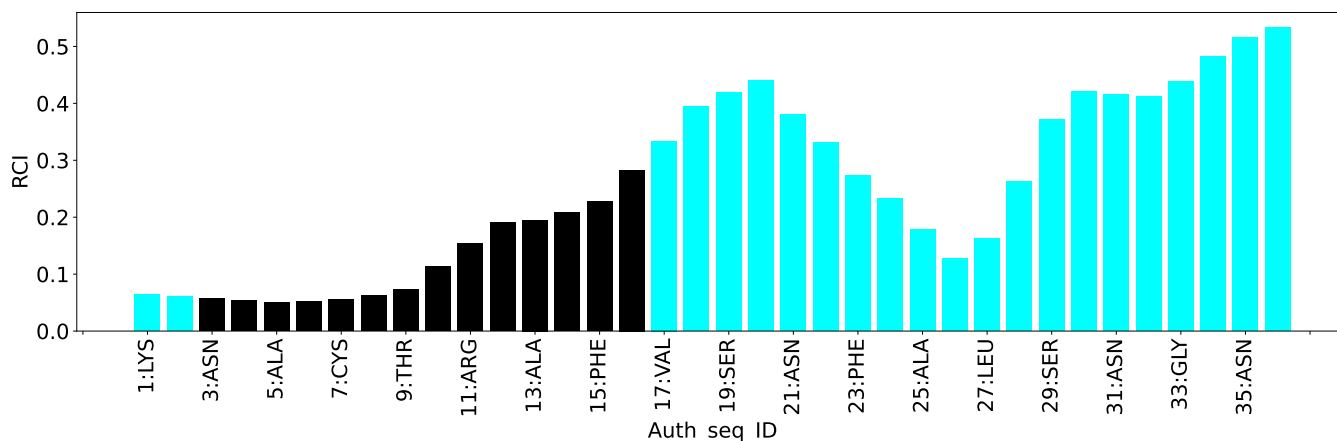
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:





## 8 NMR restraints analysis [i](#)

### 8.1 Conformationally restricting restraints [i](#)

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	542
Intra-residue ( $ i-j =0$ )	136
Sequential ( $ i-j =1$ )	218
Medium range ( $ i-j >1$ and $ i-j <5$ )	184
Long range ( $ i-j \geq 5$ )	4
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	20
Number of unmapped restraints	0
Number of restraints per residue	15.2
Number of long range restraints per residue <sup>1</sup>	0.1

<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 [i](#)

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 [i](#)

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)	12.8	0.2
0.2-0.5 (Medium)	2.2	0.29
>0.5 (Large)	None	None

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	3.2	3.0
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

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

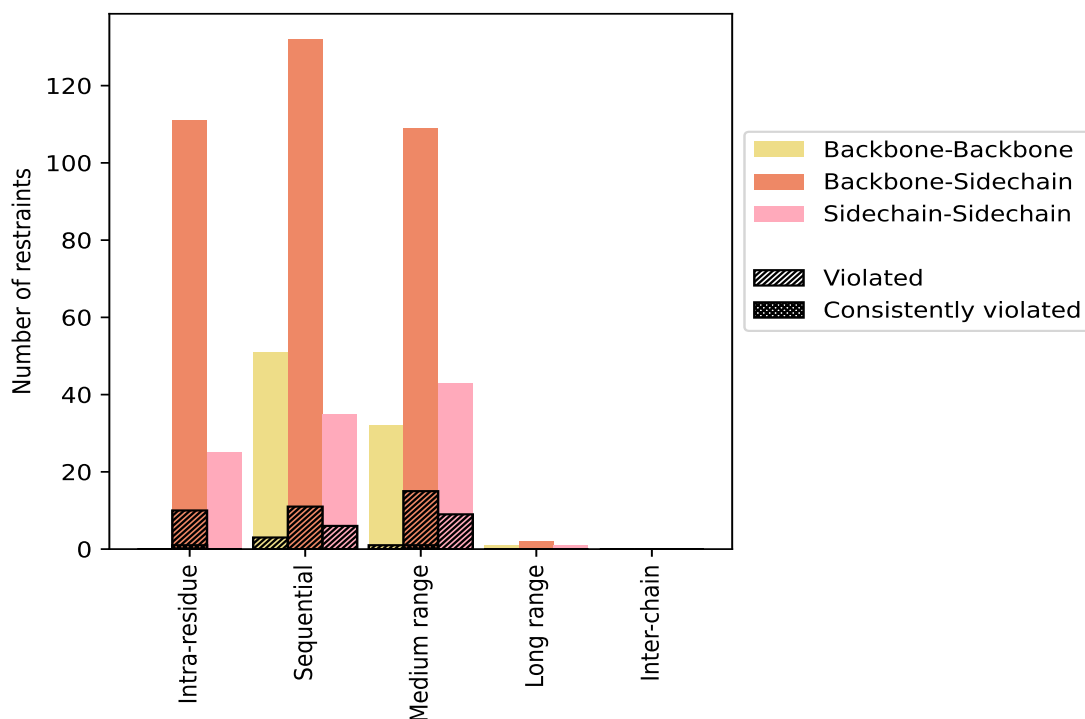
### 9.1 Summary of distance violations [i](#)

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>136</b>	<b>25.1</b>	<b>10</b>	<b>7.4</b>	<b>1.8</b>	<b>1</b>	<b>0.7</b>	<b>0.2</b>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	111	20.5	10	9.0	1.8	1	0.9	0.2
Sidechain-Sidechain	25	4.6	0	0.0	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>218</b>	<b>40.2</b>	<b>20</b>	<b>9.2</b>	<b>3.7</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	51	9.4	3	5.9	0.6	0	0.0	0.0
Backbone-Sidechain	132	24.4	11	8.3	2.0	0	0.0	0.0
Sidechain-Sidechain	35	6.5	6	17.1	1.1	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>184</b>	<b>33.9</b>	<b>25</b>	<b>13.6</b>	<b>4.6</b>	<b>1</b>	<b>0.5</b>	<b>0.2</b>
Backbone-Backbone	32	5.9	1	3.1	0.2	0	0.0	0.0
Backbone-Sidechain	109	20.1	15	13.8	2.8	1	0.9	0.2
Sidechain-Sidechain	43	7.9	9	20.9	1.7	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>4</b>	<b>0.7</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	1	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	0.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	1	0.2	0	0.0	0.0	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>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>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>542</b>	<b>100.0</b>	<b>55</b>	<b>10.1</b>	<b>10.1</b>	<b>2</b>	<b>0.4</b>	<b>0.4</b>
Backbone-Backbone	84	15.5	4	4.8	0.7	0	0.0	0.0
Backbone-Sidechain	354	65.3	36	10.2	6.6	2	0.6	0.4
Sidechain-Sidechain	104	19.2	15	14.4	2.8	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	4	7	7	0	0	18	0.16	0.26	0.05	0.16
2	3	3	8	0	0	14	0.14	0.23	0.03	0.14
3	2	2	7	0	0	11	0.16	0.22	0.04	0.15
4	2	4	6	0	0	12	0.15	0.26	0.04	0.15
5	4	8	4	0	0	16	0.16	0.24	0.04	0.16
6	3	7	8	0	0	18	0.15	0.24	0.04	0.15
7	3	4	5	0	0	12	0.17	0.25	0.04	0.17
8	4	4	6	0	0	14	0.17	0.23	0.04	0.18
9	4	9	6	0	0	19	0.16	0.26	0.05	0.14
10	5	7	4	0	0	16	0.16	0.21	0.03	0.16
11	3	2	7	0	0	12	0.15	0.23	0.04	0.15

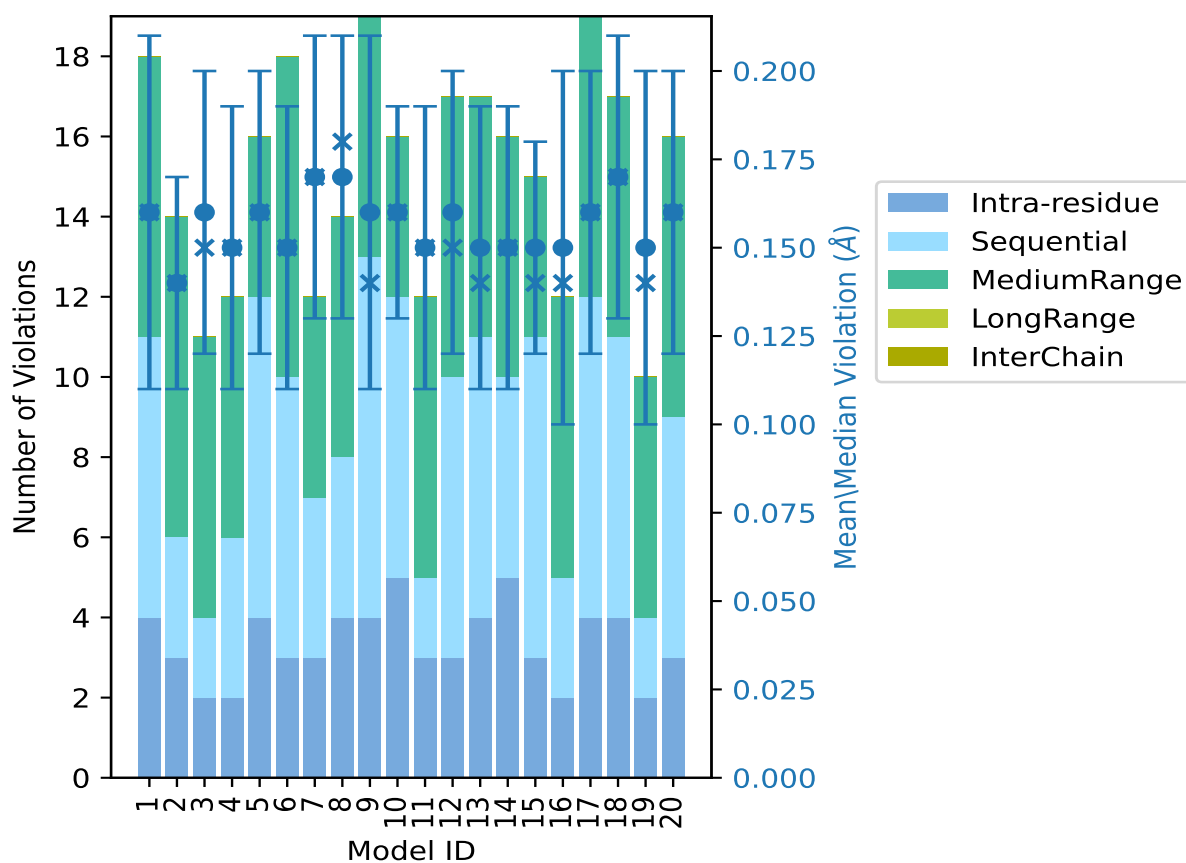
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>					
12	3	7	7	0	0	17	0.16	0.23	0.04	0.15
13	4	7	6	0	0	17	0.15	0.23	0.04	0.14
14	5	5	6	0	0	16	0.15	0.28	0.04	0.15
15	3	8	4	0	0	15	0.15	0.22	0.03	0.14
16	2	3	7	0	0	12	0.15	0.29	0.05	0.14
17	4	8	7	0	0	19	0.16	0.26	0.04	0.16
18	4	7	6	0	0	17	0.17	0.23	0.04	0.17
19	2	2	6	0	0	10	0.15	0.27	0.05	0.14
20	3	6	7	0	0	16	0.16	0.22	0.04	0.16

<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

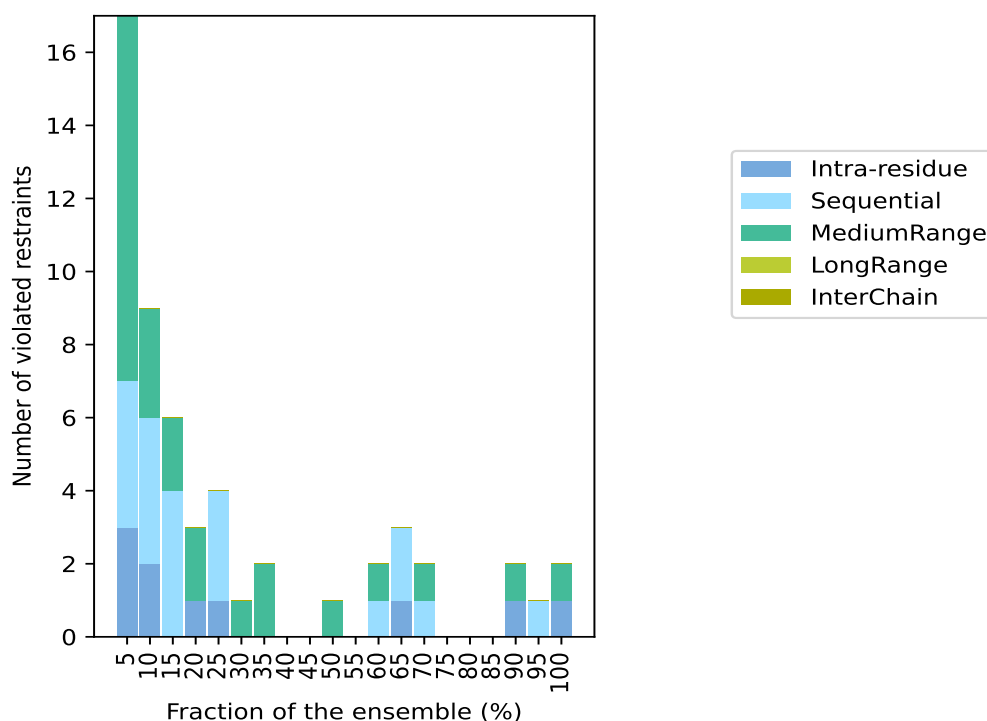
### 9.3 Distance violation statistics for the ensemble

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, 487(IR:126, SQ:198, MR:159, LR:4, 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>	%
3	4	10	0	0	17	1	5.0
2	4	3	0	0	9	2	10.0
0	4	2	0	0	6	3	15.0
1	0	2	0	0	3	4	20.0
1	3	0	0	0	4	5	25.0
0	0	1	0	0	1	6	30.0
0	0	2	0	0	2	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	1	0	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	1	1	0	0	2	12	60.0
1	2	0	0	0	3	13	65.0
0	1	1	0	0	2	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
1	0	1	0	0	2	18	90.0
0	1	0	0	0	1	19	95.0
1	0	1	0	0	2	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

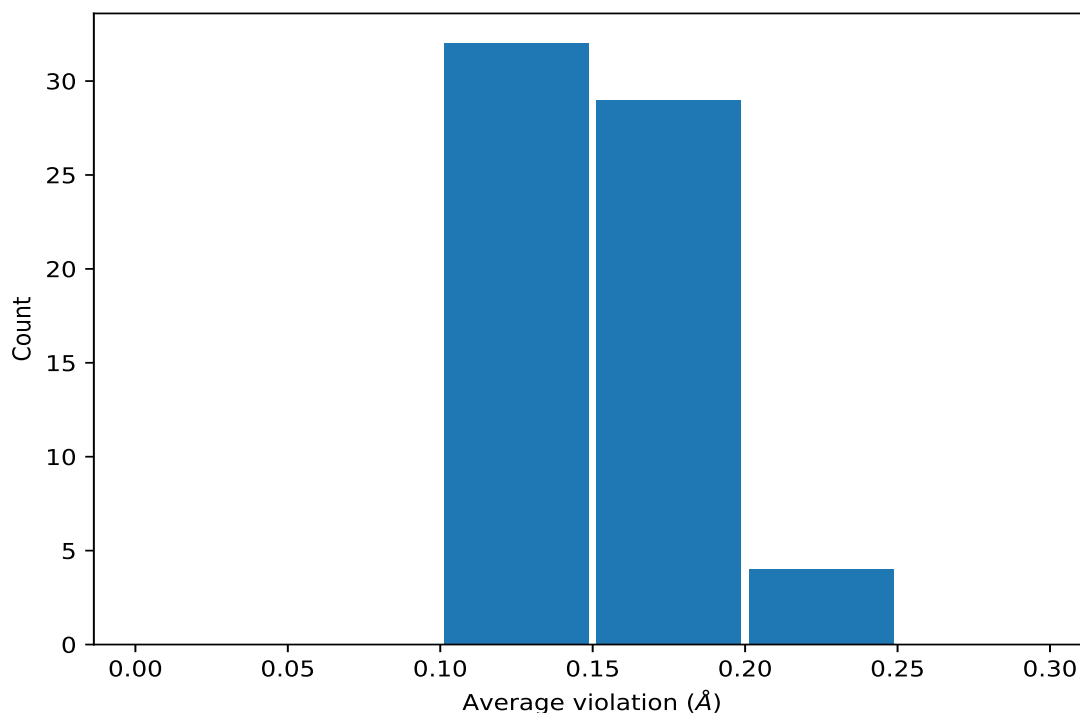
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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)
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	20	0.2	0.01	0.2
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	20	0.14	0.02	0.14
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	19	0.24	0.03	0.23
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	18	0.14	0.01	0.14
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	18	0.14	0.02	0.14
(1,72)	1:A:20:SER:H	1:A:23:PHE:HB3	14	0.16	0.04	0.16
(1,42)	1:A:25:ALA:HA	1:A:26:ILE:H	14	0.12	0.01	0.12
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD1	13	0.19	0.04	0.19
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD2	13	0.19	0.04	0.19
(1,231)	1:A:22:ASN:H	1:A:23:PHE:HB2	13	0.19	0.03	0.2
(1,197)	1:A:22:ASN:H	1:A:22:ASN:HD22	13	0.15	0.03	0.13
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD11	12	0.16	0.03	0.16
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD12	12	0.16	0.03	0.16
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD13	12	0.16	0.03	0.16
(1,31)	1:A:25:ALA:H	1:A:26:ILE:HA	12	0.13	0.02	0.12
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE1	10	0.18	0.03	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE2	10	0.18	0.03	0.18
(1,458)	1:A:17:VAL:HG11	1:A:19:SER:HA	7	0.16	0.02	0.17
(1,458)	1:A:17:VAL:HG12	1:A:19:SER:HA	7	0.16	0.02	0.17
(1,458)	1:A:17:VAL:HG13	1:A:19:SER:HA	7	0.16	0.02	0.17
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB1	7	0.14	0.02	0.15
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB2	7	0.14	0.02	0.15
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB3	7	0.14	0.02	0.15
(1,194)	1:A:21:ASN:H	1:A:23:PHE:HB3	6	0.15	0.02	0.15
(1,67)	1:A:18:HIS:H	1:A:18:HIS:HB2	5	0.16	0.02	0.16
(1,70)	1:A:17:VAL:H	1:A:18:HIS:HB2	5	0.13	0.02	0.12
(1,66)	1:A:23:PHE:HB3	1:A:24:GLY:H	5	0.13	0.01	0.12
(1,96)	1:A:20:SER:H	1:A:21:ASN:HB2	5	0.12	0.0	0.12
(1,520)	1:A:31:ASN:HA	1:A:31:ASN:HD22	4	0.18	0.02	0.18
(1,463)	1:A:19:SER:HB3	1:A:23:PHE:HE1	4	0.16	0.02	0.15
(1,463)	1:A:19:SER:HB3	1:A:23:PHE:HE2	4	0.16	0.02	0.15
(1,243)	1:A:18:HIS:HD2	1:A:20:SER:H	4	0.12	0.0	0.12
(1,422)	1:A:27:LEU:HB3	1:A:28:SER:HA	3	0.2	0.05	0.22
(1,48)	1:A:36:THR:HA	1:A:37:TYC:H	3	0.17	0.06	0.13
(1,187)	1:A:31:ASN:H	1:A:32:VAL:HB	3	0.15	0.03	0.16
(1,56)	1:A:28:SER:HB3	1:A:29:SER:H	3	0.14	0.02	0.15
(1,59)	1:A:24:GLY:HA3	1:A:27:LEU:H	3	0.12	0.01	0.11
(1,176)	1:A:26:ILE:HG21	1:A:28:SER:H	3	0.11	0.0	0.11
(1,176)	1:A:26:ILE:HG22	1:A:28:SER:H	3	0.11	0.0	0.11
(1,176)	1:A:26:ILE:HG23	1:A:28:SER:H	3	0.11	0.0	0.11
(1,215)	1:A:21:ASN:H	1:A:21:ASN:HD22	2	0.22	0.02	0.22
(1,126)	1:A:27:LEU:H	1:A:27:LEU:HB2	2	0.17	0.01	0.17
(1,438)	1:A:22:ASN:HB2	1:A:25:ALA:HB1	2	0.16	0.02	0.16
(1,438)	1:A:22:ASN:HB2	1:A:25:ALA:HB2	2	0.16	0.02	0.16
(1,438)	1:A:22:ASN:HB2	1:A:25:ALA:HB3	2	0.16	0.02	0.16
(1,190)	1:A:35:ASN:H	1:A:36:THR:HG21	2	0.16	0.02	0.16
(1,190)	1:A:35:ASN:H	1:A:36:THR:HG22	2	0.16	0.02	0.16
(1,190)	1:A:35:ASN:H	1:A:36:THR:HG23	2	0.16	0.02	0.16
(1,394)	1:A:11:ARG:HD2	1:A:14:ASN:HD21	2	0.15	0.0	0.15
(1,394)	1:A:11:ARG:HD3	1:A:14:ASN:HD21	2	0.15	0.0	0.15
(1,500)	1:A:17:VAL:HG21	1:A:18:HIS:HB3	2	0.13	0.02	0.13
(1,500)	1:A:17:VAL:HG22	1:A:18:HIS:HB3	2	0.13	0.02	0.13
(1,500)	1:A:17:VAL:HG23	1:A:18:HIS:HB3	2	0.13	0.02	0.13
(1,345)	1:A:24:GLY:HA2	1:A:25:ALA:HB1	2	0.12	0.0	0.12
(1,345)	1:A:24:GLY:HA2	1:A:25:ALA:HB2	2	0.12	0.0	0.12
(1,345)	1:A:24:GLY:HA2	1:A:25:ALA:HB3	2	0.12	0.0	0.12
(1,444)	1:A:6:THR:HG21	1:A:7:CYS:HB3	2	0.12	0.0	0.12
(1,444)	1:A:6:THR:HG22	1:A:7:CYS:HB3	2	0.12	0.0	0.12

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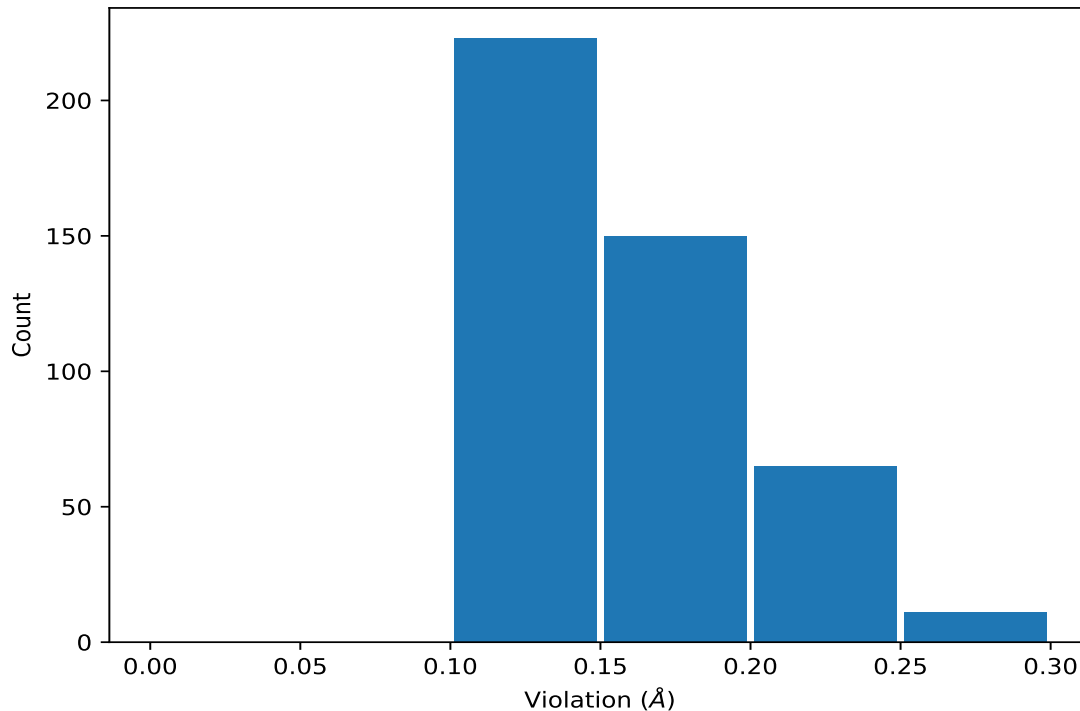
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,444)	1:A:6:THR:HG23	1:A:7:CYS:HB3	2	0.12	0.0	0.12
(1,350)	1:A:14:ASN:HB2	1:A:17:VAL:HG21	2	0.11	0.0	0.11
(1,350)	1:A:14:ASN:HB2	1:A:17:VAL:HG22	2	0.11	0.0	0.11
(1,350)	1:A:14:ASN:HB2	1:A:17:VAL:HG23	2	0.11	0.0	0.11
(1,350)	1:A:14:ASN:HB3	1:A:17:VAL:HG21	2	0.11	0.0	0.11
(1,350)	1:A:14:ASN:HB3	1:A:17:VAL:HG22	2	0.11	0.0	0.11
(1,350)	1:A:14:ASN:HB3	1:A:17:VAL:HG23	2	0.11	0.0	0.11

<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)
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	16	0.29
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	14	0.28
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	19	0.27
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD1	1	0.26
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD2	1	0.26
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	4	0.26
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	9	0.26
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	17	0.26
(1,48)	1:A:36:THR:HA	1:A:37:TYC:H	9	0.25
(1,215)	1:A:21:ASN:H	1:A:21:ASN:HD22	7	0.25
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	7	0.25
(1,72)	1:A:20:SER:H	1:A:23:PHE:HB3	6	0.24
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE1	9	0.24
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE2	9	0.24
(1,422)	1:A:27:LEU:HB3	1:A:28:SER:HA	17	0.24
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD1	5	0.24
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD2	5	0.24
(1,72)	1:A:20:SER:H	1:A:23:PHE:HB3	1	0.23
(1,72)	1:A:20:SER:H	1:A:23:PHE:HB3	12	0.23
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD1	8	0.23
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD2	8	0.23
(1,231)	1:A:22:ASN:H	1:A:23:PHE:HB2	6	0.23
(1,231)	1:A:22:ASN:H	1:A:23:PHE:HB2	18	0.23
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	18	0.23
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	2	0.23
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	5	0.23
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	8	0.23
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	11	0.23
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	13	0.23
(1,422)	1:A:27:LEU:HB3	1:A:28:SER:HA	1	0.22
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD1	13	0.22
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD2	13	0.22
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD1	15	0.22
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD2	15	0.22
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	3	0.22
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	20	0.22
(1,197)	1:A:22:ASN:H	1:A:22:ASN:HD22	20	0.22
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	12	0.22
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	18	0.22
(1,520)	1:A:31:ASN:HA	1:A:31:ASN:HD22	10	0.21
(1,231)	1:A:22:ASN:H	1:A:23:PHE:HB2	12	0.21
(1,231)	1:A:22:ASN:H	1:A:23:PHE:HB2	17	0.21
(1,231)	1:A:22:ASN:H	1:A:23:PHE:HB2	20	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	1	0.21
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	9	0.21
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	16	0.21
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	17	0.21
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	1	0.21
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	3	0.21
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	10	0.21
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE1	8	0.2
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE2	8	0.2
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE1	20	0.2
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE2	20	0.2
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD11	3	0.2
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD12	3	0.2
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD13	3	0.2
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD11	8	0.2
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD12	8	0.2
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD13	8	0.2
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD11	13	0.2
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD12	13	0.2
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD13	13	0.2
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD1	10	0.2
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD2	10	0.2
(1,231)	1:A:22:ASN:H	1:A:23:PHE:HB2	1	0.2
(1,231)	1:A:22:ASN:H	1:A:23:PHE:HB2	8	0.2
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	2	0.2
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	4	0.2
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	6	0.2
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	10	0.2
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	11	0.2
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	12	0.2
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	13	0.2
(1,215)	1:A:21:ASN:H	1:A:21:ASN:HD22	8	0.2
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	20	0.2
(1,463)	1:A:19:SER:HB3	1:A:23:PHE:HE1	6	0.19
(1,463)	1:A:19:SER:HB3	1:A:23:PHE:HE2	6	0.19
(1,458)	1:A:17:VAL:HG11	1:A:19:SER:HA	3	0.19
(1,458)	1:A:17:VAL:HG12	1:A:19:SER:HA	3	0.19
(1,458)	1:A:17:VAL:HG13	1:A:19:SER:HA	3	0.19
(1,438)	1:A:22:ASN:HB2	1:A:25:ALA:HB1	7	0.19
(1,438)	1:A:22:ASN:HB2	1:A:25:ALA:HB2	7	0.19
(1,438)	1:A:22:ASN:HB2	1:A:25:ALA:HB3	7	0.19
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD1	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD2	9	0.19
(1,231)	1:A:22:ASN:H	1:A:23:PHE:HB2	5	0.19
(1,231)	1:A:22:ASN:H	1:A:23:PHE:HB2	15	0.19
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	7	0.19
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	8	0.19
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	14	0.19
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	15	0.19
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	19	0.19
(1,197)	1:A:22:ASN:H	1:A:22:ASN:HD22	18	0.19
(1,194)	1:A:21:ASN:H	1:A:23:PHE:HB3	7	0.19
(1,187)	1:A:31:ASN:H	1:A:32:VAL:HB	15	0.19
(1,175)	1:A:22:ASN:H	1:A:26:ILE:HG21	14	0.19
(1,175)	1:A:22:ASN:H	1:A:26:ILE:HG22	14	0.19
(1,175)	1:A:22:ASN:H	1:A:26:ILE:HG23	14	0.19
(1,67)	1:A:18:HIS:H	1:A:18:HIS:HB2	10	0.18
(1,67)	1:A:18:HIS:H	1:A:18:HIS:HB2	13	0.18
(1,520)	1:A:31:ASN:HA	1:A:31:ASN:HD22	11	0.18
(1,520)	1:A:31:ASN:HA	1:A:31:ASN:HD22	18	0.18
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE1	1	0.18
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE2	1	0.18
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE1	17	0.18
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE2	17	0.18
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE1	18	0.18
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE2	18	0.18
(1,458)	1:A:17:VAL:HG11	1:A:19:SER:HA	12	0.18
(1,458)	1:A:17:VAL:HG12	1:A:19:SER:HA	12	0.18
(1,458)	1:A:17:VAL:HG13	1:A:19:SER:HA	12	0.18
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD11	5	0.18
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD12	5	0.18
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD13	5	0.18
(1,31)	1:A:25:ALA:H	1:A:26:ILE:HA	17	0.18
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD1	12	0.18
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD2	12	0.18
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD1	17	0.18
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD2	17	0.18
(1,231)	1:A:22:ASN:H	1:A:23:PHE:HB2	9	0.18
(1,218)	1:A:7:CYS:HB2	1:A:9:THR:H	5	0.18
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	7	0.18
(1,129)	1:A:15:PHE:H	1:A:16:LEU:HB2	6	0.18
(1,126)	1:A:27:LEU:H	1:A:27:LEU:HB2	17	0.18
(1,72)	1:A:20:SER:H	1:A:23:PHE:HB3	9	0.17
(1,72)	1:A:20:SER:H	1:A:23:PHE:HB3	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:A:20:SER:H	1:A:23:PHE:HB3	18	0.17
(1,72)	1:A:20:SER:H	1:A:23:PHE:HB3	20	0.17
(1,70)	1:A:17:VAL:H	1:A:18:HIS:HB2	6	0.17
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE1	15	0.17
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE2	15	0.17
(1,458)	1:A:17:VAL:HG11	1:A:19:SER:HA	6	0.17
(1,458)	1:A:17:VAL:HG12	1:A:19:SER:HA	6	0.17
(1,458)	1:A:17:VAL:HG13	1:A:19:SER:HA	6	0.17
(1,458)	1:A:17:VAL:HG11	1:A:19:SER:HA	18	0.17
(1,458)	1:A:17:VAL:HG12	1:A:19:SER:HA	18	0.17
(1,458)	1:A:17:VAL:HG13	1:A:19:SER:HA	18	0.17
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD11	9	0.17
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD12	9	0.17
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD13	9	0.17
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD11	19	0.17
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD12	19	0.17
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD13	19	0.17
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD1	18	0.17
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD2	18	0.17
(1,197)	1:A:22:ASN:H	1:A:22:ASN:HD22	5	0.17
(1,197)	1:A:22:ASN:H	1:A:22:ASN:HD22	17	0.17
(1,190)	1:A:35:ASN:H	1:A:36:THR:HG21	9	0.17
(1,190)	1:A:35:ASN:H	1:A:36:THR:HG22	9	0.17
(1,190)	1:A:35:ASN:H	1:A:36:THR:HG23	9	0.17
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	4	0.17
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB1	4	0.17
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB2	4	0.17
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB3	4	0.17
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB1	11	0.17
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB2	11	0.17
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB3	11	0.17
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	5	0.17
(1,72)	1:A:20:SER:H	1:A:23:PHE:HB3	10	0.16
(1,72)	1:A:20:SER:H	1:A:23:PHE:HB3	17	0.16
(1,67)	1:A:18:HIS:H	1:A:18:HIS:HB2	5	0.16
(1,67)	1:A:18:HIS:H	1:A:18:HIS:HB2	14	0.16
(1,56)	1:A:28:SER:HB3	1:A:29:SER:H	5	0.16
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD11	20	0.16
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD12	20	0.16
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD13	20	0.16
(1,31)	1:A:25:ALA:H	1:A:26:ILE:HA	14	0.16
(1,31)	1:A:25:ALA:H	1:A:26:ILE:HA	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD1	20	0.16
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD2	20	0.16
(1,231)	1:A:22:ASN:H	1:A:23:PHE:HB2	10	0.16
(1,231)	1:A:22:ASN:H	1:A:23:PHE:HB2	14	0.16
(1,197)	1:A:22:ASN:H	1:A:22:ASN:HD22	1	0.16
(1,194)	1:A:21:ASN:H	1:A:23:PHE:HB3	16	0.16
(1,187)	1:A:31:ASN:H	1:A:32:VAL:HB	7	0.16
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	8	0.16
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	10	0.16
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	12	0.16
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	16	0.16
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB1	2	0.16
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB2	2	0.16
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB3	2	0.16
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	13	0.16
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	18	0.16
(1,126)	1:A:27:LEU:H	1:A:27:LEU:HB2	1	0.16
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	5	0.16
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	14	0.16
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	17	0.16
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	19	0.16
(1,56)	1:A:28:SER:HB3	1:A:29:SER:H	13	0.15
(1,500)	1:A:17:VAL:HG21	1:A:18:HIS:HB3	15	0.15
(1,500)	1:A:17:VAL:HG22	1:A:18:HIS:HB3	15	0.15
(1,500)	1:A:17:VAL:HG23	1:A:18:HIS:HB3	15	0.15
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE1	10	0.15
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE2	10	0.15
(1,463)	1:A:19:SER:HB3	1:A:23:PHE:HE1	12	0.15
(1,463)	1:A:19:SER:HB3	1:A:23:PHE:HE2	12	0.15
(1,462)	1:A:19:SER:HB2	1:A:23:PHE:HE1	14	0.15
(1,462)	1:A:19:SER:HB2	1:A:23:PHE:HE2	14	0.15
(1,458)	1:A:17:VAL:HG11	1:A:19:SER:HA	2	0.15
(1,458)	1:A:17:VAL:HG12	1:A:19:SER:HA	2	0.15
(1,458)	1:A:17:VAL:HG13	1:A:19:SER:HA	2	0.15
(1,394)	1:A:11:ARG:HD2	1:A:14:ASN:HD21	12	0.15
(1,394)	1:A:11:ARG:HD3	1:A:14:ASN:HD21	12	0.15
(1,394)	1:A:11:ARG:HD2	1:A:14:ASN:HD21	18	0.15
(1,394)	1:A:11:ARG:HD3	1:A:14:ASN:HD21	18	0.15
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD1	6	0.15
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD2	6	0.15
(1,197)	1:A:22:ASN:H	1:A:22:ASN:HD22	8	0.15
(1,194)	1:A:21:ASN:H	1:A:23:PHE:HB3	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:A:21:ASN:H	1:A:23:PHE:HB3	3	0.15
(1,194)	1:A:21:ASN:H	1:A:23:PHE:HB3	11	0.15
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	1	0.15
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	6	0.15
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	18	0.15
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB1	7	0.15
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB2	7	0.15
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB3	7	0.15
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	4	0.15
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	8	0.15
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	16	0.15
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	17	0.15
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	3	0.15
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	4	0.15
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	11	0.15
(1,72)	1:A:20:SER:H	1:A:23:PHE:HB3	13	0.14
(1,66)	1:A:23:PHE:HB3	1:A:24:GLY:H	9	0.14
(1,66)	1:A:23:PHE:HB3	1:A:24:GLY:H	20	0.14
(1,59)	1:A:24:GLY:HA3	1:A:27:LEU:H	16	0.14
(1,520)	1:A:31:ASN:HA	1:A:31:ASN:HD22	1	0.14
(1,476)	1:A:30:THR:HG21	1:A:31:ASN:HD21	15	0.14
(1,476)	1:A:30:THR:HG22	1:A:31:ASN:HD21	15	0.14
(1,476)	1:A:30:THR:HG23	1:A:31:ASN:HD21	15	0.14
(1,463)	1:A:19:SER:HB3	1:A:23:PHE:HE1	1	0.14
(1,463)	1:A:19:SER:HB3	1:A:23:PHE:HE2	1	0.14
(1,463)	1:A:19:SER:HB3	1:A:23:PHE:HE1	9	0.14
(1,463)	1:A:19:SER:HB3	1:A:23:PHE:HE2	9	0.14
(1,438)	1:A:22:ASN:HB2	1:A:25:ALA:HB1	4	0.14
(1,438)	1:A:22:ASN:HB2	1:A:25:ALA:HB2	4	0.14
(1,438)	1:A:22:ASN:HB2	1:A:25:ALA:HB3	4	0.14
(1,42)	1:A:25:ALA:HA	1:A:26:ILE:H	8	0.14
(1,373)	1:A:15:PHE:HE1	1:A:16:LEU:HB2	15	0.14
(1,373)	1:A:15:PHE:HE2	1:A:16:LEU:HB2	15	0.14
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD11	2	0.14
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD12	2	0.14
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD13	2	0.14
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD11	14	0.14
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD12	14	0.14
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD13	14	0.14
(1,31)	1:A:25:ALA:H	1:A:26:ILE:HA	5	0.14
(1,31)	1:A:25:ALA:H	1:A:26:ILE:HA	11	0.14
(1,231)	1:A:22:ASN:H	1:A:23:PHE:HB2	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:A:35:ASN:H	1:A:36:THR:HG21	18	0.14
(1,190)	1:A:35:ASN:H	1:A:36:THR:HG22	18	0.14
(1,190)	1:A:35:ASN:H	1:A:36:THR:HG23	18	0.14
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	2	0.14
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	5	0.14
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	13	0.14
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	15	0.14
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	20	0.14
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	3	0.14
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	7	0.14
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	9	0.14
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	10	0.14
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	12	0.14
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	14	0.14
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	19	0.14
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	20	0.14
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	6	0.14
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	7	0.14
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	8	0.14
(1,121)	1:A:9:THR:H	1:A:11:ARG:HB2	12	0.14
(1,121)	1:A:9:THR:H	1:A:11:ARG:HB3	12	0.14
(1,70)	1:A:17:VAL:H	1:A:18:HIS:HB2	10	0.13
(1,67)	1:A:18:HIS:H	1:A:18:HIS:HB2	9	0.13
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE1	6	0.13
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE2	6	0.13
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE1	12	0.13
(1,490)	1:A:19:SER:HA	1:A:23:PHE:HE2	12	0.13
(1,48)	1:A:36:THR:HA	1:A:37:TYC:H	5	0.13
(1,458)	1:A:17:VAL:HG11	1:A:19:SER:HA	8	0.13
(1,458)	1:A:17:VAL:HG12	1:A:19:SER:HA	8	0.13
(1,458)	1:A:17:VAL:HG13	1:A:19:SER:HA	8	0.13
(1,458)	1:A:17:VAL:HG11	1:A:19:SER:HA	16	0.13
(1,458)	1:A:17:VAL:HG12	1:A:19:SER:HA	16	0.13
(1,458)	1:A:17:VAL:HG13	1:A:19:SER:HA	16	0.13
(1,422)	1:A:27:LEU:HB3	1:A:28:SER:HA	4	0.13
(1,42)	1:A:25:ALA:HA	1:A:26:ILE:H	12	0.13
(1,42)	1:A:25:ALA:HA	1:A:26:ILE:H	13	0.13
(1,372)	1:A:15:PHE:HE1	1:A:16:LEU:HB3	15	0.13
(1,372)	1:A:15:PHE:HE2	1:A:16:LEU:HB3	15	0.13
(1,31)	1:A:25:ALA:H	1:A:26:ILE:HA	13	0.13
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD1	14	0.13
(1,276)	1:A:22:ASN:HB3	1:A:23:PHE:HD2	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	1:A:22:ASN:H	1:A:22:ASN:HD22	6	0.13
(1,197)	1:A:22:ASN:H	1:A:22:ASN:HD22	9	0.13
(1,197)	1:A:22:ASN:H	1:A:22:ASN:HD22	10	0.13
(1,197)	1:A:22:ASN:H	1:A:22:ASN:HD22	12	0.13
(1,169)	1:A:26:ILE:HG21	1:A:29:SER:H	13	0.13
(1,169)	1:A:26:ILE:HG22	1:A:29:SER:H	13	0.13
(1,169)	1:A:26:ILE:HG23	1:A:29:SER:H	13	0.13
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	3	0.13
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	9	0.13
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	17	0.13
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	19	0.13
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB1	20	0.13
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB2	20	0.13
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB3	20	0.13
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	2	0.13
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	6	0.13
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	2	0.13
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	13	0.13
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	16	0.13
(1,96)	1:A:20:SER:H	1:A:21:ASN:HB2	1	0.12
(1,96)	1:A:20:SER:H	1:A:21:ASN:HB2	12	0.12
(1,96)	1:A:20:SER:H	1:A:21:ASN:HB2	17	0.12
(1,72)	1:A:20:SER:H	1:A:23:PHE:HB3	4	0.12
(1,72)	1:A:20:SER:H	1:A:23:PHE:HB3	5	0.12
(1,72)	1:A:20:SER:H	1:A:23:PHE:HB3	14	0.12
(1,70)	1:A:17:VAL:H	1:A:18:HIS:HB2	13	0.12
(1,66)	1:A:23:PHE:HB3	1:A:24:GLY:H	17	0.12
(1,66)	1:A:23:PHE:HB3	1:A:24:GLY:H	18	0.12
(1,48)	1:A:36:THR:HA	1:A:37:TYC:H	18	0.12
(1,444)	1:A:6:THR:HG21	1:A:7:CYS:HB3	4	0.12
(1,444)	1:A:6:THR:HG22	1:A:7:CYS:HB3	4	0.12
(1,444)	1:A:6:THR:HG23	1:A:7:CYS:HB3	4	0.12
(1,42)	1:A:25:ALA:HA	1:A:26:ILE:H	3	0.12
(1,42)	1:A:25:ALA:HA	1:A:26:ILE:H	4	0.12
(1,42)	1:A:25:ALA:HA	1:A:26:ILE:H	6	0.12
(1,42)	1:A:25:ALA:HA	1:A:26:ILE:H	7	0.12
(1,42)	1:A:25:ALA:HA	1:A:26:ILE:H	10	0.12
(1,42)	1:A:25:ALA:HA	1:A:26:ILE:H	16	0.12
(1,345)	1:A:24:GLY:HA2	1:A:25:ALA:HB1	14	0.12
(1,345)	1:A:24:GLY:HA2	1:A:25:ALA:HB2	14	0.12
(1,345)	1:A:24:GLY:HA2	1:A:25:ALA:HB3	14	0.12
(1,345)	1:A:24:GLY:HA2	1:A:25:ALA:HB1	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,345)	1:A:24:GLY:HA2	1:A:25:ALA:HB2	17	0.12
(1,345)	1:A:24:GLY:HA2	1:A:25:ALA:HB3	17	0.12
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD11	16	0.12
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD12	16	0.12
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD13	16	0.12
(1,31)	1:A:25:ALA:H	1:A:26:ILE:HA	1	0.12
(1,31)	1:A:25:ALA:H	1:A:26:ILE:HA	9	0.12
(1,31)	1:A:25:ALA:H	1:A:26:ILE:HA	10	0.12
(1,300)	1:A:17:VAL:HG11	1:A:19:SER:HB2	1	0.12
(1,300)	1:A:17:VAL:HG12	1:A:19:SER:HB2	1	0.12
(1,300)	1:A:17:VAL:HG13	1:A:19:SER:HB2	1	0.12
(1,269)	1:A:3:ASN:H	1:A:7:CYS:HB2	3	0.12
(1,255)	1:A:23:PHE:HA	1:A:23:PHE:HD1	14	0.12
(1,255)	1:A:23:PHE:HA	1:A:23:PHE:HD2	14	0.12
(1,243)	1:A:18:HIS:HD2	1:A:20:SER:H	17	0.12
(1,243)	1:A:18:HIS:HD2	1:A:20:SER:H	19	0.12
(1,197)	1:A:22:ASN:H	1:A:22:ASN:HD22	15	0.12
(1,176)	1:A:26:ILE:HG21	1:A:28:SER:H	16	0.12
(1,176)	1:A:26:ILE:HG22	1:A:28:SER:H	16	0.12
(1,176)	1:A:26:ILE:HG23	1:A:28:SER:H	16	0.12
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	11	0.12
(1,154)	1:A:26:ILE:H	1:A:26:ILE:HG12	14	0.12
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	1	0.12
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	10	0.12
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	15	0.12
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	18	0.12
(1,96)	1:A:20:SER:H	1:A:21:ASN:HB2	6	0.11
(1,96)	1:A:20:SER:H	1:A:21:ASN:HB2	20	0.11
(1,72)	1:A:20:SER:H	1:A:23:PHE:HB3	8	0.11
(1,70)	1:A:17:VAL:H	1:A:18:HIS:HB2	5	0.11
(1,70)	1:A:17:VAL:H	1:A:18:HIS:HB2	9	0.11
(1,66)	1:A:23:PHE:HB3	1:A:24:GLY:H	10	0.11
(1,59)	1:A:24:GLY:HA3	1:A:27:LEU:H	1	0.11
(1,59)	1:A:24:GLY:HA3	1:A:27:LEU:H	17	0.11
(1,56)	1:A:28:SER:HB3	1:A:29:SER:H	12	0.11
(1,54)	1:A:29:SER:HB2	1:A:31:ASN:H	2	0.11
(1,500)	1:A:17:VAL:HG21	1:A:18:HIS:HB3	12	0.11
(1,500)	1:A:17:VAL:HG22	1:A:18:HIS:HB3	12	0.11
(1,500)	1:A:17:VAL:HG23	1:A:18:HIS:HB3	12	0.11
(1,456)	1:A:30:THR:H	1:A:30:THR:HB	15	0.11
(1,444)	1:A:6:THR:HG21	1:A:7:CYS:HB3	2	0.11
(1,444)	1:A:6:THR:HG22	1:A:7:CYS:HB3	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,444)	1:A:6:THR:HG23	1:A:7:CYS:HB3	2	0.11
(1,429)	1:A:23:PHE:H	1:A:23:PHE:HE1	2	0.11
(1,429)	1:A:23:PHE:H	1:A:23:PHE:HE2	2	0.11
(1,42)	1:A:25:ALA:HA	1:A:26:ILE:H	2	0.11
(1,42)	1:A:25:ALA:HA	1:A:26:ILE:H	5	0.11
(1,42)	1:A:25:ALA:HA	1:A:26:ILE:H	9	0.11
(1,42)	1:A:25:ALA:HA	1:A:26:ILE:H	15	0.11
(1,42)	1:A:25:ALA:HA	1:A:26:ILE:H	18	0.11
(1,418)	1:A:8:ALA:HB1	1:A:11:ARG:HD2	3	0.11
(1,418)	1:A:8:ALA:HB1	1:A:11:ARG:HD3	3	0.11
(1,418)	1:A:8:ALA:HB2	1:A:11:ARG:HD2	3	0.11
(1,418)	1:A:8:ALA:HB2	1:A:11:ARG:HD3	3	0.11
(1,418)	1:A:8:ALA:HB3	1:A:11:ARG:HD2	3	0.11
(1,418)	1:A:8:ALA:HB3	1:A:11:ARG:HD3	3	0.11
(1,360)	1:A:30:THR:HG21	1:A:32:VAL:HG21	13	0.11
(1,360)	1:A:30:THR:HG21	1:A:32:VAL:HG22	13	0.11
(1,360)	1:A:30:THR:HG21	1:A:32:VAL:HG23	13	0.11
(1,360)	1:A:30:THR:HG22	1:A:32:VAL:HG21	13	0.11
(1,360)	1:A:30:THR:HG22	1:A:32:VAL:HG22	13	0.11
(1,360)	1:A:30:THR:HG22	1:A:32:VAL:HG23	13	0.11
(1,360)	1:A:30:THR:HG23	1:A:32:VAL:HG21	13	0.11
(1,360)	1:A:30:THR:HG23	1:A:32:VAL:HG22	13	0.11
(1,360)	1:A:30:THR:HG23	1:A:32:VAL:HG23	13	0.11
(1,350)	1:A:14:ASN:HB2	1:A:17:VAL:HG21	9	0.11
(1,350)	1:A:14:ASN:HB2	1:A:17:VAL:HG22	9	0.11
(1,350)	1:A:14:ASN:HB2	1:A:17:VAL:HG23	9	0.11
(1,350)	1:A:14:ASN:HB3	1:A:17:VAL:HG21	9	0.11
(1,350)	1:A:14:ASN:HB3	1:A:17:VAL:HG22	9	0.11
(1,350)	1:A:14:ASN:HB3	1:A:17:VAL:HG23	9	0.11
(1,350)	1:A:14:ASN:HB2	1:A:17:VAL:HG21	11	0.11
(1,350)	1:A:14:ASN:HB2	1:A:17:VAL:HG22	11	0.11
(1,350)	1:A:14:ASN:HB2	1:A:17:VAL:HG23	11	0.11
(1,350)	1:A:14:ASN:HB3	1:A:17:VAL:HG21	11	0.11
(1,350)	1:A:14:ASN:HB3	1:A:17:VAL:HG22	11	0.11
(1,350)	1:A:14:ASN:HB3	1:A:17:VAL:HG23	11	0.11
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD11	6	0.11
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD12	6	0.11
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD13	6	0.11
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD11	11	0.11
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD12	11	0.11
(1,344)	1:A:24:GLY:HA3	1:A:27:LEU:HD13	11	0.11
(1,31)	1:A:25:ALA:H	1:A:26:ILE:HA	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:A:25:ALA:H	1:A:26:ILE:HA	16	0.11
(1,31)	1:A:25:ALA:H	1:A:26:ILE:HA	19	0.11
(1,297)	1:A:29:SER:HA	1:A:30:THR:HG21	7	0.11
(1,297)	1:A:29:SER:HA	1:A:30:THR:HG22	7	0.11
(1,297)	1:A:29:SER:HA	1:A:30:THR:HG23	7	0.11
(1,284)	1:A:32:VAL:HG21	1:A:34:SER:H	4	0.11
(1,284)	1:A:32:VAL:HG22	1:A:34:SER:H	4	0.11
(1,284)	1:A:32:VAL:HG23	1:A:34:SER:H	4	0.11
(1,243)	1:A:18:HIS:HD2	1:A:20:SER:H	2	0.11
(1,243)	1:A:18:HIS:HD2	1:A:20:SER:H	20	0.11
(1,197)	1:A:22:ASN:H	1:A:22:ASN:HD22	13	0.11
(1,197)	1:A:22:ASN:H	1:A:22:ASN:HD22	14	0.11
(1,194)	1:A:21:ASN:H	1:A:23:PHE:HB3	19	0.11
(1,187)	1:A:31:ASN:H	1:A:32:VAL:HB	1	0.11
(1,176)	1:A:26:ILE:HG21	1:A:28:SER:H	6	0.11
(1,176)	1:A:26:ILE:HG22	1:A:28:SER:H	6	0.11
(1,176)	1:A:26:ILE:HG23	1:A:28:SER:H	6	0.11
(1,176)	1:A:26:ILE:HG21	1:A:28:SER:H	11	0.11
(1,176)	1:A:26:ILE:HG22	1:A:28:SER:H	11	0.11
(1,176)	1:A:26:ILE:HG23	1:A:28:SER:H	11	0.11
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB1	17	0.11
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB2	17	0.11
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB3	17	0.11
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB1	19	0.11
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB2	19	0.11
(1,145)	1:A:22:ASN:HD22	1:A:25:ALA:HB3	19	0.11
(1,130)	1:A:16:LEU:H	1:A:16:LEU:HB2	11	0.11
(1,124)	1:A:10:GLN:H	1:A:12:LEU:HB3	20	0.11

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

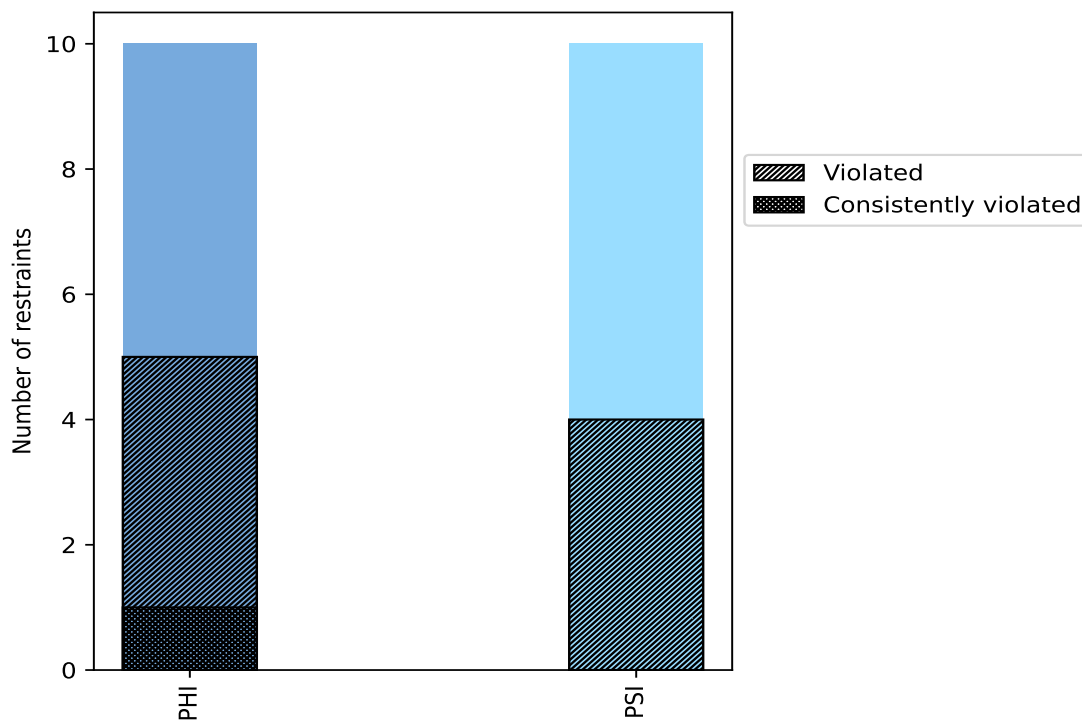
### 10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% <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>
PHI	10	50.0	5	50.0	25.0	1	10.0	5.0
PSI	10	50.0	4	40.0	20.0	0	0.0	0.0
Total	20	100.0	9	45.0	45.0	1	5.0	5.0

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

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



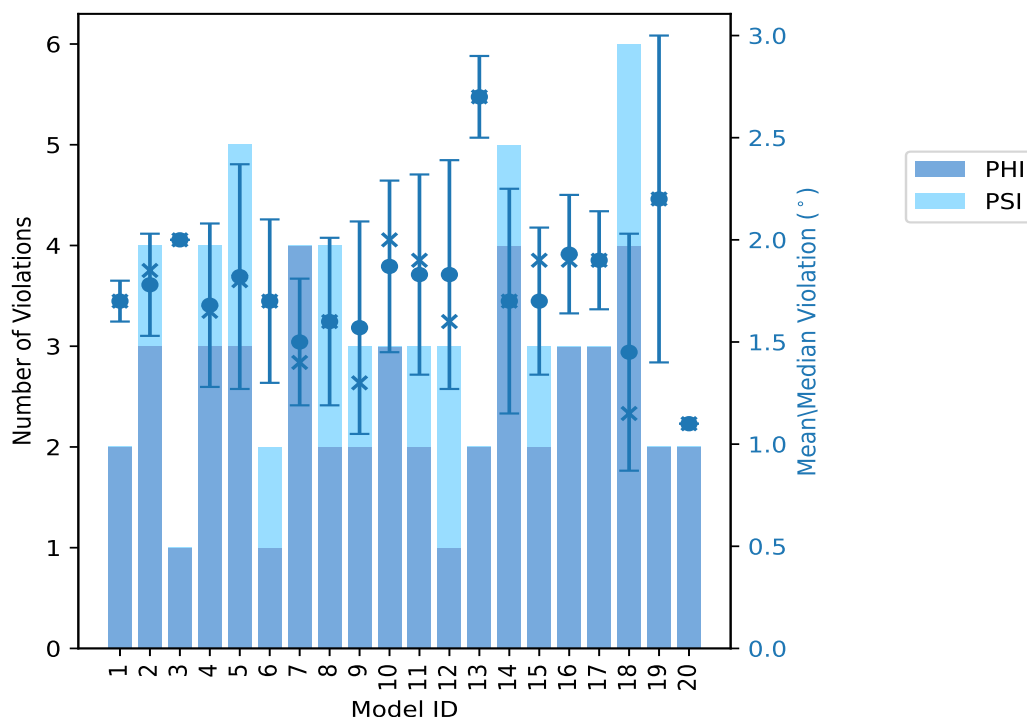
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model [i](#)

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	2	0	2	1.7	1.8	0.1	1.7
2	3	1	4	1.78	2.0	0.25	1.85
3	1	0	1	2.0	2.0	0.0	2.0
4	3	1	4	1.68	2.2	0.4	1.65
5	3	2	5	1.82	2.8	0.55	1.8
6	1	1	2	1.7	2.1	0.4	1.7
7	4	0	4	1.5	2.0	0.31	1.4
8	2	2	4	1.6	2.1	0.41	1.6
9	2	1	3	1.57	2.3	0.52	1.3
10	3	0	3	1.87	2.3	0.42	2.0
11	2	1	3	1.83	2.4	0.49	1.9
12	1	2	3	1.83	2.6	0.56	1.6
13	2	0	2	2.7	2.9	0.2	2.7
14	4	1	5	1.7	2.5	0.55	1.7
15	2	1	3	1.7	2.0	0.36	1.9
16	3	0	3	1.93	2.3	0.29	1.9
17	3	0	3	1.9	2.2	0.24	1.9
18	4	2	6	1.45	2.7	0.58	1.15
19	2	0	2	2.2	3.0	0.8	2.2
20	2	0	2	1.1	1.1	0.0	1.1

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



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

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

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

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

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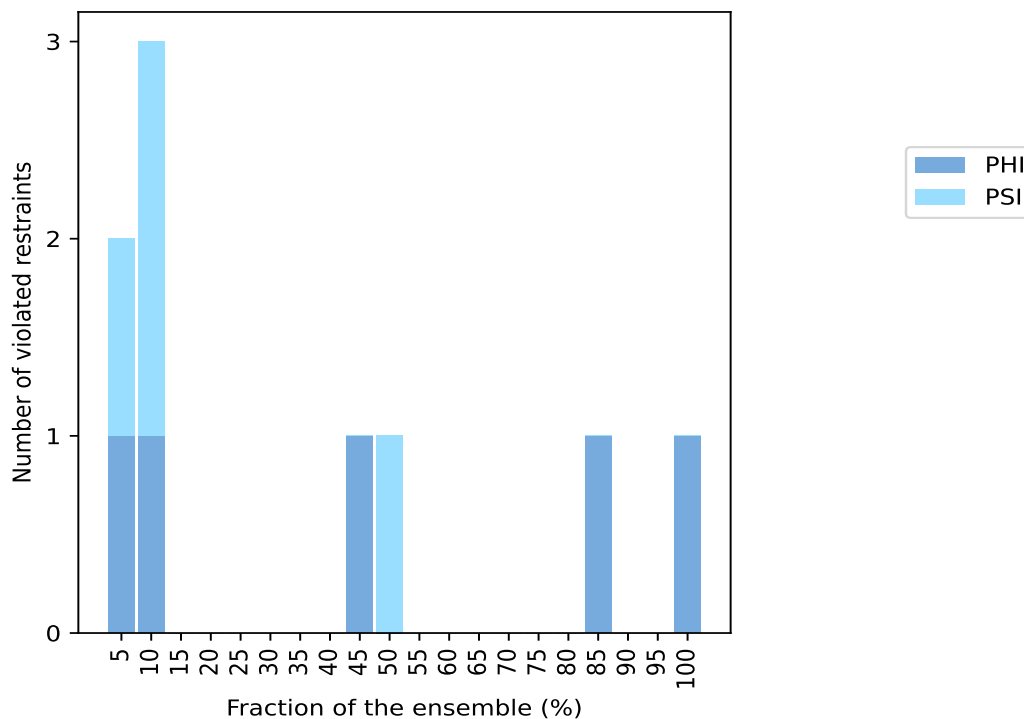


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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count <sup>1</sup>	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
1	0	1	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
1	0	1	20	100.0

<sup>1</sup> Number of models with violations

### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)

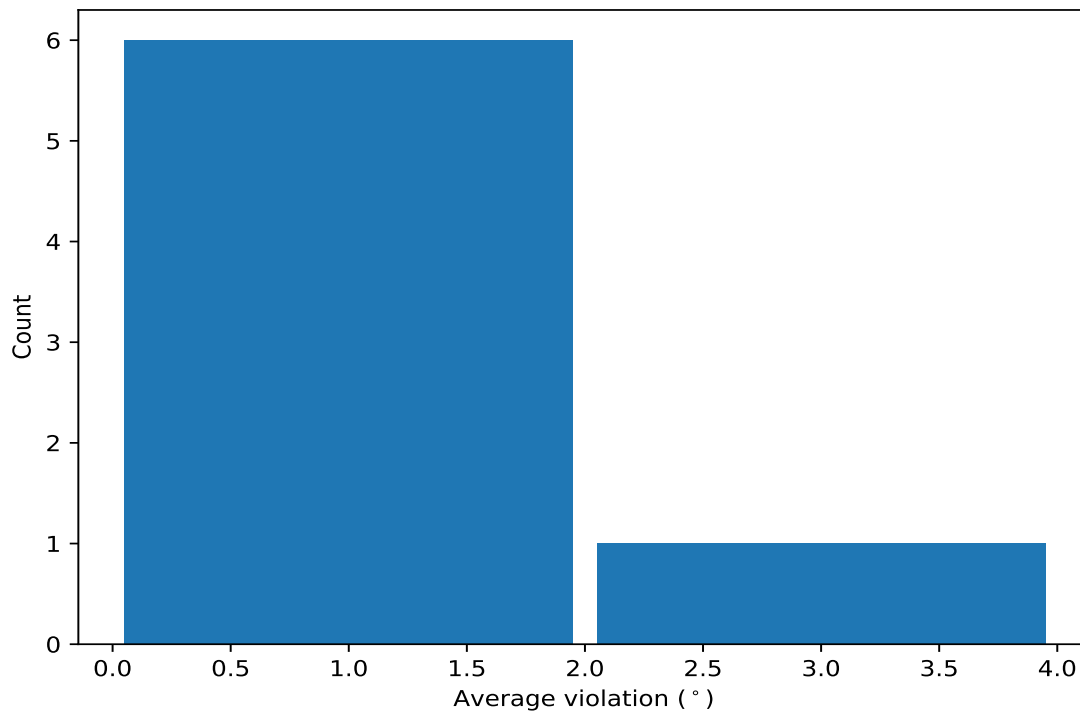


## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 10.4.1 Histogram : Distribution of mean dihedral-angle 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



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

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

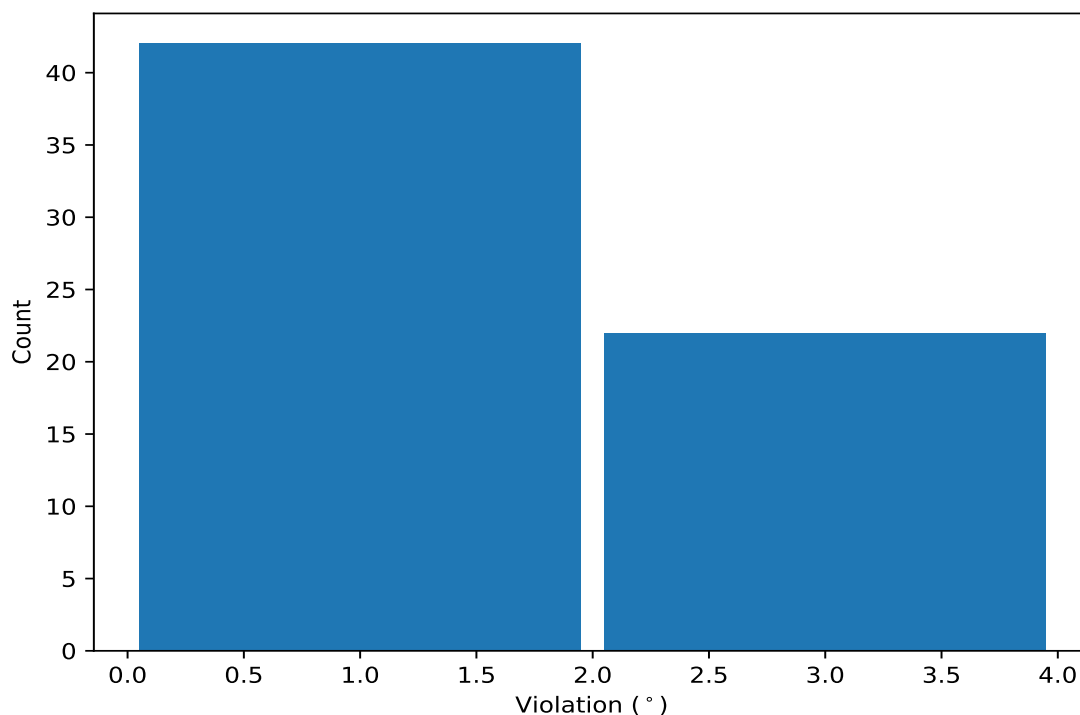
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	20	2.15	0.47	2.1
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	17	1.81	0.46	1.9
(1,6)	1:A:5:ALA:N	1:A:5:ALA:CA	1:A:5:ALA:C	1:A:6:THR:N	10	1.35	0.35	1.2
(1,11)	1:A:9:THR:C	1:A:10:GLN:N	1:A:10:GLN:CA	1:A:10:GLN:C	9	1.51	0.3	1.6
(1,14)	1:A:11:ARG:N	1:A:11:ARG:CA	1:A:11:ARG:C	1:A:12:LEU:N	2	1.55	0.05	1.55
(1,15)	1:A:11:ARG:C	1:A:12:LEU:N	1:A:12:LEU:CA	1:A:12:LEU:C	2	1.25	0.05	1.25
(1,20)	1:A:14:ASN:N	1:A:14:ASN:CA	1:A:14:ASN:C	1:A:15:PHE:N	2	1.25	0.05	1.25

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	19	3.0
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	13	2.9
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	5	2.8
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	18	2.7
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	12	2.6
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	13	2.5
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	14	2.5
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	11	2.4
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	10	2.3
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	9	2.3
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	16	2.3
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	17	2.2
(1,6)	1:A:5:ALA:N	1:A:5:ALA:CA	1:A:5:ALA:C	1:A:6:THR:N	4	2.2
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	6	2.1
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	8	2.1
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	14	2.1
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	2	2.0
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	3	2.0
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	7	2.0
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	2	2.0
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	10	2.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	15	2.0
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	4	1.9
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	15	1.9
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	16	1.9
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	8	1.9
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	11	1.9
(1,11)	1:A:9:THR:C	1:A:10:GLN:N	1:A:10:GLN:CA	1:A:10:GLN:C	5	1.9
(1,11)	1:A:9:THR:C	1:A:10:GLN:N	1:A:10:GLN:CA	1:A:10:GLN:C	17	1.9
(1,6)	1:A:5:ALA:N	1:A:5:ALA:CA	1:A:5:ALA:C	1:A:6:THR:N	5	1.8
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	1	1.8
(1,11)	1:A:9:THR:C	1:A:10:GLN:N	1:A:10:GLN:CA	1:A:10:GLN:C	2	1.7
(1,11)	1:A:9:THR:C	1:A:10:GLN:N	1:A:10:GLN:CA	1:A:10:GLN:C	14	1.7
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	1	1.6
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	17	1.6
(1,14)	1:A:11:ARG:N	1:A:11:ARG:CA	1:A:11:ARG:C	1:A:12:LEU:N	12	1.6
(1,11)	1:A:9:THR:C	1:A:10:GLN:N	1:A:10:GLN:CA	1:A:10:GLN:C	16	1.6
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	7	1.5
(1,14)	1:A:11:ARG:N	1:A:11:ARG:CA	1:A:11:ARG:C	1:A:12:LEU:N	18	1.5
(1,6)	1:A:5:ALA:N	1:A:5:ALA:CA	1:A:5:ALA:C	1:A:6:THR:N	2	1.4
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	4	1.4
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	5	1.4
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	19	1.4
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	9	1.3
(1,6)	1:A:5:ALA:N	1:A:5:ALA:CA	1:A:5:ALA:C	1:A:6:THR:N	6	1.3
(1,20)	1:A:14:ASN:N	1:A:14:ASN:CA	1:A:14:ASN:C	1:A:15:PHE:N	8	1.3
(1,15)	1:A:11:ARG:C	1:A:12:LEU:N	1:A:12:LEU:CA	1:A:12:LEU:C	7	1.3
(1,12)	1:A:10:GLN:N	1:A:10:GLN:CA	1:A:10:GLN:C	1:A:11:ARG:N	12	1.3
(1,11)	1:A:9:THR:C	1:A:10:GLN:N	1:A:10:GLN:CA	1:A:10:GLN:C	10	1.3
(1,6)	1:A:5:ALA:N	1:A:5:ALA:CA	1:A:5:ALA:C	1:A:6:THR:N	11	1.2
(1,6)	1:A:5:ALA:N	1:A:5:ALA:CA	1:A:5:ALA:C	1:A:6:THR:N	15	1.2
(1,20)	1:A:14:ASN:N	1:A:14:ASN:CA	1:A:14:ASN:C	1:A:15:PHE:N	5	1.2
(1,15)	1:A:11:ARG:C	1:A:12:LEU:N	1:A:12:LEU:CA	1:A:12:LEU:C	18	1.2
(1,11)	1:A:9:THR:C	1:A:10:GLN:N	1:A:10:GLN:CA	1:A:10:GLN:C	4	1.2
(1,11)	1:A:9:THR:C	1:A:10:GLN:N	1:A:10:GLN:CA	1:A:10:GLN:C	7	1.2
(1,9)	1:A:8:ALA:C	1:A:9:THR:N	1:A:9:THR:CA	1:A:9:THR:C	20	1.1
(1,6)	1:A:5:ALA:N	1:A:5:ALA:CA	1:A:5:ALA:C	1:A:6:THR:N	8	1.1
(1,6)	1:A:5:ALA:N	1:A:5:ALA:CA	1:A:5:ALA:C	1:A:6:THR:N	9	1.1
(1,6)	1:A:5:ALA:N	1:A:5:ALA:CA	1:A:5:ALA:C	1:A:6:THR:N	14	1.1
(1,6)	1:A:5:ALA:N	1:A:5:ALA:CA	1:A:5:ALA:C	1:A:6:THR:N	18	1.1
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	18	1.1
(1,3)	1:A:3:ASN:C	1:A:4:THR:N	1:A:4:THR:CA	1:A:4:THR:C	20	1.1
(1,11)	1:A:9:THR:C	1:A:10:GLN:N	1:A:10:GLN:CA	1:A:10:GLN:C	18	1.1
(1,1)	1:A:1:LYS:C	1:A:2:CYS:N	1:A:2:CYS:CA	1:A:2:CYS:C	14	1.1