



# wwPDB NMR Structure Validation Summary Report ⓘ

Jun 6, 2023 – 08:07 pm BST

PDB ID : 5AGQ  
BMRB ID : 26517  
Title : Solution structure of the TAM domain of human TIP5 BAZ2A involved in epigenetic regulation of rRNA genes  
Authors : Anosova, I.; Melnik, S.; Tripsianes, K.; Kateb, F.; Grummt, I.; Sattler, M.  
Deposited on : 2015-02-03

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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  
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

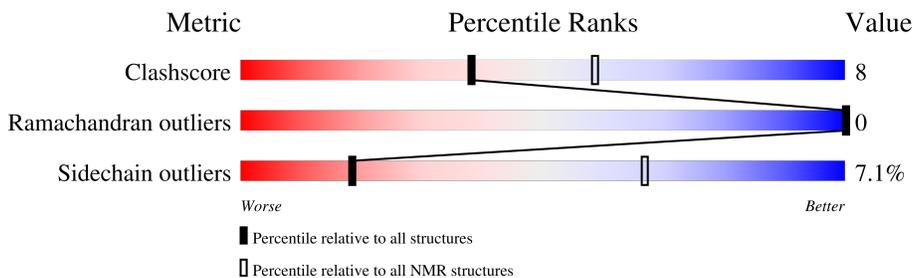
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 82%.

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	113	 68% 22% 6% .

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:520-A:621 (102)	0.28	16

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 4 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1829 atoms, of which 909 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BROMODOMAIN ADJACENT TO ZINC FINGER DOMAIN PROTEIN 2A.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	109	1829	581	909	178	158	3	0

There are 5 discrepancies between the modelled and reference sequences:

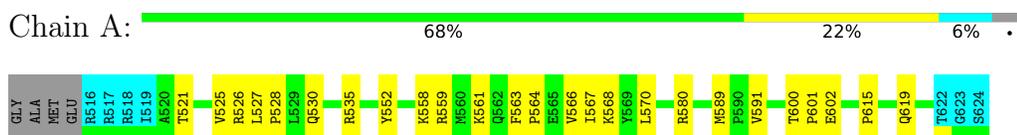
Chain	Residue	Modelled	Actual	Comment	Reference
A	512	GLY	-	expression tag	UNP Q9UIF9
A	513	ALA	-	expression tag	UNP Q9UIF9
A	514	MET	-	expression tag	UNP Q9UIF9
A	515	GLU	-	expression tag	UNP Q9UIF9
A	624	SER	-	cloning artifact	UNP Q9UIF9

## 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.

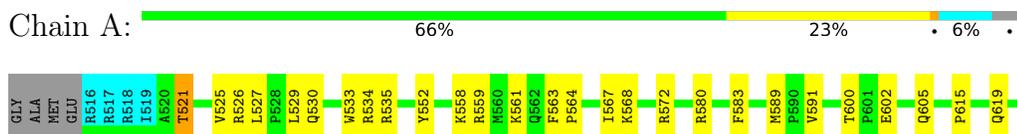
- Molecule 1: BROMODOMAIN ADJACENT TO ZINC FINGER DOMAIN PROTEIN 2A



### 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 16. Colouring as in section 4.1 above.

- Molecule 1: BROMODOMAIN ADJACENT TO ZINC FINGER DOMAIN PROTEIN 2A



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *ARIA2*, *CNS*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *BEST ENERGY*.

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

Software name	Classification	Version
CNS	refinement	
Sparky	structure solution	
CYANA	structure solution	3.0

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	1381
Number of shifts mapped to atoms	1381
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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	861	842	842	14±3
All	All	17220	16840	16840	274

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 8.

5 of 42 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:563:PHE:CE1	1:A:567:ILE:HD11	0.65	2.26	3	20
1:A:535:ARG:HG3	1:A:552:TYR:CZ	0.64	2.28	20	13
1:A:589:MET:HG3	1:A:591:VAL:HG23	0.63	1.68	17	16
1:A:535:ARG:HG3	1:A:552:TYR:CE1	0.59	2.33	9	13
1:A:525:VAL:HB	1:A:591:VAL:HG21	0.57	1.75	17	16

### 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	102/113 (90%)	97±2 (95±1%)	5±2 (5±1%)	0±0 (0±0%)	100	100
All	All	2040/2260 (90%)	1945 (95%)	95 (5%)	0 (0%)	100	100

There are no Ramachandran outliers.

### 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	92/100 (92%)	86±1 (93±1%)	6±1 (7±1%)	18	67
All	All	1840/2000 (92%)	1710 (93%)	130 (7%)	18	67

5 of 11 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	521	THR	20
1	A	527	LEU	20
1	A	558	LYS	20
1	A	580	ARG	20
1	A	561	LYS	19

### 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 82% for the well-defined parts and 80% 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	1381
Number of shifts mapped to atoms	1381
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	12

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. First 5 (of 0) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	519	ILE	HD12	0.831	0.026	1
1	A	519	ILE	HD13	0.831	0.026	1
1	A	519	ILE	HG22	0.895	0.026	1
1	A	519	ILE	HG23	0.895	0.026	1
1	A	520	ALA	HB2	1.295	0.02	1
1	A	520	ALA	HB3	1.295	0.02	1
1	A	521	THR	HG22	1.284	0.006	1
1	A	521	THR	HG23	1.284	0.006	1
1	A	525	VAL	HG12	0.819	0.001	2
1	A	525	VAL	HG13	0.819	0.001	2
1	A	525	VAL	HG22	0.804	0.019	2
1	A	525	VAL	HG23	0.804	0.019	2
1	A	527	LEU	HD12	0.672	0.005	2
1	A	527	LEU	HD13	0.672	0.005	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	527	LEU	HD22	0.442	0.008	2
1	A	527	LEU	HD23	0.442	0.008	2
1	A	529	LEU	HD12	0.873	0.004	1
1	A	529	LEU	HD13	0.873	0.004	1
1	A	529	LEU	HD22	0.873	0.004	1
1	A	529	LEU	HD23	0.873	0.004	1
1	A	537	VAL	HG12	0.509	0.005	2
1	A	537	VAL	HG13	0.509	0.005	2
1	A	537	VAL	HG22	0.312	0.02	2
1	A	537	VAL	HG23	0.312	0.02	2
1	A	539	ILE	HD12	0.827	0.011	1
1	A	539	ILE	HD13	0.827	0.011	1
1	A	539	ILE	HG22	1.049	0.003	1
1	A	539	ILE	HG23	1.049	0.003	1
1	A	550	THR	HG22	0.684	0.009	1
1	A	550	THR	HG23	0.684	0.009	1
1	A	560	MET	HE2	1.169	0.004	1
1	A	560	MET	HE3	1.169	0.004	1
1	A	566	VAL	HG12	-0.4	0.001	2
1	A	566	VAL	HG13	-0.4	0.001	2
1	A	566	VAL	HG22	0.77	0.02	2
1	A	566	VAL	HG23	0.77	0.02	2
1	A	567	ILE	HD12	0.473	0.008	1
1	A	567	ILE	HD13	0.473	0.008	1
1	A	567	ILE	HG22	0.77	0.001	1
1	A	567	ILE	HG23	0.77	0.001	1
1	A	570	LEU	HD12	0.589	0.01	2
1	A	570	LEU	HD13	0.589	0.01	2
1	A	570	LEU	HD22	0.95	0.004	2
1	A	570	LEU	HD23	0.95	0.004	2
1	A	574	VAL	HG12	0.836	0.02	2
1	A	574	VAL	HG13	0.836	0.02	2
1	A	574	VAL	HG22	0.837	0.02	2
1	A	574	VAL	HG23	0.837	0.02	2
1	A	575	VAL	HG12	1.043	0.02	2
1	A	575	VAL	HG13	1.043	0.02	2
1	A	575	VAL	HG22	1.031	0.003	2
1	A	575	VAL	HG23	1.031	0.003	2
1	A	578	VAL	HG12	0.549	0.003	2
1	A	578	VAL	HG13	0.549	0.003	2
1	A	578	VAL	HG22	0.655	0.001	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	578	VAL	HG23	0.655	0.001	2
1	A	589	MET	HE2	1.942	0.005	1
1	A	589	MET	HE3	1.942	0.005	1
1	A	591	VAL	HG12	0.771	0.007	2
1	A	591	VAL	HG13	0.771	0.007	2
1	A	591	VAL	HG22	0.768	0.002	2
1	A	591	VAL	HG23	0.768	0.002	2
1	A	600	THR	HG22	1.156	0.003	1
1	A	600	THR	HG23	1.156	0.003	1
1	A	604	LEU	HD12	0.649	0.02	2
1	A	604	LEU	HD13	0.649	0.02	2
1	A	604	LEU	HD22	0.574	0.013	2
1	A	604	LEU	HD23	0.574	0.013	2
1	A	607	VAL	HG12	0.976	0.002	2
1	A	607	VAL	HG13	0.976	0.002	2
1	A	607	VAL	HG22	0.924	0.002	2
1	A	607	VAL	HG23	0.924	0.002	2
1	A	609	LEU	HD12	0.692	0.002	2
1	A	609	LEU	HD13	0.692	0.002	2
1	A	609	LEU	HD22	0.645	0.013	2
1	A	609	LEU	HD23	0.645	0.013	2
1	A	611	ALA	HB2	1.375	0.001	1
1	A	611	ALA	HB3	1.375	0.001	1
1	A	614	ILE	HD12	0.518	0.003	1
1	A	614	ILE	HD13	0.518	0.003	1
1	A	614	ILE	HG22	-0.164	0.007	1
1	A	614	ILE	HG23	-0.164	0.007	1
1	A	618	ILE	HD12	0.52	0.003	1
1	A	618	ILE	HD13	0.52	0.003	1
1	A	618	ILE	HG22	0.816	0.008	1
1	A	618	ILE	HG23	0.816	0.008	1
1	A	620	ALA	HB2	1.124	0.02	1
1	A	620	ALA	HB3	1.124	0.02	1
1	A	621	ILE	HD12	0.693	0.006	1
1	A	621	ILE	HD13	0.693	0.006	1
1	A	621	ILE	HG22	0.84	0.013	1
1	A	621	ILE	HG23	0.84	0.013	1
1	A	622	THR	HG22	1.241	0.009	1
1	A	622	THR	HG23	1.241	0.009	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
$^{13}\text{C}_\alpha$	98	$-0.09 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	99	$-0.07 \pm 0.17$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	96	$-0.09 \pm 0.41$	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 82%, i.e. 1219 atoms were assigned a chemical shift out of a possible 1491. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	378/501 (75%)	198/203 (98%)	91/204 (45%)	89/94 (95%)
Sidechain	703/837 (84%)	477/537 (89%)	219/252 (87%)	7/48 (15%)
Aromatic	138/153 (90%)	69/77 (90%)	65/68 (96%)	4/8 (50%)
Overall	1219/1491 (82%)	744/817 (91%)	375/524 (72%)	100/150 (67%)

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

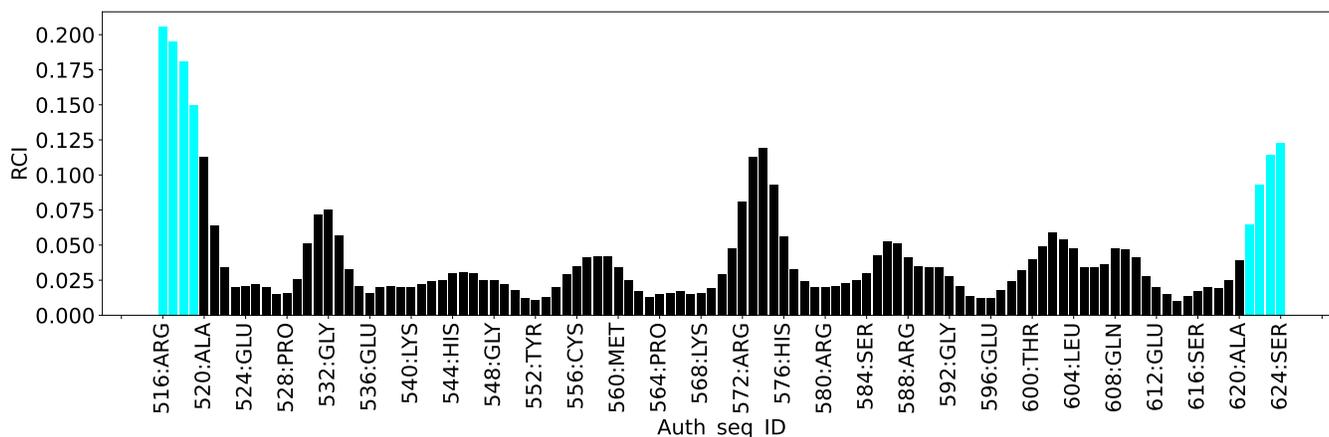
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	552	TYR	CD1	118.61	125.84 – 139.60	-10.2
1	A	552	TYR	CD2	118.61	125.28 – 140.14	-9.5
1	A	538	ARG	HD2	1.08	1.97 – 4.26	-8.9
1	A	538	ARG	HD3	0.97	1.81 – 4.39	-8.3
1	A	597	GLU	HG3	0.70	1.20 – 3.30	-7.4
1	A	537	VAL	HB	-0.14	0.43 – 3.54	-6.8
1	A	555	PRO	HD3	1.28	1.76 – 5.48	-6.3
1	A	561	LYS	HE3	1.71	1.92 – 3.89	-6.1
1	A	535	ARG	HG3	0.01	0.15 – 2.94	-5.5
1	A	597	GLU	HG2	1.15	1.24 – 3.30	-5.4
1	A	541	LYS	HB3	0.37	0.46 – 3.04	-5.4
1	A	538	ARG	HG2	0.18	0.26 – 2.87	-5.3

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2835
Intra-residue ( $ i-j =0$ )	662
Sequential ( $ i-j =1$ )	747
Medium range ( $ i-j >1$ and $ i-j <5$ )	501
Long range ( $ i-j \geq 5$ )	925
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	25.1
Number of long range restraints per residue <sup>1</sup>	8.2

<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)	51.5	0.2
0.2-0.5 (Medium)	66.3	0.5
>0.5 (Large)	111.2	2.9

### 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

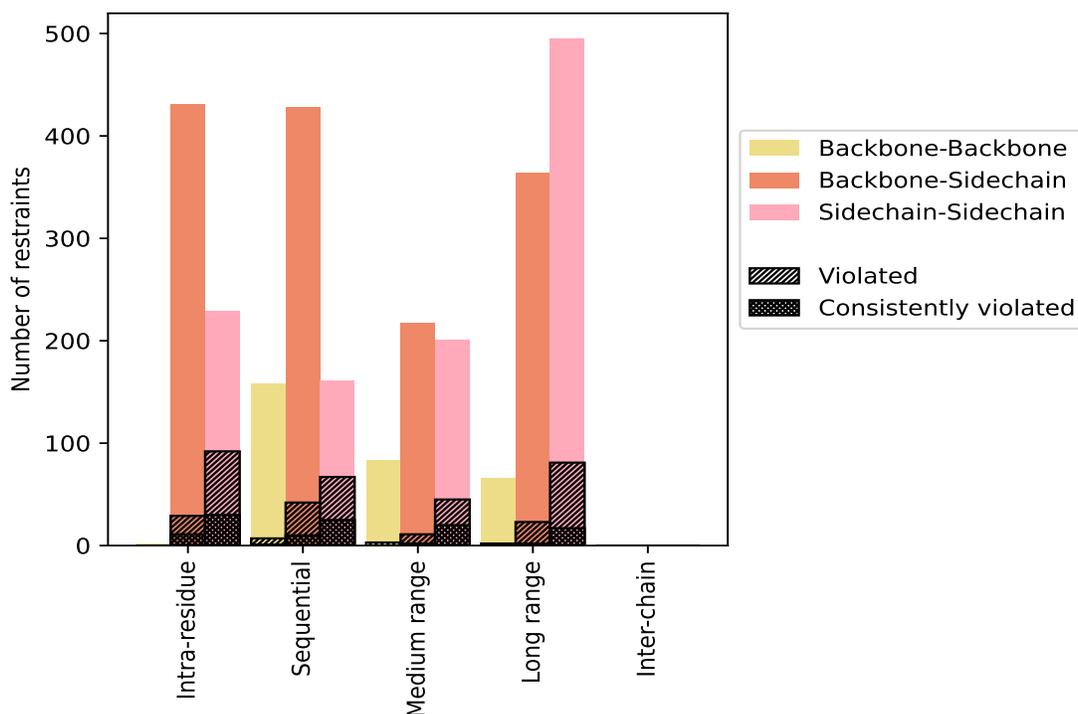
### 9.1 Summary of distance violations i

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>662</b>	<b>23.4</b>	<b>121</b>	<b>18.3</b>	<b>4.3</b>	<b>41</b>	<b>6.2</b>	<b>1.4</b>
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	431	15.2	29	6.7	1.0	11	2.6	0.4
Sidechain-Sidechain	229	8.1	92	40.2	3.2	30	13.1	1.1
<b>Sequential (<math> i-j =1</math>)</b>	<b>747</b>	<b>26.3</b>	<b>116</b>	<b>15.5</b>	<b>4.1</b>	<b>36</b>	<b>4.8</b>	<b>1.3</b>
Backbone-Backbone	158	5.6	7	4.4	0.2	1	0.6	0.0
Backbone-Sidechain	428	15.1	42	9.8	1.5	10	2.3	0.4
Sidechain-Sidechain	161	5.7	67	41.6	2.4	25	15.5	0.9
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>501</b>	<b>17.7</b>	<b>59</b>	<b>11.8</b>	<b>2.1</b>	<b>22</b>	<b>4.4</b>	<b>0.8</b>
Backbone-Backbone	83	2.9	3	3.6	0.1	0	0.0	0.0
Backbone-Sidechain	217	7.7	11	5.1	0.4	2	0.9	0.1
Sidechain-Sidechain	201	7.1	45	22.4	1.6	20	10.0	0.7
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>925</b>	<b>32.6</b>	<b>106</b>	<b>11.5</b>	<b>3.7</b>	<b>19</b>	<b>2.1</b>	<b>0.7</b>
Backbone-Backbone	66	2.3	2	3.0	0.1	0	0.0	0.0
Backbone-Sidechain	364	12.8	23	6.3	0.8	2	0.5	0.1
Sidechain-Sidechain	495	17.5	81	16.4	2.9	17	3.4	0.6
<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>2835</b>	<b>100.0</b>	<b>402</b>	<b>14.2</b>	<b>14.2</b>	<b>118</b>	<b>4.2</b>	<b>4.2</b>
Backbone-Backbone	309	10.9	12	3.9	0.4	1	0.3	0.0
Backbone-Sidechain	1440	50.8	105	7.3	3.7	25	1.7	0.9
Sidechain-Sidechain	1086	38.3	285	26.2	10.1	92	8.5	3.2

<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					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>					
1	78	73	40	45	0	236	0.62	2.54	0.49	0.46
2	72	71	33	46	0	222	0.62	2.68	0.49	0.5
3	72	67	34	46	0	219	0.63	2.86	0.52	0.47
4	77	70	36	48	0	231	0.62	2.64	0.47	0.49
5	75	72	34	44	0	225	0.63	2.49	0.51	0.45
6	72	65	33	54	0	224	0.61	2.54	0.5	0.43
7	71	69	36	55	0	231	0.66	2.45	0.52	0.49
8	76	72	34	56	0	238	0.61	2.54	0.49	0.47
9	75	62	35	54	0	226	0.64	2.75	0.51	0.5
10	77	74	31	59	0	241	0.64	2.59	0.52	0.49
11	75	72	32	51	0	230	0.64	2.67	0.5	0.52

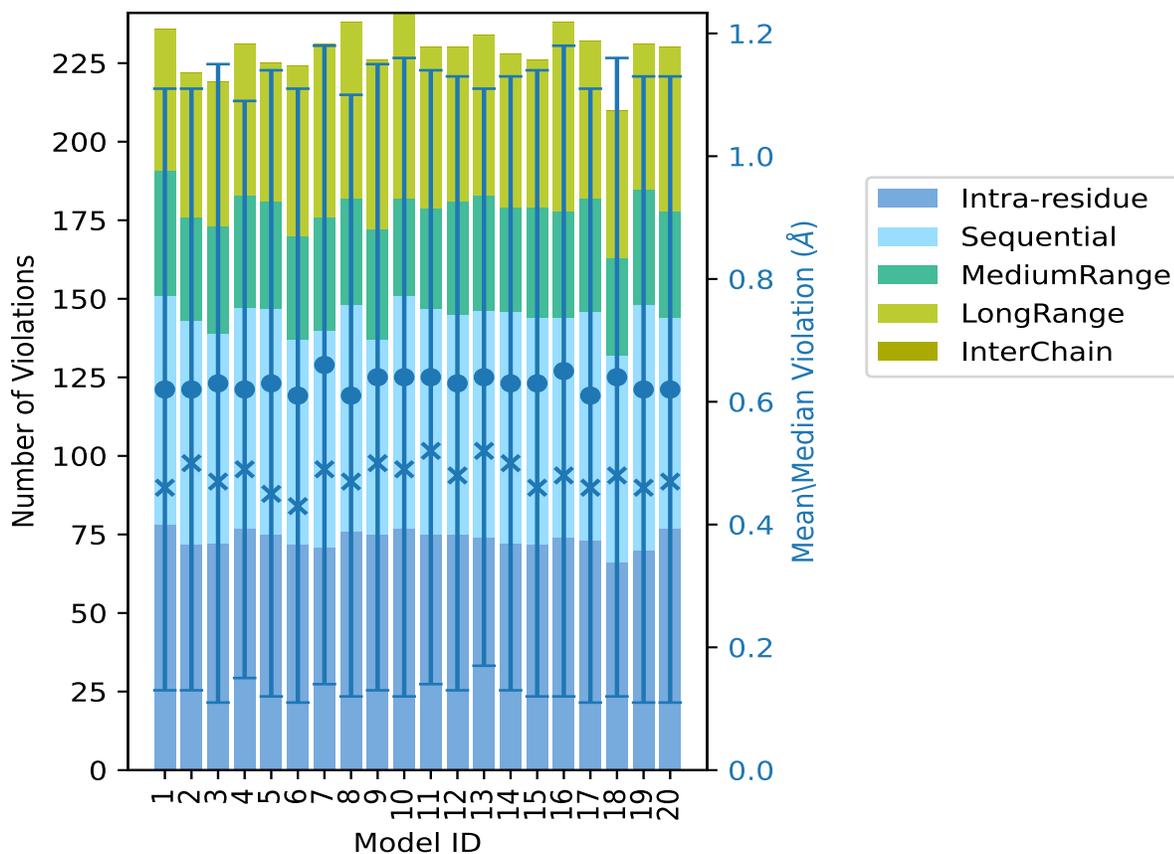
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>					
12	75	70	36	49	0	230	0.63	2.44	0.5	0.48
13	74	72	37	51	0	234	0.64	2.41	0.47	0.52
14	72	74	33	49	0	228	0.63	2.71	0.5	0.5
15	72	72	35	47	0	226	0.63	2.47	0.51	0.46
16	74	70	34	60	0	238	0.65	2.77	0.53	0.48
17	73	73	36	50	0	232	0.61	2.48	0.5	0.46
18	66	66	31	47	0	210	0.64	2.73	0.52	0.48
19	70	78	37	46	0	231	0.62	2.51	0.51	0.46
20	77	67	34	52	0	230	0.62	2.9	0.51	0.47

<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

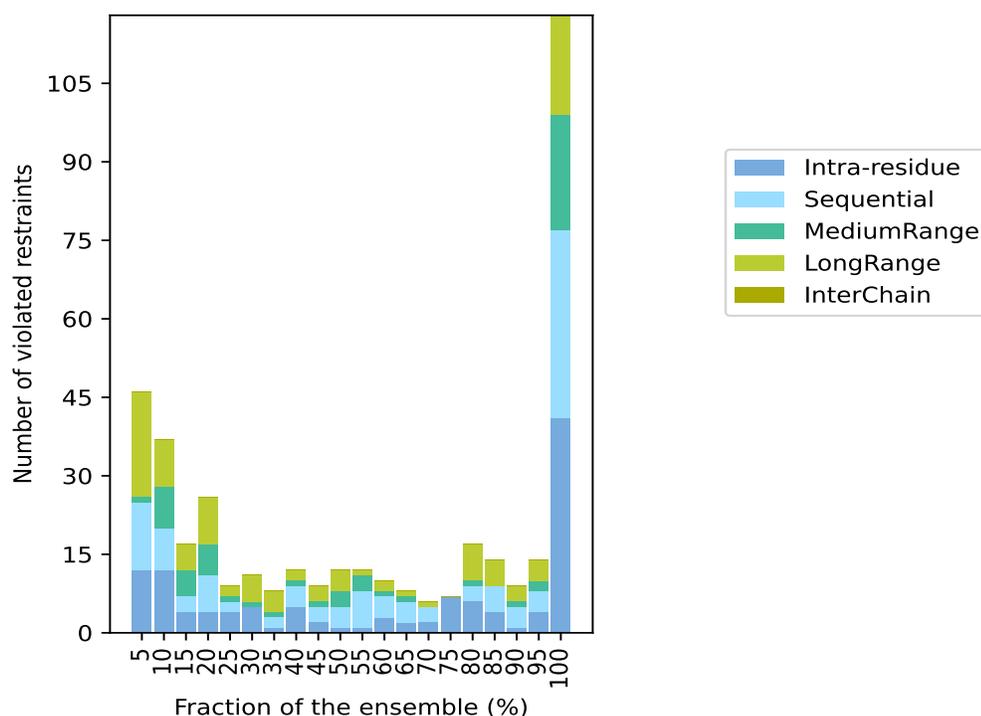
### 9.3 Distance violation statistics for the ensemble

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, 2433(IR:541, SQ:631, MR:442, LR:819, 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>	%
12	13	1	20	0	46	1	5.0
12	8	8	9	0	37	2	10.0
4	3	5	5	0	17	3	15.0
4	7	6	9	0	26	4	20.0
4	2	1	2	0	9	5	25.0
5	0	1	5	0	11	6	30.0
1	2	1	4	0	8	7	35.0
5	4	1	2	0	12	8	40.0
2	3	1	3	0	9	9	45.0
1	4	3	4	0	12	10	50.0
1	7	3	1	0	12	11	55.0
3	4	1	2	0	10	12	60.0
2	4	1	1	0	8	13	65.0
2	3	0	1	0	6	14	70.0
7	0	0	0	0	7	15	75.0
6	3	1	7	0	17	16	80.0
4	5	0	5	0	14	17	85.0
1	4	1	3	0	9	18	90.0
4	4	2	4	0	14	19	95.0
41	36	22	19	0	118	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

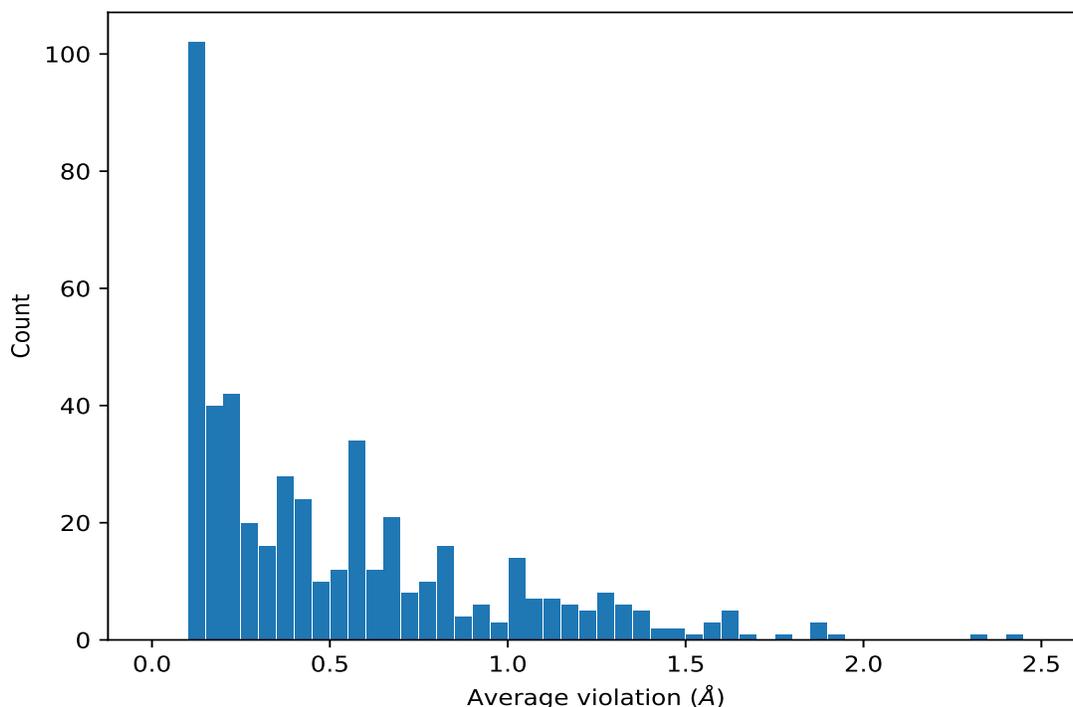
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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 violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation 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.

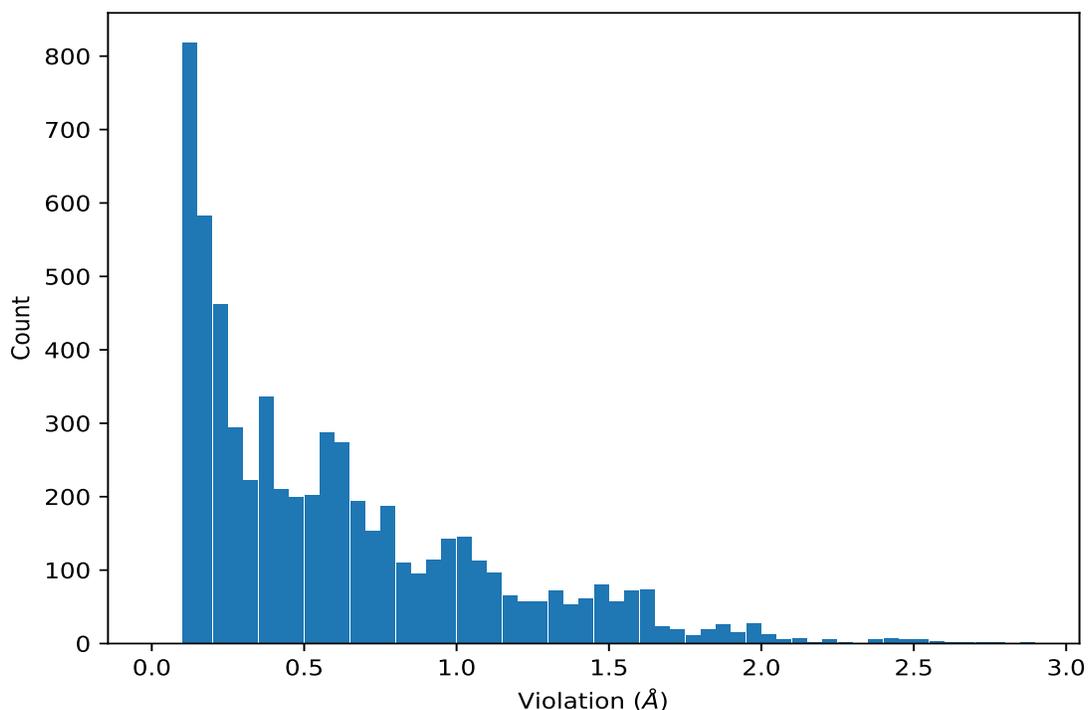
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2114)	1:A:568:LYS:HE2	1:A:562:GLN:HB3	20	2.44	0.5	2.54
(1,2831)	1:A:616:SER:HB2	1:A:619:GLN:HB3	20	2.31	0.19	2.35
(1,2346)	1:A:589:MET:HG2	1:A:590:PRO:HB2	20	1.94	0.06	1.96
(1,2829)	1:A:616:SER:HB3	1:A:619:GLN:HB3	20	1.89	0.49	1.67
(1,2100)	1:A:618:ILE:HG13	1:A:619:GLN:HG3	20	1.86	0.05	1.87
(1,828)	1:A:530:GLN:HG2	1:A:526:ARG:HB3	20	1.85	0.08	1.87
(1,2751)	1:A:568:LYS:HE2	1:A:565:GLU:HB2	20	1.79	0.46	1.95
(1,2728)	1:A:562:GLN:HE21	1:A:561:LYS:HG2	20	1.67	0.52	1.94
(1,2174)	1:A:618:ILE:HD11	1:A:619:GLN:HG3	20	1.61	0.03	1.61
(1,2174)	1:A:618:ILE:HD12	1:A:619:GLN:HG3	20	1.61	0.03	1.61
(1,2174)	1:A:618:ILE:HD13	1:A:619:GLN:HG3	20	1.61	0.03	1.61
(1,2010)	1:A:526:ARG:HB2	1:A:591:VAL:HB	20	1.61	0.09	1.63

<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 provides the 10 worst performing restraints, sorted by the violation 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)
(1,2114)	1:A:568:LYS:HE2	1:A:562:GLN:HB3	20	2.9
(1,2114)	1:A:568:LYS:HE2	1:A:562:GLN:HB3	3	2.86
(1,2114)	1:A:568:LYS:HE2	1:A:562:GLN:HB3	16	2.77
(1,2114)	1:A:568:LYS:HE2	1:A:562:GLN:HB3	9	2.75
(1,2114)	1:A:568:LYS:HE2	1:A:562:GLN:HB3	18	2.73
(1,2114)	1:A:568:LYS:HE2	1:A:562:GLN:HB3	14	2.71
(1,2114)	1:A:568:LYS:HE2	1:A:562:GLN:HB3	2	2.68
(1,2114)	1:A:568:LYS:HE2	1:A:562:GLN:HB3	11	2.67
(1,2831)	1:A:616:SER:HB2	1:A:619:GLN:HB3	4	2.64
(1,2831)	1:A:616:SER:HB2	1:A:619:GLN:HB3	11	2.62

## 10 Dihedral-angle violation analysis

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