



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 22, 2025 – 09:34 AM EST

PDB ID : 8RHM  
BMRB ID : 34888  
Title : Solution structure of sulfazecin NRPS holo-PCP domain 3  
Authors : Chagot, B.  
Deposited on : 2023-12-15

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.41.4

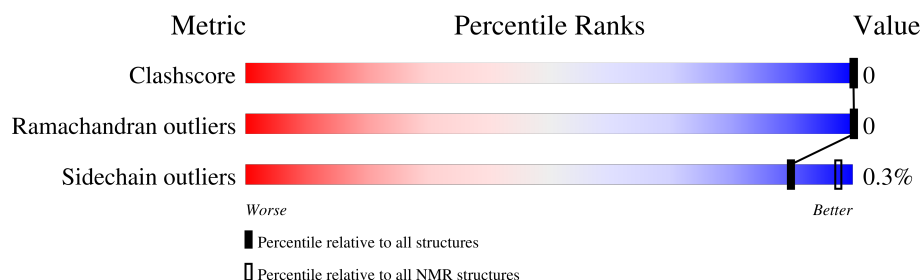
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*


The overall completeness of chemical shifts assignment is 92%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	72	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:2641-A:2670, A:2672-A:2703 (62)	0.22	6

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1149 atoms, of which 569 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Non-ribosomal peptide synthetase, putative.

Mol	Chain	Residues	Atoms							Trace
1	A	72	Total	C	H	N	O	P	S	0
			1149	370	569	97	111	1	1	

There are 4 discrepancies between the modelled and reference sequences:

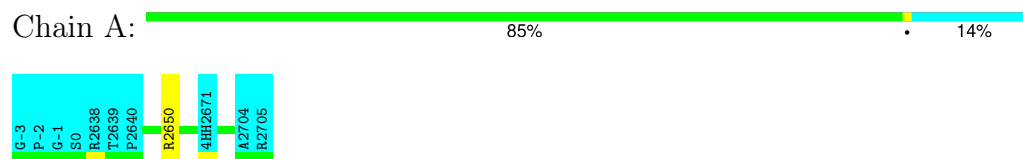
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q2SX64
A	-2	PRO	-	expression tag	UNP Q2SX64
A	-1	GLY	-	expression tag	UNP Q2SX64
A	0	SER	-	expression tag	UNP Q2SX64

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Non-ribosomal peptide synthetase, putative

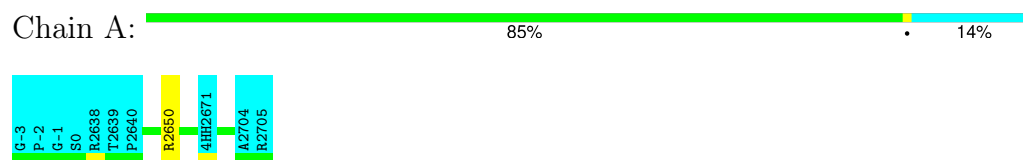


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

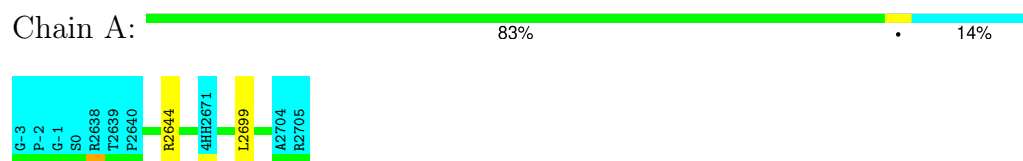
#### 4.2.1 Score per residue for model 1

- Molecule 1: Non-ribosomal peptide synthetase, putative



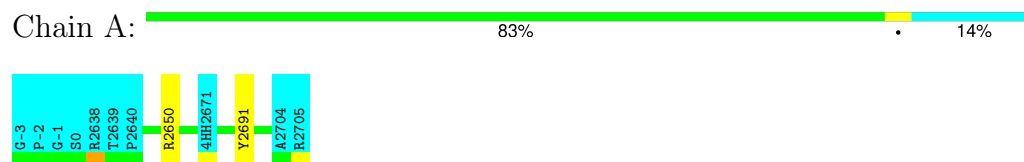
#### 4.2.2 Score per residue for model 2

- Molecule 1: Non-ribosomal peptide synthetase, putative



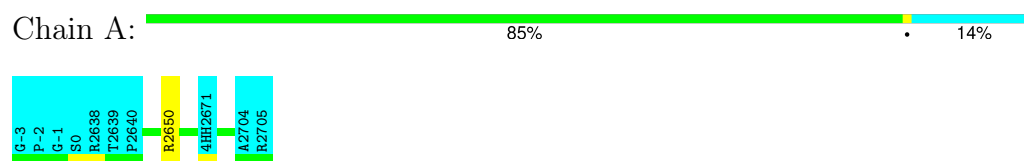
### 4.2.3 Score per residue for model 3

- Molecule 1: Non-ribosomal peptide synthetase, putative



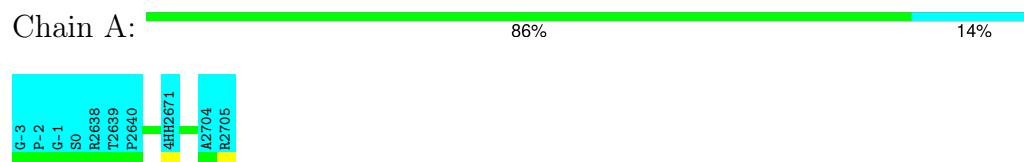
### 4.2.4 Score per residue for model 4

- Molecule 1: Non-ribosomal peptide synthetase, putative



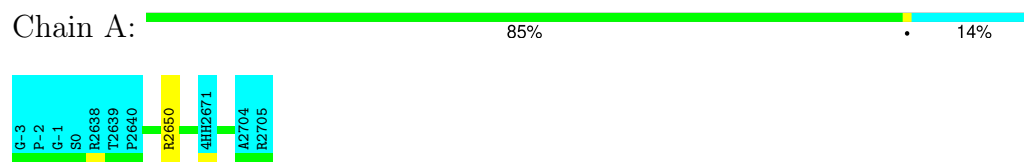
### 4.2.5 Score per residue for model 5

- Molecule 1: Non-ribosomal peptide synthetase, putative



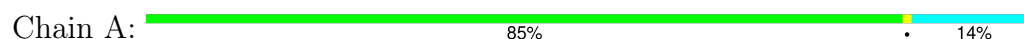
### 4.2.6 Score per residue for model 6 (medoid)

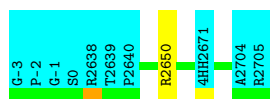
- Molecule 1: Non-ribosomal peptide synthetase, putative



### 4.2.7 Score per residue for model 7

- Molecule 1: Non-ribosomal peptide synthetase, putative

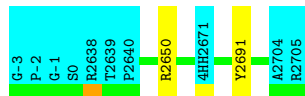




#### 4.2.8 Score per residue for model 8

- Molecule 1: Non-ribosomal peptide synthetase, putative

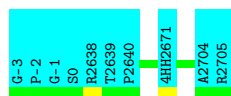
Chain A: 83% 14%



#### 4.2.9 Score per residue for model 9

- Molecule 1: Non-ribosomal peptide synthetase, putative

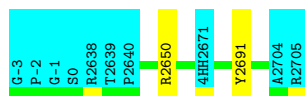
Chain A: 86% 14%



#### 4.2.10 Score per residue for model 10

- Molecule 1: Non-ribosomal peptide synthetase, putative

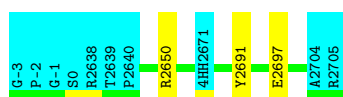
Chain A: 83% 14%



#### 4.2.11 Score per residue for model 11

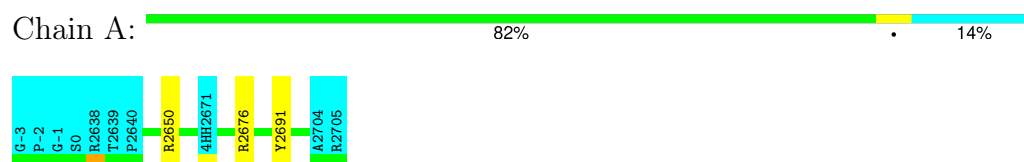
- Molecule 1: Non-ribosomal peptide synthetase, putative

Chain A: 82% 14%



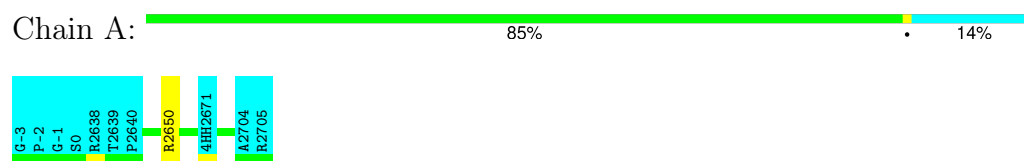
#### 4.2.12 Score per residue for model 12

- Molecule 1: Non-ribosomal peptide synthetase, putative



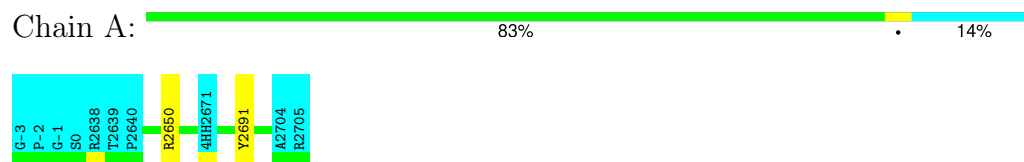
#### 4.2.13 Score per residue for model 13

- Molecule 1: Non-ribosomal peptide synthetase, putative



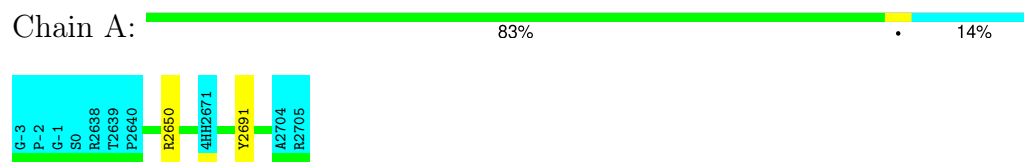
#### 4.2.14 Score per residue for model 14

- Molecule 1: Non-ribosomal peptide synthetase, putative



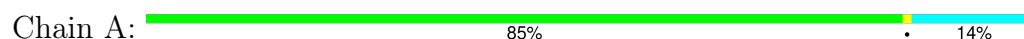
#### 4.2.15 Score per residue for model 15

- Molecule 1: Non-ribosomal peptide synthetase, putative

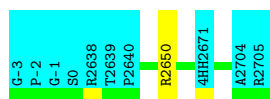


#### 4.2.16 Score per residue for model 16

- Molecule 1: Non-ribosomal peptide synthetase, putative

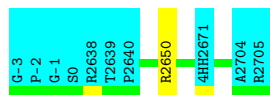
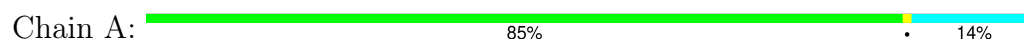






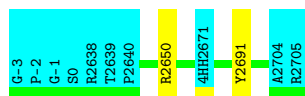
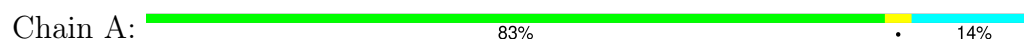
#### 4.2.17 Score per residue for model 17

- Molecule 1: Non-ribosomal peptide synthetase, putative



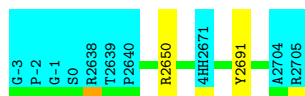
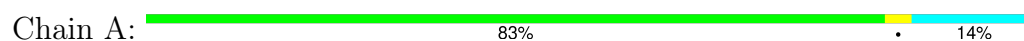
#### 4.2.18 Score per residue for model 18

- Molecule 1: Non-ribosomal peptide synthetase, putative



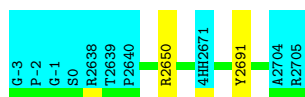
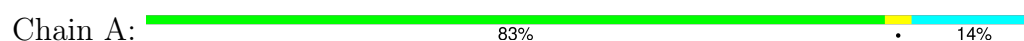
#### 4.2.19 Score per residue for model 19

- Molecule 1: Non-ribosomal peptide synthetase, putative



#### 4.2.20 Score per residue for model 20

- Molecule 1: Non-ribosomal peptide synthetase, putative



## 5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
Amber	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	906
Number of shifts mapped to atoms	869
Number of unparsed shifts	0
Number of shifts with mapping errors	37
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

## 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: 4HH

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.75±0.01	0±0/502 ( 0.0± 0.0%)	0.94±0.03	1±1/682 ( 0.2± 0.1%)
All	All	0.75	0/10040 ( 0.0%)	0.94	28/13640 ( 0.2%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	2650	ARG	NE-CZ-NH1	8.20	124.40	120.30	11	16
1	A	2691	TYR	CB-CG-CD1	-6.29	117.22	121.00	18	5
1	A	2691	TYR	CB-CG-CD2	-6.06	117.36	121.00	3	5
1	A	2644	ARG	NE-CZ-NH1	5.80	123.20	120.30	2	1
1	A	2676	ARG	NE-CZ-NH1	5.08	122.84	120.30	12	1

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
All	All	9800	9580	9560	-

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 -.

There are no clashes.

## 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	62/72 (86%)	61±1 (98±1%)	1±1 (2±1%)	0±0 (0±0%)	100	100
All	All	1240/1440 (86%)	1214 (98%)	26 (2%)	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	50/56 (89%)	50±0 (100±1%)	0±0 (0±1%)	90	97
All	All	1000/1120 (89%)	997 (100%)	3 (0%)	90	97

All 3 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	2699	LEU	1
1	A	2650	ARG	1
1	A	2697	GLU	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	4HH	A	2671	1	22,26,27	0.71±0.02	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	4HH	A	2671	1	27,35,37	1.13±0.20	2±1 (8±5%)

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	4HH	A	2671	1	-	0±0,33,35,37	-

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	2671	4HH	CJ-CK	2.03	1.55	1.52	10	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	2671	4HH	OG-CB-CA	6.00	113.99	108.14	15	17
1	A	2671	4HH	CO-NN-CL3	3.83	129.43	122.55	9	4
1	A	2671	4HH	CM-CL3-NN	3.66	123.42	116.48	9	2
1	A	2671	4HH	CS-NR-CQ	3.39	129.13	122.82	2	5
1	A	2671	4HH	ON-CL3-NN	2.89	116.87	122.98	9	2
1	A	2671	4HH	CL1-CK-CM	2.72	113.40	108.77	9	8
1	A	2671	4HH	CP-CQ-NR	2.64	121.16	116.34	17	4
1	A	2671	4HH	CL2-CK-CM	2.59	113.19	108.77	10	2
1	A	2671	4HH	OR-CQ-NR	2.18	118.76	123.03	10	4

There are no chirality outliers.

All unique torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	2671	4HH	CM-CL3-NN-CO	2

There are no ring outliers.

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 90% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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	906
Number of shifts mapped to atoms	869
Number of unparsed shifts	0
Number of shifts with mapping errors	37
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 37 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2671	SER	H	8.998	0.002	1
1	A	2671	SER	HA	4.677	0.006	1
1	A	2671	SER	HB2	4.031	0.006	2
1	A	2671	SER	HB3	4.176	0.001	2
1	A	2671	SER	C	174.984	0.000	1
1	A	2671	SER	CA	60.656	0.043	1
1	A	2671	SER	CB	65.741	0.037	1
1	A	2671	SER	N	113.573	0.013	1
1	A	2801	PNS	H281	3.564	0.003	2
1	A	2801	PNS	H282	3.231	0.000	2
1	A	2801	PNS	H301	0.71	0.003	2
1	A	2801	PNS	H302	0.71	0.003	2
1	A	2801	PNS	H303	0.71	0.003	2
1	A	2801	PNS	H311	0.631	0.004	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2801	PNS	H312	0.631	0.004	2
1	A	2801	PNS	H313	0.631	0.004	2
1	A	2801	PNS	H32	3.893	0.003	1
1	A	2801	PNS	H36	7.876	0.003	1
1	A	2801	PNS	H371	3.348	0.004	2
1	A	2801	PNS	H372	3.348	0.004	2
1	A	2801	PNS	H381	2.324	0.004	2
1	A	2801	PNS	H382	2.324	0.004	2
1	A	2801	PNS	H41	8.051	0.004	1
1	A	2801	PNS	H421	3.196	0.003	2
1	A	2801	PNS	H422	3.196	0.003	2
1	A	2801	PNS	H431	2.495	0.003	2
1	A	2801	PNS	H432	2.495	0.003	2
1	A	2801	PNS	C28	35.975	0.001	1
1	A	2801	PNS	C30	23.35	0.000	1
1	A	2801	PNS	C31	21.392	0.000	1
1	A	2801	PNS	C32	38.735	0.000	1
1	A	2801	PNS	C37	38.123	0.000	1
1	A	2801	PNS	C38	37.93	0.000	1
1	A	2801	PNS	C42	45.046	0.000	1
1	A	2801	PNS	C43	26.007	0.000	1
1	A	2801	PNS	N36	119.954	0.000	1
1	A	2801	PNS	N41	124.469	0.000	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
$^{13}\text{C}_\alpha$	72	$-0.26 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	65	$-0.11 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	65	$-0.23 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	65	$0.38 \pm 0.58$	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 92%, i.e. 785 atoms were assigned a chemical shift out of a possible 856. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.



	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	306/309 (99%)	126/126 (100%)	121/124 (98%)	59/59 (100%)
Sidechain	416/455 (91%)	285/299 (95%)	130/145 (90%)	1/11 (9%)
Aromatic	63/92 (68%)	35/45 (78%)	22/41 (54%)	6/6 (100%)
Overall	785/856 (92%)	446/470 (95%)	273/310 (88%)	66/76 (87%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 869 atoms were assigned a chemical shift out of a possible 966. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	341/352 (97%)	142/144 (99%)	135/142 (95%)	64/66 (97%)
Sidechain	465/522 (89%)	318/342 (93%)	146/163 (90%)	1/17 (6%)
Aromatic	63/92 (68%)	35/45 (78%)	22/41 (54%)	6/6 (100%)
Overall	869/966 (90%)	495/531 (93%)	303/346 (88%)	71/89 (80%)

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

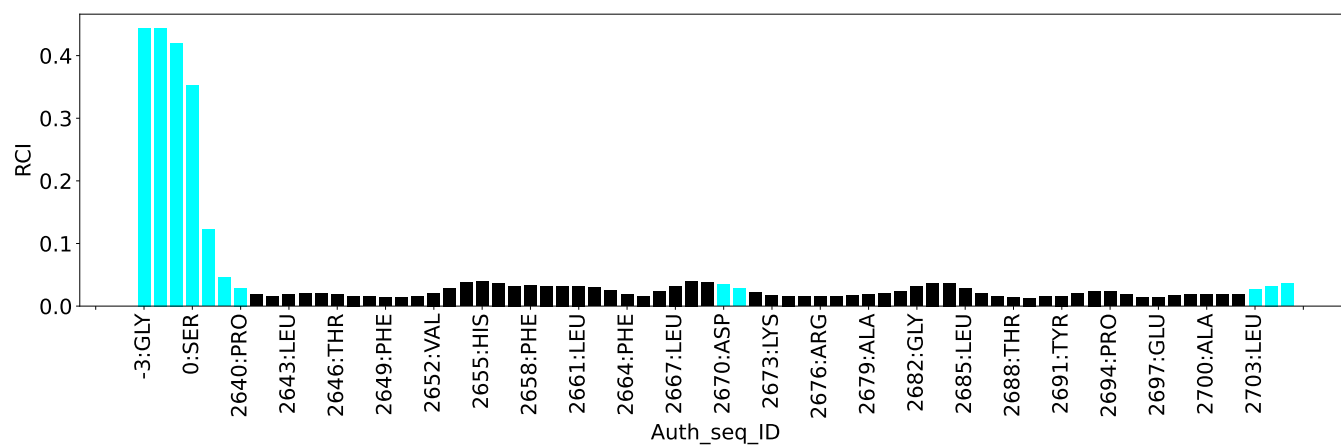
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	2669	GLY	HA2	1.11	2.15 – 5.77	-7.9

#### 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	1695
Intra-residue ( $ i-j =0$ )	237
Sequential ( $ i-j =1$ )	411
Medium range ( $ i-j >1$ and $ i-j <5$ )	550
Long range ( $ i-j \geq 5$ )	495
Inter-chain	2
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	100
Number of unmapped restraints	27
Number of restraints per residue	24.6
Number of long range restraints per residue <sup>1</sup>	6.8

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

### 8.2 Residual restraint violations

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

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

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	1.0	0.13
0.2-0.5 (Medium)	None	None
>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)	0.1	1.72
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

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

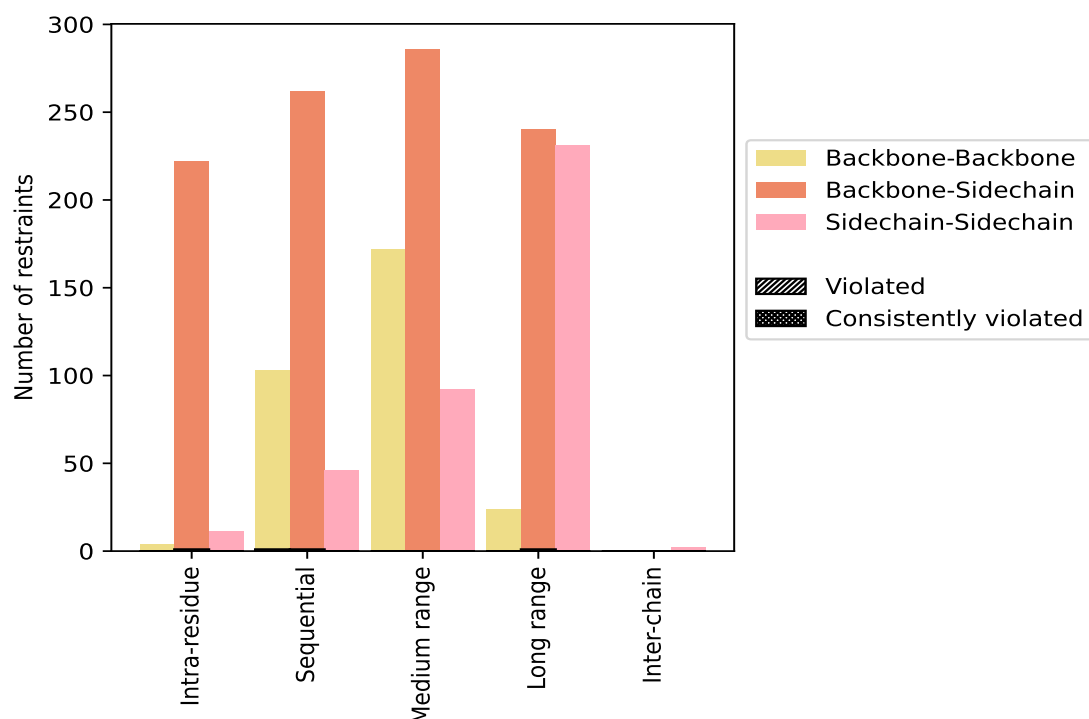
### 9.1 Summary of distance violations [i](#)

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>237</b>	<b>14.0</b>	<b>1</b>	<b>0.4</b>	<b>0.1</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	4	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	222	13.1	1	0.5	0.1	0	0.0	0.0
Sidechain-Sidechain	11	0.6	0	0.0	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>411</b>	<b>24.2</b>	<b>2</b>	<b>0.5</b>	<b>0.1</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	103	6.1	1	1.0	0.1	0	0.0	0.0
Backbone-Sidechain	262	15.5	1	0.4	0.1	0	0.0	0.0
Sidechain-Sidechain	46	2.7	0	0.0	0.0	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>550</b>	<b>32.4</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	172	10.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	286	16.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	92	5.4	0	0.0	0.0	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>495</b>	<b>29.2</b>	<b>1</b>	<b>0.2</b>	<b>0.1</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	24	1.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	240	14.2	1	0.4	0.1	0	0.0	0.0
Sidechain-Sidechain	231	13.6	0	0.0	0.0	0	0.0	0.0
<b>Inter-chain</b>	<b>2</b>	<b>0.1</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	2	0.1	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>1695</b>	<b>100.0</b>	<b>4</b>	<b>0.2</b>	<b>0.2</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	303	17.9	1	0.3	0.1	0	0.0	0.0
Backbone-Sidechain	1010	59.6	3	0.3	0.2	0	0.0	0.0
Sidechain-Sidechain	382	22.5	0	0.0	0.0	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 disulfied bonds are counted in their appropriate category on the x-axis

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	0	1	0	0	0	1	0.11	0.11	0.0	0.11
2	0	1	0	0	0	1	0.11	0.11	0.0	0.11
3	0	2	0	0	0	2	0.1	0.1	0.0	0.1
4	0	1	0	0	0	1	0.12	0.12	0.0	0.12
5	0	0	0	0	0	0	0.0	0.0	0.0	0.0
6	0	1	0	0	0	1	0.11	0.11	0.0	0.11
7	0	1	0	0	0	1	0.11	0.11	0.0	0.11
8	0	1	0	0	0	1	0.12	0.12	0.0	0.12
9	0	1	0	0	0	1	0.11	0.11	0.0	0.11
10	0	1	0	0	0	1	0.11	0.11	0.0	0.11

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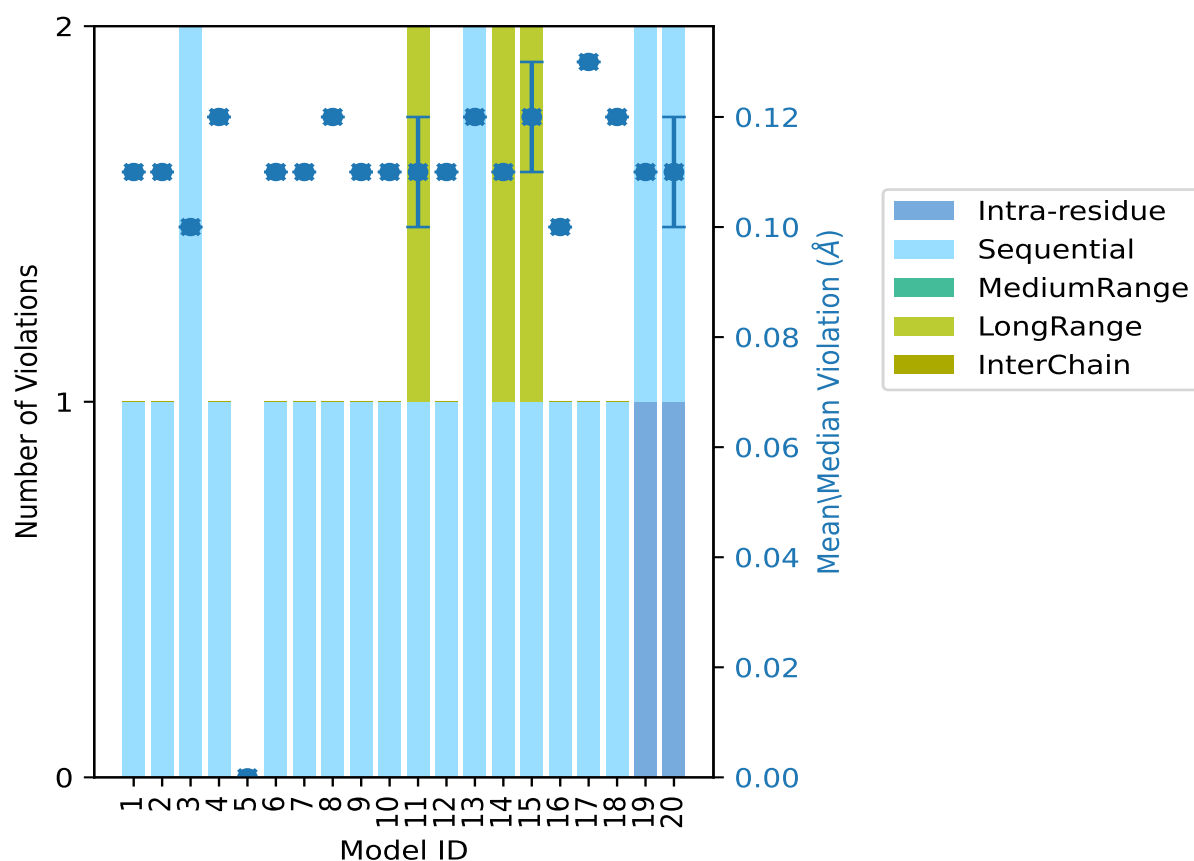
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	0	1	0	1	0	2	0.11	0.12	0.01	0.11
12	0	1	0	0	0	1	0.11	0.11	0.0	0.11
13	0	2	0	0	0	2	0.12	0.12	0.0	0.12
14	0	1	0	1	0	2	0.11	0.11	0.0	0.11
15	0	1	0	1	0	2	0.12	0.13	0.01	0.12
16	0	1	0	0	0	1	0.1	0.1	0.0	0.1
17	0	1	0	0	0	1	0.13	0.13	0.0	0.13
18	0	1	0	0	0	1	0.12	0.12	0.0	0.12
19	1	1	0	0	0	2	0.11	0.11	0.0	0.11
20	1	1	0	0	0	2	0.11	0.12	0.01	0.11

<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 ⓘ



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, 1691(IR:236, SQ:409, MR:550, LR:494, IC:2) restraints are not violated in the ensemble.

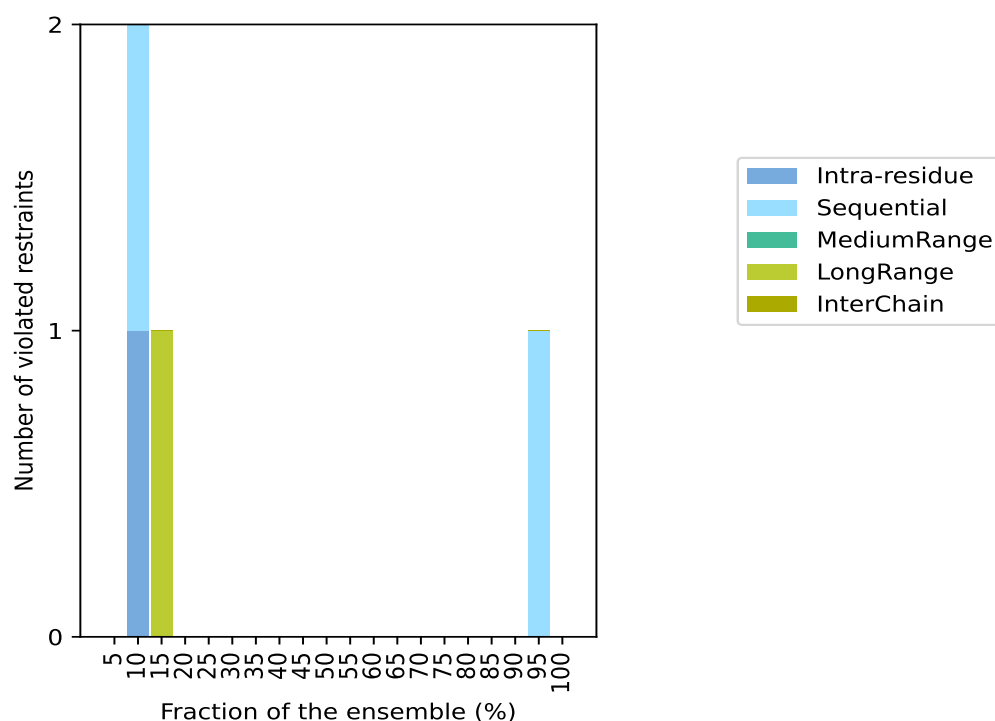
Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	0	0	0	0	0	1	5.0
1	1	0	0	0	2	2	10.0
0	0	0	1	0	1	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0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

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations



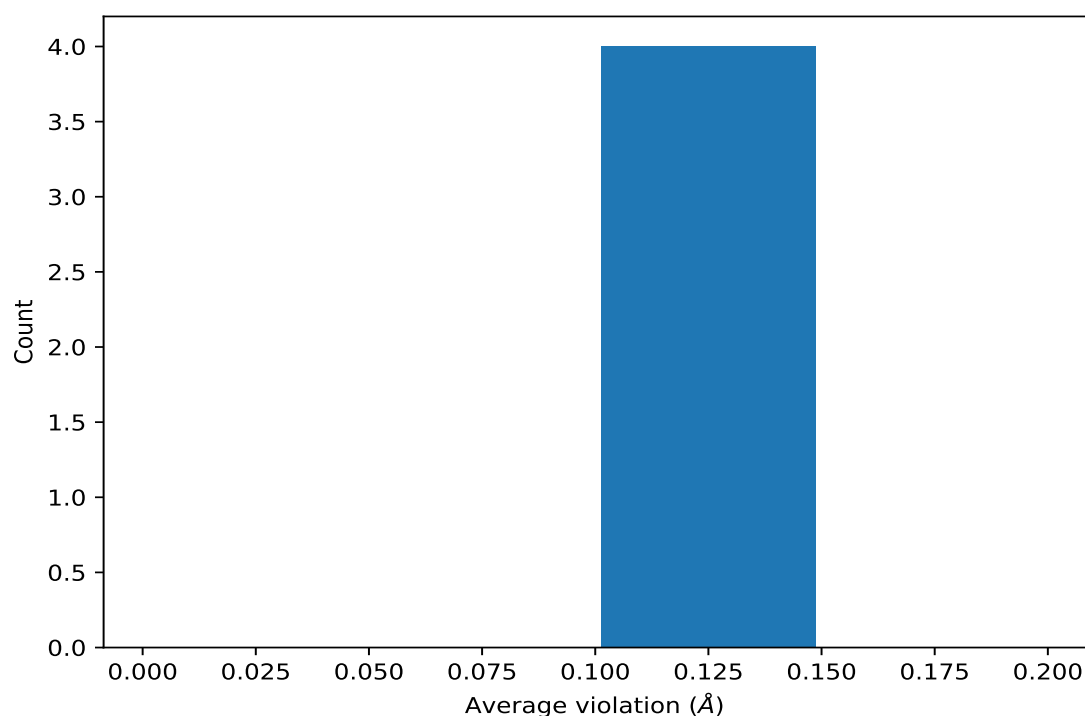
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 9.4 Most violated distance restraints in the ensemble [i](#)

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

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



#### 9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

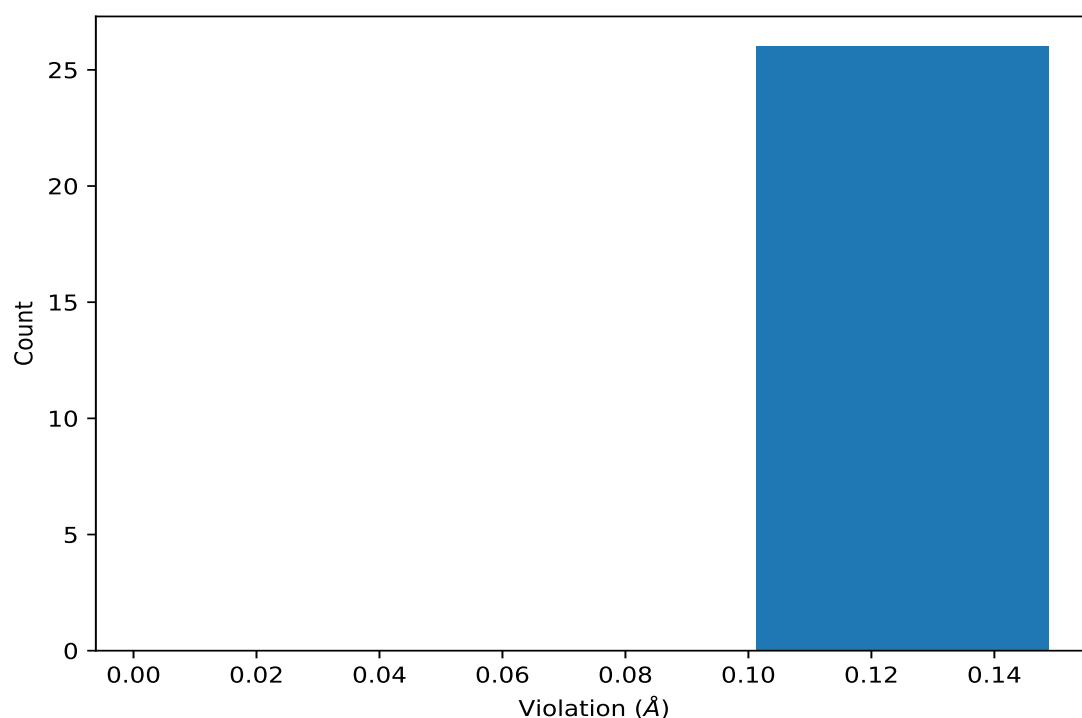
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	19	0.11	0.01	0.11
(1,1308)	1:2651:A:ASP:H	1:2677:A:ILE:HG12	3	0.11	0.0	0.11
(1,757)	1:2657:A:ALA:HA	1:2658:A:PHE:H	2	0.11	0.01	0.11
(1,1233)	1:2699:A:LEU:H	1:2699:A:LEU:HB3	2	0.1	0.0	0.1

<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)
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	15	0.13
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	17	0.13
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	4	0.12
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	8	0.12
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	11	0.12
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	18	0.12
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	20	0.12
(1,757)	1:2657:A:ALA:HA	1:2658:A:PHE:H	13	0.12
(1,1308)	1:2651:A:ASP:H	1:2677:A:ILE:HG12	14	0.11
(1,1308)	1:2651:A:ASP:H	1:2677:A:ILE:HG12	15	0.11
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	1	0.11
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	2	0.11
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	6	0.11
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	7	0.11
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	9	0.11
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	12	0.11
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	13	0.11
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	14	0.11
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	19	0.11
(1,1308)	1:2651:A:ASP:H	1:2677:A:ILE:HG12	11	0.1
(1,1233)	1:2699:A:LEU:H	1:2699:A:LEU:HB3	19	0.1
(1,1233)	1:2699:A:LEU:H	1:2699:A:LEU:HB3	20	0.1
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	3	0.1
(1,1086)	1:2688:A:THR:H	1:2689:A:ASP:HB3	16	0.1
(1,757)	1:2657:A:ALA:HA	1:2658:A:PHE:H	3	0.1

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

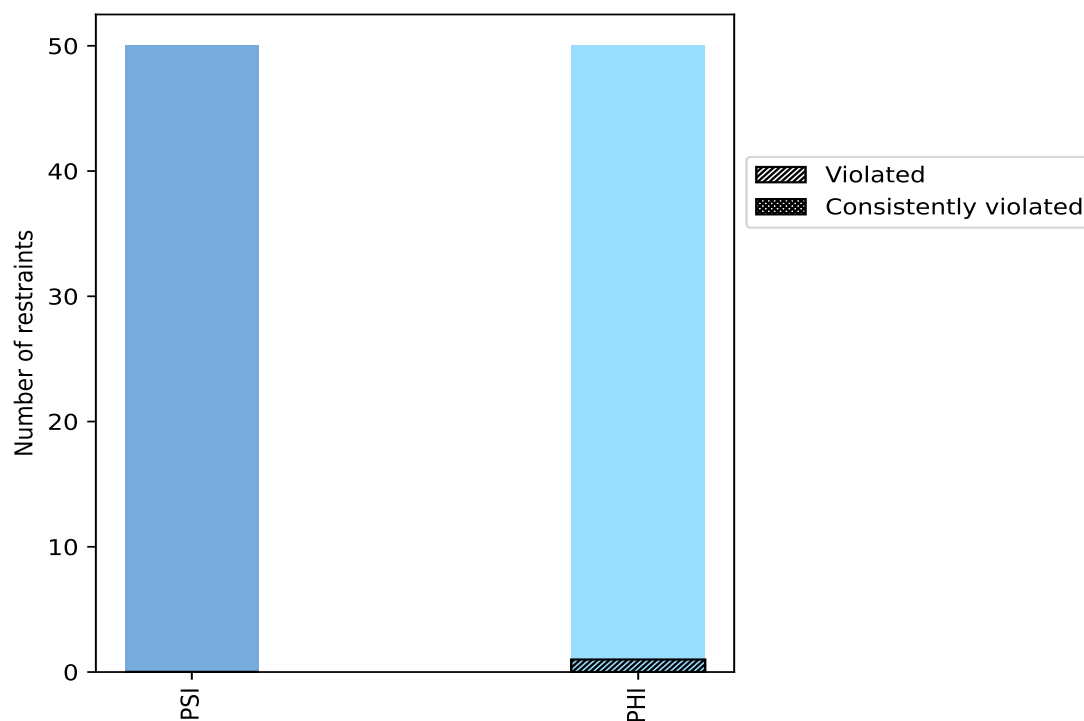
### 10.1 Summary of dihedral-angle violations [i](#)

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>
PSI	50	50.0	0	0.0	0.0	0	0.0	0.0
PHI	50	50.0	1	2.0	1.0	0	0.0	0.0
Total	100	100.0	1	1.0	1.0	0	0.0	0.0

<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](#)



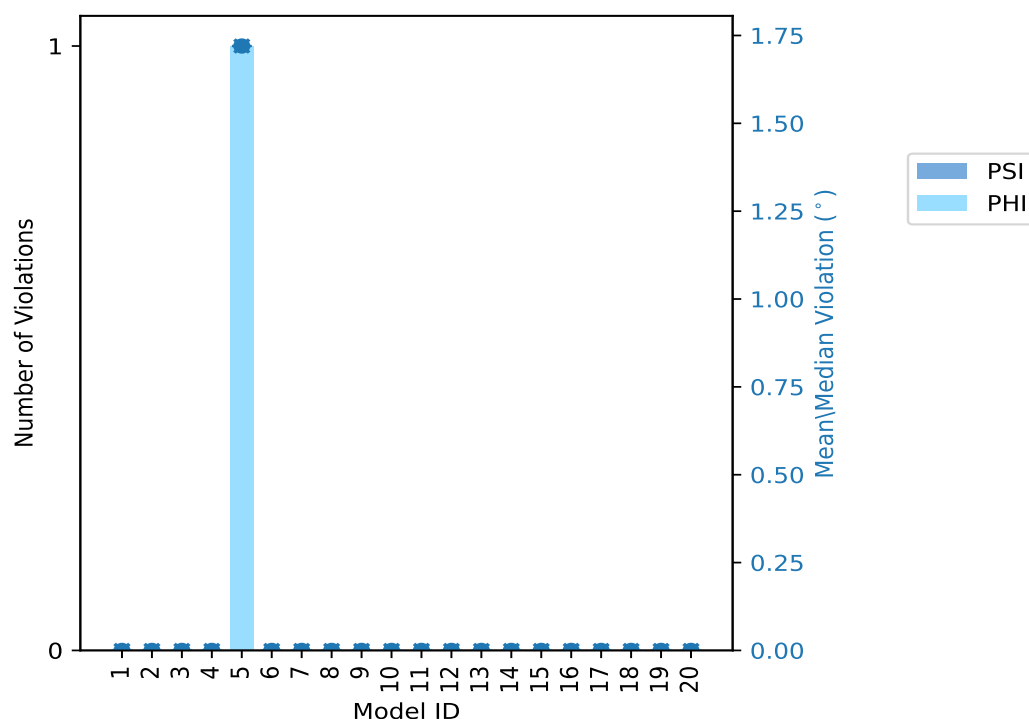
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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 (°)
	PSI	PHI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0.0	0.0	0.0	0.0
5	0	1	1	1.72	1.72	0.0	1.72
6	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0.0	0.0	0.0	0.0

### 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	
PSI	PHI	Total	Count <sup>1</sup>	%
0	1	1	1	5.0
0	0	0	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
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

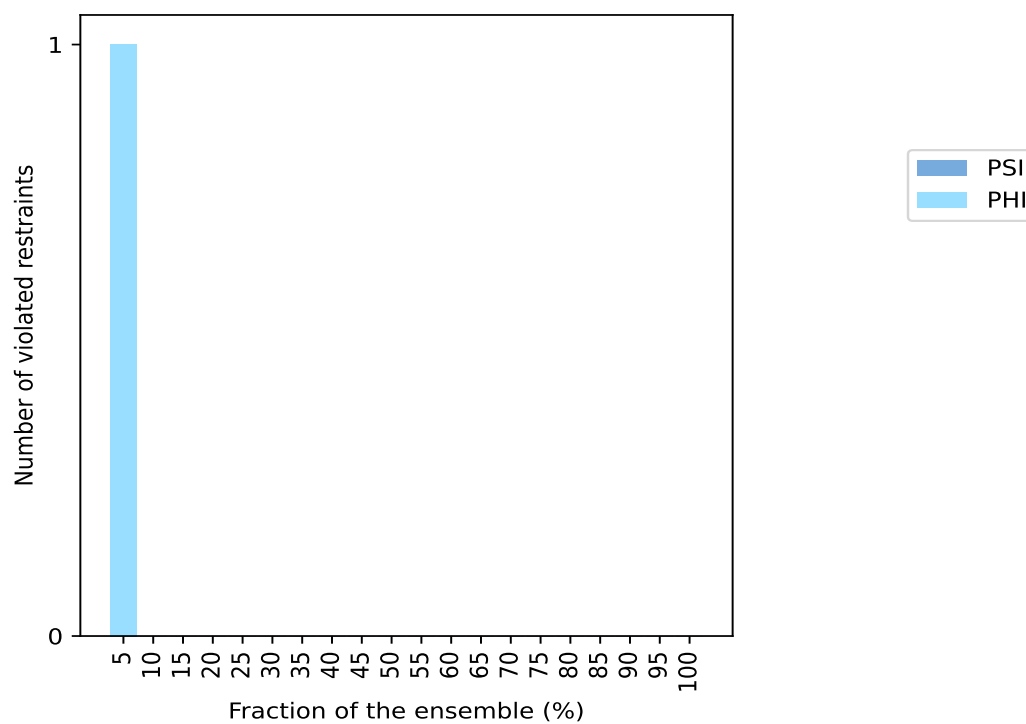
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

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

### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



## 10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

No violations found



## 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.

Data insufficient to plot histogram

### 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 (°)
(1,97)	1:2701:A:ALA:C	1:2702:A:HIS:N	1:2702:A:HIS:CA	1:2702:A:HIS:C	5	1.72