



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:00 AM UTC

PDB ID : 8RD6 / pdb_00008rd6
BMRB ID : 34887
Title : the C-terminal domain of TonB protein from Salmonella enterica.
Authors : Iwai, H.; Ciragan, A.; Oeemig, J.S.
Deposited on : 2023-12-07

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

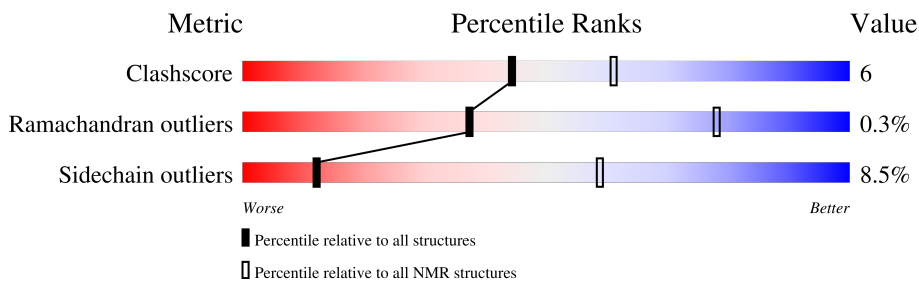
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 100%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	90	 80% 17% .

2 Ensemble composition and analysis

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:90 (87)	0.64	10

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. No single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1432 atoms, of which 726 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein TonB.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	90	1432	440	726	138	126	2	0

There is a discrepancy between the modelled and reference sequences:

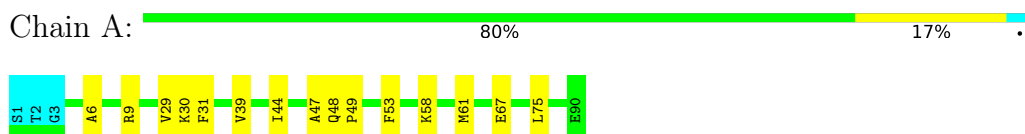
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P25945

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.

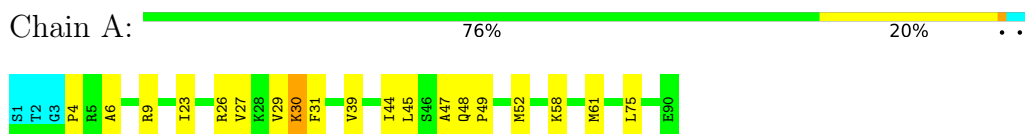
- Molecule 1: Protein TonB



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

The representative model is number 10. Colouring as in section 4.1 above.

- Molecule 1: Protein TonB



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure calculation	3.0
Amber	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1341
Number of shifts mapped to atoms	1341
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	100%

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	689	711	711	9±2
All	All	13780	14220	14220	180

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 6.

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:29:VAL:HG23	1:A:44:ILE:HD13	0.76	1.58	3	15
1:A:11:GLN:HG3	1:A:89:ILE:HD12	0.65	1.67	13	3
1:A:31:PHE:CE2	1:A:75:LEU:HD13	0.64	2.28	7	8
1:A:27:VAL:HG13	1:A:47:ALA:HB2	0.64	1.70	7	10
1:A:53:PHE:O	1:A:57:VAL:HG23	0.63	1.93	19	9

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	86/90 (96%)	75±2 (87±3%)	11±3 (12±3%)	0±1 (0±1%)	37	78
All	All	1720/1800 (96%)	1502 (87%)	213 (12%)	5 (0%)	37	78

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	67	GLU	4
1	A	74	GLY	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	71/73 (97%)	65±2 (91±3%)	6±2 (9±3%)	12	59
All	All	1420/1460 (97%)	1299 (91%)	121 (9%)	12	59

5 of 32 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	61	MET	15
1	A	30	LYS	14
1	A	58	LYS	13
1	A	9	ARG	11
1	A	67	GLU	7

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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 100% for the well-defined parts and 100% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1341
Number of shifts mapped to atoms	1341
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	161

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
$^{13}\text{C}_\alpha$	90	-0.01 \pm 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	83	-0.11 \pm 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	90	0.29 \pm 0.19	None needed (< 0.5 ppm)
^{15}N	90	0.11 \pm 0.44	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 100%, i.e. 1241 atoms were assigned a chemical shift out of a possible 1241. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	431/431 (100%)	175/175 (100%)	174/174 (100%)	82/82 (100%)
Sidechain	750/750 (100%)	484/484 (100%)	219/219 (100%)	47/47 (100%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	60/60 (100%)	29/29 (100%)	30/30 (100%)	1/1 (100%)
Overall	1241/1241 (100%)	688/688 (100%)	423/423 (100%)	130/130 (100%)

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	2	THR	HG1	999.00	0.08 – 2.19	4729.2
1	A	34	THR	HG1	999.00	0.08 – 2.19	4729.2
1	A	86	THR	HG1	999.00	0.08 – 2.19	4729.2
1	A	1	SER	HB2	999.00	2.61 – 5.13	3948.9
1	A	1	SER	HB3	999.00	2.49 – 5.20	3672.2
1	A	5	ARG	HH22	999.00	5.04 – 8.54	2834.9
1	A	9	ARG	HH22	999.00	5.04 – 8.54	2834.9
1	A	17	ARG	HH22	999.00	5.04 – 8.54	2834.9
1	A	22	ARG	HH22	999.00	5.04 – 8.54	2834.9
1	A	26	ARG	HH22	999.00	5.04 – 8.54	2834.9
1	A	38	ARG	HH22	999.00	5.04 – 8.54	2834.9
1	A	55	ARG	HH22	999.00	5.04 – 8.54	2834.9
1	A	62	ARG	HH22	999.00	5.04 – 8.54	2834.9
1	A	65	ARG	HH22	999.00	5.04 – 8.54	2834.9
1	A	82	ARG	HH22	999.00	5.04 – 8.54	2834.9
1	A	5	ARG	HH12	999.00	5.04 – 8.65	2748.4
1	A	9	ARG	HH12	999.00	5.04 – 8.65	2748.4
1	A	17	ARG	HH12	999.00	5.04 – 8.65	2748.4
1	A	22	ARG	HH12	999.00	5.04 – 8.65	2748.4
1	A	26	ARG	HH12	999.00	5.04 – 8.65	2748.4
1	A	38	ARG	HH12	999.00	5.04 – 8.65	2748.4
1	A	55	ARG	HH12	999.00	5.04 – 8.65	2748.4
1	A	62	ARG	HH12	999.00	5.04 – 8.65	2748.4
1	A	65	ARG	HH12	999.00	5.04 – 8.65	2748.4
1	A	82	ARG	HH12	999.00	5.04 – 8.65	2748.4
1	A	1	SER	HA	999.00	2.50 – 6.44	2524.2
1	A	5	ARG	HH21	999.00	4.81 – 8.80	2486.7
1	A	9	ARG	HH21	999.00	4.81 – 8.80	2486.7
1	A	17	ARG	HH21	999.00	4.81 – 8.80	2486.7
1	A	22	ARG	HH21	999.00	4.81 – 8.80	2486.7
1	A	26	ARG	HH21	999.00	4.81 – 8.80	2486.7
1	A	38	ARG	HH21	999.00	4.81 – 8.80	2486.7

Continued on next page...

Continued from previous page...

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	55	ARG	HH21	999.00	4.81 – 8.80	2486.7
1	A	62	ARG	HH21	999.00	4.81 – 8.80	2486.7
1	A	65	ARG	HH21	999.00	4.81 – 8.80	2486.7
1	A	82	ARG	HH21	999.00	4.81 – 8.80	2486.7
1	A	31	PHE	HZ	999.00	4.94 – 9.06	2407.8
1	A	53	PHE	HZ	999.00	4.94 – 9.06	2407.8
1	A	81	PHE	HZ	999.00	4.94 – 9.06	2407.8
1	A	5	ARG	HH11	999.00	4.72 – 9.08	2275.5
1	A	9	ARG	HH11	999.00	4.72 – 9.08	2275.5
1	A	17	ARG	HH11	999.00	4.72 – 9.08	2275.5
1	A	22	ARG	HH11	999.00	4.72 – 9.08	2275.5
1	A	26	ARG	HH11	999.00	4.72 – 9.08	2275.5
1	A	38	ARG	HH11	999.00	4.72 – 9.08	2275.5
1	A	55	ARG	HH11	999.00	4.72 – 9.08	2275.5
1	A	62	ARG	HH11	999.00	4.72 – 9.08	2275.5
1	A	65	ARG	HH11	999.00	4.72 – 9.08	2275.5
1	A	82	ARG	HH11	999.00	4.72 – 9.08	2275.5
1	A	35	SER	H	999.00	5.45 – 11.10	1753.5
1	A	5	ARG	HE	999.00	4.52 – 10.19	1748.9
1	A	9	ARG	HE	999.00	4.52 – 10.19	1748.9
1	A	17	ARG	HE	999.00	4.52 – 10.19	1748.9
1	A	22	ARG	HE	999.00	4.52 – 10.19	1748.9
1	A	26	ARG	HE	999.00	4.52 – 10.19	1748.9
1	A	38	ARG	HE	999.00	4.52 – 10.19	1748.9
1	A	55	ARG	HE	999.00	4.52 – 10.19	1748.9
1	A	62	ARG	HE	999.00	4.52 – 10.19	1748.9
1	A	65	ARG	HE	999.00	4.52 – 10.19	1748.9
1	A	82	ARG	HE	999.00	4.52 – 10.19	1748.9
1	A	2	THR	H	999.00	5.19 – 11.27	1629.6
1	A	30	LYS	CE	999.00	37.57 – 46.21	1107.8
1	A	1	SER	HG	999.00	0.07 – 10.62	941.9
1	A	8	SER	HG	999.00	0.07 – 10.62	941.9
1	A	35	SER	HG	999.00	0.07 – 10.62	941.9
1	A	46	SER	HG	999.00	0.07 – 10.62	941.9
1	A	73	SER	HG	999.00	0.07 – 10.62	941.9
1	A	11	GLN	CD	999.00	173.59 – 185.85	668.3
1	A	13	GLN	CD	999.00	173.59 – 185.85	668.3
1	A	19	GLN	CD	999.00	173.59 – 185.85	668.3
1	A	43	GLN	CD	999.00	173.59 – 185.85	668.3
1	A	48	GLN	CD	999.00	173.59 – 185.85	668.3
1	A	88	GLN	CD	999.00	173.59 – 185.85	668.3
1	A	1	SER	CB	999.00	56.28 – 71.32	621.8

Continued on next page...

Continued from previous page...

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	14	TYR	HH	999.00	0.99 – 17.18	611.4
1	A	66	TYR	HH	999.00	0.99 – 17.18	611.4
1	A	31	PHE	CZ	999.00	121.82 – 136.66	586.1
1	A	53	PHE	CZ	999.00	121.82 – 136.66	586.1
1	A	81	PHE	CZ	999.00	121.82 – 136.66	586.1
1	A	5	ARG	NE	999.00	76.53 – 92.65	567.2
1	A	9	ARG	NE	999.00	76.53 – 92.65	567.2
1	A	17	ARG	NE	999.00	76.53 – 92.65	567.2
1	A	22	ARG	NE	999.00	76.53 – 92.65	567.2
1	A	26	ARG	NE	999.00	76.53 – 92.65	567.2
1	A	38	ARG	NE	999.00	76.53 – 92.65	567.2
1	A	55	ARG	NE	999.00	76.53 – 92.65	567.2
1	A	62	ARG	NE	999.00	76.53 – 92.65	567.2
1	A	65	ARG	NE	999.00	76.53 – 92.65	567.2
1	A	82	ARG	NE	999.00	76.53 – 92.65	567.2
1	A	1	SER	C	999.00	166.15 – 183.14	485.2
1	A	64	TRP	CG	999.00	101.31 – 120.62	459.9
1	A	1	SER	CA	999.00	48.46 – 68.96	458.7
1	A	64	TRP	CD2	999.00	118.40 – 137.65	452.4
1	A	24	GLU	CD	999.00	171.45 – 193.13	376.7
1	A	40	GLU	CD	999.00	171.45 – 193.13	376.7
1	A	54	GLU	CD	999.00	171.45 – 193.13	376.7
1	A	56	GLU	CD	999.00	171.45 – 193.13	376.7
1	A	67	GLU	CD	999.00	171.45 – 193.13	376.7
1	A	90	GLU	CD	999.00	171.45 – 193.13	376.7
1	A	28	LYS	NZ	999.00	19.79 – 46.09	367.3
1	A	30	LYS	NZ	999.00	19.79 – 46.09	367.3
1	A	58	LYS	NZ	999.00	19.79 – 46.09	367.3
1	A	63	LYS	NZ	999.00	19.79 – 46.09	367.3
1	A	70	LYS	NZ	999.00	19.79 – 46.09	367.3
1	A	10	ASN	CG	999.00	164.52 – 188.90	337.3
1	A	41	ASN	CG	999.00	164.52 – 188.90	337.3
1	A	51	ASN	CG	999.00	164.52 – 188.90	337.3
1	A	59	ASN	CG	999.00	164.52 – 188.90	337.3
1	A	78	ASN	CG	999.00	164.52 – 188.90	337.3
1	A	84	ASN	CG	999.00	164.52 – 188.90	337.3
1	A	14	TYR	CZ	999.00	143.41 – 170.10	315.6
1	A	66	TYR	CZ	999.00	143.41 – 170.10	315.6
1	A	5	ARG	NH2	999.00	57.68 – 87.89	306.6
1	A	9	ARG	NH2	999.00	57.68 – 87.89	306.6
1	A	17	ARG	NH2	999.00	57.68 – 87.89	306.6
1	A	22	ARG	NH2	999.00	57.68 – 87.89	306.6

Continued on next page...

Continued from previous page...

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	26	ARG	NH2	999.00	57.68 – 87.89	306.6
1	A	38	ARG	NH2	999.00	57.68 – 87.89	306.6
1	A	55	ARG	NH2	999.00	57.68 – 87.89	306.6
1	A	62	ARG	NH2	999.00	57.68 – 87.89	306.6
1	A	65	ARG	NH2	999.00	57.68 – 87.89	306.6
1	A	82	ARG	NH2	999.00	57.68 – 87.89	306.6
1	A	31	PHE	CG	999.00	123.09 – 153.41	284.0
1	A	53	PHE	CG	999.00	123.09 – 153.41	284.0
1	A	81	PHE	CG	999.00	123.09 – 153.41	284.0
1	A	1	SER	N	999.00	99.14 – 133.45	257.3
1	A	35	SER	N	999.00	99.14 – 133.45	257.3
1	A	14	TYR	CG	999.00	112.42 – 146.96	251.7
1	A	66	TYR	CG	999.00	112.42 – 146.96	251.7
1	A	5	ARG	CZ	999.00	141.81 – 177.93	232.3
1	A	9	ARG	CZ	999.00	141.81 – 177.93	232.3
1	A	17	ARG	CZ	999.00	141.81 – 177.93	232.3
1	A	22	ARG	CZ	999.00	141.81 – 177.93	232.3
1	A	26	ARG	CZ	999.00	141.81 – 177.93	232.3
1	A	38	ARG	CZ	999.00	141.81 – 177.93	232.3
1	A	55	ARG	CZ	999.00	141.81 – 177.93	232.3
1	A	62	ARG	CZ	999.00	141.81 – 177.93	232.3
1	A	65	ARG	CZ	999.00	141.81 – 177.93	232.3
1	A	82	ARG	CZ	999.00	141.81 – 177.93	232.3
1	A	2	THR	N	999.00	91.89 – 138.78	188.4
1	A	5	ARG	NH1	999.00	49.05 – 99.42	183.6
1	A	9	ARG	NH1	999.00	49.05 – 99.42	183.6
1	A	17	ARG	NH1	999.00	49.05 – 99.42	183.6
1	A	22	ARG	NH1	999.00	49.05 – 99.42	183.6
1	A	26	ARG	NH1	999.00	49.05 – 99.42	183.6
1	A	38	ARG	NH1	999.00	49.05 – 99.42	183.6
1	A	55	ARG	NH1	999.00	49.05 – 99.42	183.6
1	A	62	ARG	NH1	999.00	49.05 – 99.42	183.6
1	A	65	ARG	NH1	999.00	49.05 – 99.42	183.6
1	A	82	ARG	NH1	999.00	49.05 – 99.42	183.6
1	A	4	PRO	N	999.00	108.67 – 162.11	161.6
1	A	12	PRO	N	999.00	108.67 – 162.11	161.6
1	A	15	PRO	N	999.00	108.67 – 162.11	161.6
1	A	49	PRO	N	999.00	108.67 – 162.11	161.6
1	A	71	PRO	N	999.00	108.67 – 162.11	161.6
1	A	32	ASP	CG	999.00	149.18 – 208.82	137.5
1	A	64	TRP	CE2	999.00	105.29 – 170.61	131.8
1	A	9	ARG	HB2	-0.59	0.52 – 3.08	-9.3

Continued on next page...

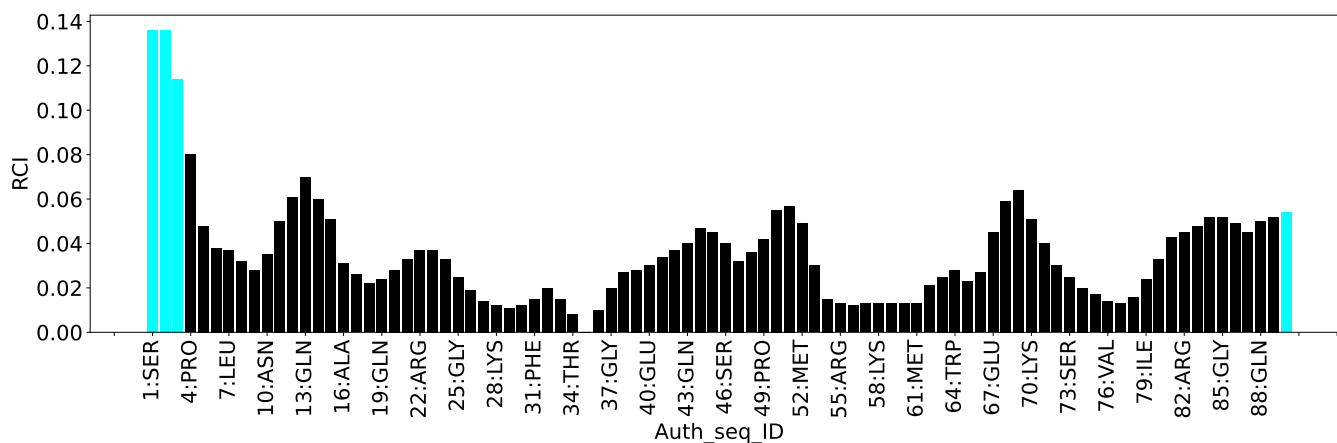
Continued from previous page...

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	61	MET	HG2	-0.44	0.65 – 4.19	-8.1
1	A	9	ARG	HD2	1.56	1.97 – 4.26	-6.8
1	A	61	MET	HA	1.89	2.11 – 6.67	-5.5

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	1541
Intra-residue ($ i-j =0$)	366
Sequential ($ i-j =1$)	436
Medium range ($ i-j >1$ and $ i-j <5$)	190
Long range ($ i-j \geq 5$)	549
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	273
Number of unmapped restraints	0
Number of restraints per residue	20.2
Number of long range restraints per residue ¹	6.1

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	17.8	0.2
0.2-0.5 (Medium)	25.9	0.5
>0.5 (Large)	24.4	2.35

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)	0.8	5.12
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis [i](#)

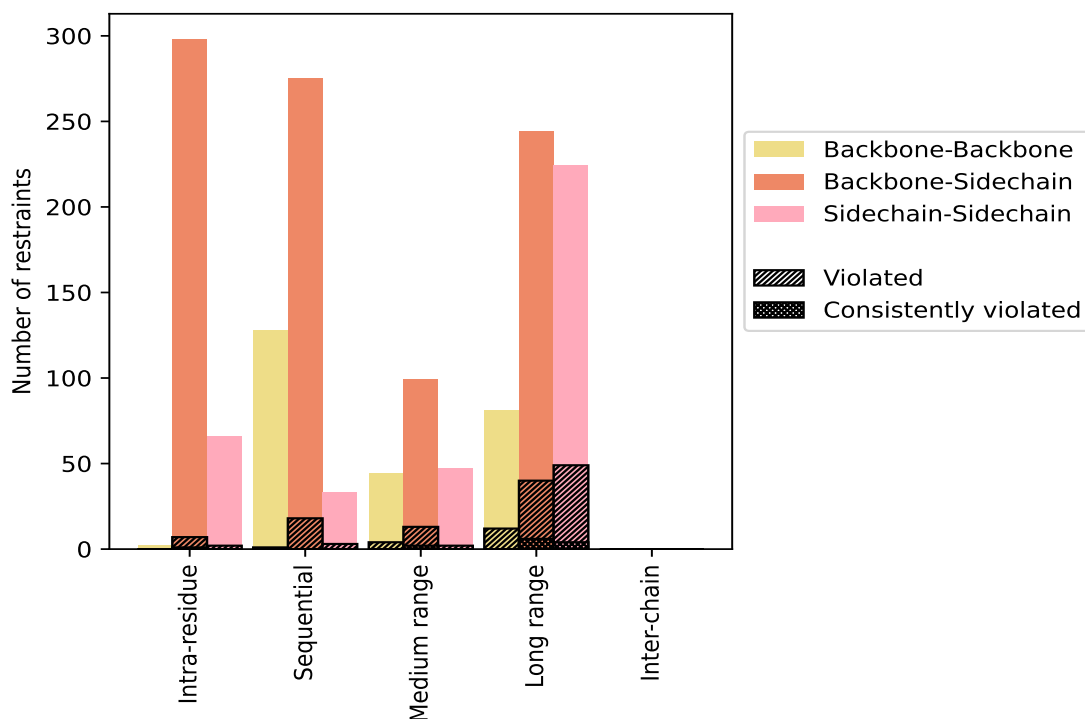
9.1 Summary of distance violations [i](#)

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	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	366	23.8	9	2.5	0.6	1	0.3	0.1
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	298	19.3	7	2.3	0.5	1	0.3	0.1
Sidechain-Sidechain	66	4.3	2	3.0	0.1	0	0.0	0.0
Sequential ($i-j =1$)	436	28.3	22	5.0	1.4	0	0.0	0.0
Backbone-Backbone	128	8.3	1	0.8	0.1	0	0.0	0.0
Backbone-Sidechain	275	17.8	18	6.5	1.2	0	0.0	0.0
Sidechain-Sidechain	33	2.1	3	9.1	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	190	12.3	19	10.0	1.2	2	1.1	0.1
Backbone-Backbone	44	2.9	4	9.1	0.3	0	0.0	0.0
Backbone-Sidechain	99	6.4	13	13.1	0.8	2	2.0	0.1
Sidechain-Sidechain	47	3.0	2	4.3	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	549	35.6	101	18.4	6.6	10	1.8	0.6
Backbone-Backbone	81	5.3	12	14.8	0.8	0	0.0	0.0
Backbone-Sidechain	244	15.8	40	16.4	2.6	6	2.5	0.4
Sidechain-Sidechain	224	14.5	49	21.9	3.2	4	1.8	0.3
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1541	100.0	151	9.8	9.8	13	0.8	0.8
Backbone-Backbone	255	16.5	17	6.7	1.1	0	0.0	0.0
Backbone-Sidechain	916	59.4	78	8.5	5.1	9	1.0	0.6
Sidechain-Sidechain	370	24.0	56	15.1	3.6	4	1.1	0.3

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfid bonds are counted in their appropriate category on the x-axis

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	5	10	9	46	0	70	0.55	2.27	0.48	0.4
2	3	11	9	48	0	71	0.56	2.21	0.46	0.39
3	5	11	10	48	0	74	0.53	2.22	0.48	0.32
4	4	11	7	48	0	70	0.55	2.29	0.5	0.32
5	6	8	9	42	0	65	0.54	2.25	0.48	0.34
6	5	8	7	45	0	65	0.52	2.32	0.45	0.34
7	1	11	8	36	0	56	0.47	2.2	0.44	0.3
8	5	11	12	49	0	77	0.53	2.24	0.49	0.32
9	6	10	11	47	0	74	0.45	2.21	0.44	0.28
10	5	10	12	54	0	81	0.52	2.24	0.47	0.32

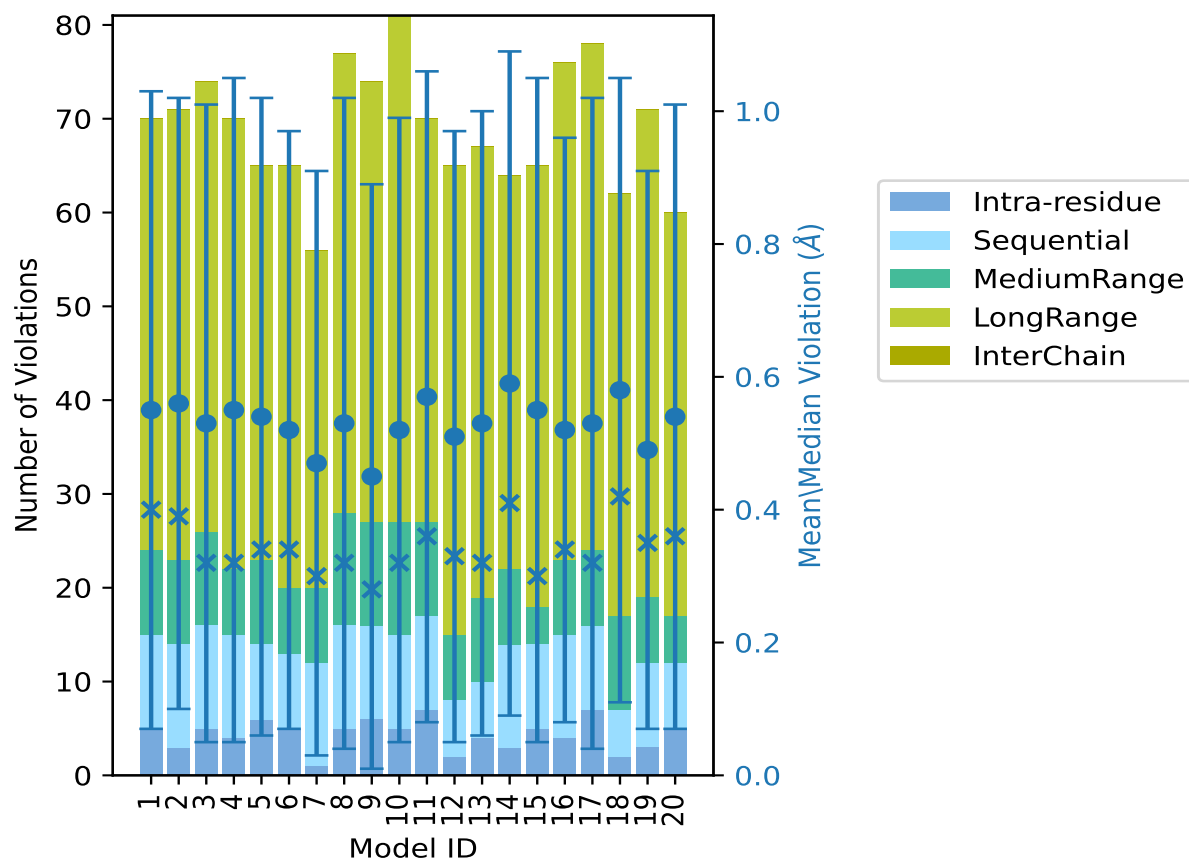
Continued on next page...

Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	7	10	10	43	0	70	0.57	2.25	0.49	0.36
12	2	6	7	50	0	65	0.51	2.3	0.46	0.33
13	4	6	9	48	0	67	0.53	2.16	0.47	0.32
14	3	11	8	42	0	64	0.59	2.26	0.5	0.41
15	5	9	4	47	0	65	0.55	2.29	0.5	0.3
16	4	11	8	53	0	76	0.52	2.27	0.44	0.34
17	7	9	8	54	0	78	0.53	2.26	0.49	0.32
18	2	5	10	45	0	62	0.58	2.25	0.47	0.42
19	3	9	7	52	0	71	0.49	2.23	0.42	0.35
20	5	7	5	43	0	60	0.54	2.35	0.47	0.36

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

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



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

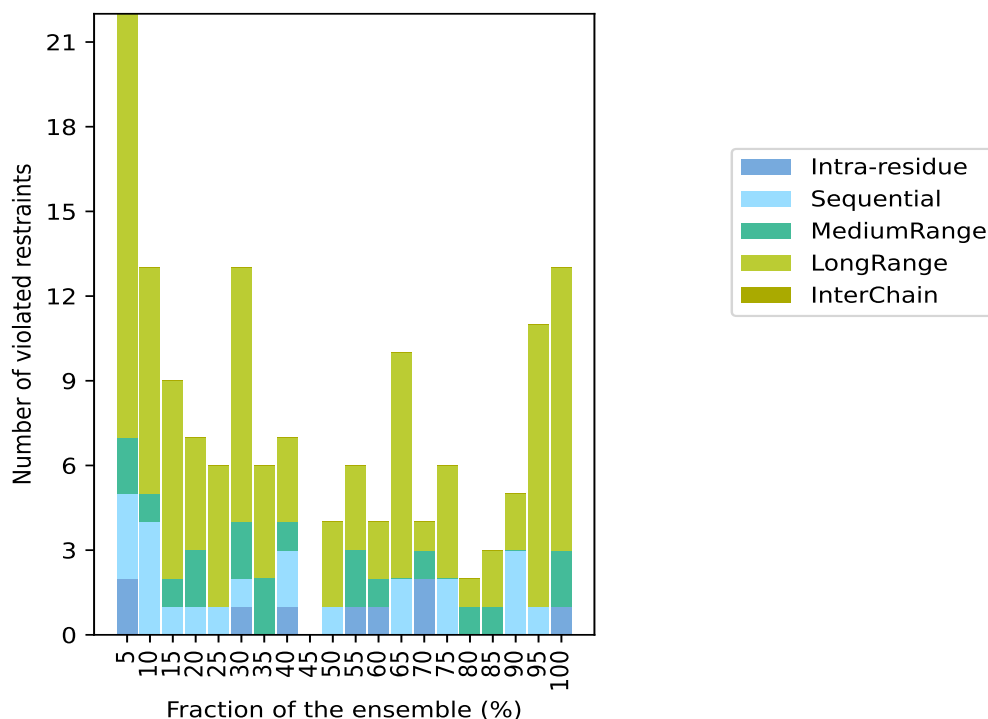
9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1390(IR:357, SQ:414, MR:171, LR:448, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
2	3	2	15	0	22	1	5.0
0	4	1	8	0	13	2	10.0
0	1	1	7	0	9	3	15.0
0	1	2	4	0	7	4	20.0
0	1	0	5	0	6	5	25.0
1	1	2	9	0	13	6	30.0
0	0	2	4	0	6	7	35.0
1	2	1	3	0	7	8	40.0
0	0	0	0	0	0	9	45.0
0	1	0	3	0	4	10	50.0
1	0	2	3	0	6	11	55.0
1	0	1	2	0	4	12	60.0
0	2	0	8	0	10	13	65.0
2	0	1	1	0	4	14	70.0
0	2	0	4	0	6	15	75.0
0	0	1	1	0	2	16	80.0
0	0	1	2	0	3	17	85.0
0	3	0	2	0	5	18	90.0
0	1	0	10	0	11	19	95.0
1	0	2	10	0	13	20	100.0

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

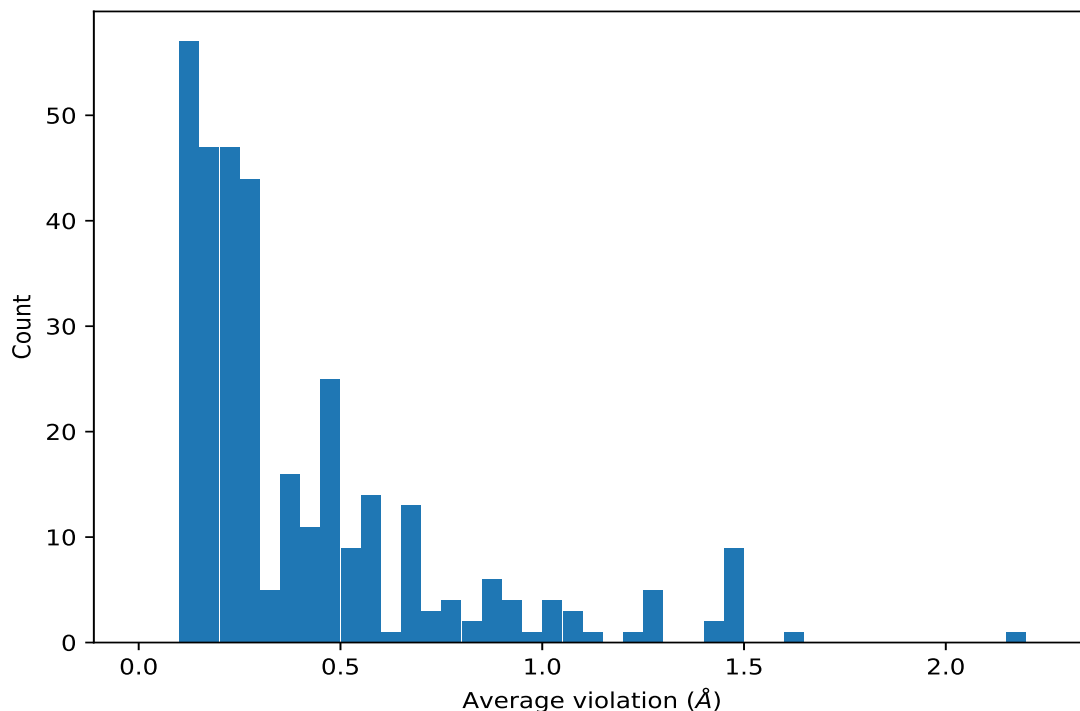
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

The following table provides the mean and the standard deviation of the 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 ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,646)	1:9:A:ARG:HG2	1:64:A:TRP:H	20	2.19	0.27	2.25
(1,737)	1:9:A:ARG:HG3	1:66:A:TYR:HA	20	1.61	0.28	1.67
(1,1130)	1:79:A:ILE:HG21	1:89:A:ILE:HD11	20	1.48	0.38	1.4
(1,1130)	1:79:A:ILE:HG21	1:89:A:ILE:HD12	20	1.48	0.38	1.4
(1,1130)	1:79:A:ILE:HG21	1:89:A:ILE:HD13	20	1.48	0.38	1.4
(1,1130)	1:79:A:ILE:HG22	1:89:A:ILE:HD11	20	1.48	0.38	1.4
(1,1130)	1:79:A:ILE:HG22	1:89:A:ILE:HD12	20	1.48	0.38	1.4
(1,1130)	1:79:A:ILE:HG22	1:89:A:ILE:HD13	20	1.48	0.38	1.4
(1,1130)	1:79:A:ILE:HG23	1:89:A:ILE:HD11	20	1.48	0.38	1.4
(1,1130)	1:79:A:ILE:HG23	1:89:A:ILE:HD12	20	1.48	0.38	1.4
(1,1130)	1:79:A:ILE:HG23	1:89:A:ILE:HD13	20	1.48	0.38	1.4
(1,1191)	1:12:A:PRO:HG2	1:57:A:VAL:HA	20	1.28	0.16	1.25
(1,1191)	1:12:A:PRO:HG3	1:57:A:VAL:HA	20	1.28	0.16	1.25
(1,1085)	1:10:A:ASN:HB2	1:63:A:LYS:HB2	20	1.26	0.4	1.44
(1,678)	1:64:A:TRP:H	1:66:A:TYR:HE1	20	1.25	0.24	1.4
(1,678)	1:64:A:TRP:H	1:66:A:TYR:HE2	20	1.25	0.24	1.4

Continued on next page...

Continued from previous page...

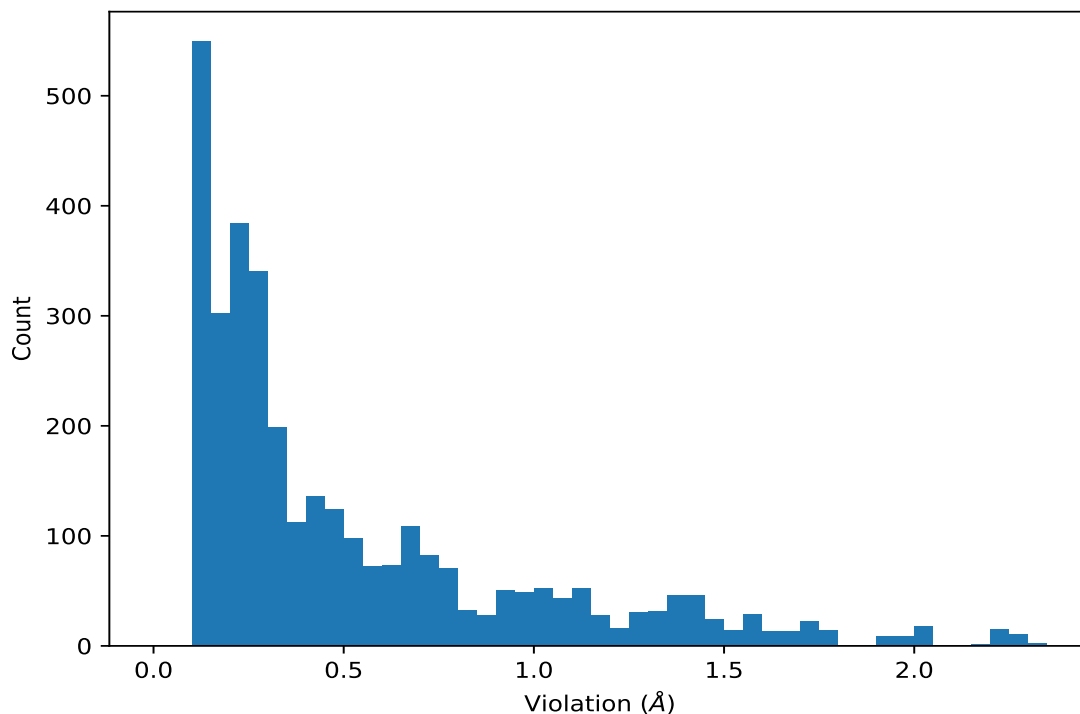
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,546)	1:10:A:ASN:HB2	1:64:A:TRP:HE1	20	1.24	0.18	1.34
(1,1133)	1:40:A:GLU:H	1:61:A:MET:HE1	20	1.06	0.26	1.02
(1,1133)	1:40:A:GLU:H	1:61:A:MET:HE2	20	1.06	0.26	1.02
(1,1133)	1:40:A:GLU:H	1:61:A:MET:HE3	20	1.06	0.26	1.02
(1,761)	1:18:A:ALA:HA	1:23:A:ILE:HB	20	1.01	0.3	1.12
(1,727)	1:7:A:LEU:HD11	1:65:A:ARG:HB2	20	0.66	0.3	0.69

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

The following table 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)
(1,646)	1:9:A:ARG:HG2	1:64:A:TRP:H	20	2.35
(1,646)	1:9:A:ARG:HG2	1:64:A:TRP:H	6	2.32
(1,646)	1:9:A:ARG:HG2	1:64:A:TRP:H	12	2.3
(1,646)	1:9:A:ARG:HG2	1:64:A:TRP:H	4	2.29
(1,646)	1:9:A:ARG:HG2	1:64:A:TRP:H	15	2.29
(1,646)	1:9:A:ARG:HG2	1:64:A:TRP:H	1	2.27
(1,646)	1:9:A:ARG:HG2	1:64:A:TRP:H	16	2.27
(1,646)	1:9:A:ARG:HG2	1:64:A:TRP:H	14	2.26
(1,646)	1:9:A:ARG:HG2	1:64:A:TRP:H	17	2.26
(1,646)	1:9:A:ARG:HG2	1:64:A:TRP:H	5	2.25

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

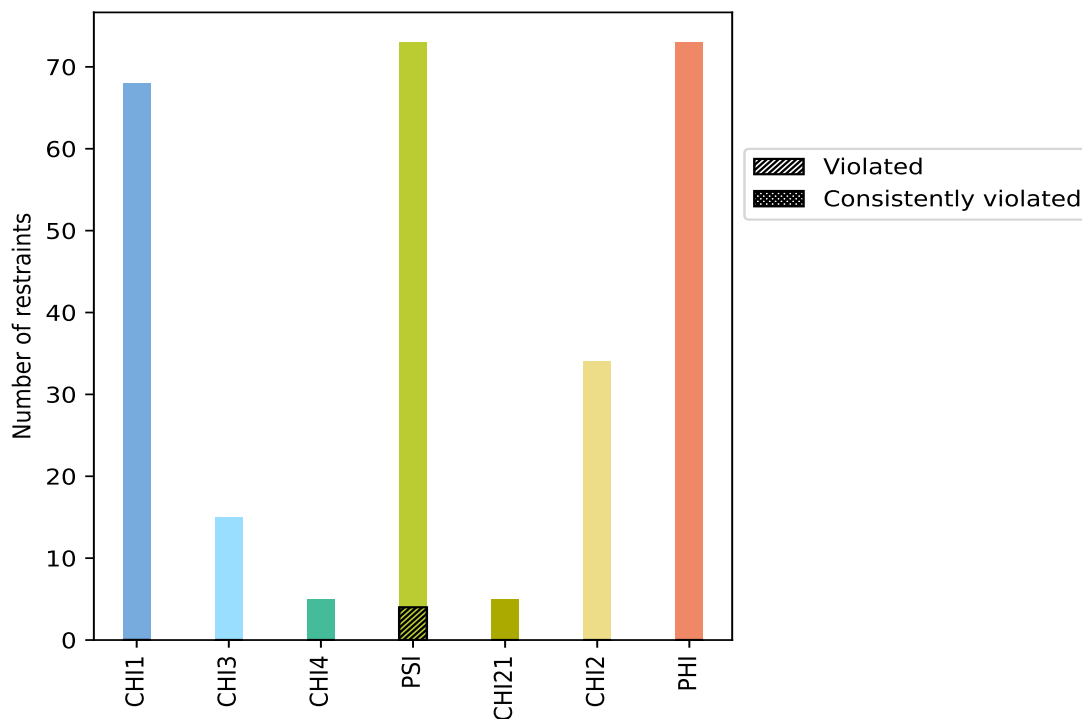
10.1 Summary of dihedral-angle violations [i](#)

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	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
CHI1	68	24.9	0	0.0	0.0	0	0.0	0.0
CHI3	15	5.5	0	0.0	0.0	0	0.0	0.0
CHI4	5	1.8	0	0.0	0.0	0	0.0	0.0
PSI	73	26.7	4	5.5	1.5	0	0.0	0.0
CHI21	5	1.8	0	0.0	0.0	0	0.0	0.0
CHI2	34	12.5	0	0.0	0.0	0	0.0	0.0
PHI	73	26.7	0	0.0	0.0	0	0.0	0.0
Total	273	100.0	4	1.5	1.5	0	0.0	0.0

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

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



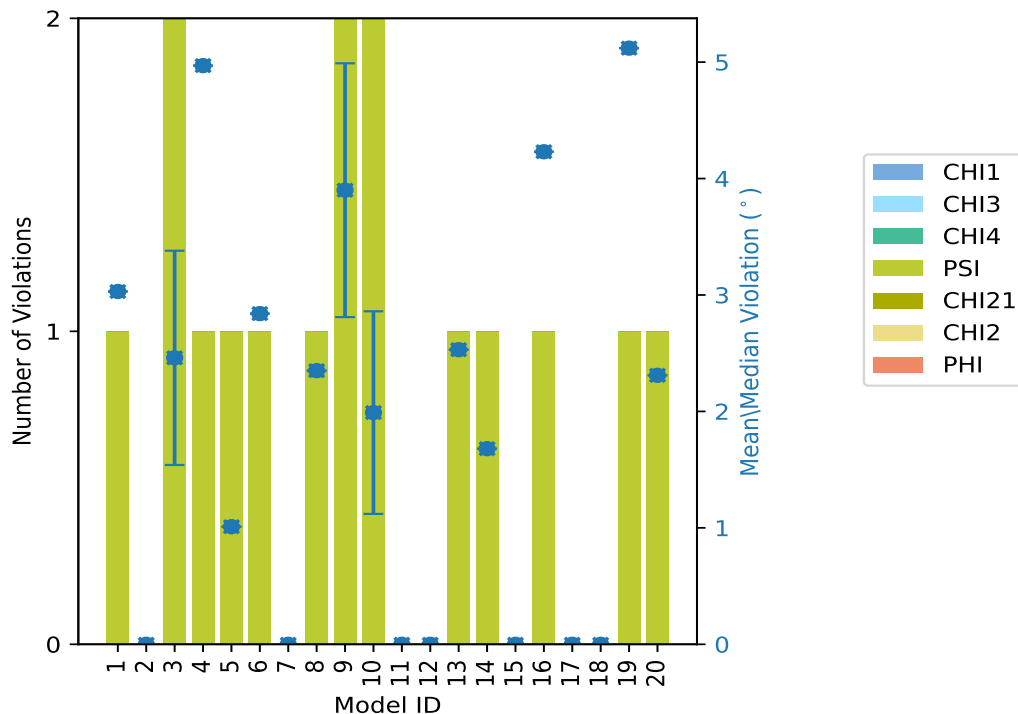
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	CHI1	CHI3	CHI4	PSI	CHI21	CHI2	PHI	Total				
1	0	0	0	1	0	0	0	1	3.03	3.03	0.0	3.03
2	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	2	0	0	0	2	2.46	3.37	0.92	2.46
4	0	0	0	1	0	0	0	1	4.97	4.97	0.0	4.97
5	0	0	0	1	0	0	0	1	1.01	1.01	0.0	1.01
6	0	0	0	1	0	0	0	1	2.84	2.84	0.0	2.84
7	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	1	0	0	0	1	2.35	2.35	0.0	2.35
9	0	0	0	2	0	0	0	2	3.9	4.99	1.09	3.9
10	0	0	0	2	0	0	0	2	1.99	2.86	0.87	1.99
11	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	1	0	0	0	1	2.53	2.53	0.0	2.53
14	0	0	0	1	0	0	0	1	1.68	1.68	0.0	1.68
15	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	1	0	0	0	1	4.23	4.23	0.0	4.23
17	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	1	0	0	0	1	5.12	5.12	0.0	5.12
20	0	0	0	1	0	0	0	1	2.31	2.31	0.0	2.31

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

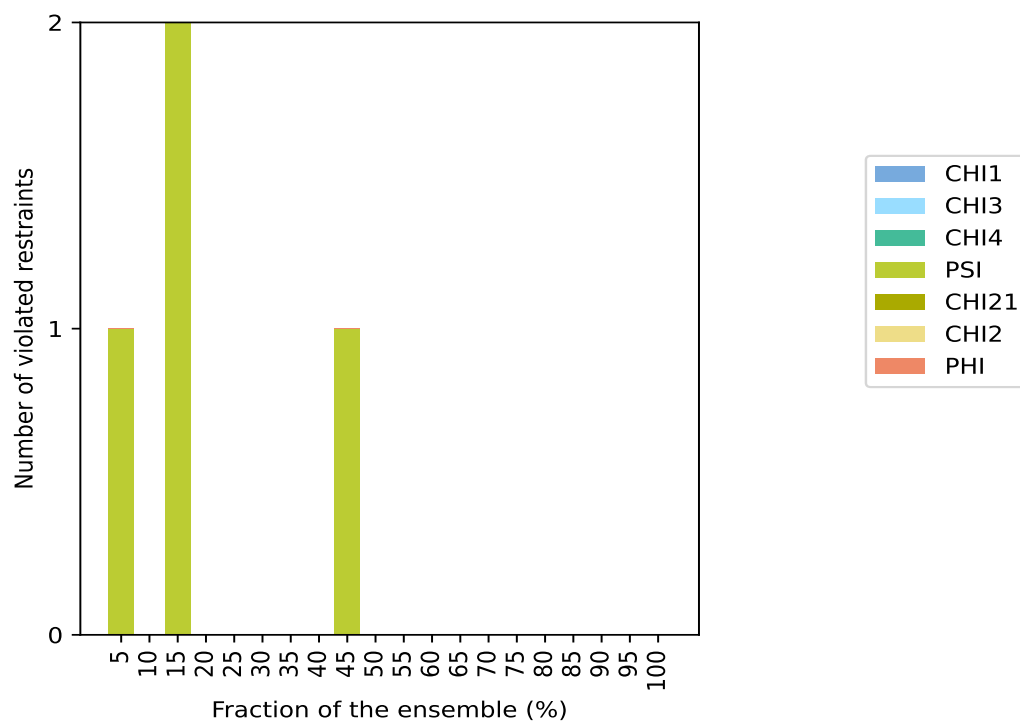
10.3 Dihedral-angle violation statistics for the ensemble

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	
CHI1	CHI3	CHI4	PSI	CHI21	CHI2	PHI	Total	Count ¹	%
0	0	0	1	0	0	0	1	1	5.0
0	0	0	0	0	0	0	0	2	10.0
0	0	0	2	0	0	0	2	3	15.0
0	0	0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	0	0	8	40.0
0	0	0	1	0	0	0	1	9	45.0
0	0	0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	0	0	20	100.0

¹ Number of models with violations

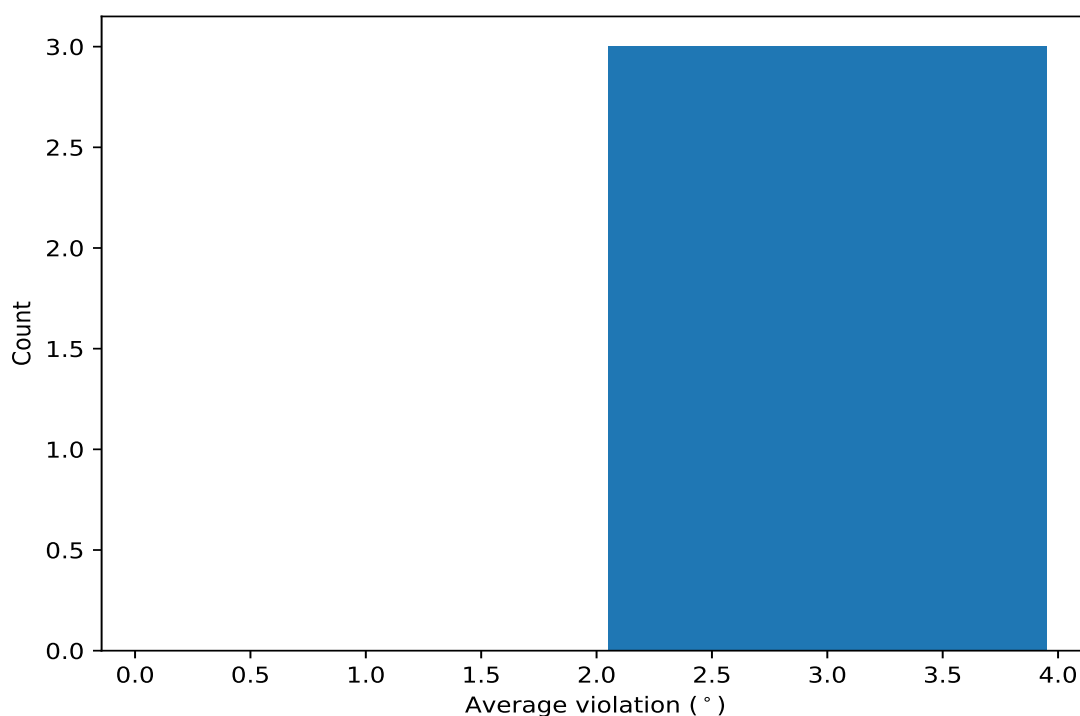
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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.

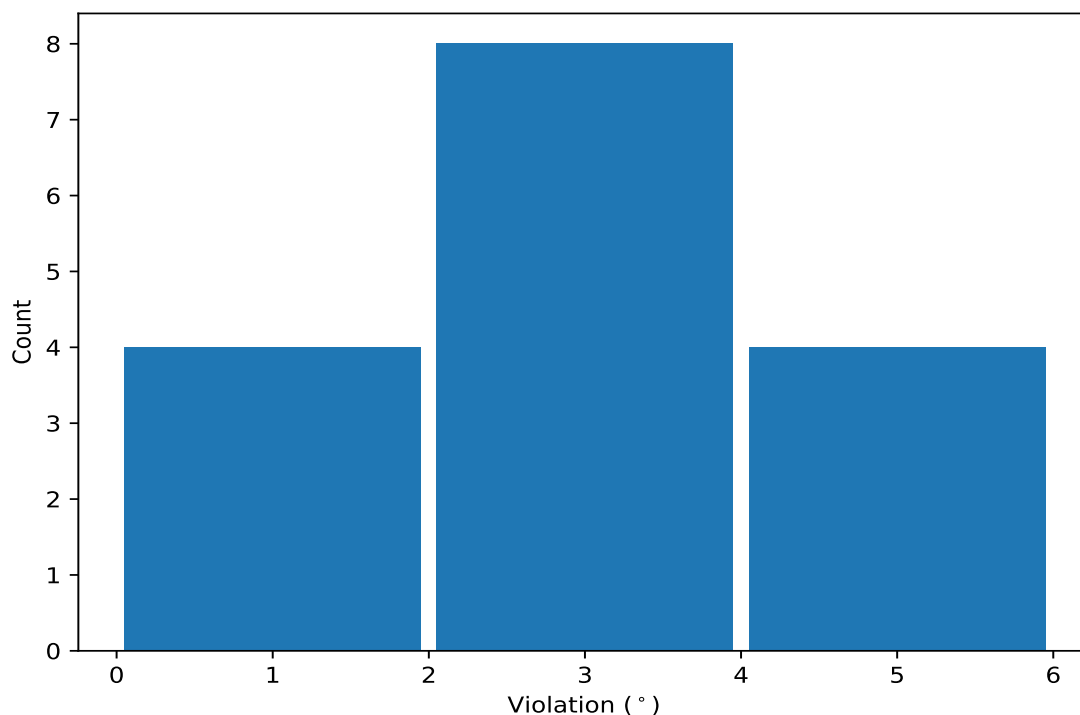
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,141)	1:87:A:ALA:N	1:87:A:ALA:CA	1:87:A:ALA:C	1:88:A:GLN:N	9	3.32	1.46	3.03
(1,15)	1:10:A:ASN:N	1:10:A:ASN:CA	1:10:A:ASN:C	1:11:A:GLN:N	3	2.46	0.55	2.84
(1,113)	1:67:A:GLU:N	1:67:A:GLU:CA	1:67:A:GLU:C	1:68:A:ALA:N	3	2.4	1.01	2.81

¹ Number of violated models, ²Standard 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 provides the list of violations for 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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,141)	1:87:A:ALA:N	1:87:A:ALA:CA	1:87:A:ALA:C	1:88:A:GLN:N	19	5.12
(1,141)	1:87:A:ALA:N	1:87:A:ALA:CA	1:87:A:ALA:C	1:88:A:GLN:N	9	4.99
(1,141)	1:87:A:ALA:N	1:87:A:ALA:CA	1:87:A:ALA:C	1:88:A:GLN:N	4	4.97
(1,141)	1:87:A:ALA:N	1:87:A:ALA:CA	1:87:A:ALA:C	1:88:A:GLN:N	16	4.23
(1,113)	1:67:A:GLU:N	1:67:A:GLU:CA	1:67:A:GLU:C	1:68:A:ALA:N	3	3.37
(1,141)	1:87:A:ALA:N	1:87:A:ALA:CA	1:87:A:ALA:C	1:88:A:GLN:N	1	3.03
(1,15)	1:10:A:ASN:N	1:10:A:ASN:CA	1:10:A:ASN:C	1:11:A:GLN:N	10	2.86
(1,15)	1:10:A:ASN:N	1:10:A:ASN:CA	1:10:A:ASN:C	1:11:A:GLN:N	6	2.84
(1,113)	1:67:A:GLU:N	1:67:A:GLU:CA	1:67:A:GLU:C	1:68:A:ALA:N	9	2.81
(1,141)	1:87:A:ALA:N	1:87:A:ALA:CA	1:87:A:ALA:C	1:88:A:GLN:N	13	2.53