wwPDB NMR Structure Validation Summary Report

May 23, 2024 – 11:11 AM EDT

PDB ID	:	8UNG
BMRB ID	:	31120
Title	:	Solution structure of toxin, U-RDTX-Pp19, from assassin bug Pristhesancus plagipennis
Authors	:	Chin, Y.K.Y.; Walker, A.A.; King, G.F.
Deposited on	:	2023-10-18

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 (i) 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 (1)) were used in the production of this report:

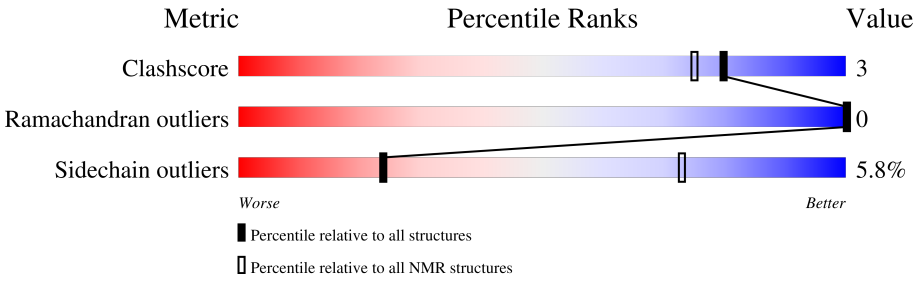
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	41	76% 5% 20%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:5-A:37 (33)	0.23	4

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 5 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 579 atoms, of which 276 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Venom peptide Pp19a.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	41	579	184	276	54	57	8	0

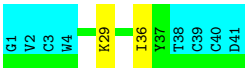
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Venom peptide Pp19a

Chain A:

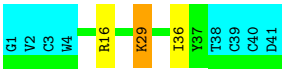


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 4. Colouring as in section 4.1 above.

- Molecule 1: Venom peptide Pp19a

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 30 calculated structures, 20 were deposited, based on the following criterion: *Stereochemical properties*.

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

Software name	Classification	Version
CYANA	structure calculation	
CYANA	refinement	
TALOS-N	geometry optimization	

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	594
Number of shifts mapped to atoms	594
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

6.1 Standard geometry

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

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	245	231	231	1±1
All	All	4900	4620	4620	26

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:LYS:HB3	1:A:36:ILE:HD12	0.58	1.75	17	12
1:A:29:LYS:CB	1:A:36:ILE:HD12	0.45	2.40	2	12
1:A:6:THR:O	1:A:36:ILE:HG23	0.41	2.16	2	2

6.3 Torsion angles

6.3.1 Protein backbone

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	33/41 (80%)	31±0 (95±1%)	2±0 (5±1%)	0±0 (0±0%)	100	100
All	All	660/820 (80%)	624 (95%)	36 (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	25/32 (78%)	24±1 (94±4%)	1±1 (6±4%)	24	73
All	All	500/640 (78%)	471 (94%)	29 (6%)	24	73

5 of 9 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	16	ARG	9
1	A	29	LYS	9
1	A	18	CYS	4
1	A	6	THR	2
1	A	23	MET	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

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_chemical_shifts_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	594
Number of shifts mapped to atoms	594
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	97

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	2	VAL	HG11	999.000	0.000	1
1	A	2	VAL	HG12	999.000	0.000	1
1	A	2	VAL	HG13	999.000	0.000	1
1	A	2	VAL	HG21	999.000	0.000	1
1	A	2	VAL	HG22	999.000	0.000	1
1	A	2	VAL	HG23	999.000	0.000	1
1	A	6	THR	HG21	999.000	0.000	1
1	A	6	THR	HG22	999.000	0.000	1
1	A	6	THR	HG23	999.000	0.000	1
1	A	10	LEU	HD11	999.000	0.000	2
1	A	10	LEU	HD12	999.000	0.000	2
1	A	10	LEU	HD13	999.000	0.000	2
1	A	10	LEU	HD21	999.000	0.000	2
1	A	10	LEU	HD22	999.000	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	10	LEU	HD23	999.000	0.000	2
1	A	12	ALA	HB1	999.000	0.000	1
1	A	12	ALA	HB2	999.000	0.000	1
1	A	12	ALA	HB3	999.000	0.000	1
1	A	14	ALA	HB1	999.000	0.000	1
1	A	14	ALA	HB2	999.000	0.000	1
1	A	14	ALA	HB3	999.000	0.000	1
1	A	15	VAL	HG11	999.000	0.000	1
1	A	15	VAL	HG12	999.000	0.000	1
1	A	15	VAL	HG13	999.000	0.000	1
1	A	15	VAL	HG21	999.000	0.000	1
1	A	15	VAL	HG22	999.000	0.000	1
1	A	15	VAL	HG23	999.000	0.000	1
1	A	19	ALA	HB1	999.000	0.000	1
1	A	19	ALA	HB2	999.000	0.000	1
1	A	19	ALA	HB3	999.000	0.000	1
1	A	23	MET	HE1	999.000	0.000	1
1	A	23	MET	HE2	999.000	0.000	1
1	A	23	MET	HE3	999.000	0.000	1
1	A	26	VAL	HG11	999.000	0.000	2
1	A	26	VAL	HG12	999.000	0.000	2
1	A	26	VAL	HG13	999.000	0.000	2
1	A	26	VAL	HG21	999.000	0.000	2
1	A	26	VAL	HG22	999.000	0.000	2
1	A	26	VAL	HG23	999.000	0.000	2
1	A	28	MET	HE1	999.000	0.000	1
1	A	28	MET	HE2	999.000	0.000	1
1	A	28	MET	HE3	999.000	0.000	1
1	A	35	ILE	HD11	999.000	0.000	1
1	A	35	ILE	HD12	999.000	0.000	1
1	A	35	ILE	HD13	999.000	0.000	1
1	A	35	ILE	HG21	999.000	0.000	1
1	A	35	ILE	HG22	999.000	0.000	1
1	A	35	ILE	HG23	999.000	0.000	1
1	A	36	ILE	HD11	999.000	0.000	1
1	A	36	ILE	HD12	999.000	0.000	1
1	A	36	ILE	HD13	999.000	0.000	1
1	A	36	ILE	HG21	999.000	0.000	1
1	A	36	ILE	HG22	999.000	0.000	1
1	A	36	ILE	HG23	999.000	0.000	1
1	A	38	THR	HG21	999.000	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	38	THR	HG22	999.000	0.000	1
1	A	38	THR	HG23	999.000	0.000	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	41	-0.12 ± 0.27	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	35	-0.06 ± 0.23	None needed (< 0.5 ppm)
$^{13}C'$	41	0.00 ± 0.00	None needed (< 0.5 ppm)
^{15}N	41	1.03 ± 0.89	None needed (imprecise)

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. 412 atoms were assigned a chemical shift out of a possible 412. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	170/170 (100%)	71/71 (100%)	66/66 (100%)	33/33 (100%)
Sidechain	212/212 (100%)	138/138 (100%)	63/63 (100%)	11/11 (100%)
Aromatic	30/30 (100%)	14/14 (100%)	15/15 (100%)	1/1 (100%)
Overall	412/412 (100%)	223/223 (100%)	144/144 (100%)	45/45 (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	6	THR	HG1	999.00	0.08 – 2.19	4729.2
1	A	38	THR	HG1	999.00	0.08 – 2.19	4729.2
1	A	24	ARG	HG3	999.00	0.15 – 2.94	3575.1
1	A	16	ARG	HH22	999.00	5.04 – 8.54	2834.9
1	A	24	ARG	HH22	999.00	5.04 – 8.54	2834.9
1	A	16	ARG	HH12	999.00	5.04 – 8.65	2748.4
1	A	24	ARG	HH12	999.00	5.04 – 8.65	2748.4

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List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	1	GLY	HA3	999.00	2.08 – 5.71	2741.3
1	A	28	MET	HE1	999.00	-0.03 – 3.80	2603.4
1	A	28	MET	HE2	999.00	-0.03 – 3.80	2603.4
1	A	28	MET	HE3	999.00	-0.03 – 3.80	2603.4
1	A	16	ARG	HH21	999.00	4.81 – 8.80	2486.7
1	A	24	ARG	HH21	999.00	4.81 – 8.80	2486.7
1	A	16	ARG	HH11	999.00	4.72 – 9.08	2275.5
1	A	24	ARG	HH11	999.00	4.72 – 9.08	2275.5
1	A	10	LEU	H	999.00	5.09 – 11.34	1585.3
1	A	30	SER	HG	999.00	0.07 – 10.62	941.9
1	A	32	SER	HG	999.00	0.07 – 10.62	941.9
1	A	21	TYR	CE2	999.00	111.68 – 124.17	705.4
1	A	37	TYR	CE2	999.00	111.68 – 124.17	705.4
1	A	9	GLN	CD	999.00	173.59 – 185.85	668.3
1	A	20	GLN	CD	999.00	173.59 – 185.85	668.3
1	A	21	TYR	HH	999.00	0.99 – 17.18	611.4
1	A	37	TYR	HH	999.00	0.99 – 17.18	611.4
1	A	21	TYR	CD2	999.00	125.28 – 140.14	583.0
1	A	37	TYR	CD2	999.00	125.28 – 140.14	583.0
1	A	28	MET	CE	999.00	8.39 – 25.85	562.4
1	A	5	ASP	C	999.00	168.07 – 184.82	491.1
1	A	25	ASP	C	999.00	168.07 – 184.82	491.1
1	A	41	ASP	C	999.00	168.07 – 184.82	491.1
1	A	6	THR	C	999.00	166.08 – 183.07	485.2
1	A	38	THR	C	999.00	166.08 – 183.07	485.2
1	A	30	SER	C	999.00	166.15 – 183.14	485.2
1	A	32	SER	C	999.00	166.15 – 183.14	485.2
1	A	11	ASN	C	999.00	166.56 – 184.06	470.7
1	A	27	ASN	C	999.00	166.56 – 184.06	470.7
1	A	4	TRP	CG	999.00	101.31 – 120.62	459.9
1	A	13	TRP	CG	999.00	101.31 – 120.62	459.9
1	A	1	GLY	C	999.00	164.92 – 182.89	459.1
1	A	7	GLY	C	999.00	164.92 – 182.89	459.1
1	A	17	GLY	C	999.00	164.92 – 182.89	459.1
1	A	22	GLY	C	999.00	164.92 – 182.89	459.1
1	A	33	GLY	C	999.00	164.92 – 182.89	459.1
1	A	34	GLY	C	999.00	164.92 – 182.89	459.1
1	A	4	TRP	CD2	999.00	118.40 – 137.65	452.4
1	A	13	TRP	CD2	999.00	118.40 – 137.65	452.4
1	A	2	VAL	C	999.00	166.52 – 184.93	447.2
1	A	15	VAL	C	999.00	166.52 – 184.93	447.2
1	A	26	VAL	C	999.00	166.52 – 184.93	447.2

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List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	35	ILE	C	999.00	166.59 – 185.34	438.9
1	A	36	ILE	C	999.00	166.59 – 185.34	438.9
1	A	9	GLN	C	999.00	166.94 – 185.80	436.2
1	A	20	GLN	C	999.00	166.94 – 185.80	436.2
1	A	29	LYS	C	999.00	167.28 – 186.22	433.9
1	A	10	LEU	C	999.00	167.56 – 186.66	430.3
1	A	21	TYR	C	999.00	165.86 – 185.23	425.1
1	A	37	TYR	C	999.00	165.86 – 185.23	425.1
1	A	16	ARG	C	999.00	166.60 – 186.40	415.4
1	A	24	ARG	C	999.00	166.60 – 186.40	415.4
1	A	4	TRP	C	999.00	166.32 – 186.14	415.1
1	A	13	TRP	C	999.00	166.32 – 186.14	415.1
1	A	3	CYS	C	999.00	164.77 – 184.97	408.0
1	A	8	CYS	C	999.00	164.77 – 184.97	408.0
1	A	18	CYS	C	999.00	164.77 – 184.97	408.0
1	A	31	CYS	C	999.00	164.77 – 184.97	408.0
1	A	39	CYS	C	999.00	164.77 – 184.97	408.0
1	A	40	CYS	C	999.00	164.77 – 184.97	408.0
1	A	23	MET	C	999.00	166.12 – 186.43	405.1
1	A	28	MET	C	999.00	166.12 – 186.43	405.1
1	A	12	ALA	C	999.00	167.61 – 188.05	401.8
1	A	14	ALA	C	999.00	167.61 – 188.05	401.8
1	A	19	ALA	C	999.00	167.61 – 188.05	401.8
1	A	37	TYR	CA	999.00	45.75 – 70.63	378.1
1	A	4	TRP	CA	999.00	45.21 – 70.26	375.8
1	A	13	TRP	CA	999.00	45.21 – 70.26	375.8
1	A	29	LYS	NZ	999.00	19.79 – 46.09	367.3
1	A	11	ASN	CG	999.00	164.52 – 188.90	337.3
1	A	27	ASN	CG	999.00	164.52 – 188.90	337.3
1	A	21	TYR	CZ	999.00	143.41 – 170.10	315.6
1	A	37	TYR	CZ	999.00	143.41 – 170.10	315.6
1	A	16	ARG	NH2	999.00	57.68 – 87.89	306.6
1	A	24	ARG	NH2	999.00	57.68 – 87.89	306.6
1	A	21	TYR	CG	999.00	112.42 – 146.96	251.7
1	A	37	TYR	CG	999.00	112.42 – 146.96	251.7
1	A	1	GLY	N	999.00	91.59 – 127.52	247.6
1	A	16	ARG	CZ	999.00	141.81 – 177.93	232.3
1	A	24	ARG	CZ	999.00	141.81 – 177.93	232.3
1	A	10	LEU	N	999.00	102.77 – 140.89	230.1
1	A	16	ARG	NH1	999.00	49.05 – 99.42	183.6
1	A	24	ARG	NH1	999.00	49.05 – 99.42	183.6
1	A	5	ASP	CG	999.00	149.18 – 208.82	137.5

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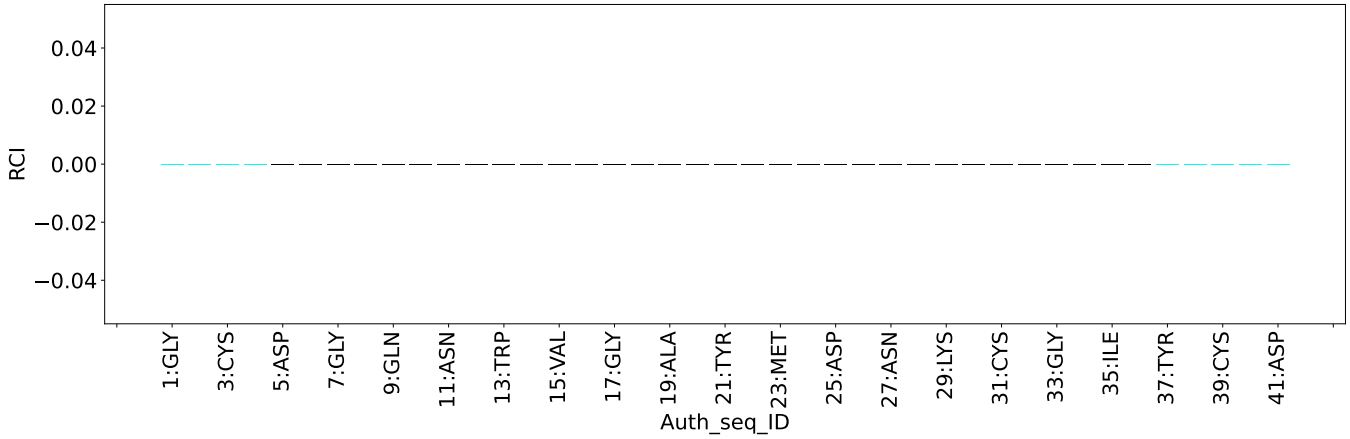
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	25	ASP	CG	999.00	149.18 – 208.82	137.5
1	A	41	ASP	CG	999.00	149.18 – 208.82	137.5
1	A	4	TRP	CE2	999.00	105.29 – 170.61	131.8
1	A	13	TRP	CE2	999.00	105.29 – 170.61	131.8
1	A	20	GLN	HG3	0.30	0.91 – 3.68	-7.2
1	A	17	GLY	HA2	1.72	2.15 – 5.77	-6.2

7.1.5 Random Coil Index (RCI) plots

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	451
Intra-residue (|i-j|=0)	112
Sequential (|i-j|=1)	134
Medium range (|i-j|>1 and |i-j|<5)	57
Long range (|i-j|≥5)	145
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	3
Total dihedral-angle restraints	115
Number of unmapped restraints	0
Number of restraints per residue	13.8
Number of long range restraints per residue[1]	3.6

[1]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.There are no distance violations

8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

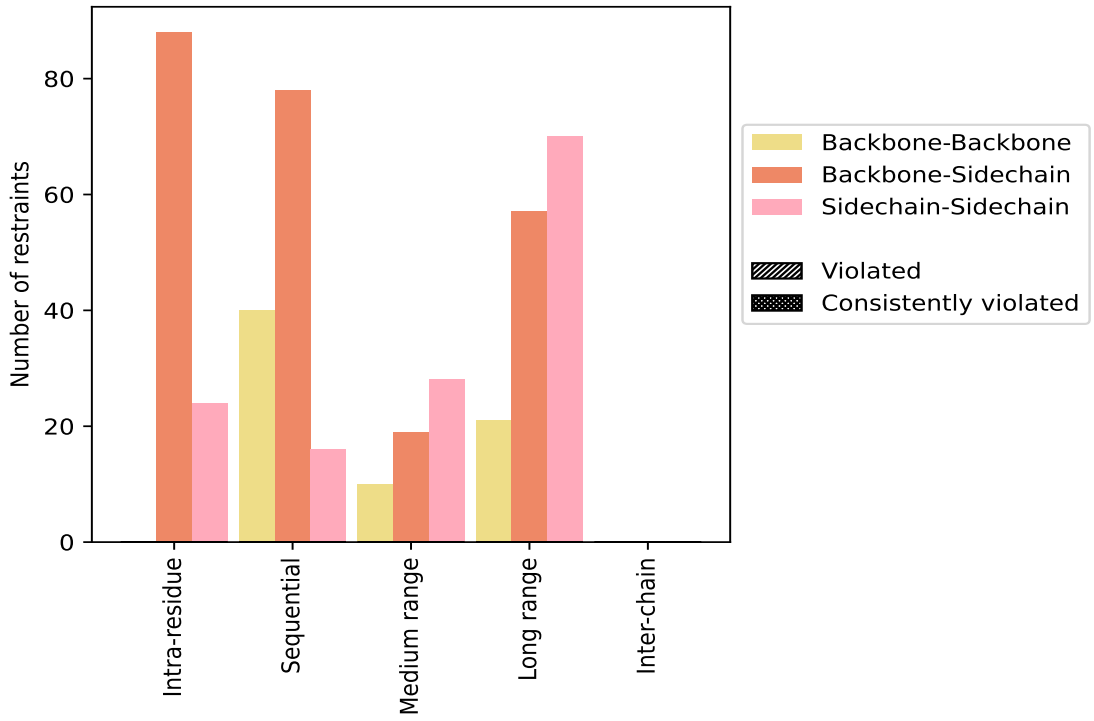
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	112	24.8	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	88	19.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	24	5.3	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	134	29.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	40	8.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	78	17.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	16	3.5	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	57	12.6	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	10	2.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	19	4.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	28	6.2	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	145	32.2	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	21	4.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	57	12.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	67	14.9	0	0.0	0.0	0	0.0	0.0
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	3	0.7	0	0.0	0.0	0	0.0	0.0
Total	451	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	71	15.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	242	53.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	138	30.6	0	0.0	0.0	0	0.0	0.0

[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



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

No violations found

9.3 Distance violation statistics for the ensemble

No violations found

9.4 Most violated distance restraints in the ensemble

No violations found

9.5 All violated distance restraints

No violations found

10 Dihedral-angle violation analysis

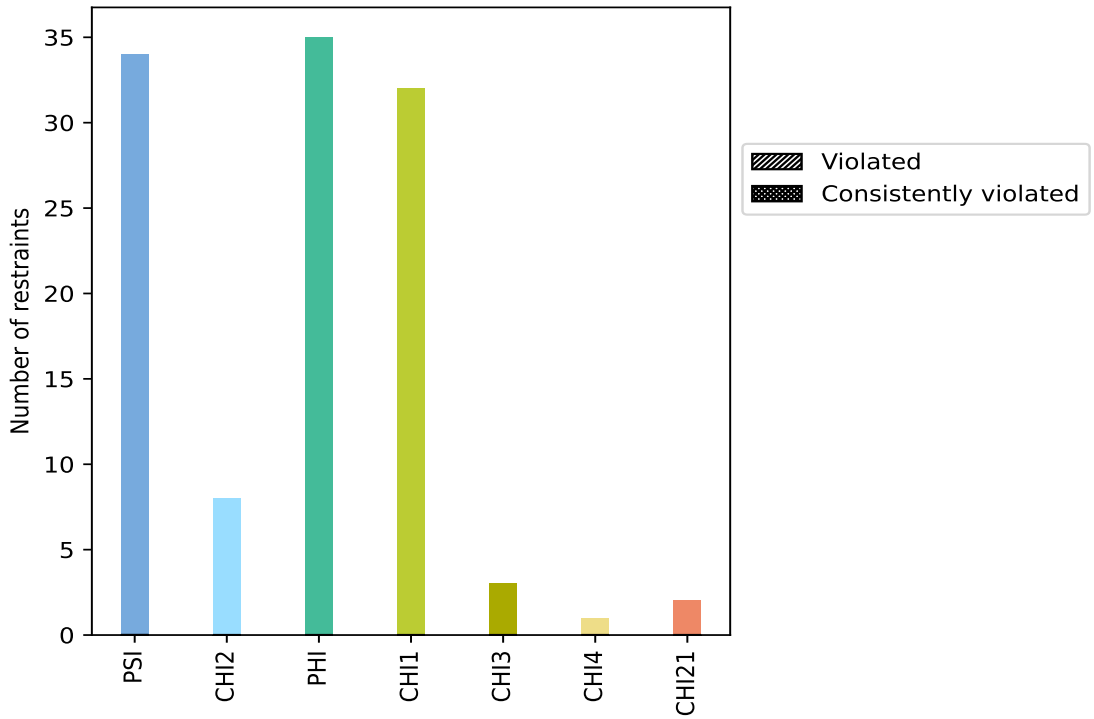
10.1 Summary of dihedral-angle violations

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]
PSI	34	29.6	0	0.0	0.0	0	0.0	0.0
CHI2	8	7.0	0	0.0	0.0	0	0.0	0.0
PHI	35	30.4	0	0.0	0.0	0	0.0	0.0
CHI1	32	27.8	0	0.0	0.0	0	0.0	0.0
CHI3	3	2.6	0	0.0	0.0	0	0.0	0.0
CHI4	1	0.9	0	0.0	0.0	0	0.0	0.0
CHI21	2	1.7	0	0.0	0.0	0	0.0	0.0
Total	115	100.0	0	0.0	0.0	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



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

10.2 Dihedral-angle violation statistics for each model

No violations found

10.3 Dihedral-angle violation statistics for the ensemble

No violations found

10.4 Most violated dihedral-angle restraints in the ensemble

No violations found

10.5 All violated dihedral-angle restraints

No violations found