wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	6YTS
BMRB ID	:	27989
Title	:	Solution NMR structure of type-I ribosome-inactivating protein trichobakin (TBK)
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Deposited on	:	2020-04-24

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:

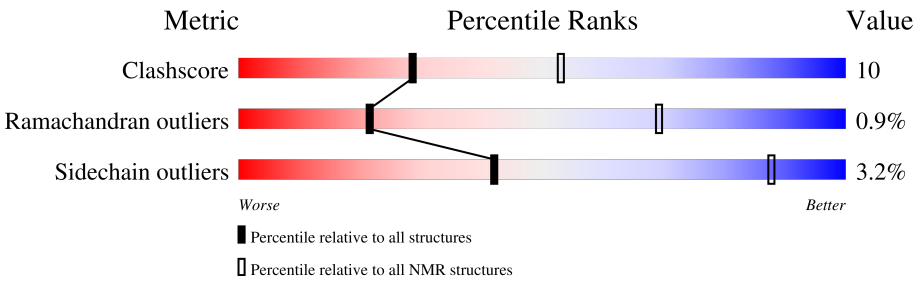
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 84%.

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	247	

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:1-A:230, A:235-A:242 (238)	0.40	1

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3862 atoms, of which 1942 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Trichobakin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	247	3862	1220	1942	328	369	3	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: Trichobakin

Chain A: 70% 25%

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

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Trichobakin

Chain A: 68% 28%

5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure calculation	2.3
CNS	structure calculation	1.21
CNS	refinement	1.21

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	2820
Number of shifts mapped to atoms	2820
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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	1854	1875	1874	39±5
All	All	37080	37500	37480	776

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 10.

5 of 185 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:SER:HA	1:A:171:ILE:HD13	0.73	1.58	17	20
1:A:129:LEU:HD12	1:A:175:VAL:HA	0.71	1.61	11	12
1:A:184:ALA:O	1:A:188:LEU:HG	0.69	1.87	15	14
1:A:47:TYR:HA	1:A:64:ILE:O	0.62	1.95	19	20
1:A:169:GLN:O	1:A:173:LYS:HG2	0.61	1.96	20	12

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	237/247 (96%)	220±2 (93±1%)	14±2 (6±1%)	2±0 (1±0%)	21 69
All	All	4740/4940 (96%)	4407 (93%)	290 (6%)	43 (1%)	21 69

All 4 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	69	VAL	20
1	A	142	TYR	20
1	A	220	ASN	2
1	A	238	ALA	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	201/208 (97%)	194±2 (97±1%)	6±2 (3±1%)	42 88
All	All	4020/4160 (97%)	3890 (97%)	130 (3%)	42 88

5 of 33 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	30	LYS	20
1	A	177	LYS	19
1	A	160	GLU	10
1	A	89	THR	9
1	A	149	SER	8

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 84% 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	2820
Number of shifts mapped to atoms	2820
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	244	-0.27 ± 0.05	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	229	0.10 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	240	-0.06 ± 0.12	None needed (< 0.5 ppm)
^{15}N	228	0.84 ± 0.18	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 84%, i.e. 2730 atoms were assigned a chemical shift out of a possible 3246. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1154/1182 (98%)	464/477 (97%)	469/476 (99%)	221/229 (97%)
Sidechain	1461/1828 (80%)	987/1198 (82%)	458/557 (82%)	16/73 (22%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	115/236 (49%)	76/111 (68%)	38/122 (31%)	1/3 (33%)
Overall	2730/3246 (84%)	1527/1786 (85%)	965/1155 (84%)	238/305 (78%)

7.1.4 Statistically unusual chemical shifts (i)

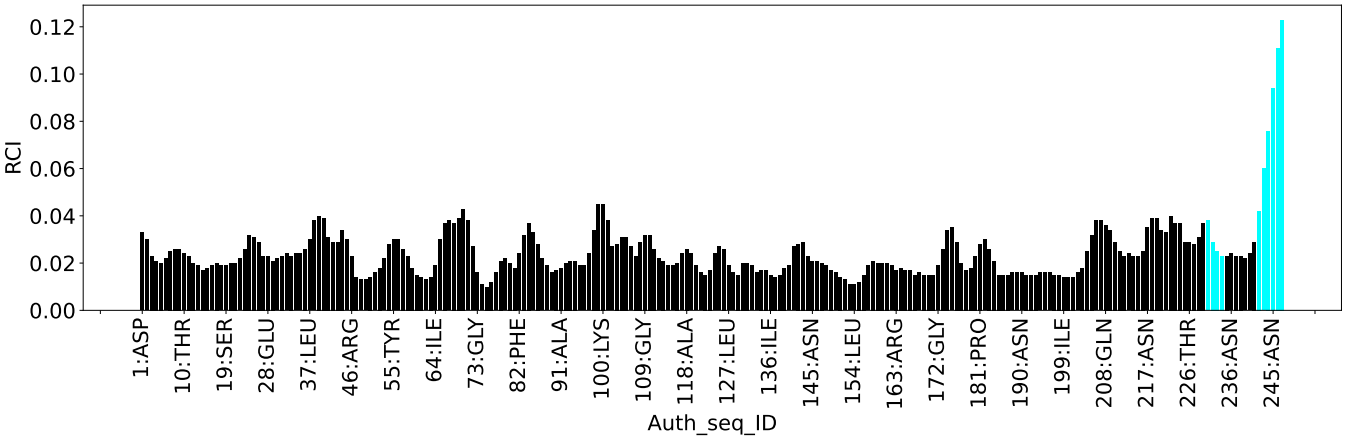
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	58	GLU	HB2	-0.12	1.00 – 3.05	-10.4
1	A	75	ARG	HB2	-0.33	0.52 – 3.08	-8.3
1	A	25	LEU	HD11	2.38	-0.61 – 2.12	5.9
1	A	25	LEU	HD12	2.38	-0.61 – 2.12	5.9
1	A	25	LEU	HD13	2.38	-0.61 – 2.12	5.9
1	A	209	PHE	CZ	120.62	121.82 – 136.66	-5.8
1	A	198	GLN	CG	27.69	28.36 – 39.21	-5.6
1	A	54	ASN	HB3	4.46	1.12 – 4.38	5.2
1	A	177	LYS	CD	23.37	23.50 – 34.42	-5.1

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:


RCI
0.12
0.10
0.08
0.06
0.04
0.02
0.00
1:ASP
10:THR
19:SER
28:GLU
37:LEU
46:ARG
55:TYR
64:ILE
73:GLY
82:PHE
91:ALA
100:LYS
109:GLY
118:ALA
127:LEU
136:ILE
145:ASN
154:LEU
163:ARG
172:GLY
181:PRO
190:ASN
199:ILE
208:GLN
217:ASN
226:THR
236:ASN
245:ASN
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	3693
Intra-residue (|i-j|=0)	1391
Sequential (|i-j|=1)	823
Medium range (|i-j|>1 and |i-j|<5)	647
Long range (|i-j|≥5)	715
Inter-chain	0
Hydrogen bond restraints	117
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	15.0
Number of long range restraints per residue[1]	3.0

[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 (i)

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

8.2.1 Average number of distance violations per model (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	168.3	0.2
0.2-0.5 (Medium)	339.1	0.5
>0.5 (Large)	289.8	9.99

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

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

9 Distance violation analysis (i)

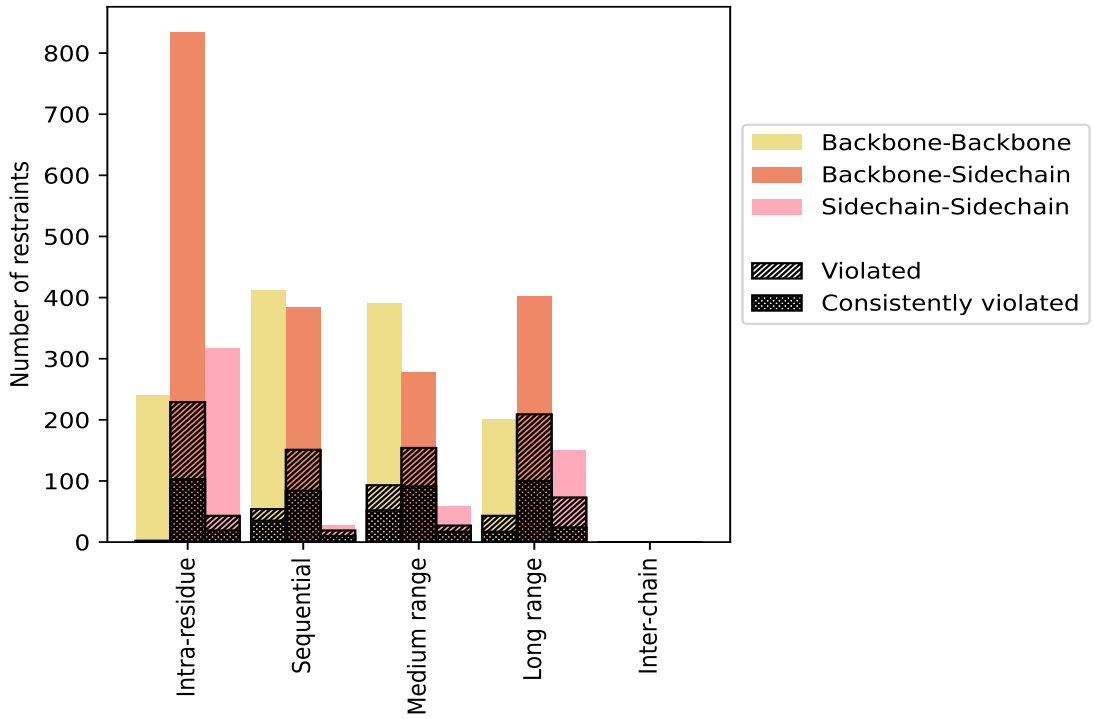
9.1 Summary of distance violations (i)

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)	1391	37.7	274	19.7	7.4	124	8.9	3.4
Backbone-Backbone	240	6.5	2	0.8	0.1	2	0.8	0.1
Backbone-Sidechain	834	22.6	229	27.5	6.2	103	12.4	2.8
Sidechain-Sidechain	317	8.6	43	13.6	1.2	19	6.0	0.5
Sequential (|i-j|=1)	823	22.3	224	27.2	6.1	129	15.7	3.5
Backbone-Backbone	411	11.1	54	13.1	1.5	35	8.5	0.9
Backbone-Sidechain	384	10.4	151	39.3	4.1	84	21.9	2.3
Sidechain-Sidechain	28	0.8	19	67.9	0.5	10	35.7	0.3
Medium range (|i-j|>1 & |i-j|<5)	647	17.5	272	42.0	7.4	160	24.7	4.3
Backbone-Backbone	311	8.4	91	29.3	2.5	52	16.7	1.4
Backbone-Sidechain	278	7.5	154	55.4	4.2	91	32.7	2.5
Sidechain-Sidechain	58	1.6	27	46.6	0.7	17	29.3	0.5
Long range (|i-j|≥5)	715	19.4	325	45.5	8.8	141	19.7	3.8
Backbone-Backbone	163	4.4	43	26.4	1.2	17	10.4	0.5
Backbone-Sidechain	402	10.9	209	52.0	5.7	100	24.9	2.7
Sidechain-Sidechain	150	4.1	73	48.7	2.0	24	16.0	0.6
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	117	3.2	2	1.7	0.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3693	100.0	1097	29.7	29.7	554	15.0	15.0
Backbone-Backbone	1242	33.6	192	15.5	5.2	106	8.5	2.9
Backbone-Sidechain	1898	51.4	743	39.1	20.1	378	19.9	10.2
Sidechain-Sidechain	553	15.0	162	29.3	4.4	70	12.7	1.9

[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 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[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	191	176	207	213	0	787	1.19	9.99	1.66	0.35
2	185	172	211	217	0	785	1.21	9.64	1.69	0.34
3	201	179	208	226	0	814	1.17	9.6	1.64	0.35
4	188	175	202	222	0	787	1.2	9.63	1.67	0.36
5	190	183	208	217	0	798	1.19	9.59	1.64	0.35
6	197	178	209	221	0	805	1.17	9.79	1.64	0.34
7	197	181	215	210	0	803	1.17	9.96	1.66	0.34
8	188	179	214	215	0	796	1.19	9.87	1.68	0.34
9	194	182	216	215	0	807	1.17	9.49	1.64	0.34
10	193	176	212	225	0	806	1.17	9.47	1.64	0.34
11	198	188	208	217	0	811	1.18	9.74	1.68	0.34

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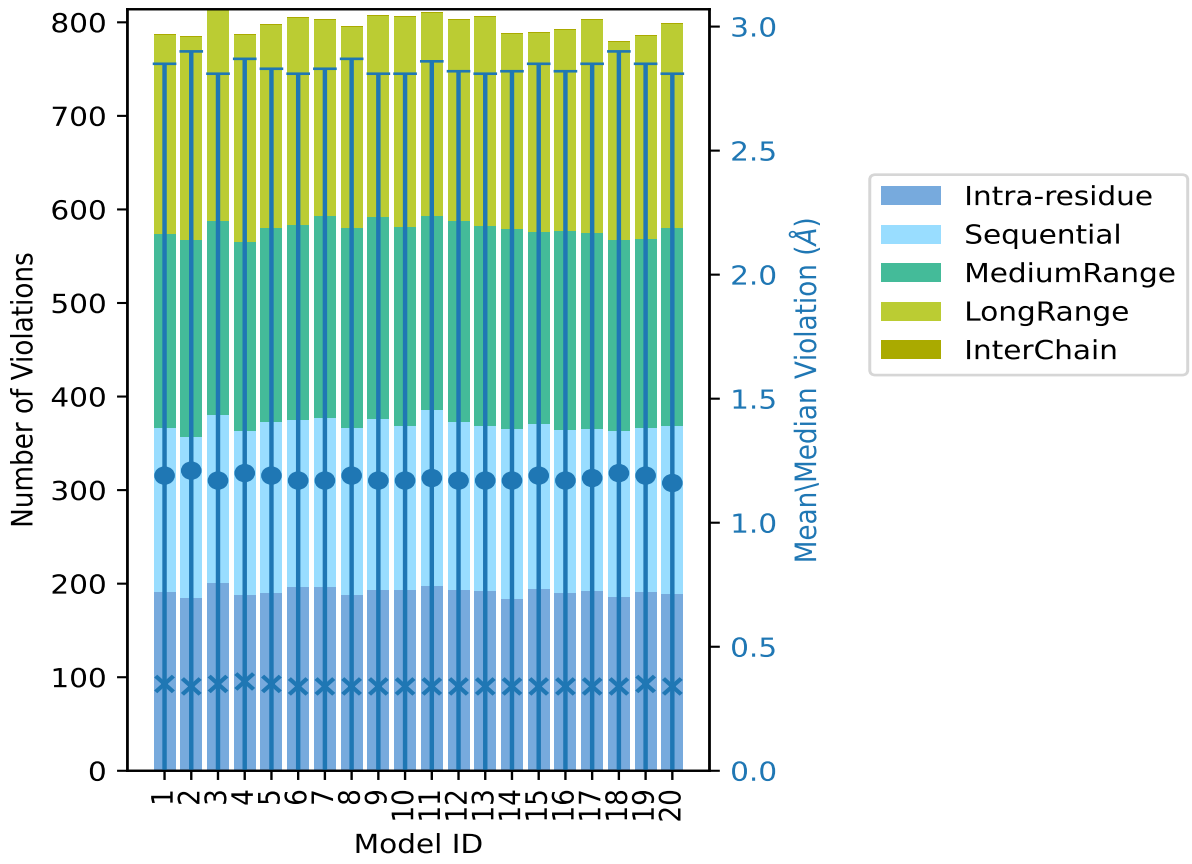
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	194	179	215	215	0	803	1.17	9.96	1.65	0.34
13	192	177	214	223	0	806	1.17	9.74	1.64	0.34
14	184	182	213	209	0	788	1.17	9.78	1.65	0.34
15	194	177	205	213	0	789	1.19	9.45	1.66	0.34
16	190	175	212	215	0	792	1.17	9.33	1.65	0.34
17	192	174	209	228	0	803	1.18	9.75	1.67	0.34
18	186	177	205	211	0	779	1.2	9.73	1.7	0.34
19	191	175	203	217	0	786	1.19	9.81	1.66	0.35
20	189	180	211	219	0	799	1.16	9.68	1.65	0.34

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

9.2.1 Bar graph : Distance Violation statistics for each model (i)



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

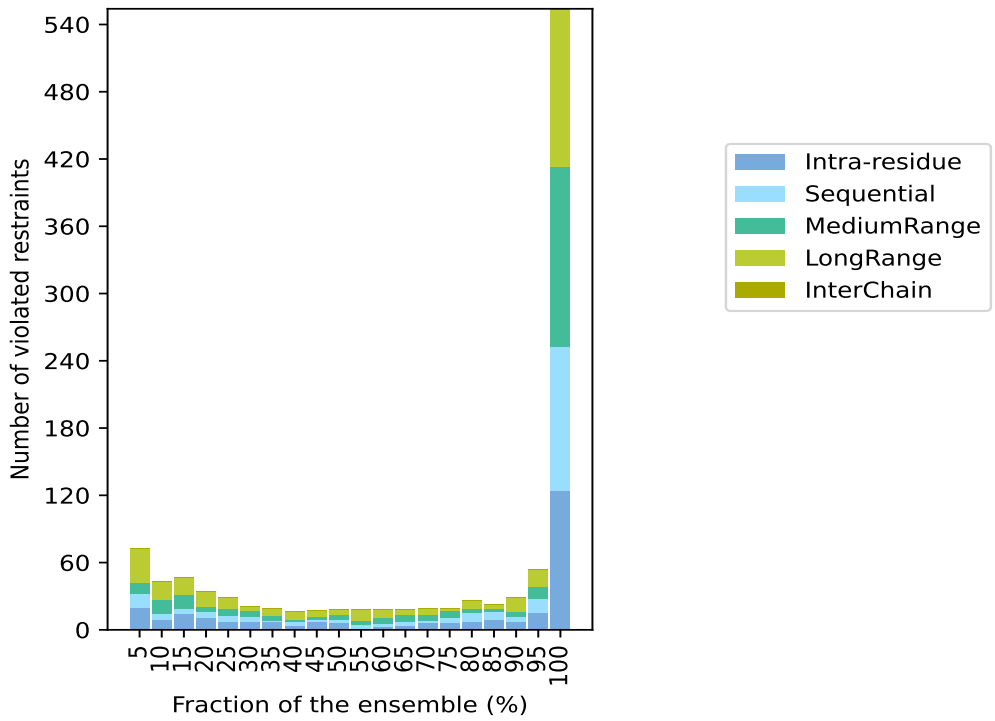
9.3 Distance violation statistics for the ensemble (i)

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, 2481(IR:1117, SQ:599, MR:375, LR:390, 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]	%
20	12	10	31	0	73	1	5.0
9	5	13	16	0	43	2	10.0
14	5	12	16	0	47	3	15.0
11	5	5	13	0	34	4	20.0
7	5	7	10	0	29	5	25.0
7	5	5	4	0	21	6	30.0
7	1	4	7	0	19	7	35.0
4	3	2	7	0	16	8	40.0
7	2	3	5	0	17	9	45.0
6	3	4	5	0	18	10	50.0
1	4	3	10	0	18	11	55.0
3	2	6	7	0	18	12	60.0
4	3	6	5	0	18	13	65.0
6	2	5	6	0	19	14	70.0
6	5	6	2	0	19	15	75.0
7	8	4	7	0	26	16	80.0
9	7	3	4	0	23	17	85.0
7	5	4	13	0	29	18	90.0
15	13	10	16	0	54	19	95.0
124	129	160	141	0	554	20	100.0

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

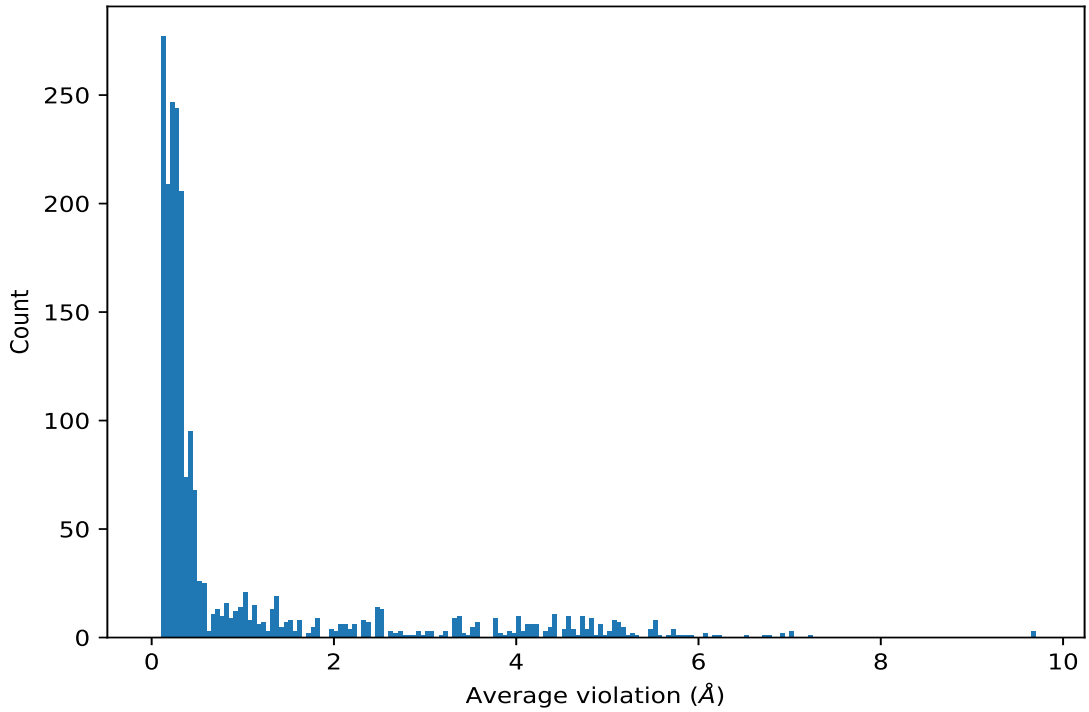
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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.

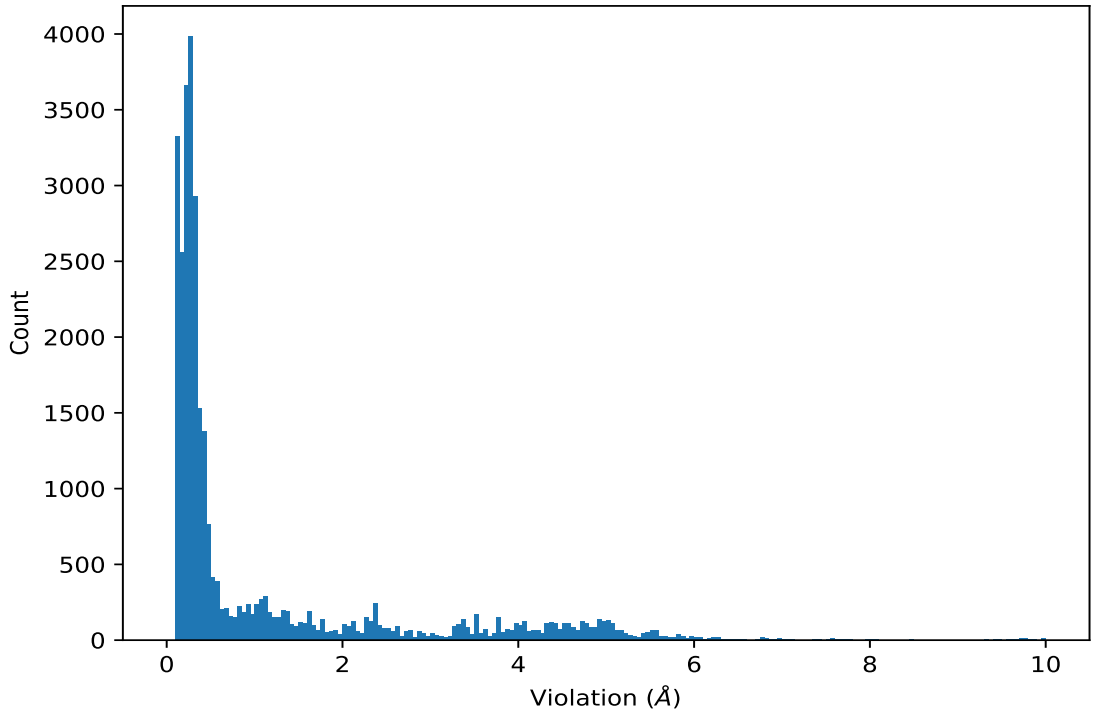
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,140)	1:A:66:VAL:HG11	1:A:242:ASN:H	20	9.7	0.17	9.74
(4,140)	1:A:66:VAL:HG12	1:A:242:ASN:H	20	9.7	0.17	9.74
(4,140)	1:A:66:VAL:HG13	1:A:242:ASN:H	20	9.7	0.17	9.74
(4,139)	1:A:242:ASN:H	1:A:240:LEU:HG	20	7.22	1.23	7.77
(4,253)	1:A:36:LEU:HD21	1:A:241:PRO:HD3	20	7.04	1.04	7.51
(4,253)	1:A:36:LEU:HD22	1:A:241:PRO:HD3	20	7.04	1.04	7.51
(4,253)	1:A:36:LEU:HD23	1:A:241:PRO:HD3	20	7.04	1.04	7.51
(4,242)	1:A:61:SER:H	1:A:140:PHE:HE1	20	6.94	0.1	6.94
(4,242)	1:A:61:SER:H	1:A:140:PHE:HE2	20	6.94	0.1	6.94
(4,227)	1:A:64:ILE:H	1:A:47:TYR:H	20	6.79	0.06	6.8
(4,138)	1:A:242:ASN:H	1:A:240:LEU:HB2	20	6.7	0.65	6.54
(4,249)	1:A:62:VAL:H	1:A:60:ILE:HG12	20	6.52	0.12	6.53
(4,196)	1:A:109:GLY:HA3	1:A:108:SER:H	20	6.22	0.1	6.24
(4,167)	1:A:183:LEU:HB2	1:A:217:ASN:H	20	6.17	0.18	6.16
(4,91)	1:A:74:TYR:H	1:A:80:SER:HB3	20	6.08	0.07	6.07

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

The following table provides the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,140)	1:A:66:VAL:HG11	1:A:242:ASN:H	1	9.99
(4,140)	1:A:66:VAL:HG12	1:A:242:ASN:H	1	9.99
(4,140)	1:A:66:VAL:HG13	1:A:242:ASN:H	1	9.99
(4,140)	1:A:66:VAL:HG11	1:A:242:ASN:H	7	9.96
(4,140)	1:A:66:VAL:HG12	1:A:242:ASN:H	7	9.96
(4,140)	1:A:66:VAL:HG13	1:A:242:ASN:H	7	9.96
(4,140)	1:A:66:VAL:HG11	1:A:242:ASN:H	12	9.96
(4,140)	1:A:66:VAL:HG12	1:A:242:ASN:H	12	9.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,140)	1:A:66:VAL:HG13	1:A:242:ASN:H	12	9.96
(4,140)	1:A:66:VAL:HG11	1:A:242:ASN:H	8	9.87
(4,140)	1:A:66:VAL:HG12	1:A:242:ASN:H	8	9.87
(4,140)	1:A:66:VAL:HG13	1:A:242:ASN:H	8	9.87
(4,140)	1:A:66:VAL:HG11	1:A:242:ASN:H	19	9.81
(4,140)	1:A:66:VAL:HG12	1:A:242:ASN:H	19	9.81
(4,140)	1:A:66:VAL:HG13	1:A:242:ASN:H	19	9.81
(4,140)	1:A:66:VAL:HG11	1:A:242:ASN:H	6	9.79
(4,140)	1:A:66:VAL:HG12	1:A:242:ASN:H	6	9.79
(4,140)	1:A:66:VAL:HG13	1:A:242:ASN:H	6	9.79
(4,140)	1:A:66:VAL:HG11	1:A:242:ASN:H	14	9.78
(4,140)	1:A:66:VAL:HG12	1:A:242:ASN:H	14	9.78
(4,140)	1:A:66:VAL:HG13	1:A:242:ASN:H	14	9.78
(4,140)	1:A:66:VAL:HG11	1:A:242:ASN:H	17	9.75
(4,140)	1:A:66:VAL:HG12	1:A:242:ASN:H	17	9.75
(4,140)	1:A:66:VAL:HG13	1:A:242:ASN:H	17	9.75
(4,140)	1:A:66:VAL:HG11	1:A:242:ASN:H	11	9.74
(4,140)	1:A:66:VAL:HG12	1:A:242:ASN:H	11	9.74
(4,140)	1:A:66:VAL:HG13	1:A:242:ASN:H	11	9.74
(4,140)	1:A:66:VAL:HG11	1:A:242:ASN:H	13	9.74

10 Dihedral-angle violation analysis (i)

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