Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2N5K
BMRB ID	:	25719
Title	:	Regnase-1 Zinc finger domain
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Deposited on	:	2015-07-18

This is a Full wwPDB NMR Structure Validation 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 (i)) were used in the production of this report:

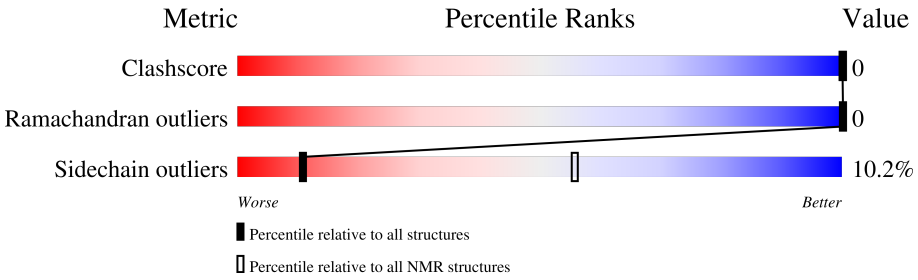
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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	29	83% . 14%

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: *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:300-A:324 (25)	0.44	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 and 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 483 atoms, of which 239 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ribonuclease ZC3H12A.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	29	482	154	239	47	39	3	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

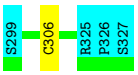
4 Residue-property plots

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: Ribonuclease ZC3H12A

Chain A: 



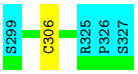
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Ribonuclease ZC3H12A

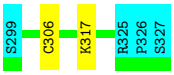
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: Ribonuclease ZC3H12A

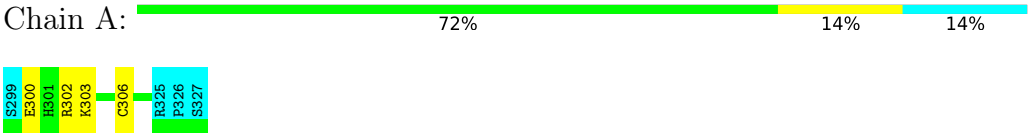
Chain A: 



4.2.3 Score per residue for model 3

• Molecule 1: Ribonuclease ZC3H12A

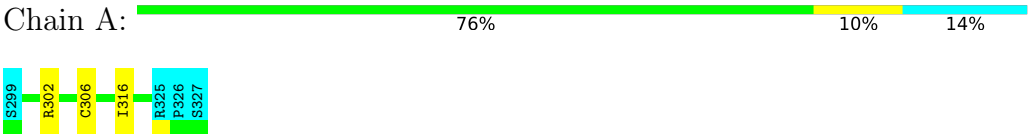
Chain A:



4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Ribonuclease ZC3H12A

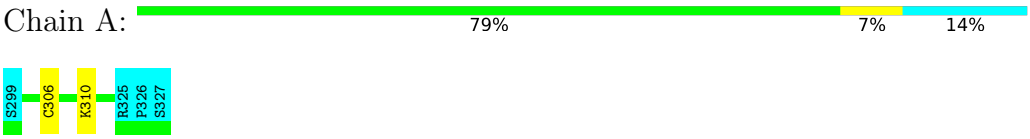
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Ribonuclease ZC3H12A

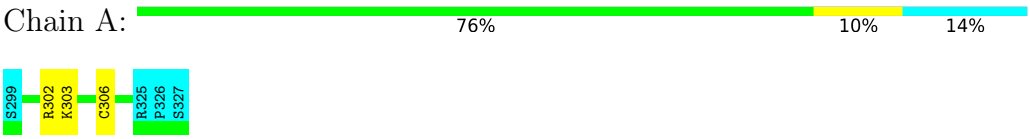
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Ribonuclease ZC3H12A

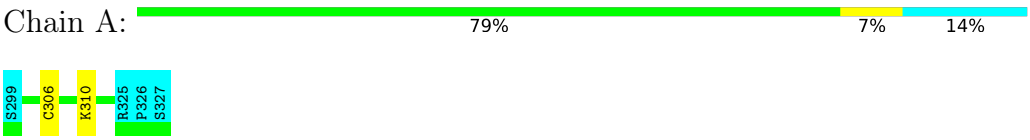
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Ribonuclease ZC3H12A

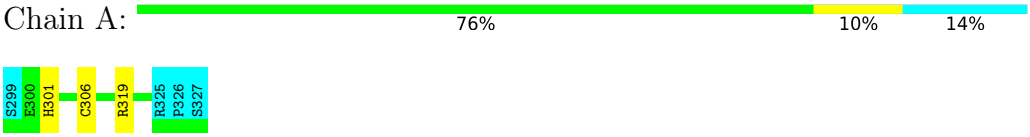
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Ribonuclease ZC3H12A

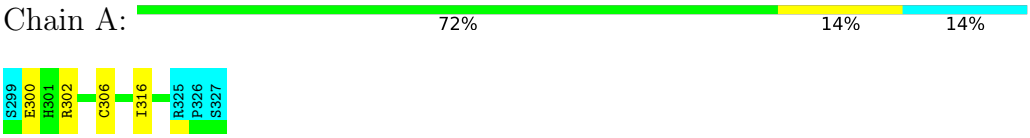
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Ribonuclease ZC3H12A

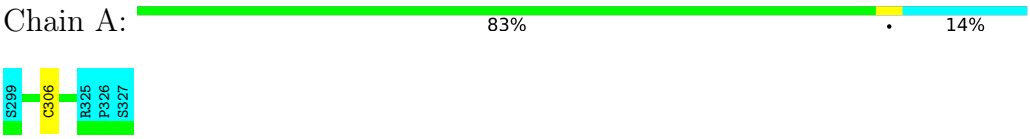
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Ribonuclease ZC3H12A

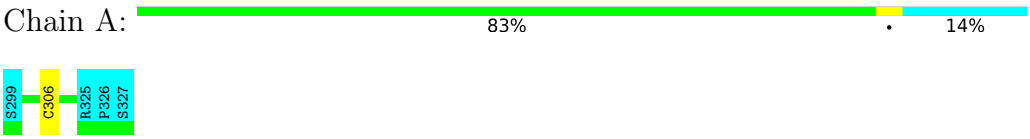
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Ribonuclease ZC3H12A

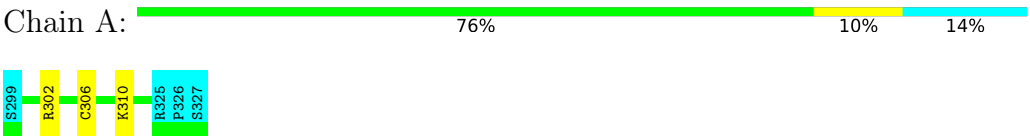
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Ribonuclease ZC3H12A

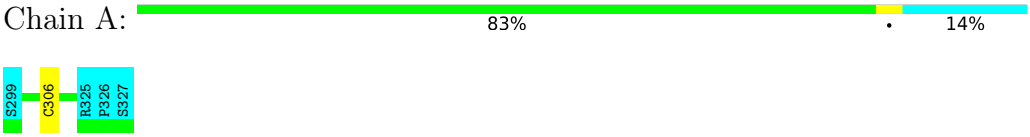
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Ribonuclease ZC3H12A

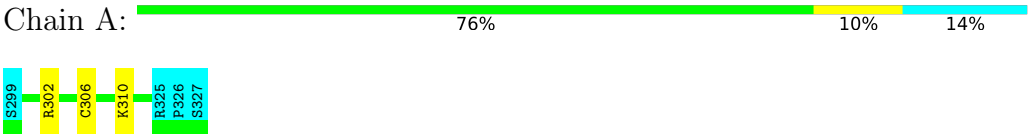
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Ribonuclease ZC3H12A

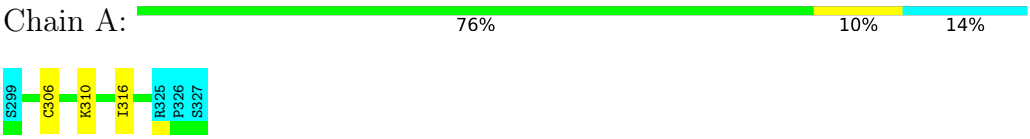
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Ribonuclease ZC3H12A

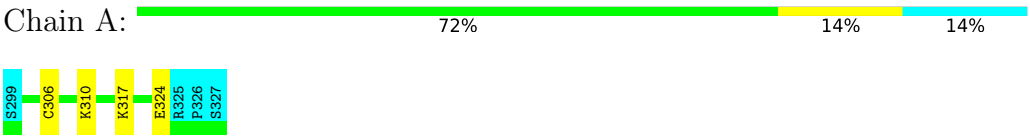
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Ribonuclease ZC3H12A

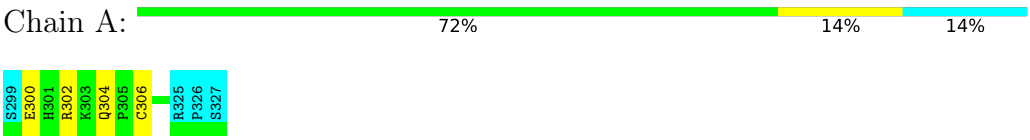
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Ribonuclease ZC3H12A

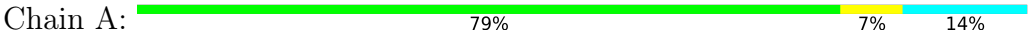
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Ribonuclease ZC3H12A

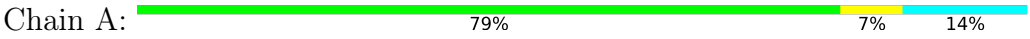
Chain A:

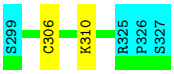


4.2.19 Score per residue for model 19

• Molecule 1: Ribonuclease ZC3H12A

Chain A:

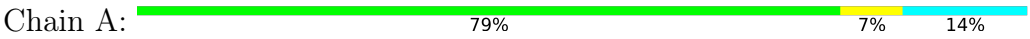




4.2.20 Score per residue for model 20

• Molecule 1: Ribonuclease ZC3H12A

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry, 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 solution	2.1
CYANA	refinement	2.1

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	338
Number of shifts mapped to atoms	338
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	213	209	205	0±0
All	All	4280	4180	4100	-

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

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	25/29 (86%)	20±1 (81±6%)	5±1 (19±6%)	0±0 (0±0%)	100	100
All	All	500/580 (86%)	406 (81%)	94 (19%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains

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	23/27 (85%)	21±1 (90±4%)	2±1 (10±4%)	11 56
All	All	460/540 (85%)	413 (90%)	47 (10%)	11 56

All 10 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	306	CYS	20
1	A	302	ARG	7
1	A	310	LYS	7
1	A	300	GLU	4
1	A	317	LYS	3
1	A	303	LYS	2
1	A	301	HIS	1
1	A	319	ARG	1
1	A	324	GLU	1
1	A	304	GLN	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 83% for the well-defined parts and 82% 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	338
Number of shifts mapped to atoms	338
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	29	-0.25 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	27	0.73 ± 0.15	Should be checked
$^{13}C'$	0	—	None (insufficient data)
^{15}N	25	-1.51 ± 0.68	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 83%, i.e. 300 atoms were assigned a chemical shift out of a possible 360. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	96/121 (79%)	49/49 (100%)	25/50 (50%)	22/22 (100%)
Sidechain	160/185 (86%)	107/117 (91%)	52/57 (91%)	1/11 (9%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	44/54 (81%)	22/26 (85%)	22/24 (92%)	0/4 (0%)
Overall	300/360 (83%)	178/192 (93%)	99/131 (76%)	23/37 (62%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 337 atoms were assigned a chemical shift out of a possible 411. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	109/139 (78%)	55/56 (98%)	29/58 (50%)	25/25 (100%)
Sidechain	184/218 (84%)	123/138 (89%)	60/66 (91%)	1/14 (7%)
Aromatic	44/54 (81%)	22/26 (85%)	22/24 (92%)	0/4 (0%)
Overall	337/411 (82%)	200/220 (91%)	111/148 (75%)	26/43 (60%)

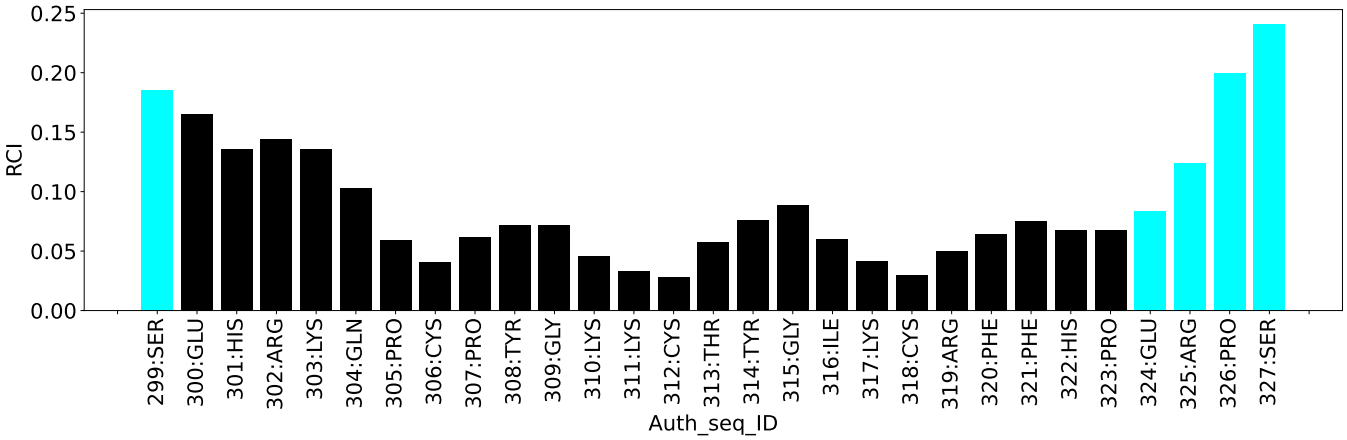
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

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	284
Intra-residue (|i-j|=0)	67
Sequential (|i-j|=1)	92
Medium range (|i-j|>1 and |i-j|<5)	79
Long range (|i-j|≥5)	46
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	9.8
Number of long range restraints per residue[1]	1.6

[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.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.1	0.18
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.There are no dihedral-angle violations

9 Distance violation analysis (i)

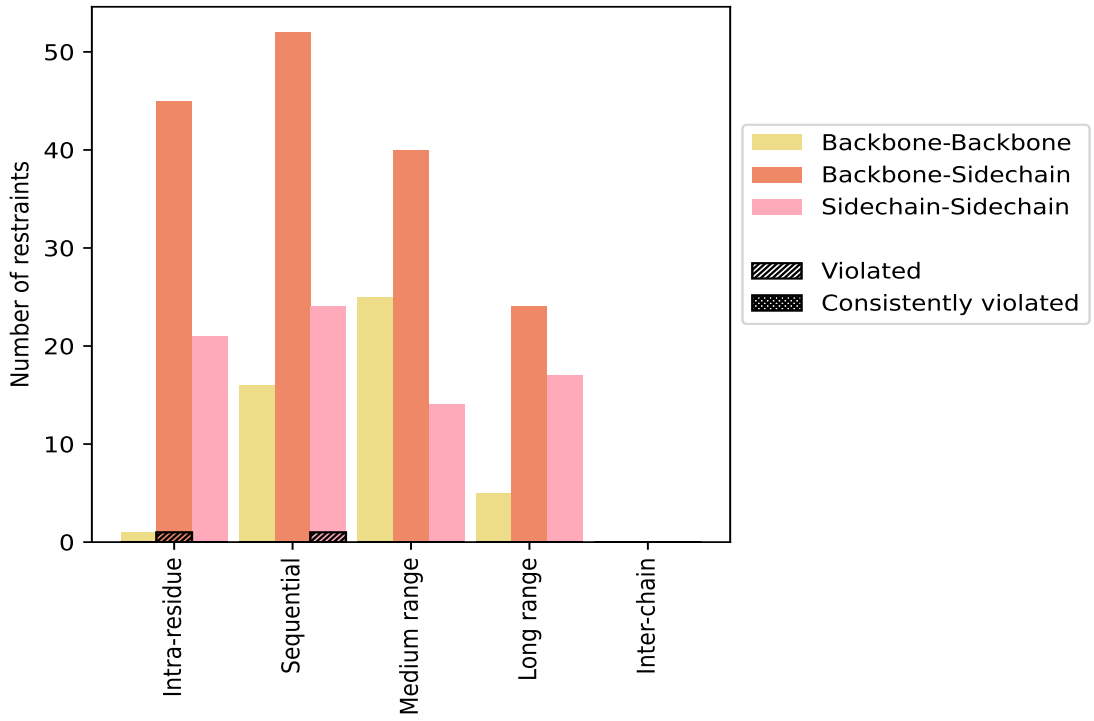
9.1 Summary of distance violations (i)

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)	67	23.6	1	1.5	0.4	0	0.0	0.0
Backbone-Backbone	1	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	45	15.8	1	2.2	0.4	0	0.0	0.0
Sidechain-Sidechain	21	7.4	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	92	32.4	1	1.1	0.4	0	0.0	0.0
Backbone-Backbone	16	5.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	52	18.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	24	8.5	1	4.2	0.4	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	79	27.8	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	25	8.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	40	14.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	14	4.9	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	46	16.2	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	5	1.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	24	8.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	17	6.0	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	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	284	100.0	2	0.7	0.7	0	0.0	0.0
Backbone-Backbone	47	16.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	161	56.7	1	0.6	0.4	0	0.0	0.0
Sidechain-Sidechain	76	26.8	1	1.3	0.4	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

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	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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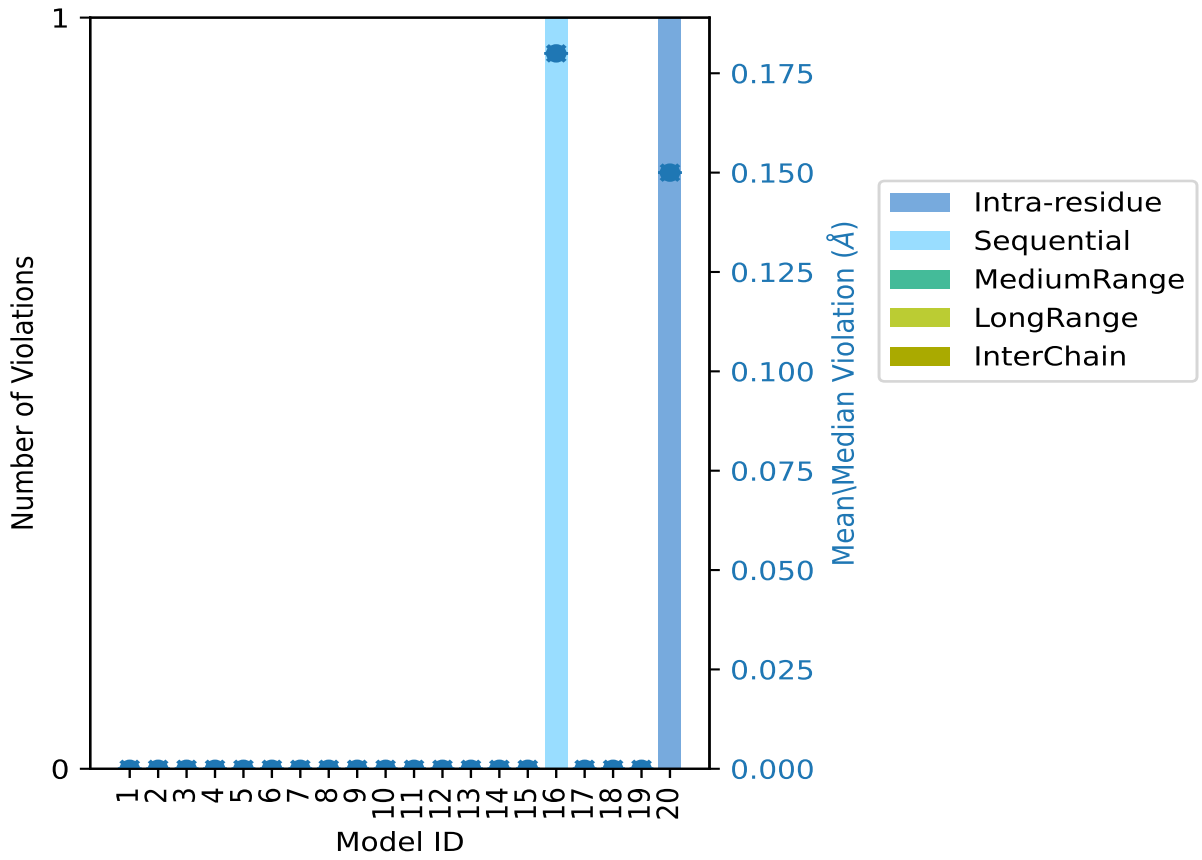
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0	0	0	0.0	0.0	0.0	0.0
16	0	1	0	0	0	1	0.18	0.18	0.0	0.18
17	0	0	0	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0	0	0	0.0	0.0	0.0	0.0
20	1	0	0	0	0	1	0.15	0.15	0.0	0.15

[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



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

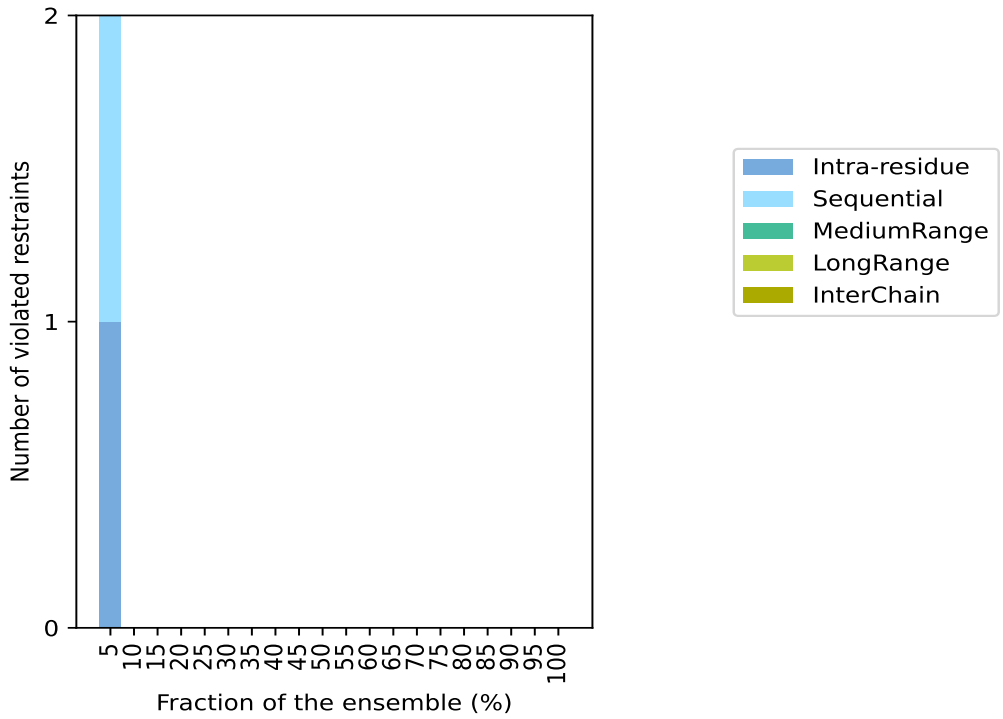
9.3 Distance violation statistics for the ensemble (i)

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, 282(IR:66, SQ:91, MR:79, LR:46, 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]	%
1	1	0	0	0	2	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	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	0	0	0	0	0	19	95.0
0	0	0	0	0	0	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



9.4 Most violated distance restraints in the ensemble

No violations found

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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

9.5.2 Table : All distance violations

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)
(1,280)	1:A:323:PRO:HB2	1:A:324:GLU:HG2	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,280)	1:A:323:PRO:HB2	1:A:324:GLU:HG3	16	0.18
(1,277)	1:A:319:ARG:HA	1:A:319:ARG:HG2	20	0.15
(1,277)	1:A:319:ARG:HA	1:A:319:ARG:HG3	20	0.15

10 Dihedral-angle violation analysis (i)

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