wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	7N45
BMRB ID	:	50507
Title	:	Solution NMR structure of the N-terminal globular domain of the endemic HKU1 coronavirus nucleocapsid protein
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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 (i)) were used in the production of this report:

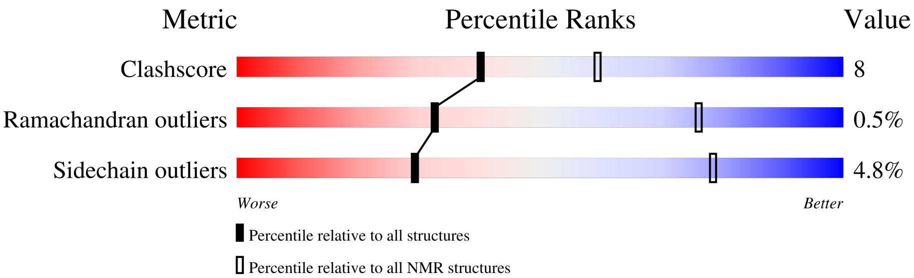
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 87%.

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	138	 76% 8% • 15%

2 Ensemble composition and analysis (i)

This entry contains 19 models. Model 2 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:8-A:49, A:64-A:138 (117)	1.01	2

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2121 atoms, of which 1020 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	138	2121	705	1020	189	207	0

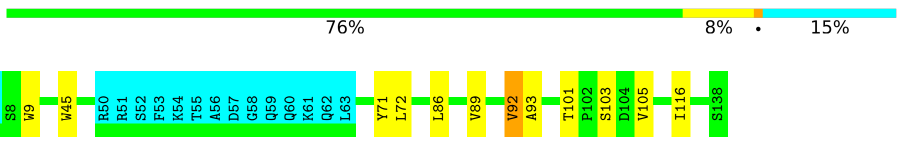
4 Residue-property plots (i)

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: Nucleoprotein

Chain A:

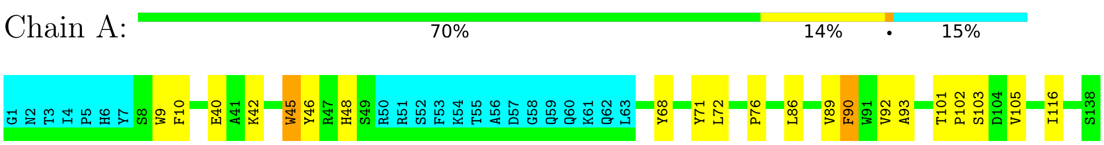


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 2. Colouring as in section 4.1 above.

- Molecule 1: Nucleoprotein

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry*.

Of the 150000 calculated structures, 19 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	
CS-ROSETTA	structure calculation	
CS-ROSETTA	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	1571
Number of shifts mapped to atoms	1571
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.62±0.01	0±0/966 (0.0± 0.0%)	0.48±0.01	0±0/1318 (0.0± 0.0%)
All	All	0.62	4/18354 (0.0%)	0.48	0/25042 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.8±0.7
All	All	0	35

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	102	PRO	N-CD	-5.34	1.40	1.47	9	4

There are no bond-angle outliers.

There are no chirality outliers.

5 of 8 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	92	VAL	Peptide	17
1	A	45	TRP	Peptide	6
1	A	33	ALA	Peptide	3
1	A	10	PHE	Peptide	3
1	A	130	TYR	Peptide	3

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	929	849	851	13±3
All	All	17651	16131	16169	256

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 8.

5 of 83 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:ILE:HD12	1:A:116:ILE:N	0.93	1.77	13	19
1:A:116:ILE:HD12	1:A:116:ILE:H	0.74	1.36	13	5
1:A:14:THR:OG1	1:A:66:ARG:NH1	0.74	2.21	4	1
1:A:131:TYR:C	1:A:131:TYR:CD1	0.72	2.60	8	1
1:A:116:ILE:N	1:A:116:ILE:CD1	0.72	2.50	13	17

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	116/138 (84%)	109±2 (94±1%)	7±2 (6±1%)	1±1 (0±1%)	32	76
All	All	2204/2622 (84%)	2070 (94%)	124 (6%)	10 (0%)	32	76

5 of 6 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	84	GLU	5
1	A	105	VAL	1
1	A	107	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	122	PRO	1
1	A	123	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	96/114 (84%)	91±1 (95±1%)	5±1 (5±1%)	29	78
All	All	1824/2166 (84%)	1736 (95%)	88 (5%)	29	78

5 of 24 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	101	THR	16
1	A	9	TRP	13
1	A	105	VAL	10
1	A	112	THR	9
1	A	116	ILE	6

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 87% for the well-defined parts and 86% 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 (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	1571
Number of shifts mapped to atoms	1571
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	13

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	138	0.17 ± 0.07	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	122	0.13 ± 0.17	None needed (< 0.5 ppm)
$^{13}C'$	117	0.33 ± 0.10	None needed (< 0.5 ppm)
^{15}N	120	-1.25 ± 0.48	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 87%, i.e. 1325 atoms were assigned a chemical shift out of a possible 1521. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	550/577 (95%)	232/237 (98%)	217/234 (93%)	101/106 (95%)
Sidechain	635/723 (88%)	430/469 (92%)	197/225 (88%)	8/29 (28%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	140/221 (63%)	73/108 (68%)	63/109 (58%)	4/4 (100%)
Overall	1325/1521 (87%)	735/814 (90%)	477/568 (84%)	113/139 (81%)

7.1.4 Statistically unusual chemical shifts (i)

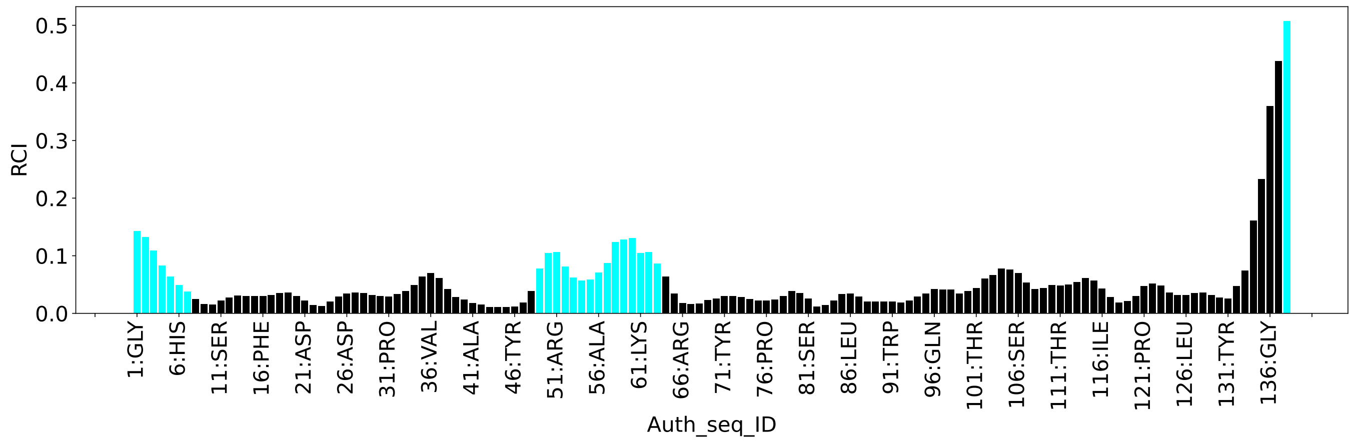
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	47	ARG	HD2	0.10	1.97 – 4.26	-13.2
1	A	47	ARG	HB2	-1.36	0.52 – 3.08	-12.3
1	A	47	ARG	HB3	-1.35	0.43 – 3.11	-11.6
1	A	47	ARG	HD3	0.10	1.81 – 4.39	-11.6
1	A	108	ARG	HB3	-0.84	0.43 – 3.11	-9.7
1	A	83	GLY	H	3.04	5.23 – 11.42	-8.5
1	A	29	GLY	HA2	1.47	2.15 – 5.77	-6.9
1	A	31	PRO	HD3	1.15	1.76 – 5.48	-6.6
1	A	127	PRO	HG3	-0.09	0.33 – 3.48	-6.3
1	A	31	PRO	HG2	0.13	0.41 – 3.45	-5.9
1	A	31	PRO	HB3	0.12	0.25 – 3.76	-5.4
1	A	82	TYR	HA	1.78	1.87 – 7.33	-5.2
1	A	76	PRO	HD3	1.74	1.76 – 5.48	-5.0

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
0.0
0.1
0.2
0.3
0.4
0.5
1:GLY
6:HIS
11:SER
16:PHE
21:ASP
26:ASP
31:PRO
36:VAL
41:ALA
46:TYR
51:ARG
56:ALA
61:LYS
66:ARG
71:TYR
76:PRO
81:SER
86:LEU
91:TRP
96:GLN
101:THR
106:SER
111:THR
116:ILE
121:PRO
126:LEU
131:TYR
136:GLY
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	2568
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	1221
Medium range (|i-j|>1 and |i-j|<5)	444
Long range (|i-j|≥5)	903
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	18.6
Number of long range restraints per residue[1]	6.5

[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)	42.6	0.2
0.2-0.5 (Medium)	72.6	0.5
>0.5 (Large)	234.1	6.55

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)

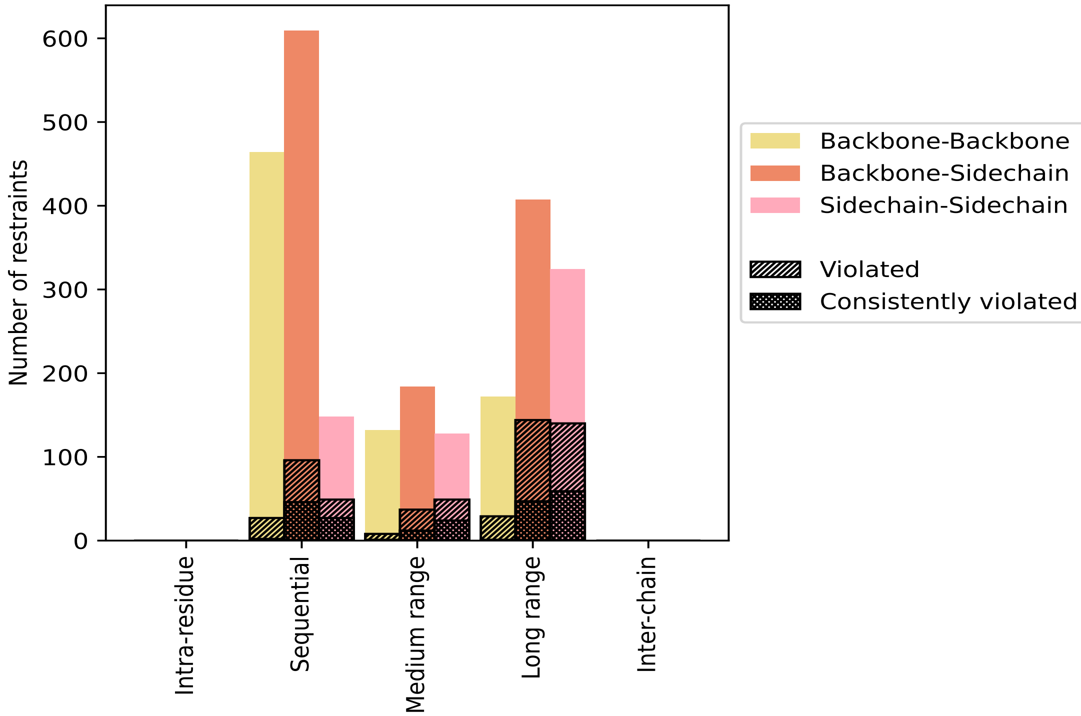
9.1 Summary of distance violations (i)

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)	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
Sequential (|i-j|=1)	1221	47.5	172	14.1	6.7	75	6.1	2.9
Backbone-Backbone	464	18.1	27	5.8	1.1	2	0.4	0.1
Backbone-Sidechain	609	23.7	96	15.8	3.7	46	7.6	1.8
Sidechain-Sidechain	148	5.8	49	33.1	1.9	27	18.2	1.1
Medium range (|i-j|>1 & |i-j|<5)	444	17.3	94	21.2	3.7	37	8.3	1.4
Backbone-Backbone	132	5.1	8	6.1	0.3	1	0.8	0.0
Backbone-Sidechain	184	7.2	37	20.1	1.4	12	6.5	0.5
Sidechain-Sidechain	128	5.0	49	38.3	1.9	24	18.8	0.9
Long range (|i-j|≥5)	903	35.2	313	34.7	12.2	107	11.8	4.2
Backbone-Backbone	172	6.7	29	16.9	1.1	1	0.6	0.0
Backbone-Sidechain	407	15.8	144	35.4	5.6	47	11.5	1.8
Sidechain-Sidechain	324	12.6	140	43.2	5.5	59	18.2	2.3
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	2568	100.0	579	22.5	22.5	219	8.5	8.5
Backbone-Backbone	768	29.9	64	8.3	2.5	4	0.5	0.2
Backbone-Sidechain	1200	46.7	277	23.1	10.8	105	8.8	4.1
Sidechain-Sidechain	600	23.4	238	39.7	9.3	110	18.3	4.3

[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 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	0	105	61	170	0	336	0.99	4.74	0.82	0.75
2	0	110	57	183	0	350	1.0	6.17	0.83	0.82
3	0	116	54	176	0	346	1.0	6.12	0.84	0.76
4	0	115	53	180	0	348	1.0	5.65	0.86	0.76
5	0	109	54	185	0	348	1.02	6.48	0.85	0.83
6	0	105	50	187	0	342	0.99	6.11	0.84	0.77
7	0	113	53	185	0	351	0.96	5.96	0.83	0.74
8	0	108	59	188	0	355	0.96	5.22	0.84	0.72
9	0	110	59	188	0	357	0.99	6.13	0.83	0.77
10	0	105	60	195	0	360	0.98	6.08	0.84	0.76
11	0	105	57	184	0	346	1.02	4.71	0.83	0.82

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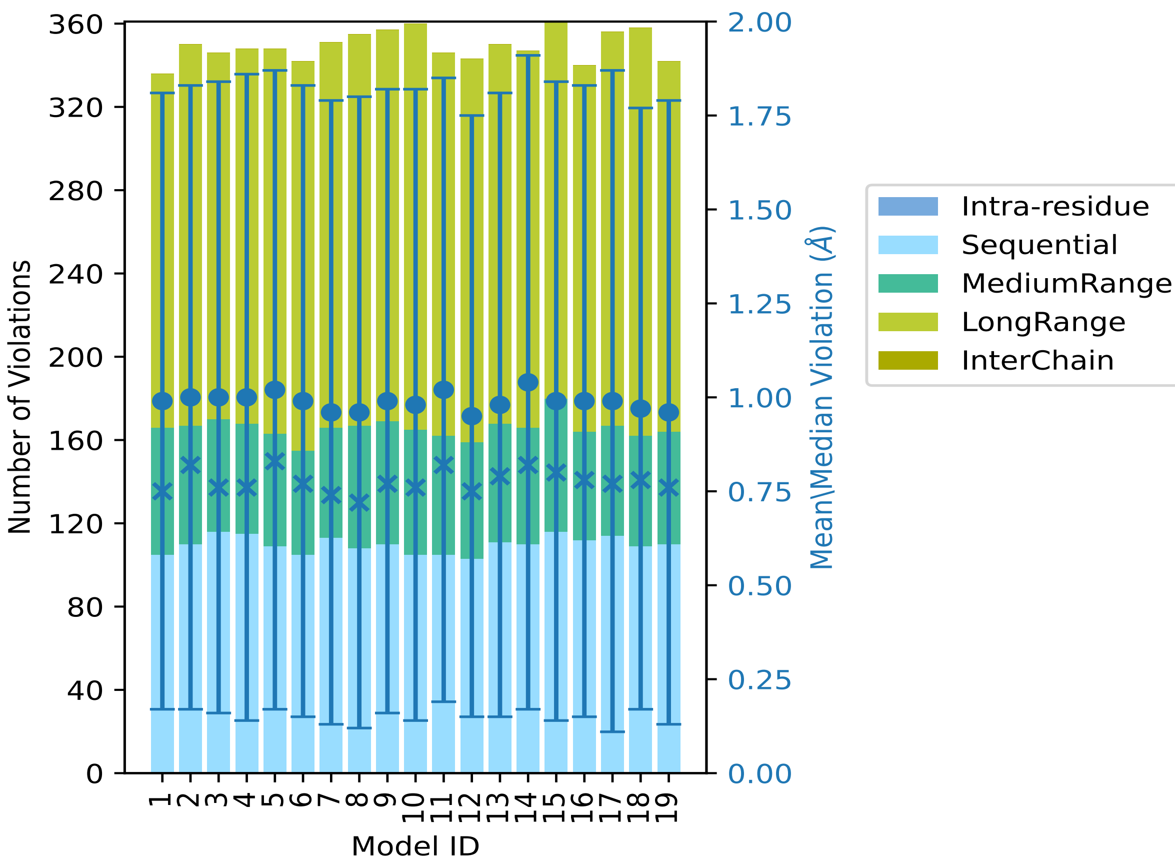
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	103	56	184	0	343	0.95	4.73	0.8	0.75
13	0	111	57	182	0	350	0.98	6.21	0.83	0.79
14	0	110	56	181	0	347	1.04	6.55	0.87	0.82
15	0	116	64	181	0	361	0.99	5.88	0.85	0.8
16	0	112	52	176	0	340	0.99	5.51	0.84	0.78
17	0	114	53	189	0	356	0.99	5.93	0.88	0.77
18	0	109	53	196	0	358	0.97	4.6	0.8	0.78
19	0	110	54	178	0	342	0.96	5.7	0.83	0.76

[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

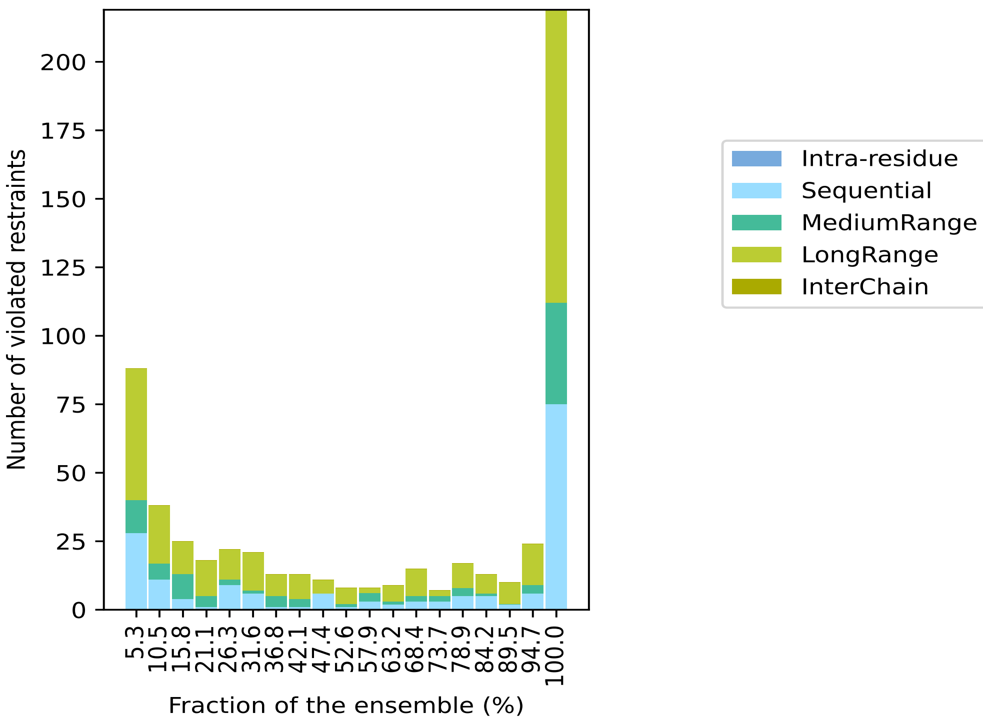
9.3 Distance violation statistics for the ensemble (i)

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, 1989(IR:0, SQ:1049, MR:350, LR:590, 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]	%
0	28	12	48	0	88	1	5.3
0	11	6	21	0	38	2	10.5
0	4	9	12	0	25	3	15.8
0	1	4	13	0	18	4	21.1
0	9	2	11	0	22	5	26.3
0	6	1	14	0	21	6	31.6
0	1	4	8	0	13	7	36.8
0	1	3	9	0	13	8	42.1
0	6	0	5	0	11	9	47.4
0	1	1	6	0	8	10	52.6
0	3	3	2	0	8	11	57.9
0	2	1	6	0	9	12	63.2
0	3	2	10	0	15	13	68.4
0	3	2	2	0	7	14	73.7
0	5	3	9	0	17	15	78.9
0	5	1	7	0	13	16	84.2
0	2	0	8	0	10	17	89.5
0	6	3	15	0	24	18	94.7
0	75	37	107	0	219	19	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

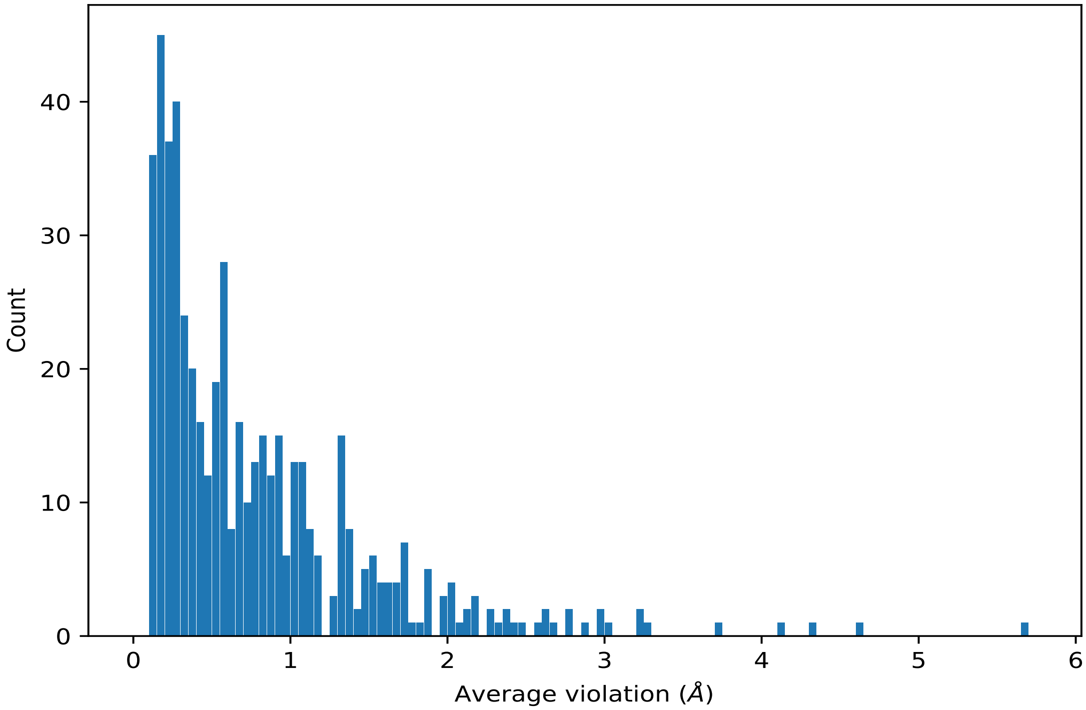
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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.

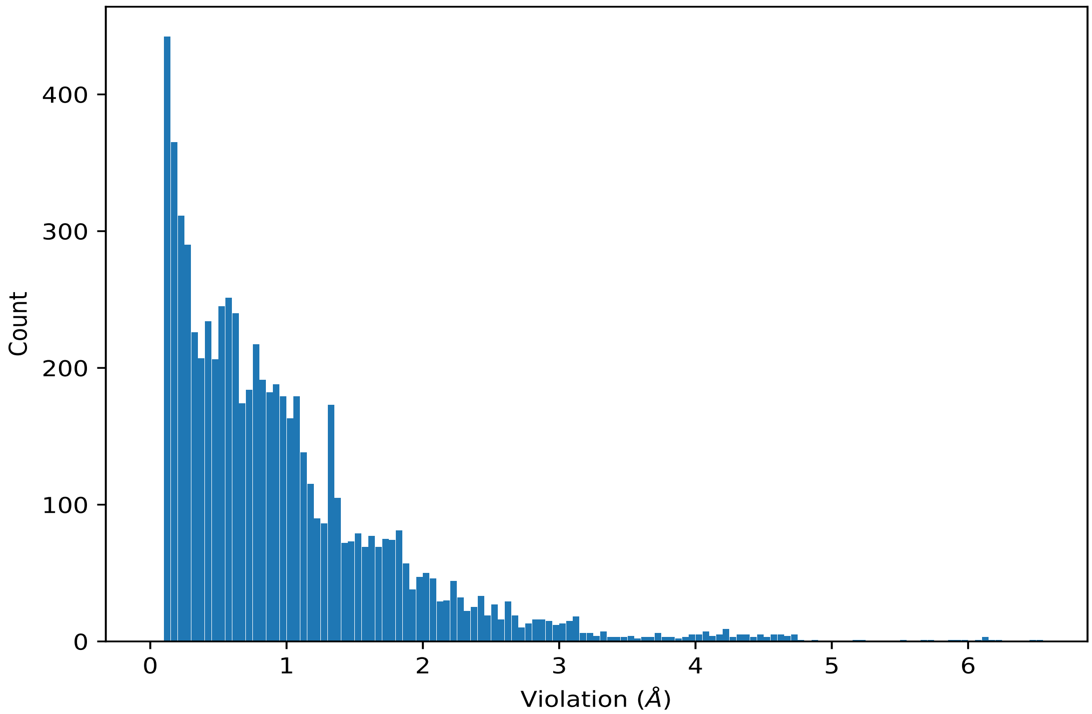
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,88)	1:A:34:PHE:CB	1:A:71:TYR:CB	19	5.68	0.65	5.93
(2,286)	1:A:91:TRP:CB	1:A:72:LEU:CB	19	4.63	0.1	4.62
(2,937)	1:A:91:TRP:CB	1:A:72:LEU:CB	19	4.35	0.1	4.34
(2,878)	1:A:91:TRP:CB	1:A:72:LEU:CB	19	4.12	0.1	4.11
(2,781)	1:A:124:THR:CB	1:A:127:PRO:CB	19	3.73	0.18	3.71
(2,80)	1:A:113:GLN:CB	1:A:9:TRP:CB	19	3.27	1.05	3.64
(2,728)	1:A:113:GLN:CB	1:A:116:ILE:CB	19	3.21	1.0	3.3
(2,548)	1:A:80:ALA:CB	1:A:91:TRP:CB	19	3.21	0.14	3.24
(2,87)	1:A:46:TYR:CB	1:A:44:TYR:CB	19	3.05	0.09	3.06
(2,879)	1:A:80:ALA:CB	1:A:91:TRP:CB	19	2.98	0.14	3.01

[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)
(2,88)	1:A:34:PHE:CB	1:A:71:TYR:CB	14	6.55
(2,88)	1:A:34:PHE:CB	1:A:71:TYR:CB	5	6.48
(2,88)	1:A:34:PHE:CB	1:A:71:TYR:CB	13	6.21
(2,88)	1:A:34:PHE:CB	1:A:71:TYR:CB	2	6.17
(2,88)	1:A:34:PHE:CB	1:A:71:TYR:CB	9	6.13
(2,88)	1:A:34:PHE:CB	1:A:71:TYR:CB	3	6.12
(2,88)	1:A:34:PHE:CB	1:A:71:TYR:CB	6	6.11
(2,88)	1:A:34:PHE:CB	1:A:71:TYR:CB	10	6.08
(2,88)	1:A:34:PHE:CB	1:A:71:TYR:CB	7	5.96
(2,88)	1:A:34:PHE:CB	1:A:71:TYR:CB	17	5.93

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found