wwPDB NMR Structure Validation Summary Report

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PDB ID	:	6SVH
BMRB ID	:	34434
Title	:	Protein allostery of the WW domain at atomic resolution: FFpSPR bound structure
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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 (1)) were used in the production of this report:

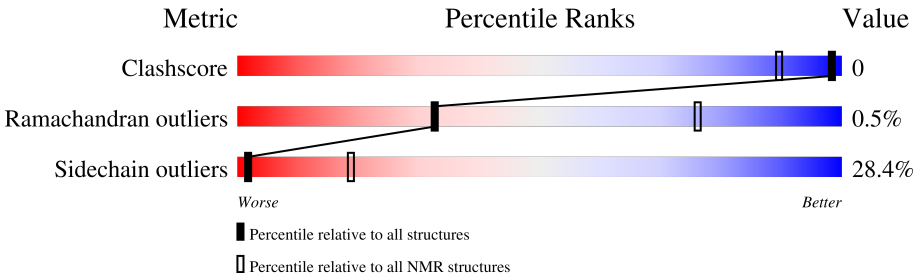
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 79%.

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	35	71% 20% · 6%

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:7-A:39 (33)	0.43	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 2 clusters and 14 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1130 atoms, of which 552 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	35	1130	362	552	112	102	2	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	SER	-	expression tag	UNP Q13526
A	18	ASN	SER	engineered mutation	UNP Q13526
A	34	PHE	TRP	engineered mutation	UNP Q13526

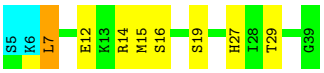
4 Residue-property plots (i)

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: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:

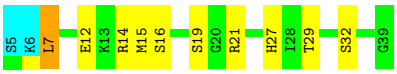


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

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

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure calculation	3.98.12

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	378
Number of shifts mapped to atoms	378
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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	518	480	516	0±0
All	All	10360	9600	10320	4

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7[B]:LEU:HD21	1:A:24[B]:TYR:CD1	0.47	2.44	16	1
1:A:7[A]:LEU:HD21	1:A:24[A]:TYR:CE2	0.45	2.46	6	1
1:A:7[B]:LEU:HD21	1:A:24[B]:TYR:CD2	0.45	2.47	11	1
1:A:8[A]:PRO:HB2	1:A:9[A]:PRO:HD2	0.40	1.94	13	1

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	64/35 (183%)	56±3 (87±4%)	8±3 (12±4%)	0±1 (0±1%)	32 76
All	All	1280/700 (183%)	1118 (87%)	156 (12%)	6 (0%)	32 76

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

Mol	Chain	Res	Type	Models (Total)
1	A	16[A]	SER	3
1	A	16[B]	SER	3

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	58/31 (187%)	42±4 (72±7%)	16±4 (28±7%)	2 19
All	All	1160/620 (187%)	830 (72%)	330 (28%)	2 19

5 of 36 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	15[A]	MET	18
1	A	15[B]	MET	18
1	A	27[A]	HIS	17
1	A	27[B]	HIS	17
1	A	14[A]	ARG	16

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

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 77% 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	378
Number of shifts mapped to atoms	378
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	30	0.33 ± 0.27	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	31	0.02 ± 0.21	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	30	-0.77 ± 0.97	None needed (imprecise)

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 79%, i.e. 364 atoms were assigned a chemical shift out of a possible 462. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	123/162 (76%)	64/66 (97%)	30/66 (45%)	29/30 (97%)
Sidechain	204/243 (84%)	139/155 (90%)	59/71 (83%)	6/17 (35%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	37/57 (65%)	22/28 (79%)	14/27 (52%)	1/2 (50%)
Overall	364/462 (79%)	225/249 (90%)	103/164 (63%)	36/49 (73%)

7.1.4 Statistically unusual chemical shifts (i)

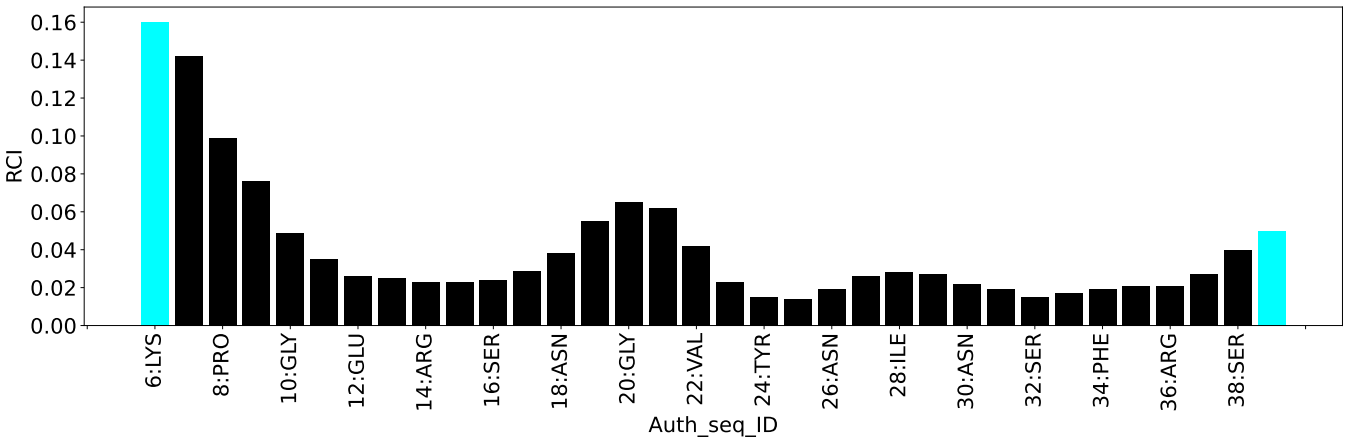
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	26	ASN	HB2	-0.83	1.27 – 4.34	-11.8
1	A	14	ARG	HB2	-0.07	0.52 – 3.08	-7.3
1	A	37	PRO	HG3	-0.27	0.33 – 3.48	-6.9
1	A	26	ASN	HD21	4.06	4.94 – 9.72	-6.8

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	1312
Intra-residue (|i-j|=0)	351
Sequential (|i-j|=1)	356
Medium range (|i-j|>1 and |i-j|<5)	179
Long range (|i-j|≥5)	426
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	37.5
Number of long range restraints per residue[1]	12.2

[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)	24.6	0.2
0.2-0.5 (Medium)	93.4	0.5
>0.5 (Large)	1061.5	7.17

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)

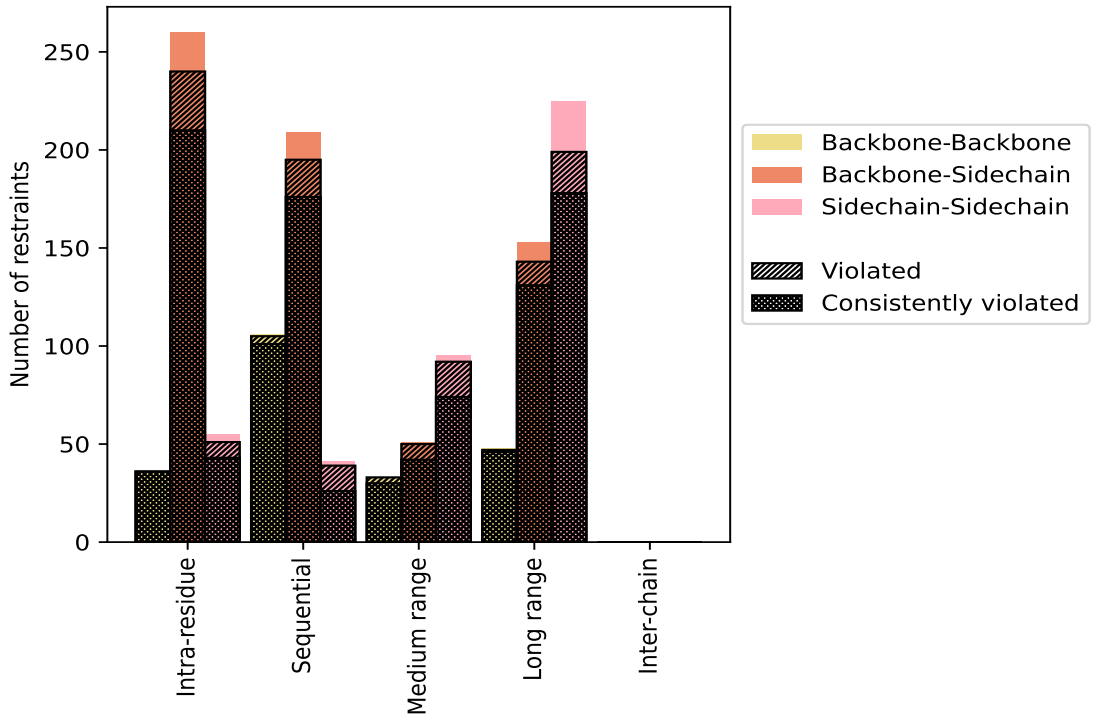
9.1 Summary of distance violations (i)

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)	351	26.8	327	93.2	24.9	289	82.3	22.0
Backbone-Backbone	36	2.7	36	100.0	2.7	36	100.0	2.7
Backbone-Sidechain	260	19.8	240	92.3	18.3	210	80.8	16.0
Sidechain-Sidechain	55	4.2	51	92.7	3.9	43	78.2	3.3
Sequential (|i-j|=1)	356	27.1	339	95.2	25.8	303	85.1	23.1
Backbone-Backbone	106	8.1	105	99.1	8.0	101	95.3	7.7
Backbone-Sidechain	209	15.9	195	93.3	14.9	176	84.2	13.4
Sidechain-Sidechain	41	3.1	39	95.1	3.0	26	63.4	2.0
Medium range (|i-j|>1 & |i-j|<5)	179	13.6	175	97.8	13.3	146	81.6	11.1
Backbone-Backbone	33	2.5	33	100.0	2.5	30	90.9	2.3
Backbone-Sidechain	51	3.9	50	98.0	3.8	42	82.4	3.2
Sidechain-Sidechain	95	7.2	92	96.8	7.0	74	77.9	5.6
Long range (|i-j|≥5)	426	32.5	389	91.3	29.6	355	83.3	27.1
Backbone-Backbone	48	3.7	47	97.9	3.6	46	95.8	3.5
Backbone-Sidechain	153	11.7	143	93.5	10.9	131	85.6	10.0
Sidechain-Sidechain	225	17.1	199	88.4	15.2	178	79.1	13.6
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	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	1312	100.0	1230	93.8	93.8	1093	83.3	83.3
Backbone-Backbone	223	17.0	221	99.1	16.8	213	95.5	16.2
Backbone-Sidechain	673	51.3	628	93.3	47.9	559	83.1	42.6
Sidechain-Sidechain	416	31.7	381	91.6	29.0	321	77.2	24.5

[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	307	329	166	376	0	1178	1.35	5.28	0.83	1.13
2	314	328	164	375	0	1181	1.35	5.37	0.84	1.13
3	312	328	166	376	0	1182	1.34	5.15	0.82	1.13
4	308	328	165	377	0	1178	1.35	5.49	0.85	1.15
5	312	322	166	375	0	1175	1.34	6.16	0.84	1.14
6	308	330	170	372	0	1180	1.38	5.35	0.88	1.13
7	315	319	170	373	0	1177	1.42	7.17	0.91	1.17
8	312	328	167	376	0	1183	1.34	5.25	0.83	1.13
9	311	330	169	370	0	1180	1.37	6.11	0.89	1.15
10	311	332	165	376	0	1184	1.33	5.08	0.82	1.13
11	312	327	165	376	0	1180	1.35	5.66	0.82	1.14

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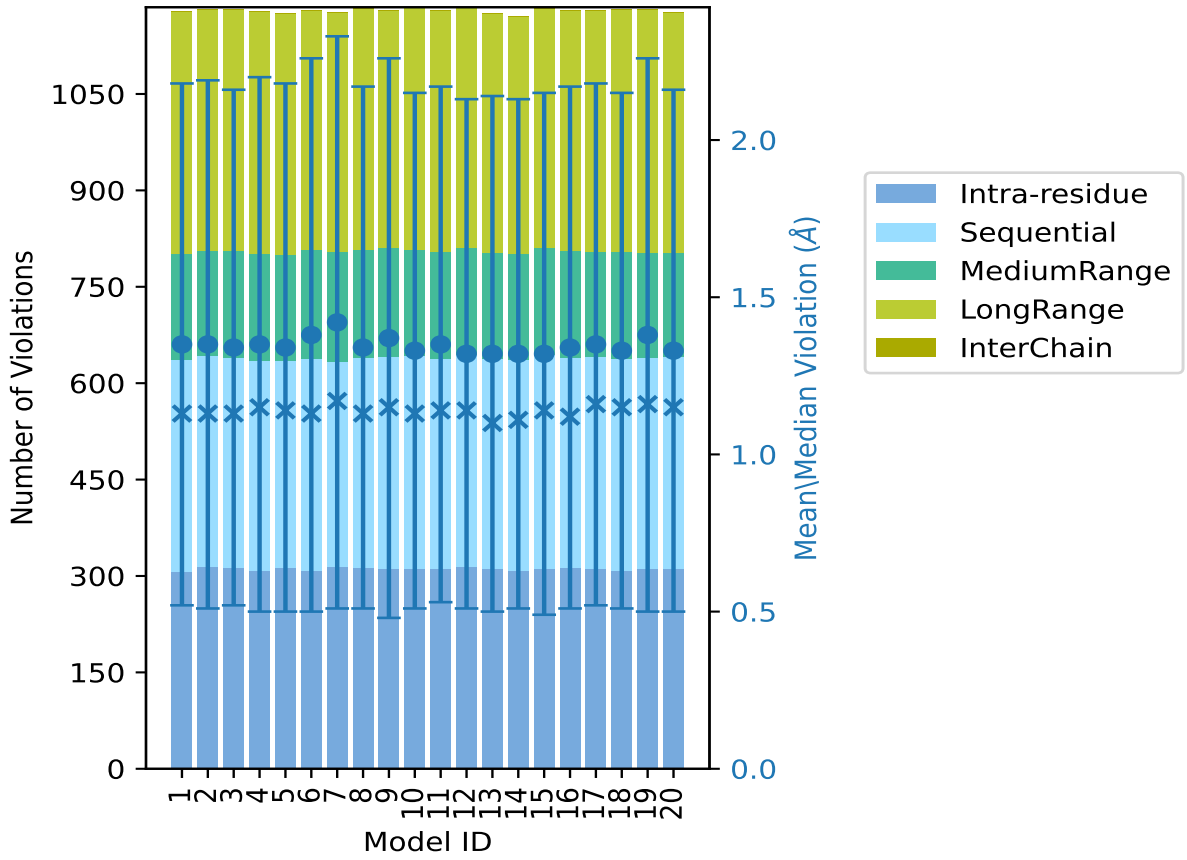
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	314	330	166	375	0	1185	1.32	4.85	0.81	1.14
13	311	327	165	372	0	1175	1.32	5.3	0.82	1.1
14	308	329	165	368	0	1170	1.32	5.12	0.81	1.11
15	312	333	165	373	0	1183	1.32	7.1	0.83	1.14
16	312	328	165	375	0	1180	1.34	4.88	0.83	1.12
17	311	330	163	376	0	1180	1.35	7.02	0.83	1.16
18	308	330	167	376	0	1181	1.33	5.37	0.82	1.15
19	311	329	163	378	0	1181	1.38	5.8	0.88	1.16
20	311	330	162	374	0	1177	1.33	4.94	0.83	1.15

[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

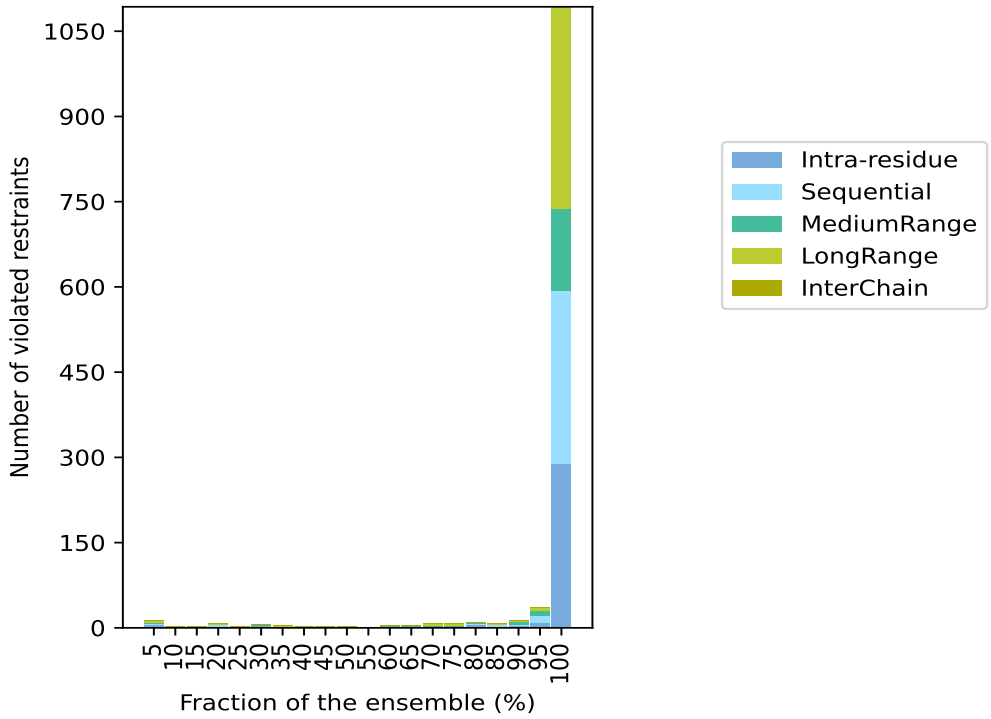
9.3 Distance violation statistics for the ensemble (i)

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, 82(IR:24, SQ:17, MR:4, LR:37, 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]	%
6	1	1	5	0	13	1	5.0
1	1	1	0	0	3	2	10.0
0	2	1	0	0	3	3	15.0
2	4	0	2	0	8	4	20.0
0	0	0	2	0	2	5	25.0
3	1	2	0	0	6	6	30.0
1	0	1	2	0	4	7	35.0
1	0	1	1	0	3	8	40.0
0	0	2	1	0	3	9	45.0
1	1	0	1	0	3	10	50.0
0	0	0	0	0	0	11	55.0
2	0	1	1	0	4	12	60.0
3	0	0	1	0	4	13	65.0
0	1	3	3	0	7	14	70.0
1	1	1	5	0	8	15	75.0
5	2	2	1	0	10	16	80.0
1	5	0	1	0	7	17	85.0
3	3	5	2	0	13	18	90.0
8	14	8	6	0	36	19	95.0
289	303	146	355	0	1093	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

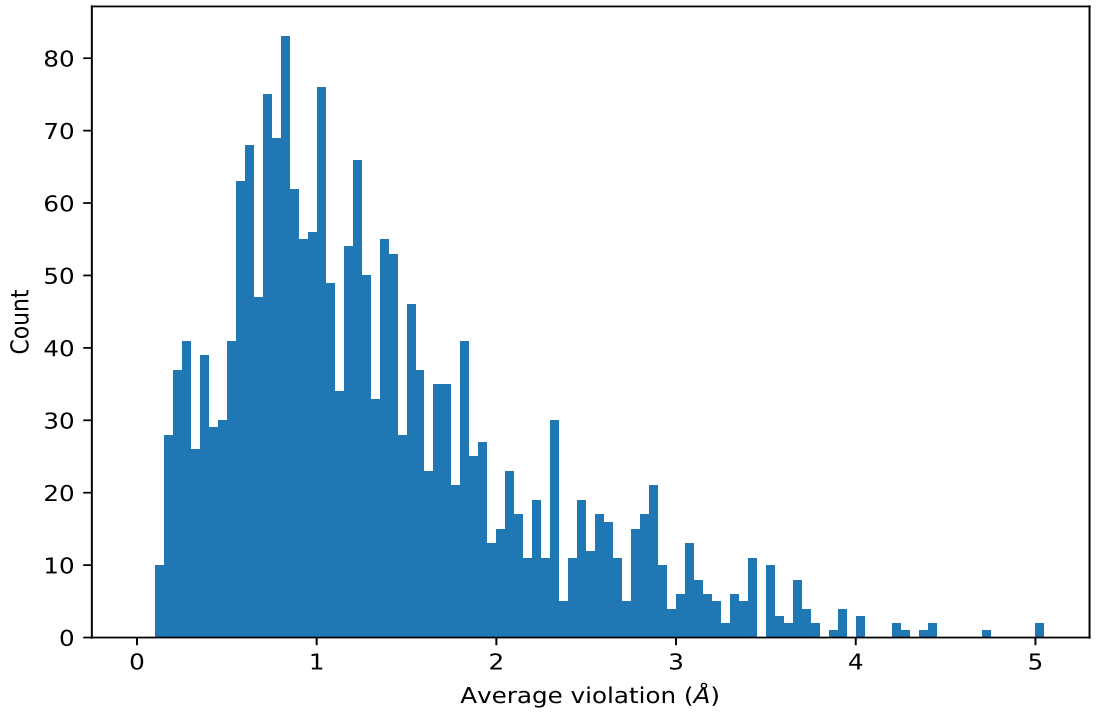
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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)
(2,517)	1:A:17:ARG:HG2	1:A:18:ASN:HD22	20	5.0	1.28	4.9
(2,517)	1:A:17:ARG:HG3	1:A:18:ASN:HD22	20	5.0	1.28	4.9
(2,584)	1:A:8:PRO:HG2	1:A:39:GLY:HA2	20	4.7	0.71	4.94
(2,381)	1:A:32:SER:HB3	1:A:34:PHE:HE1	20	4.44	0.49	4.34
(2,381)	1:A:32:SER:HB3	1:A:34:PHE:HE2	20	4.44	0.49	4.34
(2,525)	1:A:9:PRO:HB3	1:A:10:GLY:HA3	20	4.37	0.02	4.36
(2,431)	1:A:37:PRO:HB3	1:A:39:GLY:H	20	4.27	0.51	4.36
(2,512)	1:A:17:ARG:HB2	1:A:18:ASN:HD21	20	4.2	0.75	4.27
(2,512)	1:A:17:ARG:HB3	1:A:18:ASN:HD21	20	4.2	0.75	4.27
(2,16)	1:A:7:LEU:HD11	1:A:11:TRP:HB3	20	4.0	0.4	4.1
(2,16)	1:A:7:LEU:HD12	1:A:11:TRP:HB3	20	4.0	0.4	4.1
(2,16)	1:A:7:LEU:HD13	1:A:11:TRP:HB3	20	4.0	0.4	4.1
(2,468)	1:A:14:ARG:HD3	1:A:25:PHE:H	20	3.94	0.22	3.99
(2,195)	1:A:7:LEU:HD11	1:A:37:PRO:HG3	20	3.91	0.31	3.98
(2,195)	1:A:7:LEU:HD12	1:A:37:PRO:HG3	20	3.91	0.31	3.98
(2,195)	1:A:7:LEU:HD13	1:A:37:PRO:HG3	20	3.91	0.31	3.98

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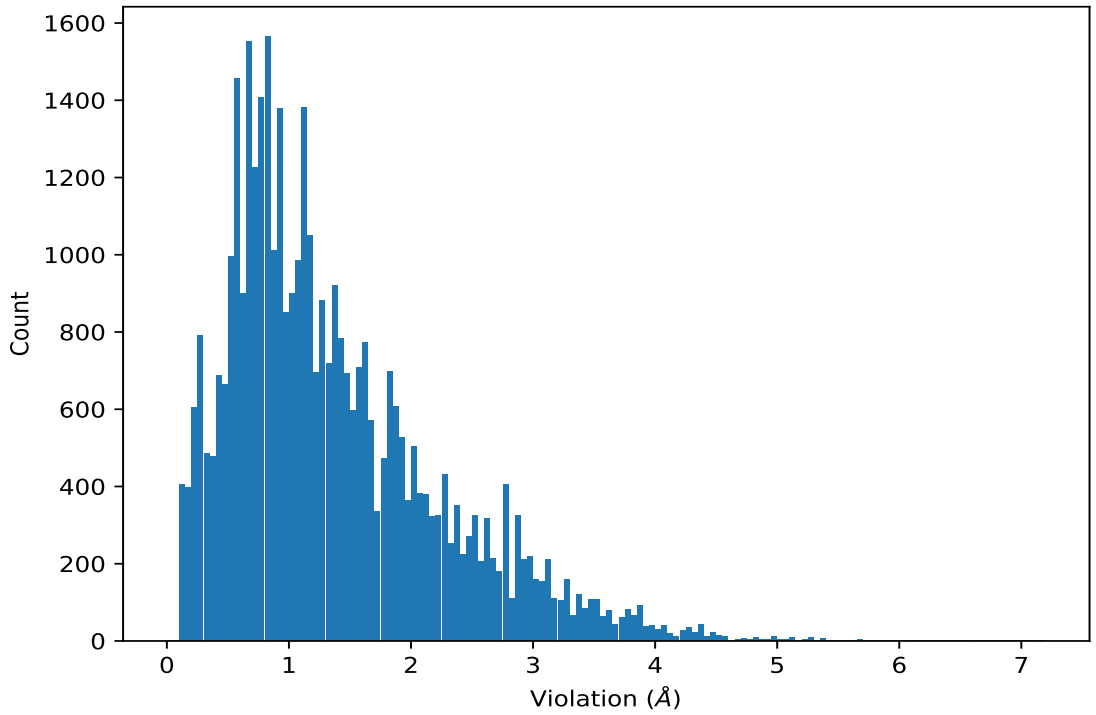
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,404)	1:A:14:ARG:HD2	1:A:25:PHE:HB2	20	3.89	0.22	3.9

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

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.



9.5.2 Table : All distance violations

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)
(2,517)	1:A:17:ARG:HG2	1:A:18:ASN:HD22	7	7.17
(2,517)	1:A:17:ARG:HG3	1:A:18:ASN:HD22	7	7.17
(2,517)	1:A:17:ARG:HG2	1:A:18:ASN:HD22	15	7.1
(2,517)	1:A:17:ARG:HG3	1:A:18:ASN:HD22	15	7.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,517)	1:A:17:ARG:HG2	1:A:18:ASN:HD22	17	7.02
(2,517)	1:A:17:ARG:HG3	1:A:18:ASN:HD22	17	7.02
(2,481)	1:A:12:GLU:H	1:A:27:HIS:HD2	5	6.16
(2,517)	1:A:17:ARG:HG2	1:A:18:ASN:HD22	9	6.11
(2,517)	1:A:17:ARG:HG3	1:A:18:ASN:HD22	9	6.11
(2,390)	1:A:12:GLU:HB2	1:A:27:HIS:HD2	5	5.81
(2,390)	1:A:12:GLU:HB3	1:A:27:HIS:HD2	5	5.81
(2,517)	1:A:17:ARG:HG2	1:A:18:ASN:HD22	19	5.8
(2,517)	1:A:17:ARG:HG3	1:A:18:ASN:HD22	19	5.8
(2,517)	1:A:17:ARG:HG2	1:A:18:ASN:HD22	11	5.66
(2,517)	1:A:17:ARG:HG3	1:A:18:ASN:HD22	11	5.66
(2,505)	1:A:33:GLN:HE21	1:A:37:PRO:HD2	9	5.65
(2,466)	1:A:33:GLN:HE21	1:A:36:ARG:HA	9	5.61

10 Dihedral-angle violation analysis (i)

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