



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 5TVZ / pdb_00005tvz
BMRB ID : 30201
Title : Solution NMR structure of Saccharomyces cerevisiae Pom152 Ig-like repeat, residues 718-820
Authors : Dutta, K.; Sampathkumar, P.; Cowburn, D.; Almo, S.C.; Rout, M.P.; Fernandez-Martinez, J.
Deposited on : 2016-11-10

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

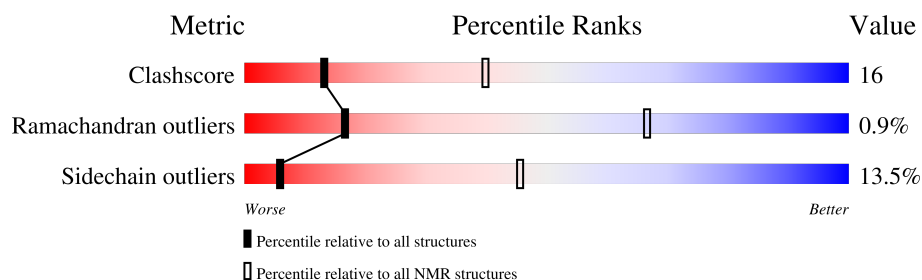
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	114	

2 Ensemble composition and analysis

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:720-A:760, A:765-A:818 (95)	0.42	4

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1637 atoms, of which 837 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nucleoporin POM152.

Mol	Chain	Residues	Atoms						Trace
1	A	103	Total	C	H	N	O	S	0
			1637	511	837	136	151	2	

There are 11 discrepancies between the modelled and reference sequences:

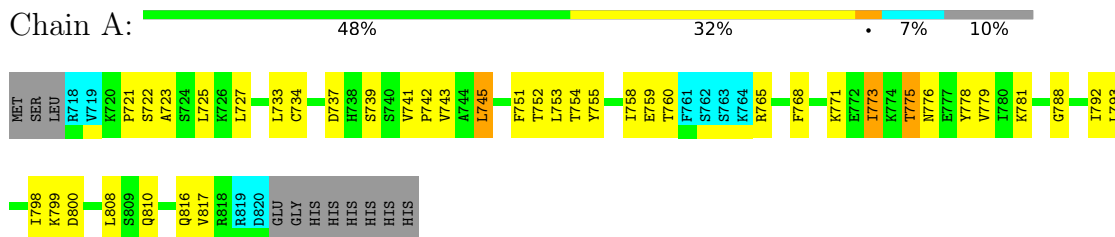
Chain	Residue	Modelled	Actual	Comment	Reference
A	715	MET	-	expression tag	UNP P39685
A	716	SER	-	expression tag	UNP P39685
A	717	LEU	-	expression tag	UNP P39685
A	821	GLU	-	expression tag	UNP P39685
A	822	GLY	-	expression tag	UNP P39685
A	823	HIS	-	expression tag	UNP P39685
A	824	HIS	-	expression tag	UNP P39685
A	825	HIS	-	expression tag	UNP P39685
A	826	HIS	-	expression tag	UNP P39685
A	827	HIS	-	expression tag	UNP P39685
A	828	HIS	-	expression tag	UNP P39685

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.

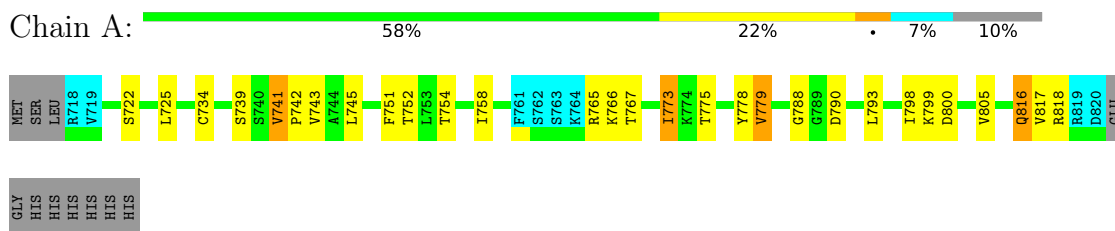
- Molecule 1: Nucleoporin POM152



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

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

- Molecule 1: Nucleoporin POM152



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 2048 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
ARIA	structure calculation	
CNS	refinement	
CNS	structure calculation	

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	1337
Number of shifts mapped to atoms	1287
Number of unparsed shifts	0
Number of shifts with mapping errors	50
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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	731	766	763	24±6
All	All	14620	15320	15260	487

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 16.

5 of 129 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:788:GLY:HA2	1:A:817:VAL:HG22	0.91	1.39	16	4
1:A:745:LEU:HD13	1:A:773:ILE:HD13	0.84	1.49	3	16
1:A:725:LEU:HG	1:A:743:VAL:HG22	0.78	1.54	13	1
1:A:722:SER:HB2	1:A:810:GLN:OE1	0.76	1.81	13	2
1:A:745:LEU:HD11	1:A:778:TYR:HB3	0.76	1.55	14	20

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	95/114 (83%)	86±1 (91±1%)	8±1 (8±1%)	1±1 (1±1%)	16	66
All	All	1900/2280 (83%)	1725 (91%)	157 (8%)	18 (1%)	16	66

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	722	SER	15
1	A	776	ASN	1
1	A	786	THR	1
1	A	750	PRO	1

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	85/103 (83%)	74±2 (86±3%)	12±2 (14±3%)	6	45
All	All	1700/2060 (83%)	1470 (86%)	230 (14%)	6	45

5 of 34 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	773	ILE	20
1	A	816	GLN	20
1	A	741	VAL	17
1	A	760	THR	16
1	A	745	LEU	14

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 [i](#)

There are no oligosaccharides 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 92% for the well-defined parts and 91% 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	1337
Number of shifts mapped to atoms	1287
Number of unparsed shifts	0
Number of shifts with mapping errors	50
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 50) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	716	SER	HA	4.516	0.0000	1
1	A	716	SER	HB2	3.937	0.0000	2
1	A	716	SER	HB3	3.937	0.0000	2
1	A	716	SER	C	174.3546	0.0000	1
1	A	716	SER	CA	58.1807	0.0000	1
1	A	716	SER	CB	63.9	0.0000	1
1	A	717	LEU	H	8.1873	0.0000	1
1	A	717	LEU	HA	4.417	0.0000	1
1	A	717	LEU	HB2	1.615	0.0000	2
1	A	717	LEU	HB3	1.615	0.0000	2
1	A	717	LEU	HD11	0.916	0.0000	2
1	A	717	LEU	HD12	0.916	0.0000	2
1	A	717	LEU	HD13	0.916	0.0000	2
1	A	717	LEU	HD21	0.8778	0.0000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	717	LEU	HD22	0.8778	0.0000	2
1	A	717	LEU	HD23	0.8778	0.0000	2
1	A	717	LEU	HG	1.615	0.0000	1
1	A	717	LEU	C	177.0432	0.0000	1
1	A	717	LEU	CA	55.414	0.0000	1
1	A	717	LEU	CB	42.3929	0.0000	1
1	A	717	LEU	CD1	24.794	0.0000	2
1	A	717	LEU	CD2	23.902	0.0000	2
1	A	717	LEU	CG	26.995	0.0000	1
1	A	717	LEU	N	123.6128	0.0000	1
1	A	821	GLU	H	8.5739	0.0000	1
1	A	821	GLU	HA	4.293	0.0000	1
1	A	821	GLU	HB2	2.103	0.0000	2
1	A	821	GLU	HB3	1.893	0.0000	2
1	A	821	GLU	HG2	2.209	0.0000	2
1	A	821	GLU	HG3	2.265	0.0000	2
1	A	821	GLU	C	177.1055	0.0000	1
1	A	821	GLU	CA	56.8883	0.0000	1
1	A	821	GLU	CB	30.0196	0.0000	1
1	A	821	GLU	CG	36.305	0.0000	1
1	A	821	GLU	N	122.8553	0.0000	1
1	A	822	GLY	H	8.536	0.0000	1
1	A	822	GLY	HA2	3.864	0.0000	2
1	A	822	GLY	HA3	3.864	0.0000	2
1	A	822	GLY	C	174.1262	0.0000	1
1	A	822	GLY	CA	45.4403	0.0000	1
1	A	822	GLY	N	108.9427	0.0000	1
1	A	823	HIS	H	8.1055	0.0000	1
1	A	823	HIS	HA	4.54	0.0000	1
1	A	823	HIS	HB2	2.975	0.0000	2
1	A	823	HIS	HB3	3.03	0.0000	2
1	A	823	HIS	HD2	6.955	0.0000	1
1	A	823	HIS	C	175.0597	0.0000	1
1	A	823	HIS	CA	55.9022	0.0000	1
1	A	823	HIS	CB	29.7537	0.0000	1
1	A	823	HIS	N	118.7278	0.0000	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	108	0.00 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	100	-0.01 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	108	0.26 ± 0.11	None needed (< 0.5 ppm)
^{15}N	101	-0.98 ± 0.27	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 92%, i.e. 1191 atoms were assigned a chemical shift out of a possible 1290. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	470/472 (100%)	191/192 (99%)	190/190 (100%)	89/90 (99%)
Sidechain	690/737 (94%)	468/483 (97%)	217/234 (93%)	5/20 (25%)
Aromatic	31/81 (38%)	19/39 (49%)	12/36 (33%)	0/6 (0%)
Overall	1191/1290 (92%)	678/714 (95%)	419/460 (91%)	94/116 (81%)

7.1.4 Statistically unusual chemical shifts [i](#)

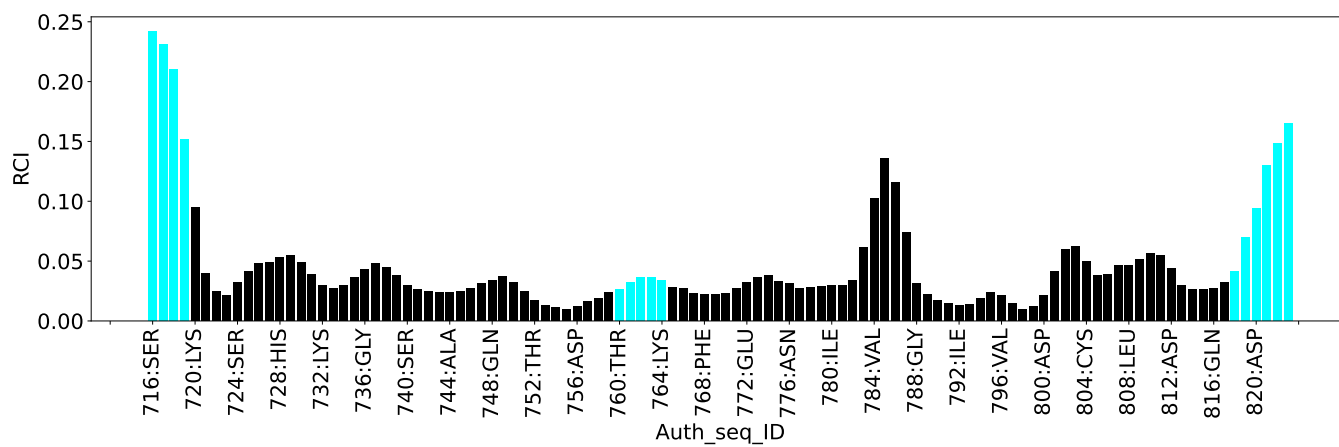
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	765	ARG	NE	111.48	76.53 – 92.65	16.7
1	A	756	ASP	HA	6.14	3.04 – 6.12	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:



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	2346
Intra-residue ($ i-j =0$)	1018
Sequential ($ i-j =1$)	515
Medium range ($ i-j >1$ and $ i-j <5$)	145
Long range ($ i-j \geq 5$)	668
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	5
Number of restraints per residue	20.6
Number of long range restraints per residue ¹	5.9

¹Long 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)	83.2	0.2
0.2-0.5 (Medium)	116.5	0.5
>0.5 (Large)	152.2	4.96

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 ⓘ

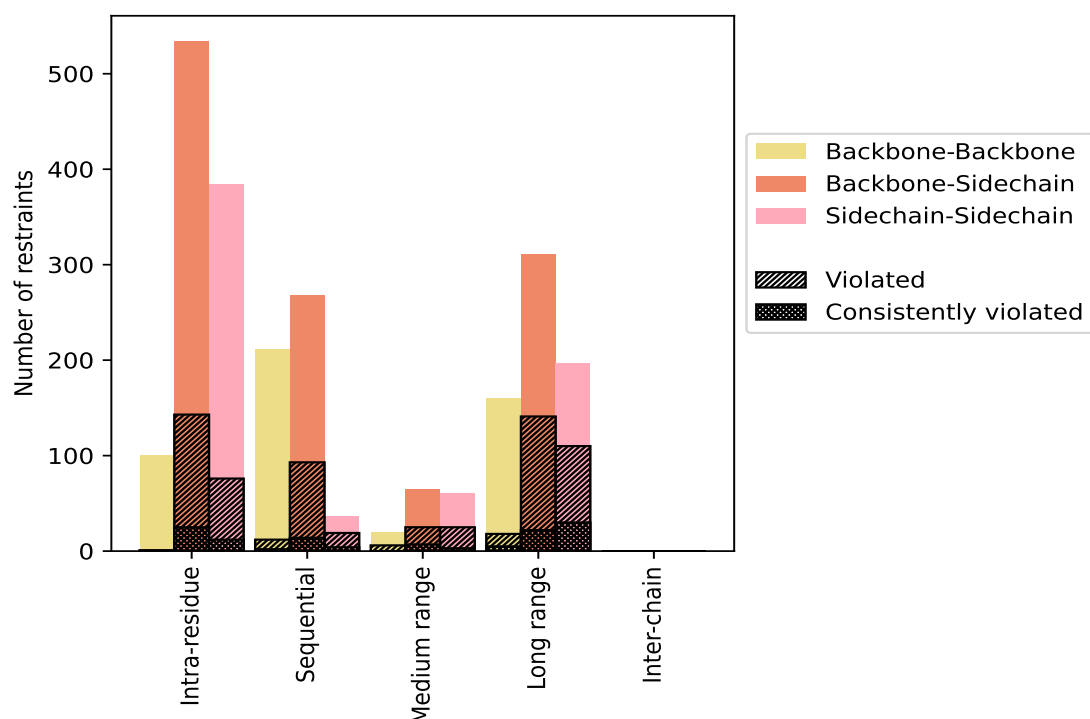
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	1018	43.4	220	21.6	9.4	37	3.6	1.6
Backbone-Backbone	100	4.3	1	1.0	0.0	0	0.0	0.0
Backbone-Sidechain	534	22.8	143	26.8	6.1	25	4.7	1.1
Sidechain-Sidechain	384	16.4	76	19.8	3.2	12	3.1	0.5
Sequential ($i-j =1$)	515	22.0	124	24.1	5.3	20	3.9	0.9
Backbone-Backbone	211	9.0	12	5.7	0.5	2	0.9	0.1
Backbone-Sidechain	268	11.4	93	34.7	4.0	14	5.2	0.6
Sidechain-Sidechain	36	1.5	19	52.8	0.8	4	11.1	0.2
Medium range ($i-j >1$ & $i-j <5$)	145	6.2	56	38.6	2.4	10	6.9	0.4
Backbone-Backbone	20	0.9	6	30.0	0.3	0	0.0	0.0
Backbone-Sidechain	65	2.8	25	38.5	1.1	7	10.8	0.3
Sidechain-Sidechain	60	2.6	25	41.7	1.1	3	5.0	0.1
Long range ($i-j \geq 5$)	668	28.5	269	40.3	11.5	57	8.5	2.4
Backbone-Backbone	160	6.8	18	11.2	0.8	5	3.1	0.2
Backbone-Sidechain	311	13.3	141	45.3	6.0	22	7.1	0.9
Sidechain-Sidechain	197	8.4	110	55.8	4.7	30	15.2	1.3
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	2346	100.0	669	28.5	28.5	124	5.3	5.3
Backbone-Backbone	491	20.9	37	7.5	1.6	7	1.4	0.3
Backbone-Sidechain	1178	50.2	402	34.1	17.1	68	5.8	2.9
Sidechain-Sidechain	677	28.9	230	34.0	9.8	49	7.2	2.1

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	110	62	29	148	0	349	0.63	3.63	0.63	0.41
2	110	68	31	149	0	358	0.63	3.1	0.58	0.42
3	112	68	31	139	0	350	0.62	3.67	0.58	0.4
4	115	56	29	129	0	329	0.54	3.86	0.51	0.36
5	102	68	34	143	0	347	0.64	4.26	0.61	0.41
6	100	67	26	143	0	336	0.65	4.96	0.64	0.43
7	114	64	30	150	0	358	0.62	3.14	0.58	0.42
8	114	67	28	151	0	360	0.66	3.73	0.62	0.43
9	108	64	23	138	0	333	0.57	3.02	0.51	0.4
10	127	73	28	166	0	394	0.65	3.79	0.61	0.4

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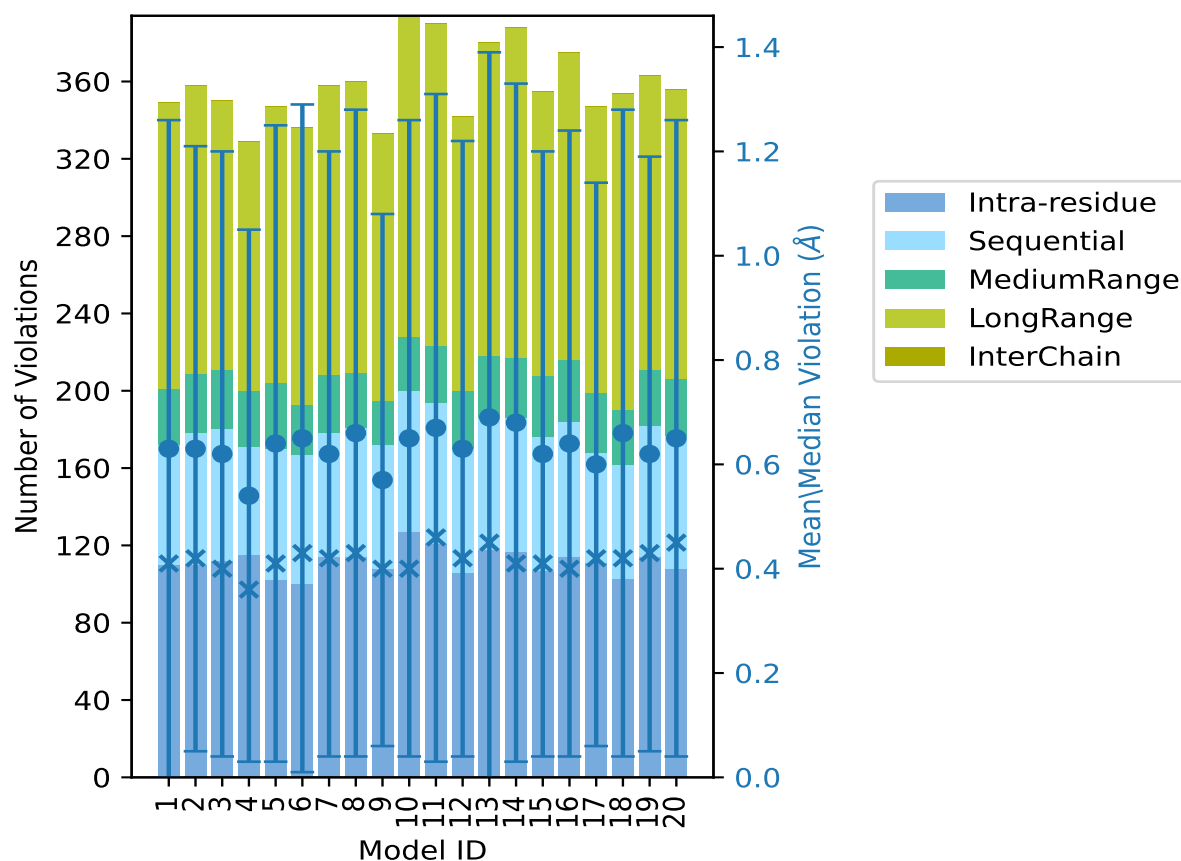
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	121	73	29	167	0	390	0.67	3.59	0.64	0.46
12	106	64	30	142	0	342	0.63	3.82	0.59	0.42
13	118	68	32	162	0	380	0.69	4.94	0.7	0.45
14	117	69	31	171	0	388	0.68	3.6	0.65	0.41
15	107	69	32	147	0	355	0.62	3.32	0.58	0.41
16	114	70	32	159	0	375	0.64	3.24	0.6	0.4
17	111	57	31	148	0	347	0.6	2.95	0.54	0.42
18	103	59	28	164	0	354	0.66	3.32	0.62	0.42
19	114	68	29	152	0	363	0.62	3.71	0.57	0.43
20	108	69	29	150	0	356	0.65	3.79	0.61	0.45

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard 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

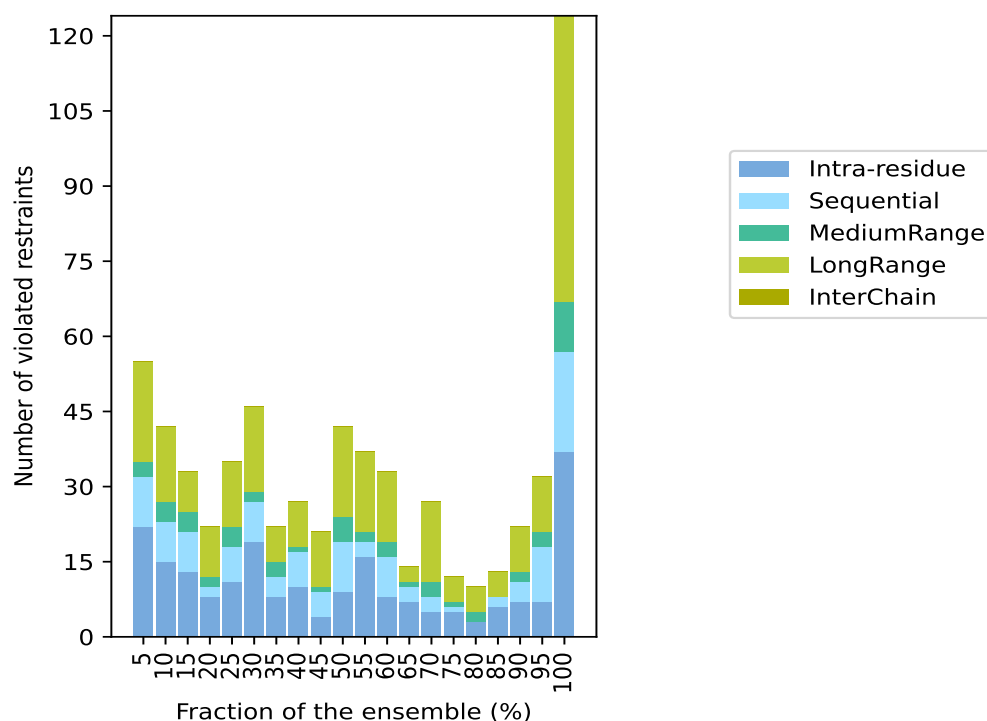
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1677(IR:798, SQ:391, MR:89, LR:399, IC:0) restraints are 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	%
22	10	3	20	0	55	1	5.0
15	8	4	15	0	42	2	10.0
13	8	4	8	0	33	3	15.0
8	2	2	10	0	22	4	20.0
11	7	4	13	0	35	5	25.0
19	8	2	17	0	46	6	30.0
8	4	3	7	0	22	7	35.0
10	7	1	9	0	27	8	40.0
4	5	1	11	0	21	9	45.0
9	10	5	18	0	42	10	50.0
16	3	2	16	0	37	11	55.0
8	8	3	14	0	33	12	60.0
7	3	1	3	0	14	13	65.0
5	3	3	16	0	27	14	70.0
5	1	1	5	0	12	15	75.0
3	0	2	5	0	10	16	80.0
6	2	0	5	0	13	17	85.0
7	4	2	9	0	22	18	90.0
7	11	3	11	0	32	19	95.0
37	20	10	57	0	124	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

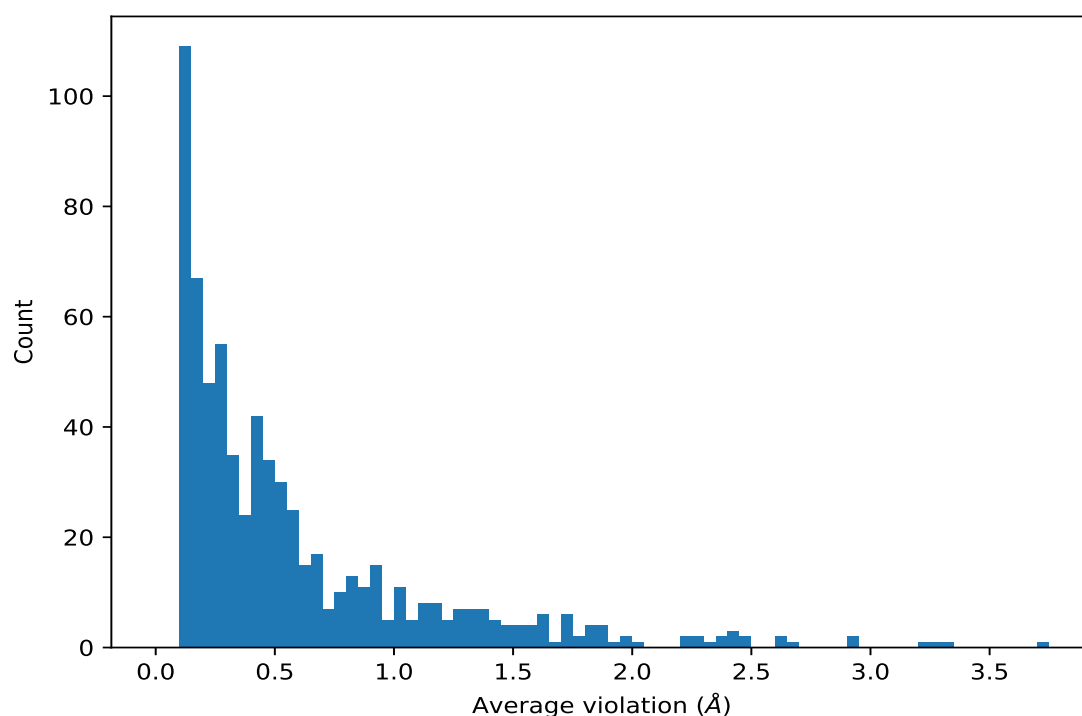
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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.

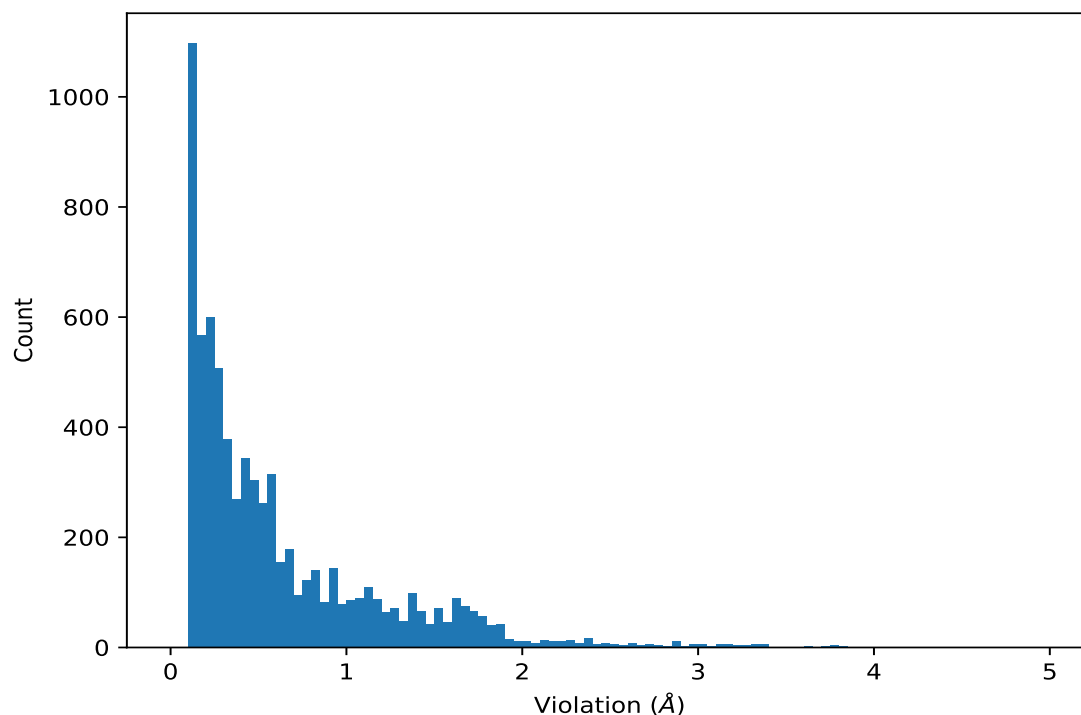
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2251)	1:754:A:THR:HG23	1:773:A:ILE:HG21	20	2.93	0.07	2.94
(1,2251)	1:754:A:THR:HG21	1:780:A:ILE:HG22	20	2.93	0.07	2.94
(1,2112)	1:778:A:TYR:HA	1:753:A:LEU:HD21	20	1.87	0.26	1.78
(1,2112)	1:778:A:TYR:HA	1:770:A:ILE:HG22	20	1.87	0.26	1.78
(1,760)	1:769:A:GLU:HB3	1:754:A:THR:HG21	20	1.8	0.04	1.81
(1,715)	1:766:A:LYS:HB2	1:755:A:TYR:HD1	20	1.79	0.08	1.79
(1,1214)	1:748:A:GLN:H	1:721:A:PRO:HB2	20	1.72	0.06	1.72
(1,591)	1:751:A:PHE:HB3	1:753:A:LEU:HB3	20	1.7	0.12	1.7
(1,1088)	1:798:A:ILE:HG21	1:751:A:PHE:HB2	20	1.64	0.03	1.64
(1,507)	1:813:A:ALA:HA	1:727:A:LEU:HB2	20	1.55	0.46	1.72
(1,1189)	1:742:A:PRO:HB2	1:779:A:VAL:HG11	20	1.53	0.91	2.06
(1,426)	1:727:A:LEU:HA	1:742:A:PRO:HG3	20	1.52	0.09	1.52

¹Number of violated models, ²Standard 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)
(1,601)	1:747:A:GLY:HA3	1:719:A:VAL:HG11	6	4.96
(1,601)	1:747:A:GLY:HA3	1:719:A:VAL:HG11	13	4.94
(1,601)	1:747:A:GLY:HA3	1:719:A:VAL:HG11	5	4.26
(1,601)	1:747:A:GLY:HA3	1:719:A:VAL:HG11	4	3.86
(1,923)	1:793:A:LEU:HD11	1:782:A:THR:HG21	5	3.84
(1,923)	1:793:A:LEU:HD11	1:782:A:THR:HG21	12	3.82
(1,923)	1:793:A:LEU:HD11	1:782:A:THR:HG21	10	3.79
(1,923)	1:793:A:LEU:HD11	1:782:A:THR:HG21	20	3.79
(1,923)	1:793:A:LEU:HD11	1:782:A:THR:HG21	6	3.77
(1,923)	1:793:A:LEU:HD11	1:782:A:THR:HG21	13	3.77

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found