

wwPDB NMR Structure Validation Summary Report (i)

Jul 18, 2023 – 10:08 AM JST

PDB ID : 7YB4 BMRB ID : 51157

Title : Solution structure of homeodomain of EXTRADENTICLE

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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)

 $\begin{array}{ccc} wwPDB\text{-ShiftChecker} &:& v1.2\\ BMRB \ Restraints \ Analysis &:& v1.2 \end{array}$

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

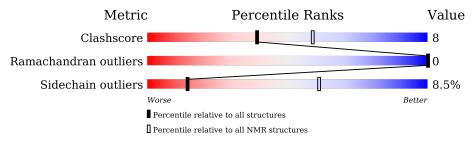
Validation Pipeline (wwPDB-VP) : 2.34

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 89%.

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 $(\# \mathrm{Entries})$	$egin{array}{c} { m NMR \ archive} \ { m (\#Entries)} \end{array}$		
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	67	57%	19%	24%			



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	Backbone RMSD (Å)	Medoid model				
1	A:246-A:296 (51)	0.42	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 2 single-model clusters were found.

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



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1120 atoms, of which 559 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Homeobox protein extradenticle.

Mol	Chain	Residues	Atoms					Trace	
1	Λ	67	Total	С	Н	N	О	S	0
1 A	67	1120	350	559	108	101	2	U	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	GLY	-	expression tag	UNP P40427
A	235	SER	-	expression tag	UNP P40427
A	236	HIS	-	expression tag	UNP P40427
A	237	MET	-	expression tag	UNP P40427

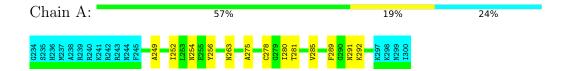


4 Residue-property plots (i)

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.

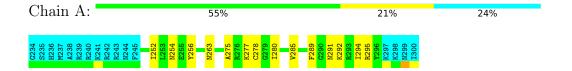
• Molecule 1: Homeobox protein extradenticle



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: Homeobox protein extradenticle





Refinement protocol and experimental data overview (i) 5



The models were refined using the following method: DGSA-distance geometry simulated annealing.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: structures with the lowest energy.

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

Software name	Classification	Version	
PONDEROSA-C/S	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	855
Number of shifts mapped to atoms	855
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%



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	В	Sond lengths	Bond angles		
Moi Chain		RMSZ	#Z>5	RMSZ	#Z>5	
1	A	0.91 ± 0.02	$0\pm0/432~(~0.0\pm~0.0\%)$	0.77 ± 0.03	$0\pm0/583~(~0.0\pm~0.1\%)$	
All	All	0.91	0/8640 (0.0%)	0.77	2/11660 (0.0%)	

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

	Mol			Chain	Pos	7 Observe	7 Observed(0)	$Ideal(^{o})$	Mod	dels
	MIOI	Chain	nes	Type	Atoms	L	Observed()	ideai()	Worst	Total
Ī	1	A	289	PHE	CB-CG-CD2	7.58	126.11	120.80	19	1
	1	A	289	PHE	CB-CG-CD1	-7.22	115.74	120.80	19	1

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	421	405	404	6±2
All	All	8420	8100	8080	129

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



Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:252:ILE:HD11	1:A:285:VAL:HG22	0.86	1.42	19	10
1:A:252:ILE:HD12	1:A:278:CYS:SG	0.80	2.17	15	5
1:A:249:ALA:O	1:A:252:ILE:HG22	0.76	1.81	6	11
1:A:252:ILE:HD11	1:A:285:VAL:CG2	0.68	2.17	13	2
1:A:252:ILE:CD1	1:A:285:VAL:HG22	0.66	2.20	15	8

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	sed Favoured Allowed		Outliers	Percentiles
1	A	51/67 (76%)	50±1 (98±2%)	1±1 (2±2%)	0±0 (0±0%)	100 100
All	All	1020/1340 (76%)	995 (98%)	25 (2%)	0 (0%)	100 100

There are no Ramachandran outliers.

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	Analysed Rotameric		Percentiles	
1	A	46/60 (77%)	42±1 (92±2%)	4±1 (8±2%)	14 61	
All	All	920/1200 (77%)	842 (92%)	78 (8%)	14 61	

5 of 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	254	ASN	20
1	A	292	LYS	19
1	A	291	ASN	18
1	A	263	ASN	9

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Mol	Chain	Res	Type	Models (Total)
1	A	277	LYS	4

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 89% 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: chem_shift_list_1

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	855
Number of shifts mapped to atoms	855
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

The following errors were found when reading this chemical shift list.

• Chemical shift has been reported more than once. First 5 (of 0) occurrences are reported below.

T:4 ID	Cl :	D	(T)	A 4		Shift Dat	a
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity
1	A	238	ALA	HB2	1.287	0.00	
1	A	238	ALA	HB3	1.287	0.00	
1	A	249	ALA	HB2	1.253	0.01	
1	A	249	ALA	HB3	1.253	0.01	•
1	A	252	ILE	HD12	0.659	0.01	
1	A	252	ILE	HD13	0.659	0.01	
1	A	252	ILE	HG22	0.792	0.04	
1	A	252	ILE	HG23	0.792	0.04	
1	A	253	LEU	HD12	-0.387	0.01	•
1	A	253	LEU	HD13	-0.387	0.01	
1	A	253	LEU	HD22	0.312	0.01	
1	A	253	LEU	HD23	0.312	0.01	
1	A	261	LEU	HD12	0.752	0.01	
1	A	261	LEU	HD13	0.752	0.01	

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	Continued from previou					Shift Data		
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity	
1	A	261	LEU	HD22	0.372	0.01		
1	A	261	LEU	HD23	0.372	0.01	•	
1	A	270	ALA	HB2	1.216	0.01		
1	A	270	ALA	HB3	1.216	0.01		
1	A	274	LEU	HD12	-0.024	0.01		
1	A	274	LEU	HD13	-0.024	0.01		
1	A	274	LEU	HD22	0.515	0.00		
1	A	274	LEU	HD23	0.515	0.00	•	
1	A	275	ALA	HB2	1.343	0.01	•	
1	A	275	ALA	HB3	1.343	0.01	•	
1	A	280	ILE	HD12	0.428	0.01	•	
1	A	280	ILE	HD13	0.428	0.01	•	
1	A	280	ILE	HG22	0.570	0.02	•	
1	A	280	ILE	HG23	0.570	0.02	•	
1	A	281	THR	HG22	1.209	0.01	•	
1	A	281	THR	HG23	1.209	0.01	•	
1	A	282	VAL	HG12	0.887	0.01	•	
1	A	282	VAL	HG13	0.887	0.01	•	
1	A	282	VAL	HG22	0.913	0.01	•	
1	A	282	VAL	HG23	0.913	0.01	•	
1	A	285	VAL	HG12	0.987	0.01	•	
1	A	285	VAL	HG13	0.987	0.01	•	
1	A	285	VAL	HG22	0.919	0.01	•	
1	A	285	VAL	HG23	0.919	0.01	•	
1	A	294	ILE	HD12	0.789	0.01	•	
1	A	294	ILE	HD13	0.789	0.01	•	
1	A	294	ILE	HG22	0.794	0.01	•	
1	A	294	ILE	HG23	0.794	0.01	•	
1	A	300	ILE	HD12	0.762	0.01	•	
1	A	300	ILE	HD13	0.762	0.01		
1	A	300	ILE	HG22	0.769	0.00	•	
1	A	300	ILE	HG23	0.769	0.00		

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\mathrm{C}_{\alpha}$	65	-0.36 ± 0.14	None needed ($< 0.5 \text{ ppm}$)
$^{13}C_{\beta}$	62	0.19 ± 0.13	None needed (< 0.5 ppm)
¹³ C′	64	-0.57 ± 0.10	Should be applied

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Nucleus	# values	Correction \pm precision, ppm	Suggested action
^{15}N	60	-0.18 ± 0.37	None needed ($< 0.5 \text{ ppm}$)

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 89%, i.e. 632 atoms were assigned a chemical shift out of a possible 707. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Backbone	$250/253 \ (99\%)$	101/102~(99%)	101/102~(99%)	48/49 (98%)
Sidechain	342/378 (90%)	$235/242 \ (97\%)$	101/117 (86%)	6/19 (32%)
Aromatic	40/76 (53%)	$26/36 \ (72\%)$	$13/37 \ (35\%)$	1/3 (33%)
Overall	632/707 (89%)	$362/380 \ (95\%)$	215/256 (84%)	55/71 (77%)

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.

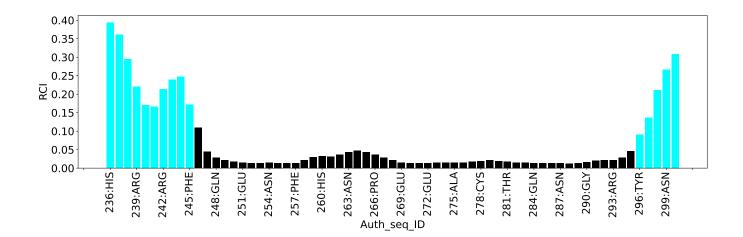
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	260	HIS	CD2	49.71	103.95 - 136.66	-21.6
1	A	237	MET	CG	16.68	25.46 - 38.60	-11.7
1	A	253	LEU	HB3	-1.18	-0.26 - 3.31	-7.6
1	A	292	LYS	HG2	-0.43	0.13 - 2.61	-7.3
1	A	292	LYS	HG3	-0.43	0.04 - 2.67	-6.8
1	A	292	LYS	HB3	0.08	0.46 - 3.04	-6.5
1	A	292	LYS	HD2	0.41	0.58 - 2.64	-5.8
1	A	266	PRO	HG3	0.22	0.33 - 3.48	-5.4

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 (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	702
Intra-residue ($ i-j =0$)	0
Sequential (i-j =1)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range (i-j ≥5)	578
Inter-chain	0
Hydrogen bond restraints	124
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	10.5
Number of long range restraints per residue ¹	8.6

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 (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)	18.2	0.2
0.2-0.5 (Medium)	5.5	0.5
>0.5 (Large)	0.1	0.99



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

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



9 Distance violation analysis (i)

9.1 Summary of distance violations (i)

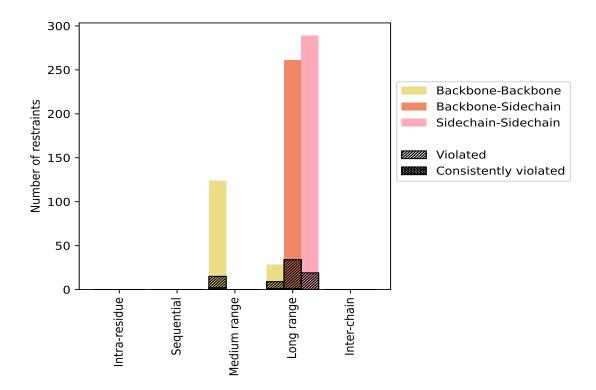
The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Doodnointe tour	C	% ¹	${f Violated}^3$			Consistently Violated		
Restraints type	Count	70	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)	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
Medium range ($ i-j >1 & i-j <5$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($ i-j \ge 5$)	578	82.3	62	10.7	8.8	2	0.3	0.3
Backbone-Backbone	28	4.0	9	32.1	1.3	1	3.6	0.1
Backbone-Sidechain	261	37.2	34	13.0	4.8	1	0.4	0.1
Sidechain-Sidechain	289	41.2	19	6.6	2.7	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	124	17.7	15	12.1	2.1	2	1.6	0.3
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	702	100.0	77	11.0	11.0	4	0.6	0.6
Backbone-Backbone	152	21.7	24	15.8	3.4	3	2.0	0.4
Backbone-Sidechain	261	37.2	34	13.0	4.8	1	0.4	0.1
Sidechain-Sidechain	289	41.2	19	6.6	2.7	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 (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.

Madal ID		Nun	nber o	f viola	ations	5	Mean (Å)	M (Å)	${ m SD}^6$ (Å)	Madian (8)
Model ID	IR^1	SQ^2	MR^3	LR^4	IC^5	Total		Max (Å)	$SD^*(A)$	Median (Å)
1	0	0	7	14	0	21	0.18	0.34	0.07	0.16
2	0	0	8	16	0	24	0.17	0.33	0.06	0.15
3	0	0	8	17	0	25	0.16	0.3	0.04	0.15
4	0	0	8	12	0	20	0.16	0.26	0.04	0.16
5	0	0	8	14	0	22	0.17	0.37	0.07	0.14
6	0	0	7	18	0	25	0.17	0.35	0.06	0.14
7	0	0	8	12	0	20	0.15	0.32	0.05	0.13
8	0	0	6	17	0	23	0.2	0.99	0.17	0.17
9	0	0	5	21	0	26	0.19	0.35	0.06	0.18
10	0	0	5	14	0	19	0.17	0.25	0.04	0.17
11	0	0	5	18	0	23	0.18	0.37	0.07	0.18

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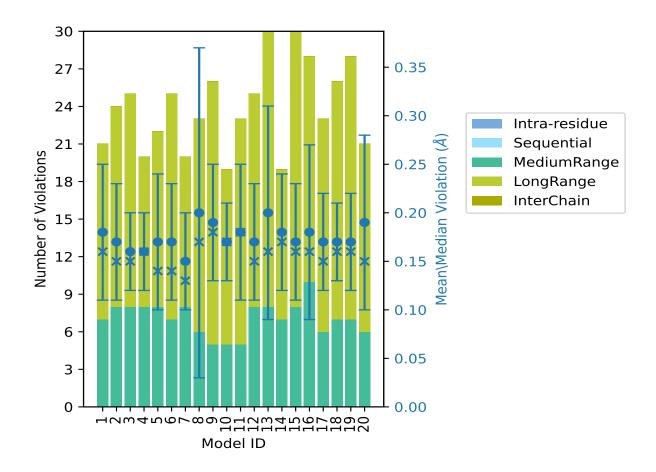


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Model ID		Nun	nber o	f viola	ations	3	Mean (Å)	Max (Å)	${ m SD}^6$ (Å)	Median (Å)
Model 1D	IR^1	SQ^2	MR^3	LR^4	IC^5	Total	al Mean (A)	Max (A)	(\mathbf{A})	Median (A)
12	0	0	8	17	0	25	0.17	0.39	0.06	0.15
13	0	0	8	22	0	30	0.2	0.58	0.11	0.16
14	0	0	7	12	0	19	0.18	0.33	0.06	0.17
15	0	0	8	22	0	30	0.17	0.34	0.06	0.16
16	0	0	10	18	0	28	0.18	0.5	0.09	0.16
17	0	0	6	17	0	23	0.17	0.31	0.05	0.15
18	0	0	7	19	0	26	0.17	0.27	0.04	0.16
19	0	0	7	21	0	28	0.17	0.3	0.05	0.16
20	0	0	6	15	0	21	0.19	0.43	0.09	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 (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)

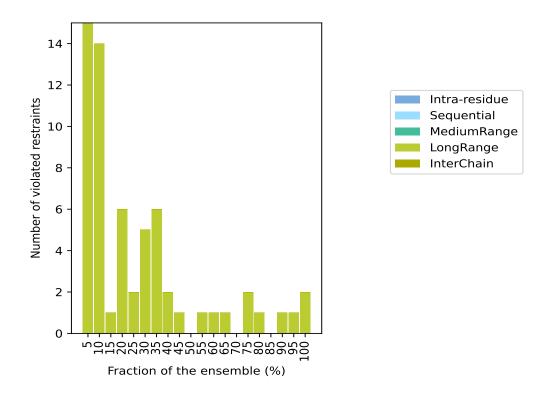
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 516(IR:0, SQ:0, MR:0, LR:516, IC:0) restraints are not violated in the ensemble.

Nu	$\overline{\mathbf{mber}}$	of vio	lated	restra	aints	Fraction	n of the ensemble
IR^1	SQ^2	MR^3	LR^4	IC^5	Total	Count ⁶	%
0	0	0	15	0	15	1	5.0
0	0	0	14	0	14	2	10.0
0	0	0	1	0	1	3	15.0
0	0	0	6	0	6	4	20.0
0	0	0	2	0	2	5	25.0
0	0	0	5	0	5	6	30.0
0	0	0	6	0	6	7	35.0
0	0	0	2	0	2	8	40.0
0	0	0	1	0	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	1	0	1	11	55.0
0	0	0	1	0	1	12	60.0
0	0	0	1	0	1	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	2	0	2	15	75.0
0	0	0	1	0	1	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	1	0	1	18	90.0
0	0	0	1	0	1	19	95.0
0	0	0	2	0	2	20	100.0

 $^{^1}$ Intra-residue restraints, 2 Sequential restraints, 3 Medium range restraints, 4 Long range restraints, 5 Inter-chain restraints, 6 Number of models with violations



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

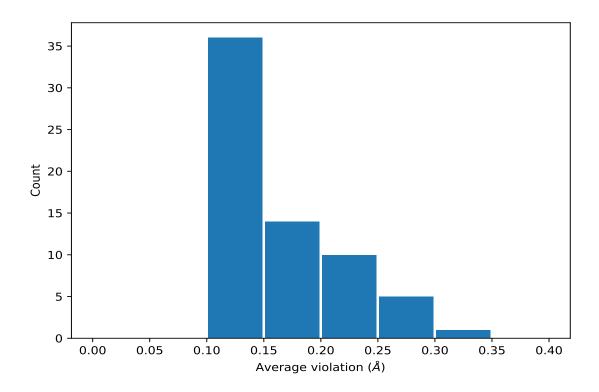


9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram: Distribution of mean distance violations (i)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble





9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	\mathbf{Models}^1	Mean (Å)	SD^1 (Å)	Median (Å)
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	20	0.29	0.09	0.3
(2,12)	1:A:256:TYR:H	1:A:252:ILE:O	20	0.24	0.03	0.24
(4,40)	1:A:253:LEU:HA	1:A:288:TRP:H	20	0.22	0.03	0.22
(2,6)	1:A:253:LEU:H	1:A:249:ALA:O	20	0.18	0.02	0.18
(4,82)	1:A:266:PRO:HA	1:A:271:LYS:H	19	0.21	0.04	0.2
(5,42)	1:A:253:LEU:HA	1:A:289:PHE:H	18	0.16	0.04	0.15
(2,45)	1:A:288:TRP:H	1:A:284:GLN:O	17	0.21	0.02	0.2
(4,148)	1:A:275:ALA:HA	1:A:281:THR:H	16	0.17	0.03	0.18
(4,57)	1:A:256:TYR:HA	1:A:292:LYS:HD2	15	0.22	0.07	0.22
(5,70)	1:A:260:HIS:HA	1:A:293:ARG:HD2	15	0.18	0.06	0.16

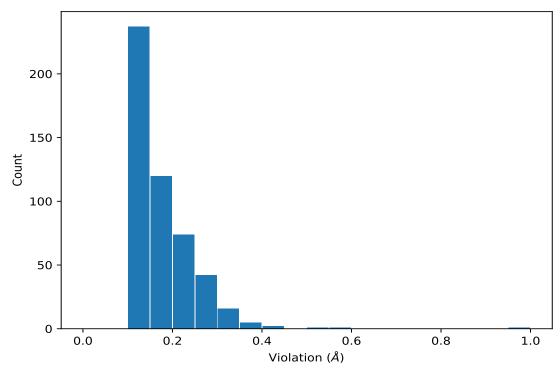
¹Number of violated models, ²Standard deviation



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)
(5,126)	1:A:281:THR:HB	1:A:286:SER:H	8	0.99
(5,54)	1:A:256:TYR:HD1	1:A:266:PRO:HB3	13	0.58
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	16	0.5
(5,87)	1:A:266:PRO:HB2	1:A:290:GLY:H	13	0.44
(4,149)	1:A:275:ALA:HA	1:A:284:GLN:HB2	20	0.43
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	12	0.39
(4,149)	1:A:275:ALA:HA	1:A:284:GLN:HB2	16	0.37
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	5	0.37
(4,101)	1:A:271:LYS:HE3	1:A:283:SER:H	11	0.37
(4,149)	1:A:275:ALA:HA	1:A:284:GLN:HB2	13	0.36



10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found

