



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 3ZTG / pdb_00003ztg
BMRB ID : 17772
Title : Solution structure of the RING finger-like domain of Retinoblastoma Binding Protein-6 (RBBP6)
Authors : Kappo, M.A.; Ab, E.; Atkinson, R.A.; Faro, A.; Muleya, V.; Mulaudzi, T.; Poole, J.O.; McKenzie, J.M.; Pugh, D.J.R.
Deposited on : 2011-07-07

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<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

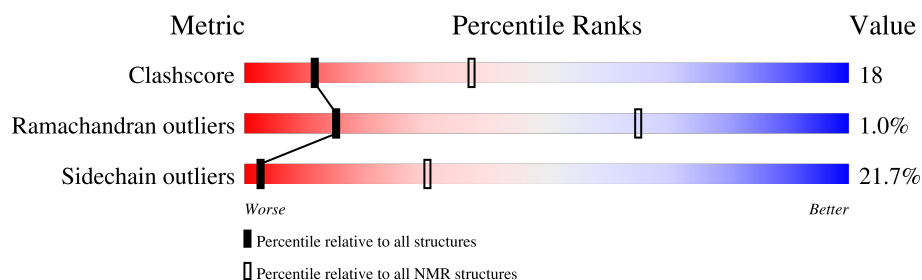
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 45%.

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	92	
1	B	92	

2 Ensemble composition and analysis

This entry contains 32 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:253-A:322, B:255-B:319 (135)	0.30	17

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 4 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 4, 5, 6, 12, 15, 16, 17, 18, 19, 21, 24, 29, 30, 31, 32
2	3, 7, 8, 9, 11, 23, 25, 26, 27, 28
3	10, 20, 22
4	2, 13
Single-model clusters	14

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2674 atoms, of which 1252 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called E3 UBIQUITIN-PROTEIN LIGASE RBBP6.

Mol	Chain	Residues	Atoms						Trace
1	A	92	Total	C	H	N	O	S	0
			1335	435	626	122	143	9	
1	B	92	Total	C	H	N	O	S	0
			1335	435	626	122	143	9	

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLY	-	expression tag	UNP Q7Z6E9
A	245	PRO	-	expression tag	UNP Q7Z6E9
A	246	LEU	-	expression tag	UNP Q7Z6E9
A	247	GLY	-	expression tag	UNP Q7Z6E9
A	248	SER	-	expression tag	UNP Q7Z6E9
B	244	GLY	-	expression tag	UNP Q7Z6E9
B	245	PRO	-	expression tag	UNP Q7Z6E9
B	246	LEU	-	expression tag	UNP Q7Z6E9
B	247	GLY	-	expression tag	UNP Q7Z6E9
B	248	SER	-	expression tag	UNP Q7Z6E9

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

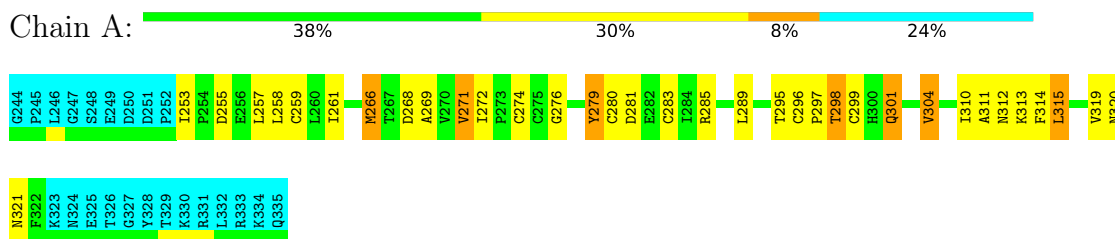
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2
2	B	2	Total	Zn
			2	2

4 Residue-property plots [i](#)

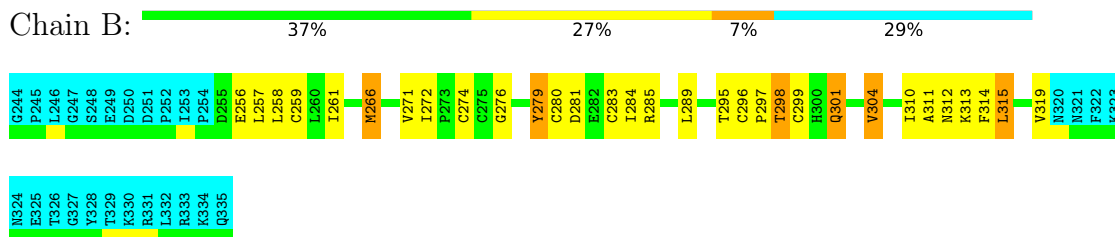
4.1 Average score per residue in the NMR ensemble

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: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



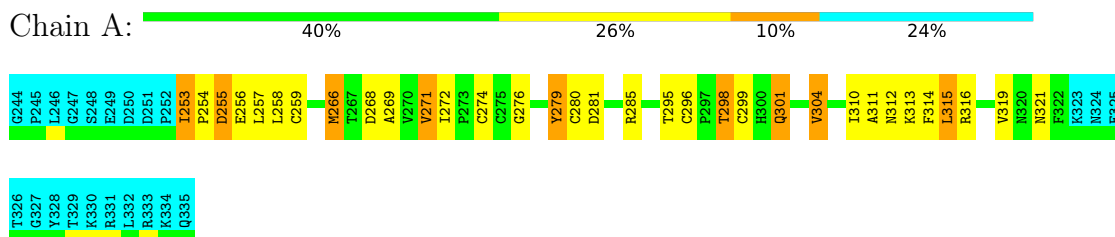
• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



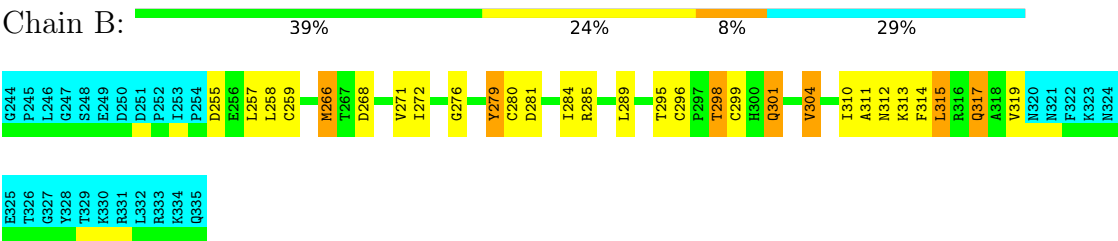
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 17. Colouring as in section 4.1 above.

• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



● Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



5 Refinement protocol and experimental data overview

The models were refined using the following method: *CYANA FOLLOWED BY HADDOCK*.

Of the 400 calculated structures, 32 were deposited, based on the following criterion: *HADDOCK ENERGY, RAMACHANDRAN QUALITY*.

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

Software name	Classification	Version
CNS	refinement	2.1
CYANA	structure solution	
NMRView	structure solution	

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	1027
Number of shifts mapped to atoms	973
Number of unparsed shifts	0
Number of shifts with mapping errors	54
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [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	535	454	510	21±3
1	B	493	420	471	20±3
All	All	33024	27968	31392	1142

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 18.

5 of 126 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:266:MET:HB3	1:A:280:CYS:SG	0.80	2.15	31	32
1:B:266:MET:HB3	1:B:280:CYS:SG	0.80	2.16	20	32
1:A:271:VAL:HG22	1:A:312:ASN:HB2	0.75	1.57	28	24
1:B:296:CYS:SG	1:B:298:THR:HG22	0.75	2.21	24	32
1:A:296:CYS:SG	1:A:298:THR:HG22	0.74	2.23	3	32

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	70/92 (76%)	62±1 (88±1%)	7±1 (11±1%)	1±1 (1±1%)	14	63
1	B	65/92 (71%)	57±1 (87±1%)	8±1 (12±2%)	1±0 (1±1%)	16	66
All	All	4320/5888 (73%)	3796 (88%)	482 (11%)	42 (1%)	15	65

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	298	THR	21
1	B	298	THR	18
1	A	304	VAL	2
1	A	303	ASP	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	64/83 (77%)	49±2 (77±2%)	15±2 (23±2%)	2	27
1	B	59/83 (71%)	47±2 (80±3%)	12±2 (20±3%)	3	33
All	All	3936/5312 (74%)	3081 (78%)	855 (22%)	3	30

5 of 59 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	266	MET	32
1	A	271	VAL	32
1	A	279	TYR	32

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Mol	Chain	Res	Type	Models (Total)
1	A	301	GLN	32
1	A	304	VAL	32

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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 45% for the well-defined parts and 43% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *rring-new.bmr.b.csh*

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	1027
Number of shifts mapped to atoms	973
Number of unparsed shifts	0
Number of shifts with mapping errors	54
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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 54) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	253	ILE	HG12	0.944	0.020	.
1	A	253	ILE	HG13	1.489	0.020	.
1	A	253	ILE	HG21	0.509	0.020	1
1	A	253	ILE	HG22	0.509	0.020	1
1	A	253	ILE	HG23	0.509	0.020	1
1	A	261	ILE	HG12	1.04	0.020	.
1	A	261	ILE	HG13	1.714	0.020	.
1	A	261	ILE	HG21	0.969	0.020	1
1	A	261	ILE	HG22	0.969	0.020	1
1	A	261	ILE	HG23	0.969	0.020	1
1	A	265	ILE	HG12	1.2	0.020	.
1	A	265	ILE	HG13	1.545	0.020	.
1	A	265	ILE	HG21	0.915	0.020	1
1	A	265	ILE	HG22	0.915	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	265	ILE	HG23	0.915	0.020	1
1	A	270	VAL	HG11	1.022	0.020	.
1	A	270	VAL	HG12	1.022	0.020	.
1	A	270	VAL	HG13	1.022	0.020	.
1	A	270	VAL	HG21	0.986	0.020	.
1	A	270	VAL	HG22	0.986	0.020	.
1	A	270	VAL	HG23	0.986	0.020	.
1	A	271	VAL	HG11	0.884	0.020	.
1	A	271	VAL	HG12	0.884	0.020	.
1	A	271	VAL	HG13	0.884	0.020	.
1	A	271	VAL	HG21	0.873	0.020	.
1	A	271	VAL	HG22	0.873	0.020	.
1	A	271	VAL	HG23	0.873	0.020	.
1	A	272	ILE	HG12	1.519	0.020	.
1	A	272	ILE	HG13	2.422	0.020	.
1	A	272	ILE	HG21	1.732	0.020	1
1	A	272	ILE	HG22	1.732	0.020	1
1	A	272	ILE	HG23	1.732	0.020	1
1	A	284	ILE	HG12	0.865	0.020	.
1	A	284	ILE	HG13	0.957	0.020	.
1	A	284	ILE	HG21	1.048	0.020	1
1	A	284	ILE	HG22	1.048	0.020	1
1	A	284	ILE	HG23	1.048	0.020	1
1	A	304	VAL	HG11	0.837	0.020	.
1	A	304	VAL	HG12	0.837	0.020	.
1	A	304	VAL	HG13	0.837	0.020	.
1	A	304	VAL	HG21	0.965	0.020	.
1	A	304	VAL	HG22	0.965	0.020	.
1	A	304	VAL	HG23	0.965	0.020	.
1	A	310	ILE	HG12	1.169	0.020	.
1	A	310	ILE	HG13	1.669	0.020	.
1	A	310	ILE	HG21	0.97	0.020	1
1	A	310	ILE	HG22	0.97	0.020	1
1	A	310	ILE	HG23	0.97	0.020	1
1	A	319	VAL	HG11	1.14	0.020	1
1	A	319	VAL	HG12	1.14	0.020	1
1	A	319	VAL	HG13	1.14	0.020	1
1	A	319	VAL	HG21	1.14	0.020	1
1	A	319	VAL	HG22	1.14	0.020	1
1	A	319	VAL	HG23	1.14	0.020	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
$^{13}\text{C}_\alpha$	92	-0.41 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	88	-0.09 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	83	-1.00 ± 0.45	Should be applied

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 45%, i.e. 787 atoms were assigned a chemical shift out of a possible 1736. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	269/663 (41%)	135/265 (51%)	70/270 (26%)	64/128 (50%)
Sidechain	488/1001 (49%)	333/653 (51%)	146/320 (46%)	9/28 (32%)
Aromatic	30/72 (42%)	18/39 (46%)	12/33 (36%)	0/0 (—%)
Overall	787/1736 (45%)	486/957 (51%)	228/623 (37%)	73/156 (47%)

7.1.4 Statistically unusual chemical shifts ⓘ

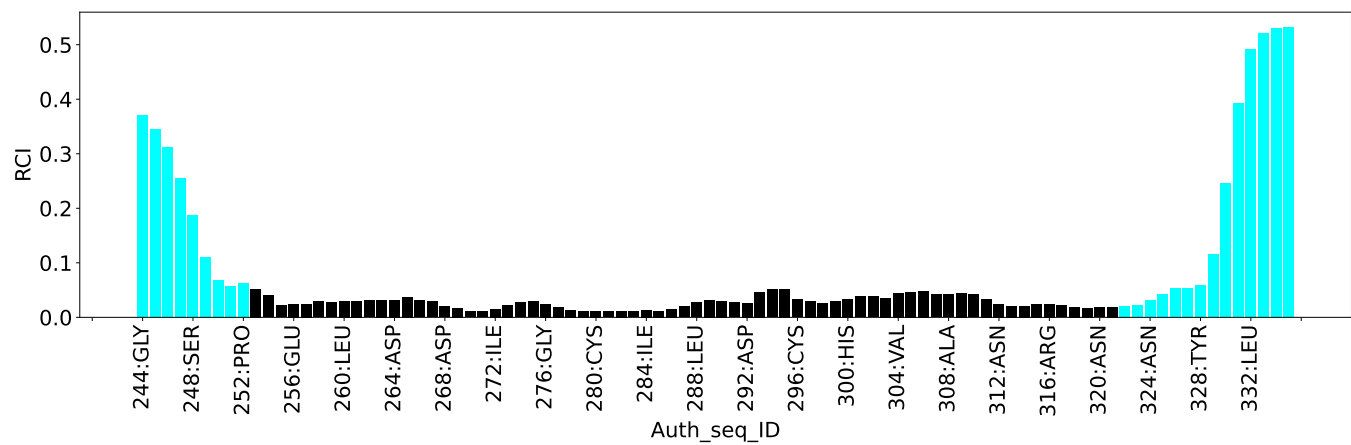
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	335	GLN	CD	21.34	173.59 – 185.85	-129.2

7.1.5 Random Coil Index (RCI) plots ⓘ

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	5274
Intra-residue ($ i-j =0$)	1031
Sequential ($ i-j =1$)	1308
Medium range ($ i-j >1$ and $ i-j <5$)	1058
Long range ($ i-j \geq 5$)	1731
Inter-chain	146
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	28.1
Number of long range restraints per residue ¹	9.2

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)	40.8	0.2
0.2-0.5 (Medium)	7.9	0.45
>0.5 (Large)	0.0	0.52

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

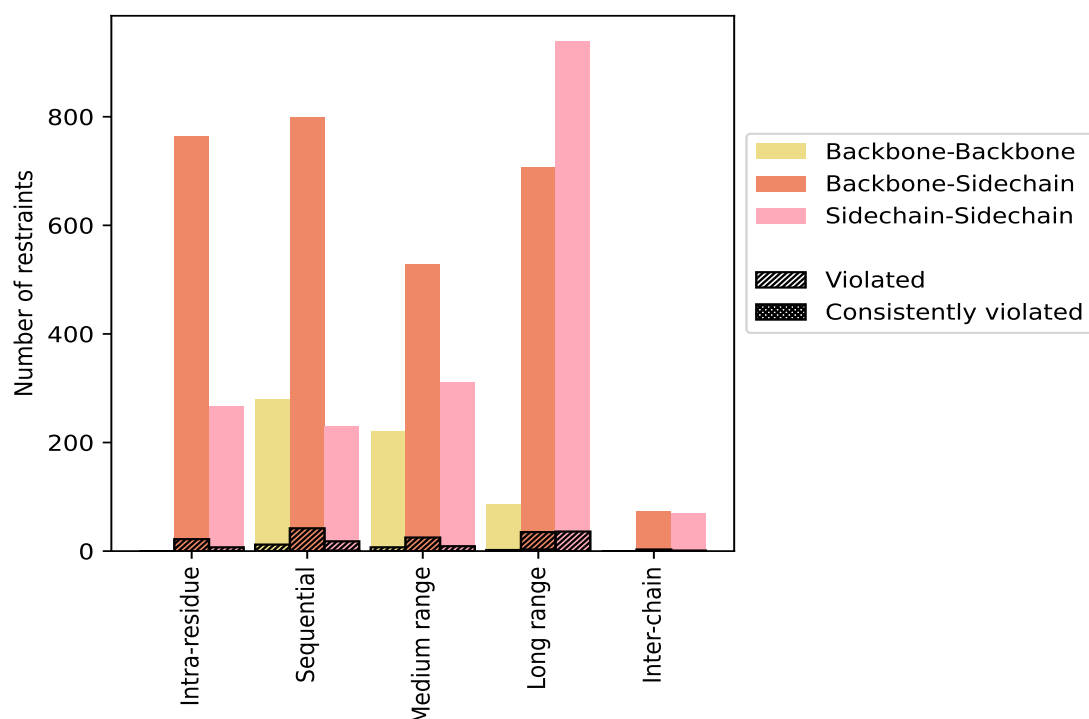
9.1 Summary of distance violations

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1031	19.5	29	2.8	0.5	0	0.0	0.0
Backbone-Backbone	2	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	763	14.5	22	2.9	0.4	0	0.0	0.0
Sidechain-Sidechain	266	5.0	7	2.6	0.1	0	0.0	0.0
Sequential ($i-j =1$)	1308	24.8	72	5.5	1.4	1	0.1	0.0
Backbone-Backbone	280	5.3	12	4.3	0.2	0	0.0	0.0
Backbone-Sidechain	799	15.1	42	5.3	0.8	0	0.0	0.0
Sidechain-Sidechain	229	4.3	18	7.9	0.3	1	0.4	0.0
Medium range ($i-j >1$ & $i-j <5$)	1058	20.1	41	3.9	0.8	0	0.0	0.0
Backbone-Backbone	220	4.2	7	3.2	0.1	0	0.0	0.0
Backbone-Sidechain	528	10.0	25	4.7	0.5	0	0.0	0.0
Sidechain-Sidechain	310	5.9	9	2.9	0.2	0	0.0	0.0
Long range ($i-j \geq 5$)	1731	32.8	73	4.2	1.4	3	0.2	0.1
Backbone-Backbone	86	1.6	2	2.3	0.0	0	0.0	0.0
Backbone-Sidechain	706	13.4	35	5.0	0.7	3	0.4	0.1
Sidechain-Sidechain	939	17.8	36	3.8	0.7	0	0.0	0.0
Inter-chain	146	2.8	4	2.7	0.1	0	0.0	0.0
Backbone-Backbone	2	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	74	1.4	3	4.1	0.1	0	0.0	0.0
Sidechain-Sidechain	70	1.3	1	1.4	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	5274	100.0	219	4.2	4.2	4	0.1	0.1
Backbone-Backbone	590	11.2	21	3.6	0.4	0	0.0	0.0
Backbone-Sidechain	2870	54.4	127	4.4	2.4	3	0.1	0.1
Sidechain-Sidechain	1814	34.4	71	3.9	1.3	1	0.1	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.

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	7	17	9	19	0	52	0.15	0.23	0.04	0.15
2	7	14	12	16	0	49	0.15	0.42	0.05	0.15
3	7	16	11	23	1	58	0.15	0.43	0.06	0.13
4	6	11	4	20	2	43	0.17	0.44	0.06	0.16
5	7	13	12	20	0	52	0.16	0.42	0.05	0.15
6	5	19	9	16	0	49	0.16	0.43	0.07	0.14
7	7	15	8	20	1	51	0.16	0.43	0.05	0.15
8	6	19	12	22	0	59	0.17	0.52	0.08	0.14
9	5	13	5	21	0	44	0.16	0.44	0.06	0.15
10	8	22	12	26	0	68	0.17	0.45	0.07	0.15

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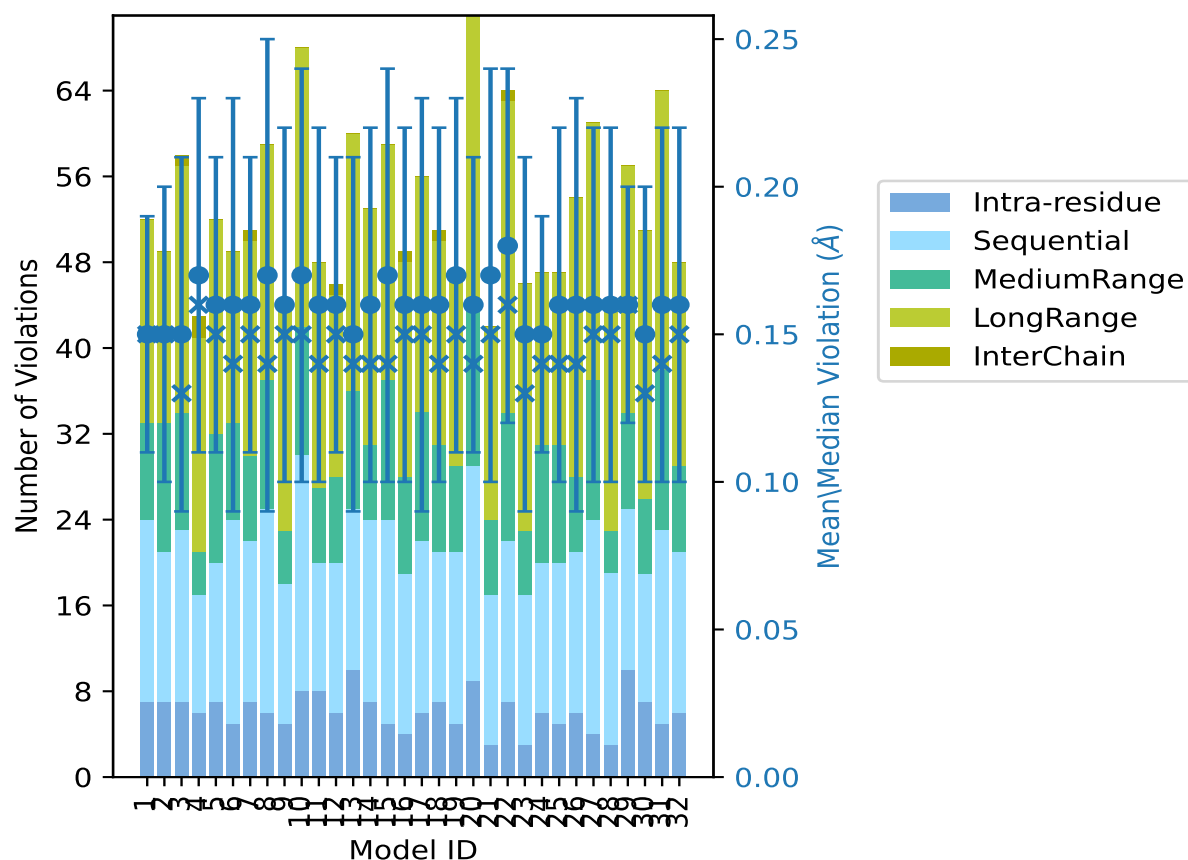
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	8	12	7	21	0	48	0.16	0.44	0.06	0.14
12	6	14	8	17	1	46	0.16	0.4	0.05	0.15
13	10	15	11	24	0	60	0.15	0.43	0.06	0.14
14	7	17	7	22	0	53	0.16	0.43	0.06	0.14
15	5	19	13	22	0	59	0.17	0.44	0.07	0.14
16	4	15	9	20	1	49	0.16	0.43	0.06	0.15
17	6	16	12	22	0	56	0.16	0.45	0.07	0.15
18	7	14	10	19	1	51	0.16	0.44	0.06	0.14
19	5	16	8	18	0	47	0.17	0.43	0.06	0.15
20	9	20	15	27	0	71	0.16	0.3	0.05	0.14
21	3	14	7	18	0	42	0.17	0.42	0.07	0.15
22	7	15	12	29	1	64	0.18	0.45	0.06	0.16
23	3	14	6	23	0	46	0.15	0.43	0.06	0.13
24	6	14	11	16	0	47	0.15	0.25	0.04	0.14
25	5	15	11	16	0	47	0.16	0.42	0.06	0.14
26	6	15	7	26	0	54	0.16	0.43	0.07	0.14
27	4	20	13	24	0	61	0.16	0.43	0.06	0.15
28	3	16	4	21	0	44	0.16	0.42	0.06	0.15
29	10	15	9	23	0	57	0.16	0.23	0.04	0.16
30	7	12	7	25	0	51	0.15	0.42	0.05	0.13
31	5	18	15	26	0	64	0.16	0.43	0.06	0.14
32	6	15	8	19	0	48	0.16	0.43	0.06	0.15

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 [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, 5055(IR:1002, SQ:1236, MR:1017, LR:1658, IC:142) 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	%
8	21	12	18	2	61	1	3.1
6	12	6	12	1	37	2	6.2
0	4	2	6	0	12	3	9.4
0	5	2	4	1	12	4	12.5
3	6	4	1	0	14	5	15.6
0	1	1	2	0	4	6	18.8

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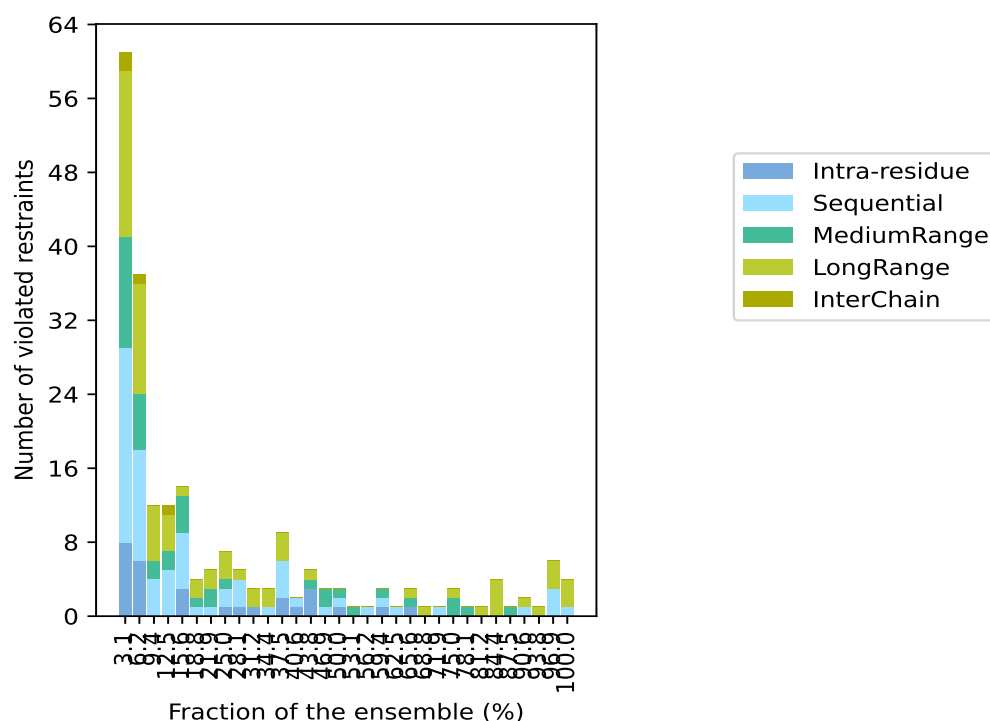
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	1	2	2	0	5	7	21.9
1	2	1	3	0	7	8	25.0
1	3	0	1	0	5	9	28.1
1	0	0	2	0	3	10	31.2
0	1	0	2	0	3	11	34.4
2	4	0	3	0	9	12	37.5
1	1	0	0	0	2	13	40.6
3	0	1	1	0	5	14	43.8
0	1	2	0	0	3	15	46.9
1	1	1	0	0	3	16	50.0
0	0	1	0	0	1	17	53.1
0	1	0	0	0	1	18	56.2
1	1	1	0	0	3	19	59.4
0	1	0	0	0	1	20	62.5
1	0	1	1	0	3	21	65.6
0	0	0	1	0	1	22	68.8
0	1	0	0	0	1	23	71.9
0	0	2	1	0	3	24	75.0
0	0	1	0	0	1	25	78.1
0	0	0	1	0	1	26	81.2
0	0	0	4	0	4	27	84.4
0	0	1	0	0	1	28	87.5
0	1	0	1	0	2	29	90.6
0	0	0	1	0	1	30	93.8
0	3	0	3	0	6	31	96.9
0	1	0	3	0	4	32	100.0

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

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

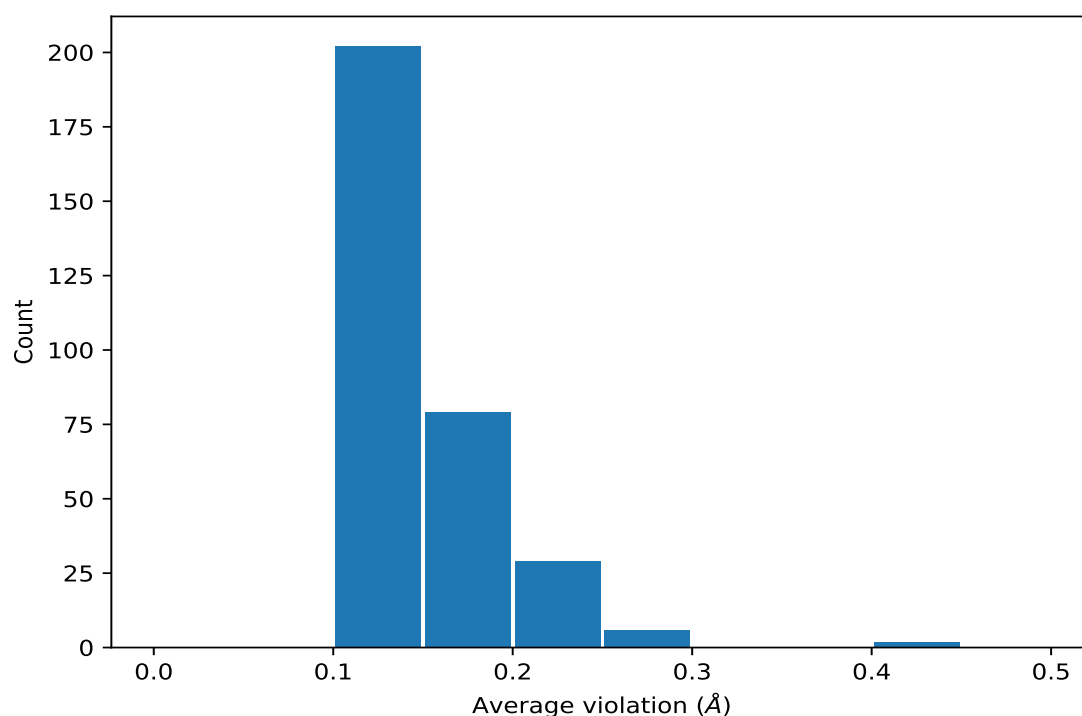
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,3560)	1:297:A:PRO:HB3	1:298:A:THR:HG21	32	0.22	0.02	0.22
(1,3560)	1:297:A:PRO:HB3	1:298:A:THR:HG22	32	0.22	0.02	0.22
(1,3560)	1:297:A:PRO:HB3	1:298:A:THR:HG23	32	0.22	0.02	0.22
(1,2424)	1:279:A:TYR:HE1	1:299:A:CYS:H	32	0.2	0.01	0.2
(1,2424)	1:279:A:TYR:HE2	1:299:A:CYS:H	32	0.2	0.01	0.2
(1,3190)	1:288:A:LEU:HG	1:305:A:SER:HA	32	0.18	0.03	0.18
(1,3562)	1:297:B:PRO:HB3	1:298:B:THR:HG21	31	0.23	0.02	0.23
(1,3562)	1:297:B:PRO:HB3	1:298:B:THR:HG22	31	0.23	0.02	0.23
(1,3562)	1:297:B:PRO:HB3	1:298:B:THR:HG23	31	0.23	0.02	0.23
(1,2439)	1:279:B:TYR:HE1	1:299:B:CYS:H	31	0.2	0.02	0.2
(1,2439)	1:279:B:TYR:HE2	1:299:B:CYS:H	31	0.2	0.02	0.2
(1,3193)	1:288:B:LEU:HG	1:305:B:SER:HA	31	0.17	0.03	0.16
(1,3557)	1:297:B:PRO:HA	1:298:B:THR:HG21	31	0.17	0.03	0.16
(1,3557)	1:297:B:PRO:HA	1:298:B:THR:HG22	31	0.17	0.03	0.16
(1,3557)	1:297:B:PRO:HA	1:298:B:THR:HG23	31	0.17	0.03	0.16
(1,3554)	1:297:A:PRO:HA	1:298:A:THR:HG21	31	0.16	0.03	0.16

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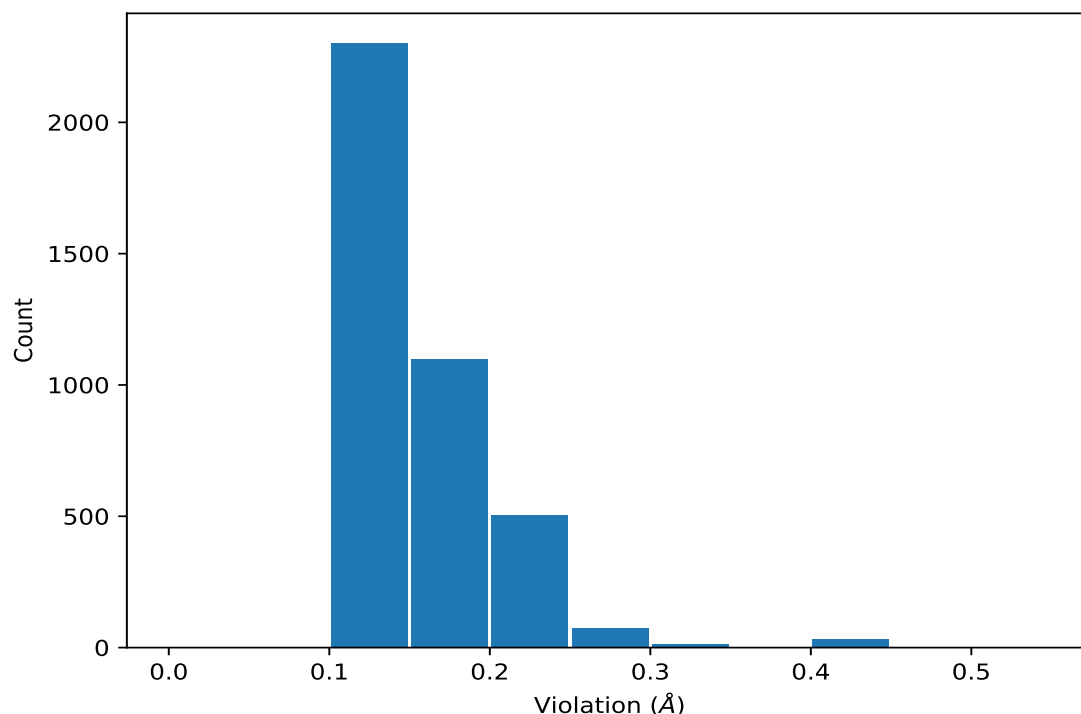
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3554)	1:297:A:PRO:HA	1:298:A:THR:HG22	31	0.16	0.03	0.16
(1,3554)	1:297:A:PRO:HA	1:298:A:THR:HG23	31	0.16	0.03	0.16
(1,842)	1:260:A:LEU:HD11	1:279:A:TYR:HB3	30	0.15	0.02	0.16
(1,842)	1:260:A:LEU:HD12	1:279:A:TYR:HB3	30	0.15	0.02	0.16
(1,842)	1:260:A:LEU:HD13	1:279:A:TYR:HB3	30	0.15	0.02	0.16
(1,842)	1:260:A:LEU:HD21	1:279:A:TYR:HB3	30	0.15	0.02	0.16
(1,842)	1:260:A:LEU:HD22	1:279:A:TYR:HB3	30	0.15	0.02	0.16
(1,842)	1:260:A:LEU:HD23	1:279:A:TYR:HB3	30	0.15	0.02	0.16
(1,4164)	1:312:A:ASN:H	1:313:A:LYS:HG2	29	0.2	0.05	0.21

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)
(1,5189)	1:333:A:ARG:HB2	1:334:A:LYS:H	8	0.52
(1,5189)	1:333:A:ARG:HB3	1:334:A:LYS:H	8	0.52
(1,4973)	1:328:A:TYR:HA	1:329:A:THR:H	10	0.45
(1,4973)	1:328:A:TYR:HA	1:329:A:THR:H	17	0.45
(1,4973)	1:328:A:TYR:HA	1:329:A:THR:H	22	0.45
(1,4976)	1:328:B:TYR:HA	1:329:B:THR:H	4	0.44
(1,4976)	1:328:B:TYR:HA	1:329:B:THR:H	9	0.44
(1,4973)	1:328:A:TYR:HA	1:329:A:THR:H	8	0.44
(1,4973)	1:328:A:TYR:HA	1:329:A:THR:H	11	0.44
(1,4973)	1:328:A:TYR:HA	1:329:A:THR:H	15	0.44
(1,4973)	1:328:A:TYR:HA	1:329:A:THR:H	18	0.44

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found