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PROTEIN DATA BANK

wwPDB NMR Structure Validation Summary Report (i)

Jan 22, 2024 – 02:20 PM JST

PDB ID	:	8IVB
BMRB ID	:	19045
Title	:	K113-Ubiquitinated BAK
Authors	:	Dong, X.; Cheng, P.; Hou, Y.Z.; Chen, Y.K.; Liu, Z.
Deposited on	:	2023-03-26

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

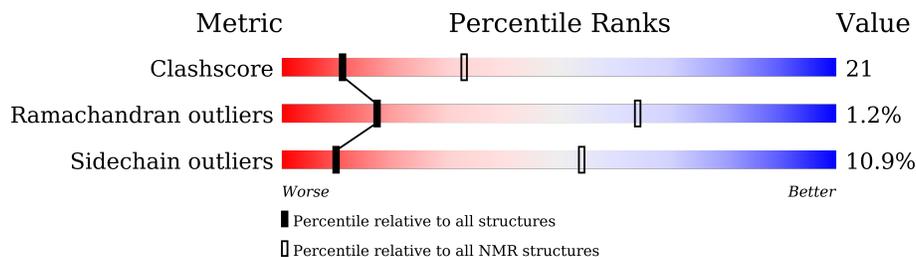|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 8%.

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	Percentile Ranks	Value
Clashscore		21
Ramachandran outliers		1.2%
Sidechain outliers		10.9%
Worse		*Better*

▮ Percentile relative to all structures
◌ Percentile relative to all NMR structures

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	76	66% 28% • 5%
2	B	169	67% 30% •

2   Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 12 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:1-A:72 (72)	0.17	11
2	B:18-B:186 (169)	0.26	12

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 4 single-model clusters were found.

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

3 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 3851 atoms, of which 1912 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	76	1235	379	631	105	118	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	CYS	GLY	conflict	UNP P62979

- Molecule 2 is a protein called Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	169	2616	847	1281	233	249	6	0

There is a discrepancy between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
B	113	CYS	LYS	engineered mutation	UNP Q16611

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.
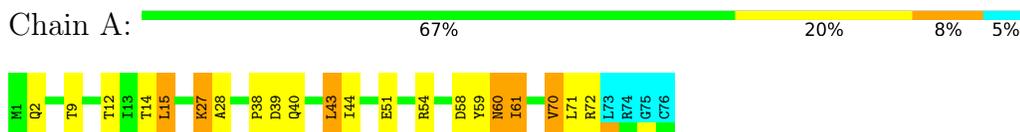
• Molecule 1: Ubiquitin

Chain A:

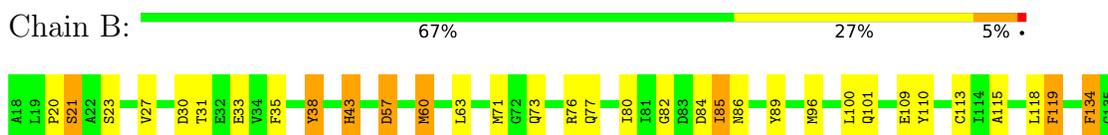• Molecule 2: Bcl-2 homologous antagonist/killer

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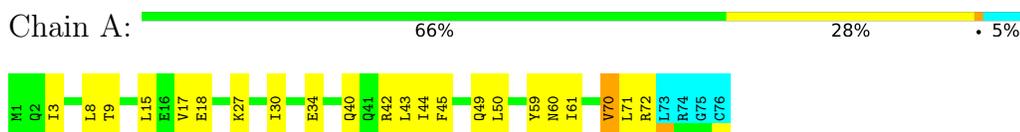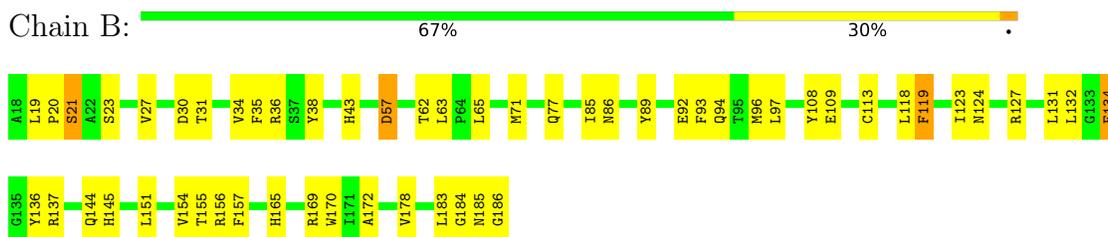
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 12. Colouring as in section 4.1 above.

• Molecule 1: Ubiquitin

Chain A:

• Molecule 2: Bcl-2 homologous antagonist/killer

Chain B:

Y136 R137 L138 A139 L140 H141 V142 Y143 Q144 H145 G146 L147 T155 R156 F157 D160 H164 R169 W170 I171 A172 V178 G184 N185 G186

5 Refinement protocol and experimental data overview ⓘ

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

Of the 240 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

The authors did not provide any information on software used for structure solution, optimization or refinement.

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	256
Number of shifts mapped to atoms	256
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	8%

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.06±0.02	0±0/581 (0.0± 0.0%)	0.84±0.02	0±0/784 (0.0± 0.0%)
2	B	1.07±0.02	0±0/1368 (0.0± 0.0%)	0.89±0.02	0±1/1858 (0.0± 0.0%)
All	All	1.07	0/38980 (0.0%)	0.87	9/52840 (0.0%)

There are no bond-length outliers.

5 of 7 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	143	TYR	CB-CG-CD1	-7.77	116.34	121.00	12	1
2	B	38	TYR	CB-CG-CD2	-7.09	116.74	121.00	8	3
1	A	45	PHE	CB-CG-CD2	-5.53	116.93	120.80	11	1
2	B	143	TYR	CB-CG-CD2	5.37	124.22	121.00	12	1
1	A	59	TYR	CA-CB-CG	-5.28	103.36	113.40	4	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	574	600	599	23±7
2	B	1335	1281	1273	57±10
All	All	38180	37620	37440	1558

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 21.

5 of 812 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
2:B:65:LEU:H	2:B:65:LEU:HD13	0.97	1.17	11	1
2:B:65:LEU:HD13	2:B:66:GLN:N	0.94	1.77	14	3
2:B:151:LEU:HD22	2:B:152:GLY:N	0.94	1.77	7	1
1:A:50:LEU:HD13	1:A:50:LEU:H	0.92	1.25	15	3
2:B:65:LEU:H	2:B:65:LEU:HD22	0.92	1.21	8	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	71/76 (93%)	63±1 (89±1%)	6±1 (9±1%)	1±0 (1±0%)	14	59
2	B	167/169 (99%)	145±3 (87±2%)	20±2 (12±1%)	2±0 (1±0%)	18	66
All	All	4760/4900 (97%)	4173 (88%)	528 (11%)	59 (1%)	17	64

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	70	VAL	20
2	B	184	GLY	20
2	B	156	ARG	18
1	A	60	ASN	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	66/69 (96%)	60±2 (91±4%)	6±2 (9±4%)	12	58
2	B	137/137 (100%)	121±4 (88±3%)	16±4 (12±3%)	9	52
All	All	4060/4120 (99%)	3619 (89%)	441 (11%)	10	54

5 of 115 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)
2	B	57	ASP	20
2	B	119	PHE	15
2	B	21	SER	15
2	B	134	PHE	15
2	B	65	LEU	13

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 ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 8% for the well-defined parts and 8% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *wk11_CS*

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	256
Number of shifts mapped to atoms	256
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	0	—	None (insufficient data)
$^{13}C_\beta$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	128	1.15 ± 0.11	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 8%, i.e. 254 atoms were assigned a chemical shift out of a possible 3317. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	254/1206 (21%)	127/492 (26%)	0/482 (0%)	127/232 (55%)
Sidechain	0/1837 (0%)	0/1196 (0%)	0/568 (0%)	0/73 (0%)

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|	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/274 (0%)	0/133 (0%)	0/124 (0%)	0/17 (0%)
Overall	254/3317 (8%)	127/1821 (7%)	0/1174 (0%)	127/322 (39%)

7.1.4　Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

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:
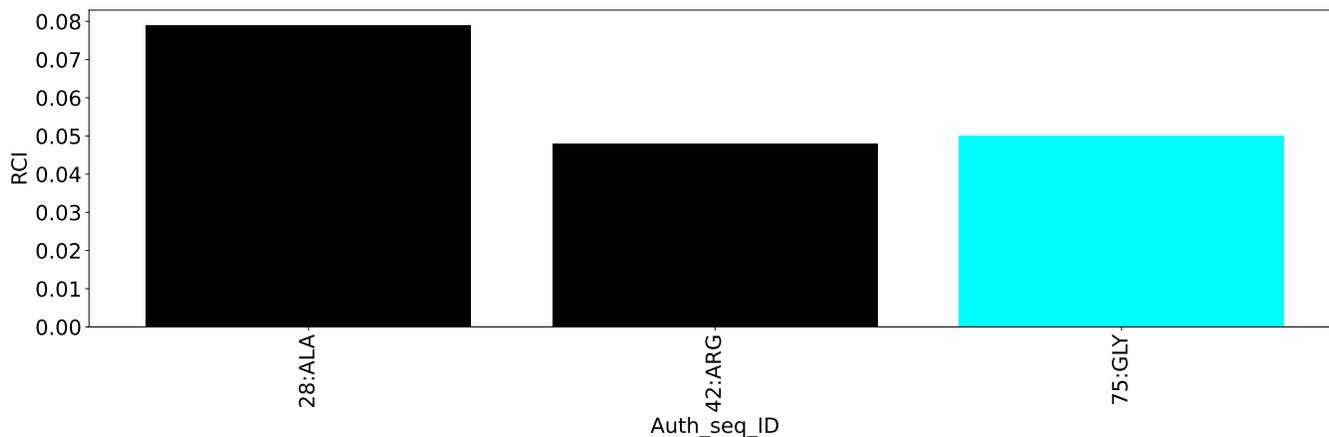
Random coil index (RCI) for chain B:
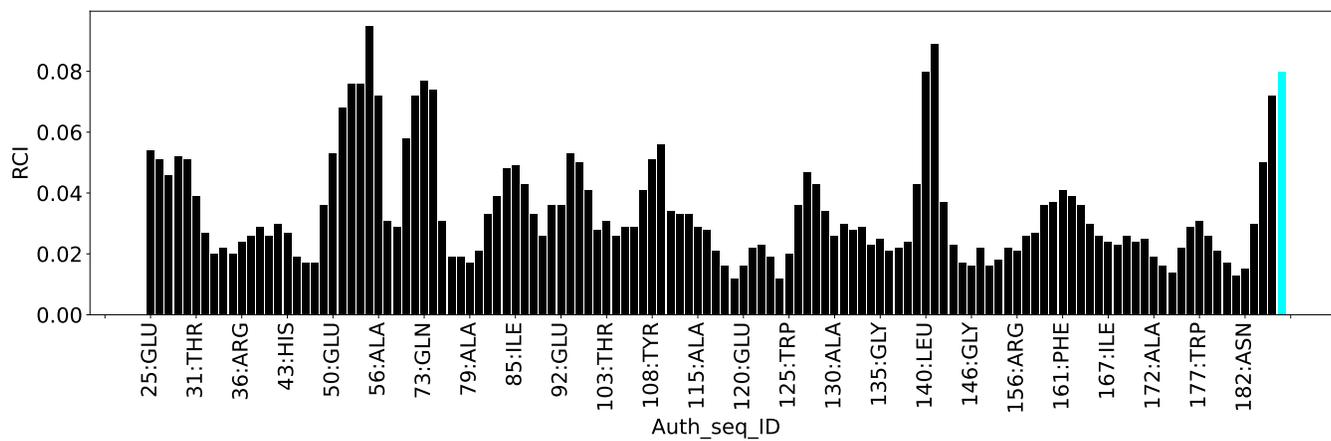
8 NMR restraints analysis ⓘ

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	14
Intra-residue ($\vert$i-j$\vert$=0)	0
Sequential ($\vert$i-j$\vert$=1)	0
Medium range ($\vert$i-j$\vert$>1 and $\vert$i-j$\vert$<5)	0
Long range ($\vert$i-j$\vert\geq$5)	0
Inter-chain	14
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.1
Number of long range restraints per residue[1]	0.0

[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)	1.4	0.2
0.2-0.5 (Medium)	3.6	0.5
>0.5 (Large)	4.2	1.68

8.2.2 Average number of dihedral-angle violations per model ⓘ

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations
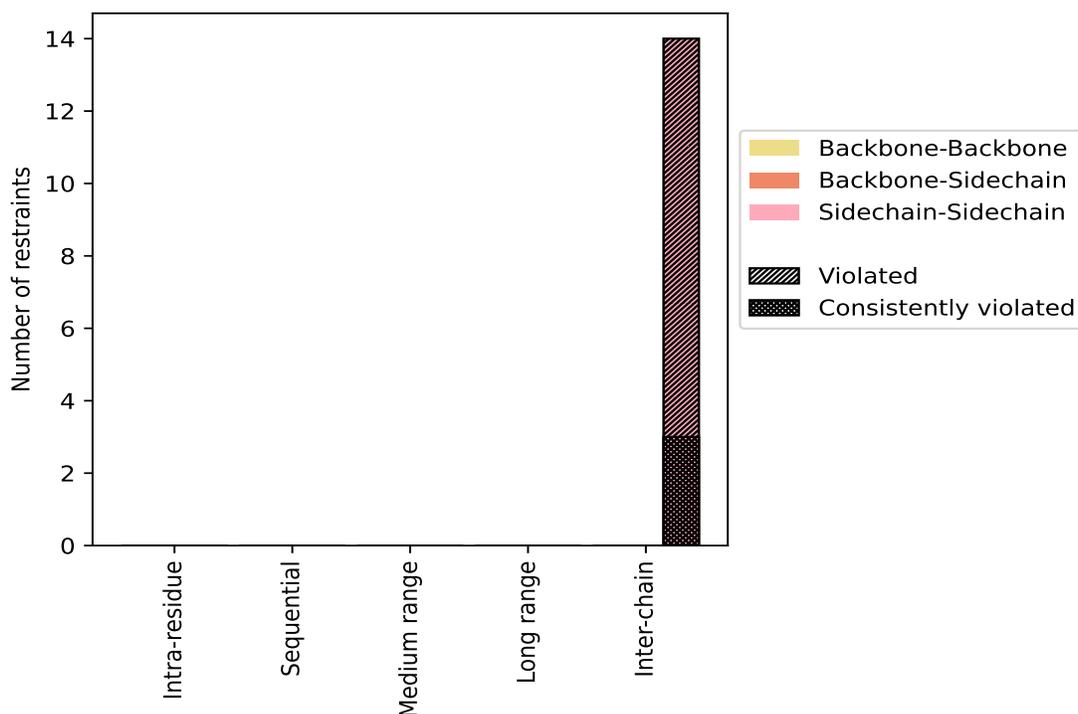
9 Distance violation analysis ⓘ

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)	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|≥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
Inter-chain	14	100.0	14	100.0	100.0	3	21.4	21.4
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	14	100.0	14	100.0	100.0	3	21.4	21.4
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	14	100.0	14	100.0	100.0	3	21.4	21.4
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	14	100.0	14	100.0	100.0	3	21.4	21.4

[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	0	0	0	0	8	8	0.56	1.15	0.33	0.43
2	0	0	0	0	10	10	0.48	1.12	0.31	0.4
3	0	0	0	0	7	7	0.58	1.1	0.36	0.5
4	0	0	0	0	10	10	0.6	1.19	0.37	0.5
5	0	0	0	0	10	10	0.58	1.68	0.5	0.4
6	0	0	0	0	8	8	0.65	1.15	0.32	0.57
7	0	0	0	0	12	12	0.59	1.55	0.44	0.48
8	0	0	0	0	8	8	0.68	1.29	0.42	0.74
9	0	0	0	0	10	10	0.56	1.02	0.28	0.44
10	0	0	0	0	9	9	0.58	1.27	0.33	0.47
11	0	0	0	0	7	7	0.65	1.22	0.33	0.63

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Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	0	0	10	10	0.59	1.17	0.35	0.46
13	0	0	0	0	10	10	0.54	1.09	0.35	0.36
14	0	0	0	0	11	11	0.5	1.16	0.39	0.24
15	0	0	0	0	10	10	0.49	1.2	0.32	0.4
16	0	0	0	0	10	10	0.4	1.05	0.32	0.26
17	0	0	0	0	10	10	0.66	1.2	0.35	0.58
18	0	0	0	0	8	8	0.71	1.47	0.49	0.74
19	0	0	0	0	10	10	0.63	1.2	0.41	0.41
20	0	0	0	0	8	8	0.54	1.12	0.33	0.48

[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 ⓘ
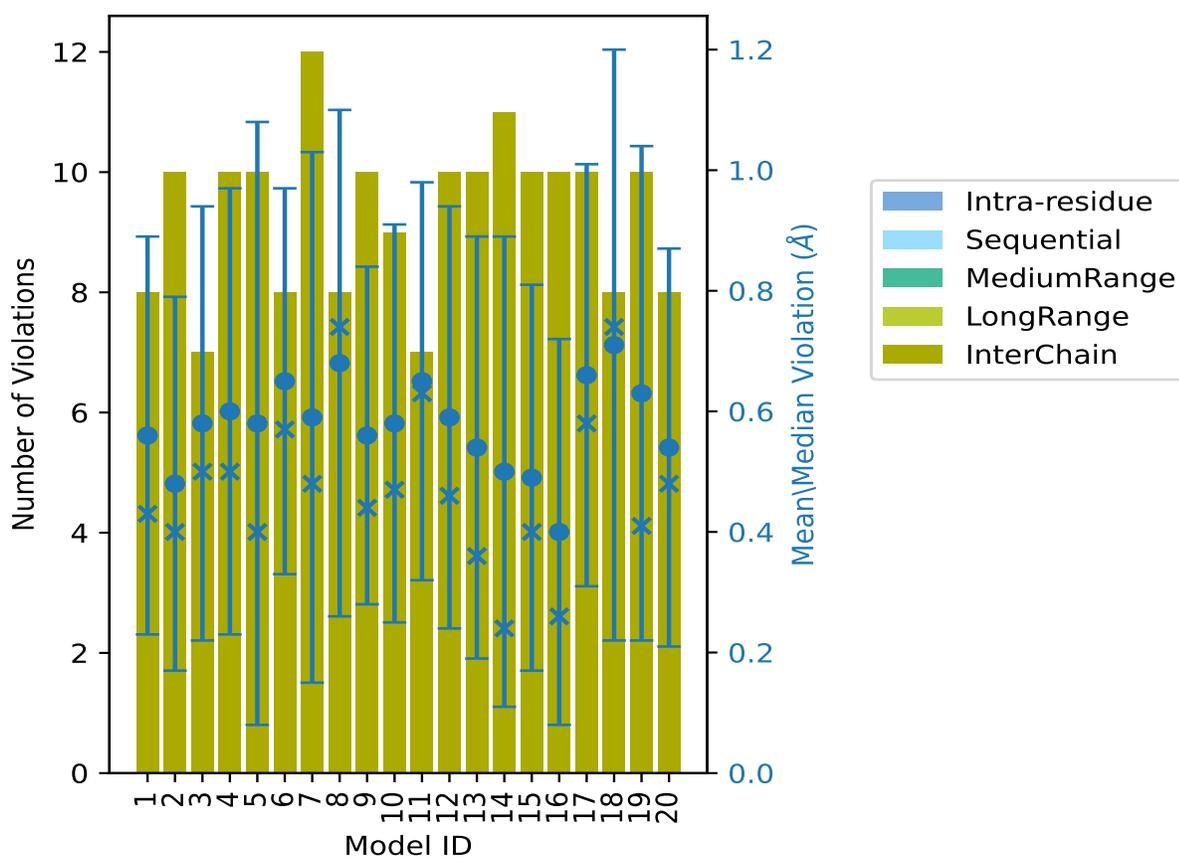
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis
on the right

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, 0(IR:0, SQ:0, MR:0, LR:0, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	1	1	1	5.0
0	0	0	0	1	1	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	1	1	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	1	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	2	2	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	1	1	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	1	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	3	3	19	95.0
0	0	0	0	3	3	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)
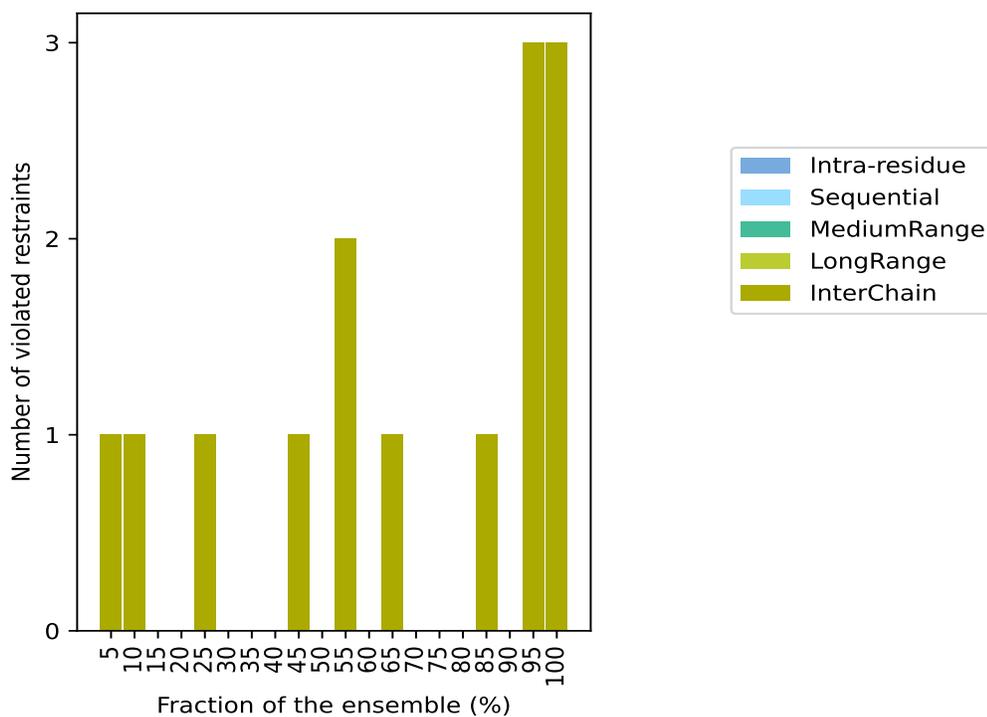
9.4 Most violated distance restraints in the ensemble (i)

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
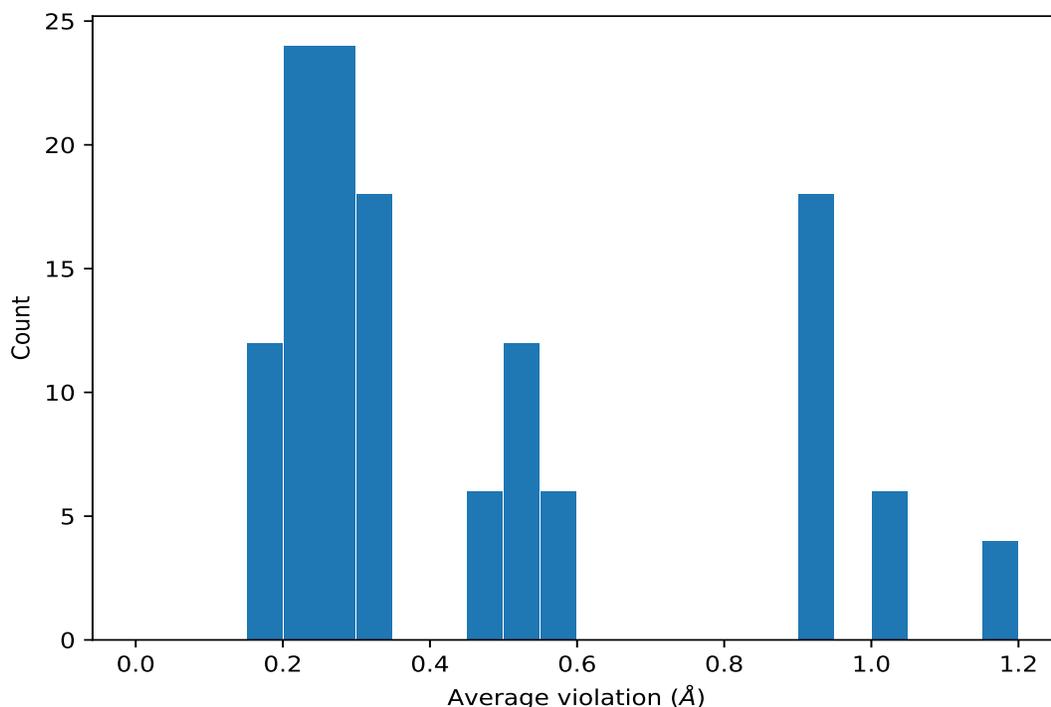
9.4.2　Table: Most violated distance restraints ⓘ

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)
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	20	1.15	0.08	1.15
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	20	1.15	0.08	1.15
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	20	1.15	0.08	1.15
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	20	1.15	0.08	1.15
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG2	20	1.03	0.11	1.04
(1,9)	2:118:B:LEU:HD11	1:42:A:ARG:HG3	20	1.03	0.11	1.04
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG2	20	1.03	0.11	1.04
(1,9)	2:118:B:LEU:HD12	1:42:A:ARG:HG3	20	1.03	0.11	1.04
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG2	20	1.03	0.11	1.04
(1,9)	2:118:B:LEU:HD13	1:42:A:ARG:HG3	20	1.03	0.11	1.04
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG11	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG12	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG13	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG21	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG22	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG21	1:70:A:VAL:HG23	20	0.34	0.1	0.36

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG11	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG12	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG13	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG21	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG22	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG22	1:70:A:VAL:HG23	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG11	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG12	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG13	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG21	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG22	20	0.34	0.1	0.36
(1,4)	2:114:B:ILE:HG23	1:70:A:VAL:HG23	20	0.34	0.1	0.36
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	19	0.91	0.41	0.93
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	19	0.91	0.41	0.93
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG11	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG12	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG13	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG21	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG22	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB2	1:70:A:VAL:HG23	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG11	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG12	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG13	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG21	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG22	19	0.53	0.1	0.55
(1,14)	2:92:B:GLU:HB3	1:70:A:VAL:HG23	19	0.53	0.1	0.55

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG11	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG12	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG13	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG21	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG22	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD11	1:70:A:VAL:HG23	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG11	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG12	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG13	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG21	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG22	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD12	1:70:A:VAL:HG23	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG11	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG12	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG13	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG21	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG22	19	0.24	0.09	0.25
(1,5)	2:114:B:ILE:HD13	1:70:A:VAL:HG23	19	0.24	0.09	0.25
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG2	17	0.56	0.24	0.48
(1,2)	2:96:B:MET:HE1	1:42:A:ARG:HG3	17	0.56	0.24	0.48
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG2	17	0.56	0.24	0.48
(1,2)	2:96:B:MET:HE2	1:42:A:ARG:HG3	17	0.56	0.24	0.48
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG2	17	0.56	0.24	0.48
(1,2)	2:96:B:MET:HE3	1:42:A:ARG:HG3	17	0.56	0.24	0.48
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG11	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG12	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG13	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG21	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG22	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD11	1:70:A:VAL:HG23	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG11	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG12	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG13	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG21	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG22	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD12	1:70:A:VAL:HG23	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG11	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG12	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG13	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG21	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG22	13	0.25	0.06	0.27
(1,8)	2:118:B:LEU:HD13	1:70:A:VAL:HG23	13	0.25	0.06	0.27

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG11	11	0.49	0.15	0.55
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG12	11	0.49	0.15	0.55
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG13	11	0.49	0.15	0.55
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG21	11	0.49	0.15	0.55
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG22	11	0.49	0.15	0.55
(1,13)	2:92:B:GLU:HG3	1:70:A:VAL:HG23	11	0.49	0.15	0.55
(1,6)	2:114:B:ILE:HD11	1:42:A:ARG:HG2	11	0.22	0.05	0.22

[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.
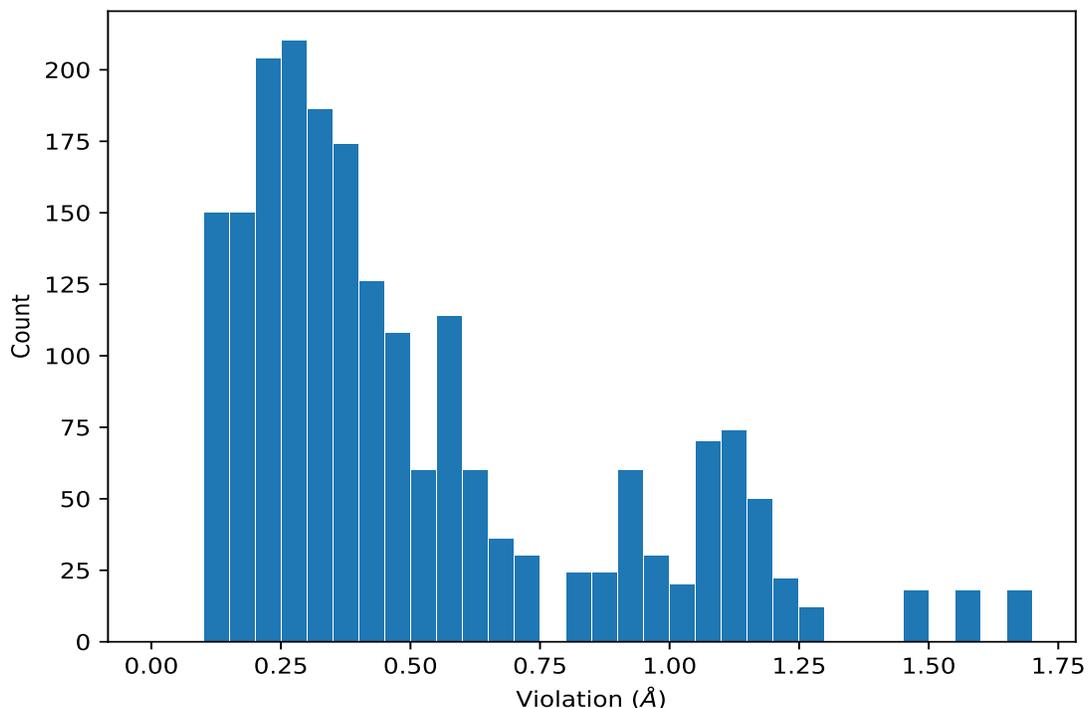
9.5.2 Table : All distance violations ⓘ

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)
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	5	1.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	5	1.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	5	1.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	5	1.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	5	1.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	5	1.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	5	1.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	5	1.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	5	1.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	5	1.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	5	1.68
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	5	1.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	5	1.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	5	1.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	5	1.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	5	1.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	5	1.68
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	5	1.68
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	7	1.55
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	7	1.55
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	7	1.55
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	7	1.55
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	7	1.55
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	7	1.55
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	7	1.55
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	7	1.55
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	7	1.55
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	7	1.55
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	7	1.55
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	7	1.55
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	7	1.55
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	7	1.55
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	7	1.55
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	7	1.55
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	7	1.55
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	7	1.55
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG11	18	1.47
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG12	18	1.47
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG13	18	1.47
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG21	18	1.47
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG22	18	1.47
(1,1)	2:96:B:MET:HE1	1:70:A:VAL:HG23	18	1.47
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG11	18	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG12	18	1.47
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG13	18	1.47
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG21	18	1.47
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG22	18	1.47
(1,1)	2:96:B:MET:HE2	1:70:A:VAL:HG23	18	1.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG11	18	1.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG12	18	1.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG13	18	1.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG21	18	1.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG22	18	1.47
(1,1)	2:96:B:MET:HE3	1:70:A:VAL:HG23	18	1.47
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	8	1.29
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	8	1.29
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	8	1.29
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	8	1.29
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	10	1.27
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	10	1.27
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	10	1.27
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	10	1.27
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	18	1.26
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	18	1.26
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	18	1.26
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	18	1.26
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	5	1.23
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	5	1.23
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	5	1.23
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	5	1.23
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	11	1.22
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	11	1.22
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	11	1.22
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	11	1.22
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	15	1.2
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG3	15	1.2
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG2	15	1.2
(1,11)	2:89:B:TYR:HB3	1:42:A:ARG:HG3	15	1.2
(1,11)	2:89:B:TYR:HB2	1:42:A:ARG:HG2	17	1.2

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found