



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 03:23 AM UTC

PDB ID : 6LZP / pdb_00006lzp
BMRB ID : 28064
Title : The solution structure of N-terminal elongated hSNF5 RPT1 domain
Authors : Lee, W.; Han, J.; Kim, I.; Suh, J.Y.
Deposited on : 2020-02-19

This is a Full wwPDB NMR Structure Validation 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

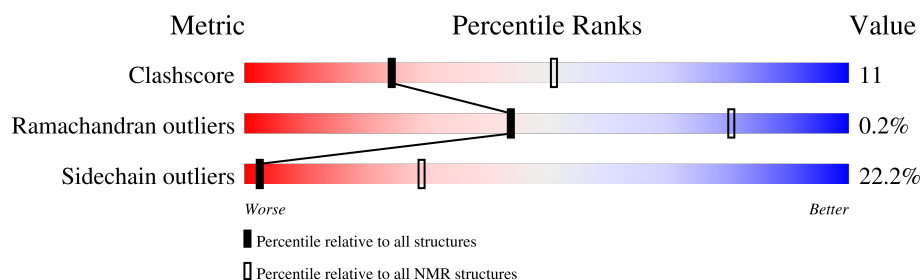
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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	89	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 3 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:184-A:246 (63)	0.63	3

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 1377 atoms, of which 677 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily B member 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	88	1377	440	677	113	142	5	0

There is a discrepancy between the modelled and reference sequences:

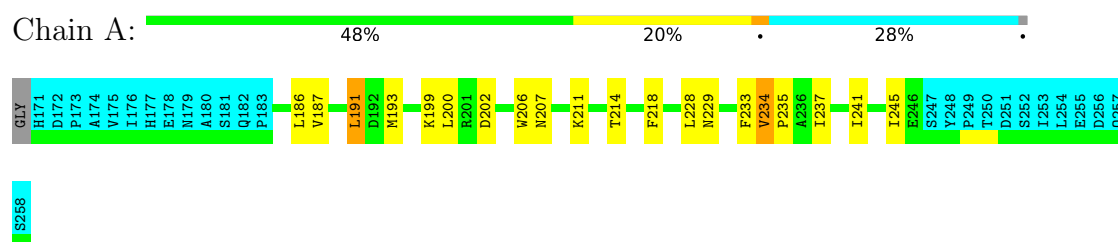
Chain	Residue	Modelled	Actual	Comment	Reference
A	170	GLY	-	expression tag	UNP A0A0G2JRV3

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: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1

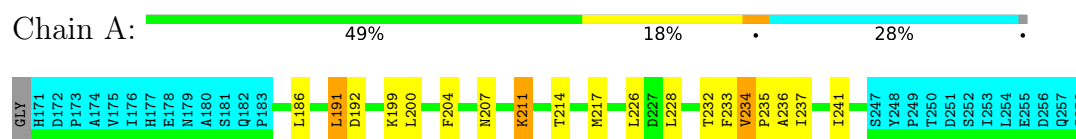


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

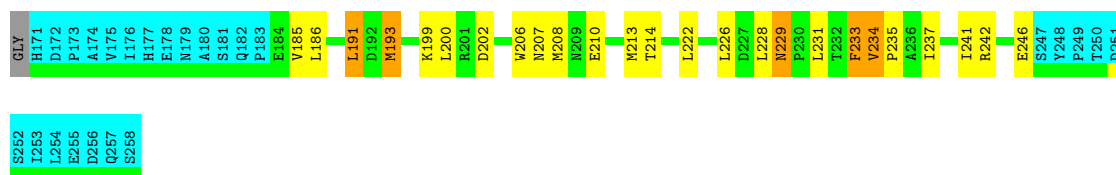
- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



4.2.2 Score per residue for model 2

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1





4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1

Chain A: 49% 18% 28%



4.2.4 Score per residue for model 4

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1

Chain A: 49% 18% 28%



4.2.5 Score per residue for model 5

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1

Chain A: 49% 19% 28%



4.2.6 Score per residue for model 6

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1

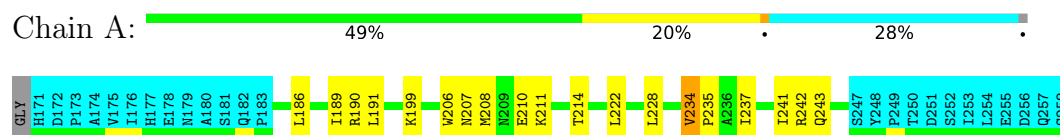
Chain A: 46% 21% 28%





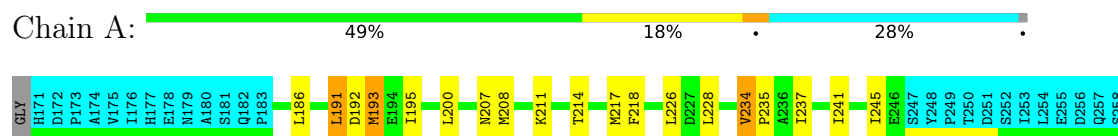
4.2.7 Score per residue for model 7

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



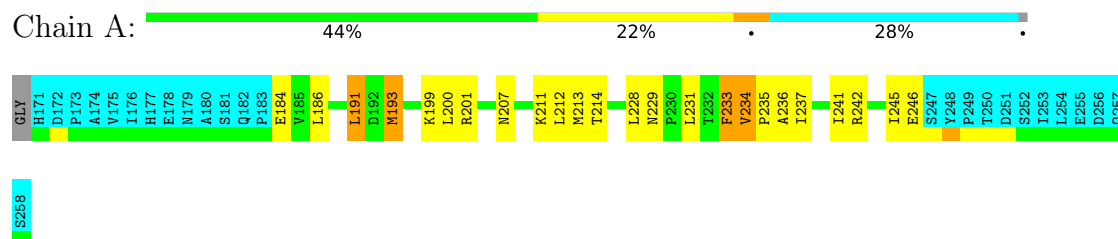
4.2.8 Score per residue for model 8

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



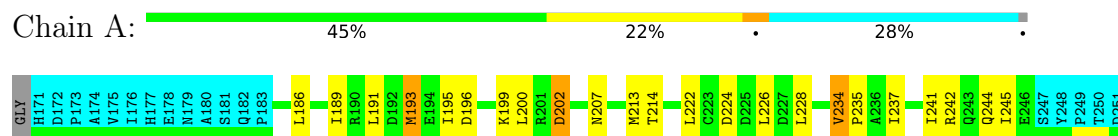
4.2.9 Score per residue for model 9

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



4.2.10 Score per residue for model 10

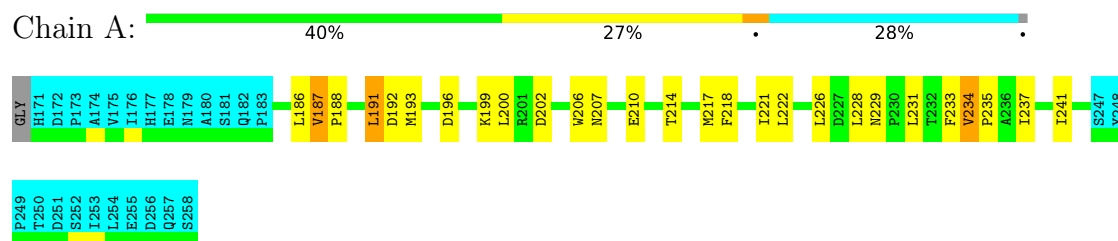
- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



S252
L253
L254
E255
D256
Q257
S258

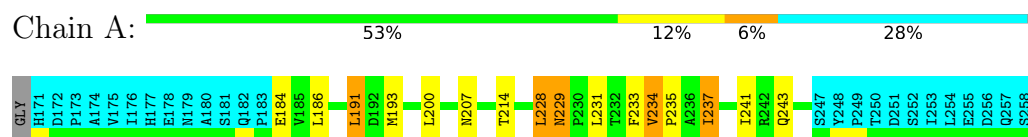
4.2.11 Score per residue for model 11

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



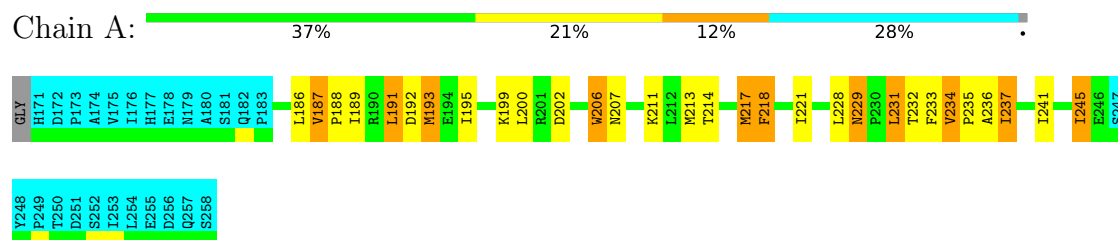
4.2.12 Score per residue for model 12

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



4.2.13 Score per residue for model 13

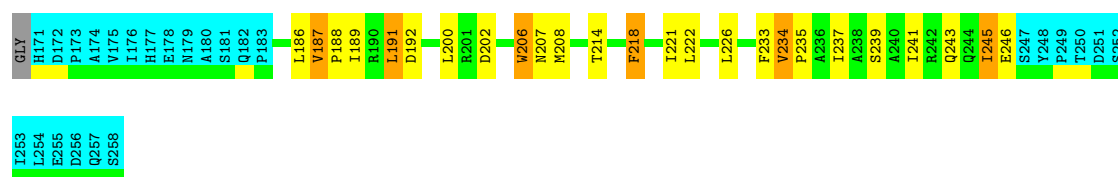
- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



4.2.14 Score per residue for model 14

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1





4.2.15 Score per residue for model 15

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1

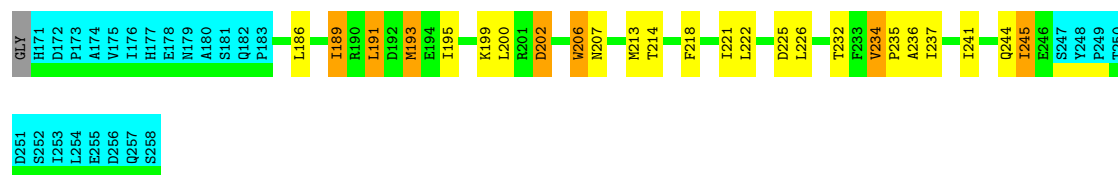
Chain A: .



4.2.16 Score per residue for model 16

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1

Chain A: .



4.2.17 Score per residue for model 17

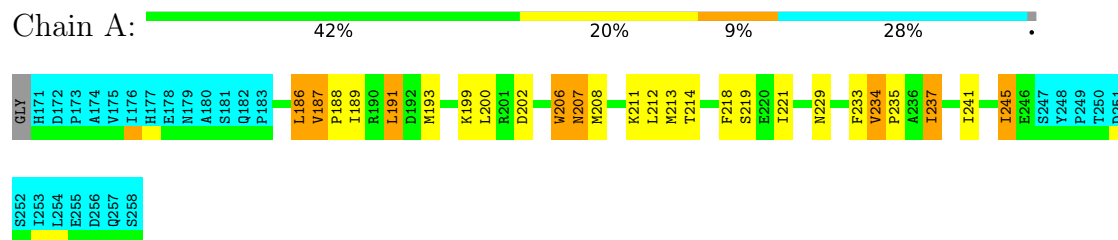
- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1

Chain A: .



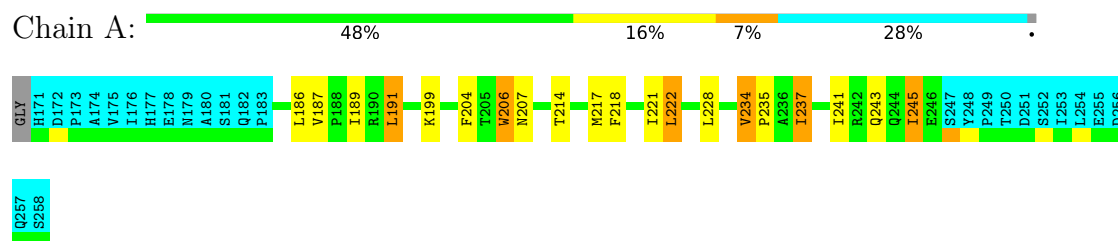
4.2.18 Score per residue for model 18

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



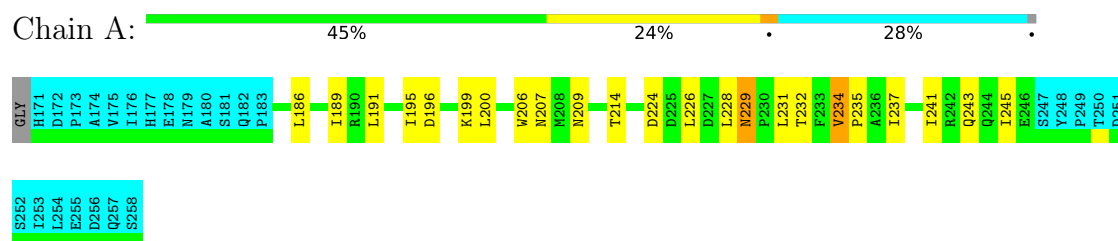
4.2.19 Score per residue for model 19

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



4.2.20 Score per residue for model 20

- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1



5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 20 were deposited, based on the following criterion: *20*.

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

Software name	Classification	Version
CYANA	structure calculation	
X-PLOR NIH	refinement	2.52

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	989
Number of shifts mapped to atoms	989
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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	507	508	508	11±4
All	All	10140	10160	10160	217

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:200:LEU:HD22	1:A:228:LEU:HD22	0.69	1.63	15	5
1:A:218:PHE:CD2	1:A:221:ILE:HD11	0.68	2.24	16	5
1:A:228:LEU:HD22	1:A:233:PHE:CE2	0.67	2.25	2	2
1:A:200:LEU:HD22	1:A:233:PHE:CE2	0.66	2.24	2	2
1:A:218:PHE:CD1	1:A:221:ILE:HD11	0.66	2.25	14	4
1:A:218:PHE:CE1	1:A:222:LEU:HD23	0.66	2.25	19	1
1:A:200:LEU:HD22	1:A:228:LEU:HD21	0.62	1.72	1	1
1:A:229:ASN:ND2	1:A:231:LEU:HD23	0.62	2.09	6	6
1:A:229:ASN:CG	1:A:231:LEU:HD23	0.61	2.20	2	3
1:A:200:LEU:CD1	1:A:228:LEU:HD22	0.61	2.25	10	2
1:A:191:LEU:HD21	1:A:204:PHE:CE2	0.61	2.30	19	2
1:A:200:LEU:HD12	1:A:228:LEU:HD22	0.60	1.73	12	3
1:A:193:MET:HG2	1:A:200:LEU:HD23	0.60	1.72	9	4
1:A:211:LYS:C	1:A:212:LEU:HD12	0.60	2.21	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:226:LEU:HB2	1:A:228:LEU:HD23	0.59	1.73	4	3
1:A:206:TRP:CE2	1:A:245:ILE:HG22	0.59	2.33	19	5
1:A:186:LEU:HD22	1:A:207:ASN:OD1	0.59	1.98	4	2
1:A:193:MET:CG	1:A:200:LEU:HD23	0.59	2.28	16	4
1:A:191:LEU:HD23	1:A:202:ASP:OD2	0.58	1.99	16	3
1:A:191:LEU:HD12	1:A:202:ASP:OD2	0.58	1.99	10	1
1:A:237:ILE:O	1:A:241:ILE:HG23	0.57	1.99	11	18
1:A:195:ILE:HD13	1:A:232:THR:OG1	0.57	1.99	6	2
1:A:189:ILE:HD11	1:A:245:ILE:HG22	0.57	1.76	10	1
1:A:195:ILE:HD13	1:A:232:THR:HB	0.55	1.77	13	1
1:A:222:LEU:HD22	1:A:233:PHE:CZ	0.55	2.37	6	1
1:A:228:LEU:HD13	1:A:233:PHE:CD2	0.54	2.37	9	2
1:A:241:ILE:O	1:A:245:ILE:HG23	0.54	2.03	10	1
1:A:200:LEU:HD22	1:A:228:LEU:CD2	0.54	2.33	15	2
1:A:191:LEU:HD11	1:A:241:ILE:HG22	0.54	1.78	14	6
1:A:200:LEU:HD13	1:A:226:LEU:HD13	0.53	1.78	1	1
1:A:211:LYS:O	1:A:212:LEU:HD22	0.53	2.04	17	1
1:A:233:PHE:CZ	1:A:237:ILE:HG21	0.52	2.39	4	4
1:A:228:LEU:HD13	1:A:233:PHE:CD1	0.52	2.39	17	1
1:A:229:ASN:HD21	1:A:231:LEU:HD12	0.51	1.66	9	2
1:A:191:LEU:HD22	1:A:237:ILE:HB	0.51	1.81	10	1
1:A:234:VAL:N	1:A:235:PRO:HD2	0.49	2.23	6	20
1:A:191:LEU:HD23	1:A:202:ASP:CG	0.49	2.32	16	1
1:A:200:LEU:HD22	1:A:233:PHE:CE1	0.49	2.42	17	1
1:A:193:MET:HE1	1:A:237:ILE:HA	0.49	1.85	2	1
1:A:193:MET:SD	1:A:195:ILE:HD12	0.49	2.48	10	4
1:A:226:LEU:HD12	1:A:228:LEU:CD2	0.49	2.38	20	1
1:A:191:LEU:HD21	1:A:204:PHE:CD2	0.49	2.43	19	1
1:A:200:LEU:CD2	1:A:228:LEU:HD22	0.48	2.38	20	2
1:A:191:LEU:HB3	1:A:237:ILE:HG22	0.48	1.85	12	5
1:A:191:LEU:HD21	1:A:241:ILE:CG2	0.48	2.39	10	2
1:A:193:MET:SD	1:A:200:LEU:HD23	0.48	2.48	6	1
1:A:187:VAL:HG21	1:A:208:MET:HE3	0.48	1.84	17	1
1:A:211:LYS:C	1:A:212:LEU:HD22	0.48	2.33	18	1
1:A:232:THR:O	1:A:236:ALA:HB2	0.48	2.08	1	3
1:A:228:LEU:HD22	1:A:233:PHE:CE1	0.48	2.43	17	1
1:A:213:MET:SD	1:A:217:MET:HE2	0.48	2.48	13	1
1:A:226:LEU:HD12	1:A:228:LEU:HD23	0.47	1.86	2	3
1:A:189:ILE:HG23	1:A:244:GLN:CD	0.47	2.34	10	1
1:A:200:LEU:HD21	1:A:233:PHE:CE1	0.46	2.46	11	5
1:A:191:LEU:CD1	1:A:241:ILE:HG22	0.46	2.40	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:228:LEU:HD13	1:A:233:PHE:HB2	0.46	1.88	1	2
1:A:187:VAL:HG12	1:A:188:PRO:HD2	0.46	1.87	14	4
1:A:191:LEU:HD21	1:A:241:ILE:HG22	0.46	1.87	17	1
1:A:200:LEU:HD13	1:A:226:LEU:HD22	0.46	1.87	15	1
1:A:218:PHE:CE1	1:A:221:ILE:HD11	0.46	2.44	15	1
1:A:228:LEU:HD22	1:A:233:PHE:CD2	0.46	2.45	9	2
1:A:222:LEU:O	1:A:226:LEU:HD12	0.46	2.10	14	2
1:A:185:VAL:HG12	1:A:208:MET:HE3	0.45	1.88	2	2
1:A:231:LEU:HD12	1:A:231:LEU:C	0.45	2.36	12	2
1:A:218:PHE:CE1	1:A:222:LEU:HD22	0.45	2.47	16	1
1:A:191:LEU:HD22	1:A:191:LEU:N	0.45	2.27	11	5
1:A:233:PHE:CE1	1:A:237:ILE:HG21	0.44	2.48	15	2
1:A:193:MET:HE2	1:A:233:PHE:HA	0.43	1.90	13	1
1:A:222:LEU:HD21	1:A:226:LEU:HD11	0.43	1.90	11	1
1:A:225:ASP:C	1:A:226:LEU:HD23	0.43	2.39	16	1
1:A:206:TRP:CZ2	1:A:245:ILE:HG22	0.42	2.49	14	2
1:A:189:ILE:HD11	1:A:244:GLN:HB2	0.42	1.92	16	1
1:A:229:ASN:ND2	1:A:231:LEU:HD12	0.42	2.28	9	1
1:A:241:ILE:HD12	1:A:242:ARG:N	0.42	2.30	10	1
1:A:200:LEU:HD21	1:A:233:PHE:HE1	0.42	1.74	18	1
1:A:228:LEU:HD12	1:A:228:LEU:C	0.42	2.40	19	4
1:A:200:LEU:HD11	1:A:226:LEU:CD1	0.42	2.45	4	1
1:A:228:LEU:O	1:A:228:LEU:HD12	0.42	2.15	1	1
1:A:193:MET:HE1	1:A:236:ALA:HB3	0.42	1.91	9	1
1:A:200:LEU:C	1:A:200:LEU:HD23	0.41	2.41	8	3
1:A:185:VAL:CG1	1:A:208:MET:HE3	0.41	2.46	6	1
1:A:218:PHE:HE1	1:A:222:LEU:HD22	0.41	1.76	16	1
1:A:200:LEU:HD13	1:A:226:LEU:CD1	0.41	2.46	1	1
1:A:234:VAL:CB	1:A:235:PRO:CD	0.40	3.00	13	3
1:A:189:ILE:HG21	1:A:241:ILE:HG22	0.40	1.93	10	1
1:A:191:LEU:N	1:A:191:LEU:HD22	0.40	2.31	19	2
1:A:202:ASP:CG	1:A:222:LEU:HD11	0.40	2.42	11	1
1:A:234:VAL:N	1:A:235:PRO:CD	0.40	2.84	14	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	63/89 (71%)	59±1 (94±2%)	4±1 (6±2%)	0±0 (0±0%)	44	80
All	All	1260/1780 (71%)	1185 (94%)	73 (6%)	2 (0%)	44	80

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	211	LYS	2

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	58/81 (72%)	45±3 (78±4%)	13±3 (22±4%)	2	29
All	All	1160/1620 (72%)	903 (78%)	257 (22%)	2	29

All 38 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	186	LEU	20
1	A	207	ASN	20
1	A	214	THR	20
1	A	234	VAL	20
1	A	191	LEU	19
1	A	199	LYS	14
1	A	245	ILE	13
1	A	193	MET	11
1	A	206	TRP	11
1	A	202	ASP	8
1	A	211	LYS	7
1	A	229	ASN	7
1	A	243	GLN	7
1	A	189	ILE	7
1	A	192	ASP	6
1	A	217	MET	6

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Mol	Chain	Res	Type	Models (Total)
1	A	213	MET	5
1	A	184	GLU	5
1	A	208	MET	5
1	A	187	VAL	5
1	A	237	ILE	5
1	A	222	LEU	4
1	A	242	ARG	4
1	A	246	GLU	4
1	A	196	ASP	4
1	A	210	GLU	3
1	A	218	PHE	3
1	A	233	PHE	2
1	A	219	SER	2
1	A	224	ASP	2
1	A	190	ARG	1
1	A	226	LEU	1
1	A	201	ARG	1
1	A	228	LEU	1
1	A	231	LEU	1
1	A	239	SER	1
1	A	212	LEU	1
1	A	209	ASN	1

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](#)

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 84% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `rpt1_all_manual.str`

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	989
Number of shifts mapped to atoms	989
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 [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	87	-0.18 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	84	0.20 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	79	-0.25 ± 0.16	None needed (< 0.5 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 84%, i.e. 748 atoms were assigned a chemical shift out of a possible 890. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	245/308 (80%)	123/123 (100%)	63/126 (50%)	59/59 (100%)
Sidechain	490/540 (91%)	337/352 (96%)	147/171 (86%)	6/17 (35%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	13/42 (31%)	12/21 (57%)	0/20 (0%)	1/1 (100%)
Overall	748/890 (84%)	472/496 (95%)	210/317 (66%)	66/77 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 989 atoms were assigned a chemical shift out of a possible 1196. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	334/427 (78%)	168/170 (99%)	87/176 (49%)	79/81 (98%)
Sidechain	640/704 (91%)	441/458 (96%)	191/226 (85%)	8/20 (40%)
Aromatic	15/65 (23%)	14/33 (42%)	0/29 (0%)	1/3 (33%)
Overall	989/1196 (83%)	623/661 (94%)	278/431 (65%)	88/104 (85%)

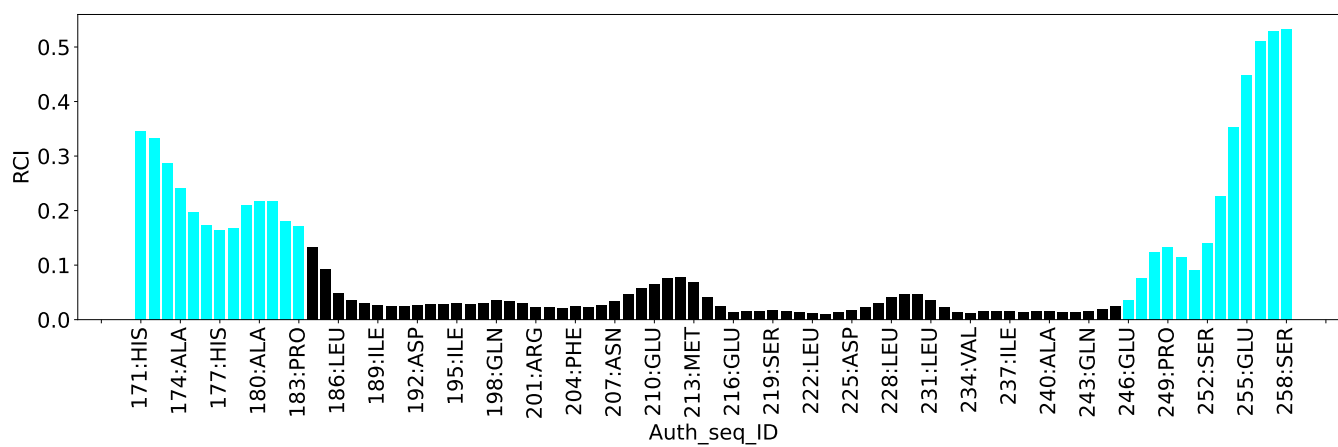
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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	872
Intra-residue ($ i-j =0$)	213
Sequential ($ i-j =1$)	337
Medium range ($ i-j >1$ and $ i-j <5$)	202
Long range ($ i-j \geq 5$)	120
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	264
Number of unmapped restraints	0
Number of restraints per residue	12.8
Number of long range restraints per residue ¹	1.3

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)	3.0	0.2
0.2-0.5 (Medium)	1.1	0.39
>0.5 (Large)	None	None

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.3	3.69
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

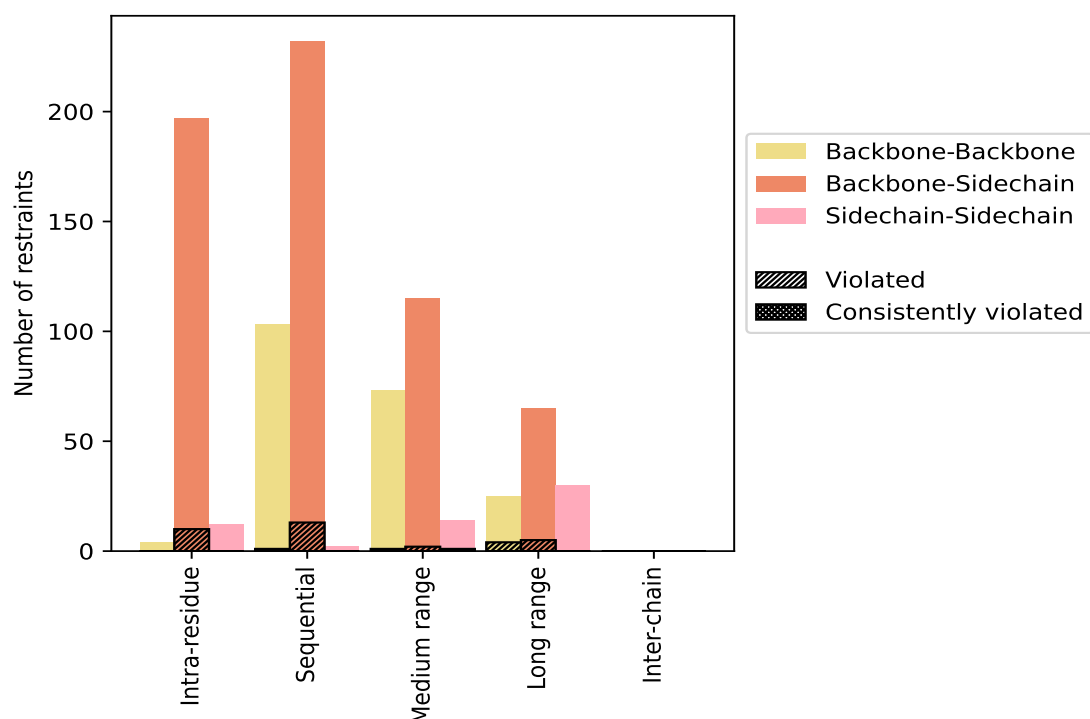
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	213	24.4	10	4.7	1.1	0	0.0	0.0
Backbone-Backbone	4	0.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	197	22.6	10	5.1	1.1	0	0.0	0.0
Sidechain-Sidechain	12	1.4	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	337	38.6	14	4.2	1.6	0	0.0	0.0
Backbone-Backbone	103	11.8	1	1.0	0.1	0	0.0	0.0
Backbone-Sidechain	232	26.6	13	5.6	1.5	0	0.0	0.0
Sidechain-Sidechain	2	0.2	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	202	23.2	4	2.0	0.5	0	0.0	0.0
Backbone-Backbone	73	8.4	1	1.4	0.1	0	0.0	0.0
Backbone-Sidechain	115	13.2	2	1.7	0.2	0	0.0	0.0
Sidechain-Sidechain	14	1.6	1	7.1	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	120	13.8	9	7.5	1.0	0	0.0	0.0
Backbone-Backbone	25	2.9	4	16.0	0.5	0	0.0	0.0
Backbone-Sidechain	65	7.5	5	7.7	0.6	0	0.0	0.0
Sidechain-Sidechain	30	3.4	0	0.0	0.0	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	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	872	100.0	37	4.2	4.2	0	0.0	0.0
Backbone-Backbone	205	23.5	6	2.9	0.7	0	0.0	0.0
Backbone-Sidechain	609	69.8	30	4.9	3.4	0	0.0	0.0
Sidechain-Sidechain	58	6.7	1	1.7	0.1	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.

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	1	0	1	0	0	2	0.16	0.18	0.02	0.16
2	0	1	0	1	0	2	0.18	0.18	0.0	0.18
3	0	2	0	0	0	2	0.18	0.25	0.06	0.18
4	2	1	1	0	0	4	0.18	0.26	0.05	0.16
5	0	3	0	0	0	3	0.12	0.15	0.02	0.1
6	0	2	0	0	0	2	0.16	0.2	0.04	0.16
7	1	4	0	0	0	5	0.18	0.25	0.04	0.17
8	1	0	1	0	0	2	0.14	0.18	0.03	0.14
9	1	1	3	0	0	5	0.14	0.18	0.03	0.14
10	0	2	3	1	0	6	0.16	0.3	0.07	0.12

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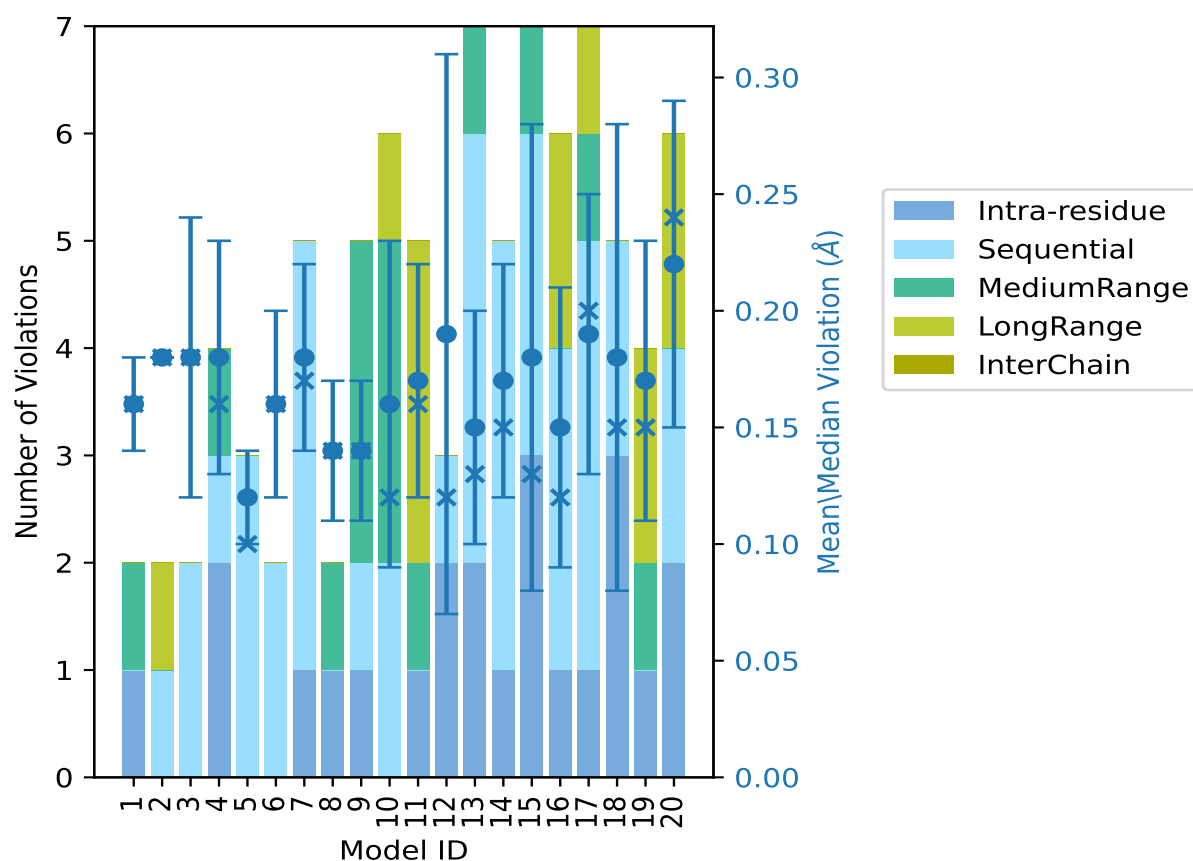
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	0	1	3	0	5	0.17	0.24	0.05	0.16
12	2	1	0	0	0	3	0.19	0.36	0.12	0.12
13	2	4	1	0	0	7	0.15	0.25	0.05	0.13
14	1	4	0	0	0	5	0.17	0.25	0.05	0.15
15	3	3	1	0	0	7	0.18	0.39	0.1	0.13
16	1	3	0	2	0	6	0.15	0.25	0.06	0.12
17	1	4	1	1	0	7	0.19	0.27	0.06	0.2
18	3	2	0	0	0	5	0.18	0.37	0.1	0.15
19	1	0	1	2	0	4	0.17	0.27	0.06	0.15
20	2	2	0	2	0	6	0.22	0.28	0.07	0.24

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

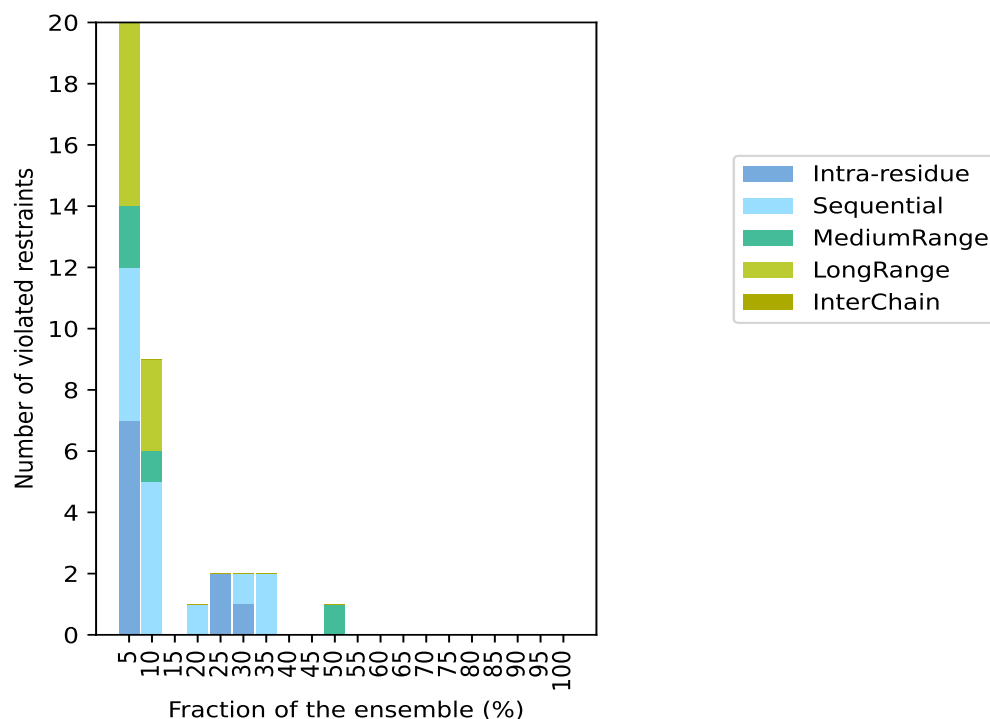
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 835(IR:203, SQ:323, MR:198, LR:111, IC:0) restraints are 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	%
7	5	2	6	0	20	1	5.0
0	5	1	3	0	9	2	10.0
0	0	0	0	0	0	3	15.0
0	1	0	0	0	1	4	20.0
2	0	0	0	0	2	5	25.0
1	1	0	0	0	2	6	30.0
0	2	0	0	0	2	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	1	0	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	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	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

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

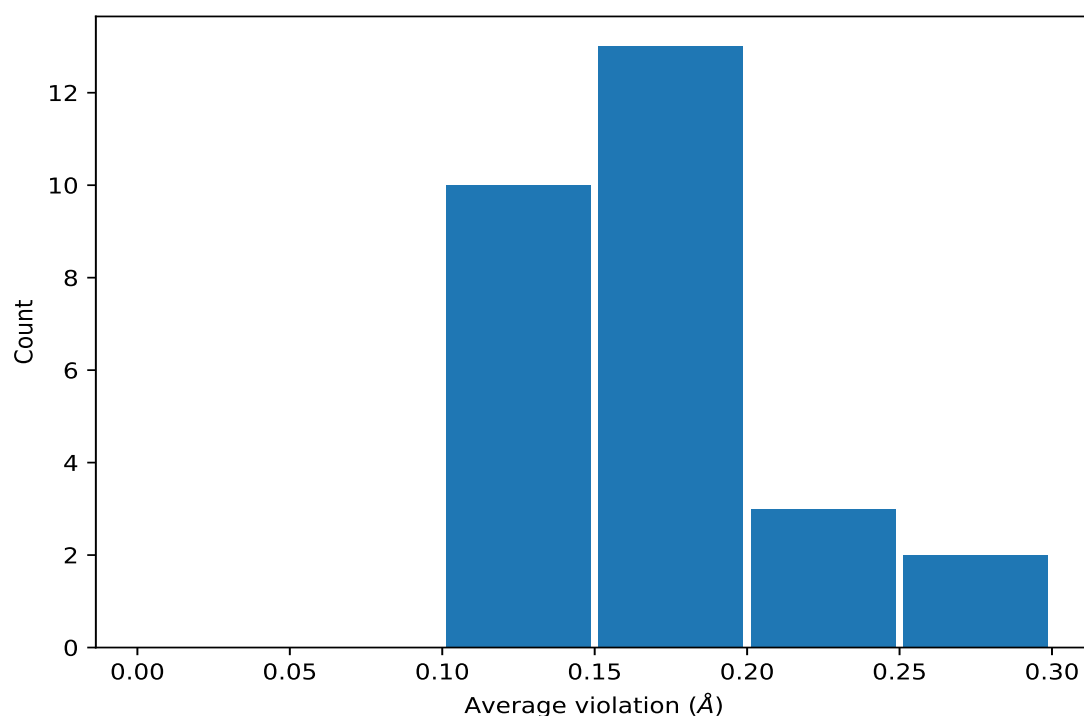
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 violation for each restraint sorted by number of violated models and the mean 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)
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG2	10	0.18	0.03	0.18
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG3	10	0.18	0.03	0.18
(1,864)	1:249:A:PRO:HD2	1:250:A:THR:H	7	0.25	0.0	0.25
(1,864)	1:249:A:PRO:HD3	1:250:A:THR:H	7	0.25	0.0	0.25
(1,565)	1:249:A:PRO:HG2	1:250:A:THR:H	7	0.11	0.0	0.11
(1,565)	1:249:A:PRO:HG3	1:250:A:THR:H	7	0.11	0.0	0.11
(1,234)	1:207:A:ASN:H	1:207:A:ASN:HD21	6	0.14	0.02	0.14
(1,728)	1:189:A:ILE:HG12	1:190:A:ARG:H	6	0.13	0.03	0.12
(1,728)	1:189:A:ILE:HG13	1:190:A:ARG:H	6	0.13	0.03	0.12
(1,850)	1:243:A:GLN:H	1:243:A:GLN:HG2	5	0.24	0.07	0.27
(1,850)	1:243:A:GLN:H	1:243:A:GLN:HG3	5	0.24	0.07	0.27
(1,102)	1:191:A:LEU:H	1:191:A:LEU:HG	5	0.13	0.02	0.11
(1,270)	1:211:A:LYS:HD2	1:212:A:LEU:H	4	0.18	0.04	0.19
(1,270)	1:211:A:LYS:HD3	1:212:A:LEU:H	4	0.18	0.04	0.19
(1,566)	1:250:A:THR:HB	1:251:A:ASP:H	2	0.22	0.08	0.22
(1,770)	1:208:A:MET:HG2	1:209:A:ASN:H	2	0.19	0.01	0.19

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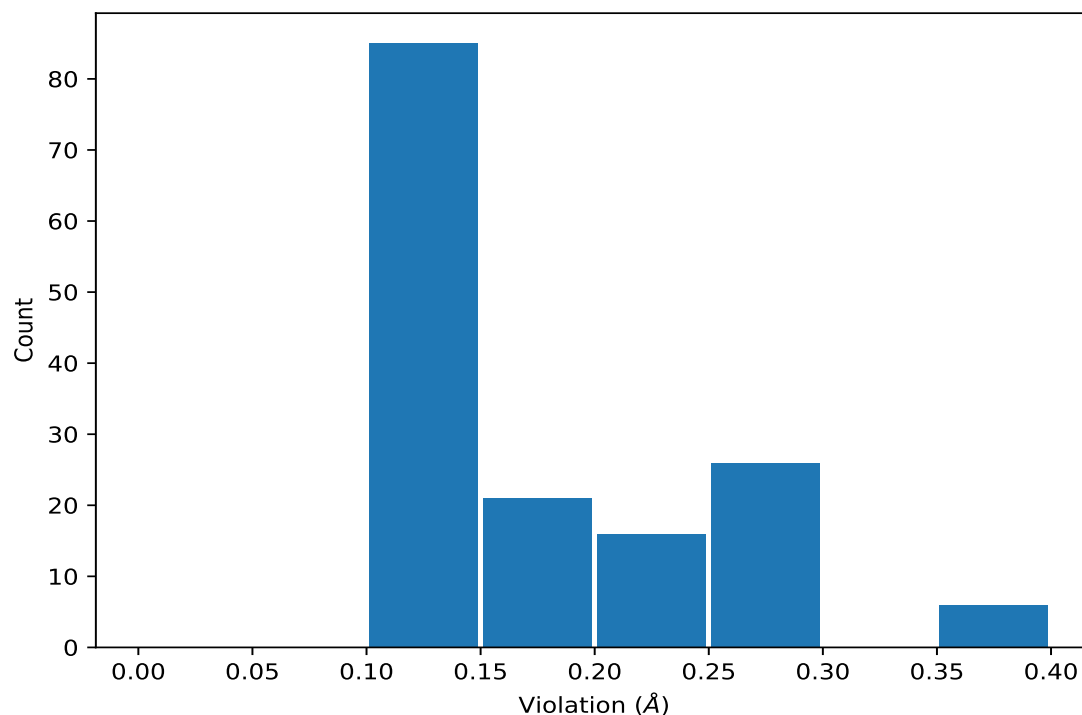
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,770)	1:208:A:MET:HG3	1:209:A:ASN:H	2	0.19	0.01	0.19
(1,699)	1:187:A:VAL:H	1:206:A:TRP:HE1	2	0.18	0.06	0.18
(1,90)	1:189:A:ILE:HD11	1:190:A:ARG:H	2	0.15	0.02	0.15
(1,90)	1:189:A:ILE:HD12	1:190:A:ARG:H	2	0.15	0.02	0.15
(1,90)	1:189:A:ILE:HD13	1:190:A:ARG:H	2	0.15	0.02	0.15
(1,601)	1:193:A:MET:H	1:202:A:ASP:H	2	0.15	0.03	0.15
(1,865)	1:251:A:ASP:HB2	1:252:A:SER:H	2	0.15	0.0	0.15
(1,865)	1:251:A:ASP:HB3	1:252:A:SER:H	2	0.15	0.0	0.15
(1,233)	1:207:A:ASN:H	1:210:A:GLU:HA	2	0.12	0.0	0.12
(1,580)	1:192:A:ASP:HA	1:202:A:ASP:H	2	0.12	0.0	0.12
(1,860)	1:246:A:GLU:HG2	1:247:A:SER:H	2	0.11	0.01	0.11
(1,860)	1:246:A:GLU:HG3	1:247:A:SER:H	2	0.11	0.01	0.11

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

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its 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)
(1,704)	1:176:A:ILE:H	1:176:A:ILE:HG12	15	0.39
(1,704)	1:176:A:ILE:H	1:176:A:ILE:HG13	15	0.39
(1,564)	1:250:A:THR:H	1:250:A:THR:HB	18	0.37
(1,563)	1:250:A:THR:H	1:250:A:THR:HG21	12	0.36
(1,563)	1:250:A:THR:H	1:250:A:THR:HG22	12	0.36
(1,563)	1:250:A:THR:H	1:250:A:THR:HG23	12	0.36
(1,566)	1:250:A:THR:HB	1:251:A:ASP:H	10	0.3
(1,871)	1:254:A:LEU:HB2	1:255:A:GLU:H	20	0.28
(1,871)	1:254:A:LEU:HB3	1:255:A:GLU:H	20	0.28
(1,850)	1:243:A:GLN:H	1:243:A:GLN:HG2	20	0.28
(1,850)	1:243:A:GLN:H	1:243:A:GLN:HG3	20	0.28
(1,850)	1:243:A:GLN:H	1:243:A:GLN:HG2	17	0.27
(1,850)	1:243:A:GLN:H	1:243:A:GLN:HG3	17	0.27
(1,850)	1:243:A:GLN:H	1:243:A:GLN:HG2	19	0.27
(1,850)	1:243:A:GLN:H	1:243:A:GLN:HG3	19	0.27
(1,850)	1:243:A:GLN:H	1:243:A:GLN:HG2	4	0.26
(1,850)	1:243:A:GLN:H	1:243:A:GLN:HG3	4	0.26
(1,864)	1:249:A:PRO:HD2	1:250:A:THR:H	3	0.25
(1,864)	1:249:A:PRO:HD3	1:250:A:THR:H	3	0.25
(1,864)	1:249:A:PRO:HD2	1:250:A:THR:H	7	0.25
(1,864)	1:249:A:PRO:HD3	1:250:A:THR:H	7	0.25
(1,864)	1:249:A:PRO:HD2	1:250:A:THR:H	13	0.25
(1,864)	1:249:A:PRO:HD3	1:250:A:THR:H	13	0.25
(1,864)	1:249:A:PRO:HD2	1:250:A:THR:H	14	0.25
(1,864)	1:249:A:PRO:HD3	1:250:A:THR:H	14	0.25
(1,864)	1:249:A:PRO:HD2	1:250:A:THR:H	15	0.25
(1,864)	1:249:A:PRO:HD3	1:250:A:THR:H	15	0.25
(1,864)	1:249:A:PRO:HD2	1:250:A:THR:H	16	0.25
(1,864)	1:249:A:PRO:HD3	1:250:A:THR:H	16	0.25
(1,864)	1:249:A:PRO:HD2	1:250:A:THR:H	17	0.25
(1,864)	1:249:A:PRO:HD3	1:250:A:THR:H	17	0.25
(1,237)	1:209:A:ASN:H	1:209:A:ASN:HB2	20	0.25
(1,699)	1:187:A:VAL:H	1:206:A:TRP:HE1	11	0.24
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG2	11	0.23
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG3	11	0.23
(1,65)	1:186:A:LEU:H	1:209:A:ASN:HD21	20	0.23
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG2	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG3	10	0.22
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG2	17	0.21
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG3	17	0.21
(1,270)	1:211:A:LYS:HD2	1:212:A:LEU:H	14	0.21
(1,270)	1:211:A:LYS:HD3	1:212:A:LEU:H	14	0.21
(1,770)	1:208:A:MET:HG2	1:209:A:ASN:H	17	0.2
(1,770)	1:208:A:MET:HG3	1:209:A:ASN:H	17	0.2
(1,415)	1:231:A:LEU:HB2	1:232:A:THR:H	13	0.2
(1,270)	1:211:A:LYS:HD2	1:212:A:LEU:H	16	0.2
(1,270)	1:211:A:LYS:HD3	1:212:A:LEU:H	16	0.2
(1,18)	1:173:A:PRO:HA	1:174:A:ALA:H	6	0.2
(1,234)	1:207:A:ASN:H	1:207:A:ASN:HD21	4	0.19
(1,770)	1:208:A:MET:HG2	1:209:A:ASN:H	7	0.18
(1,770)	1:208:A:MET:HG3	1:209:A:ASN:H	7	0.18
(1,728)	1:189:A:ILE:HG12	1:190:A:ARG:H	2	0.18
(1,728)	1:189:A:ILE:HG13	1:190:A:ARG:H	2	0.18
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG2	1	0.18
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG3	1	0.18
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG2	8	0.18
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG3	8	0.18
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG2	9	0.18
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG3	9	0.18
(1,270)	1:211:A:LYS:HD2	1:212:A:LEU:H	18	0.18
(1,270)	1:211:A:LYS:HD3	1:212:A:LEU:H	18	0.18
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG2	19	0.17
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG3	19	0.17
(1,601)	1:193:A:MET:H	1:202:A:ASP:H	2	0.17
(1,90)	1:189:A:ILE:HD11	1:190:A:ARG:H	7	0.17
(1,90)	1:189:A:ILE:HD12	1:190:A:ARG:H	7	0.17
(1,90)	1:189:A:ILE:HD13	1:190:A:ARG:H	7	0.17
(1,22)	1:176:A:ILE:H	1:176:A:ILE:HB	7	0.17
(1,102)	1:191:A:LEU:H	1:191:A:LEU:HG	11	0.16
(1,865)	1:251:A:ASP:HB2	1:252:A:SER:H	5	0.15
(1,865)	1:251:A:ASP:HB3	1:252:A:SER:H	5	0.15
(1,728)	1:189:A:ILE:HG12	1:190:A:ARG:H	9	0.15
(1,728)	1:189:A:ILE:HG13	1:190:A:ARG:H	9	0.15
(1,566)	1:250:A:THR:HB	1:251:A:ASP:H	18	0.15
(1,234)	1:207:A:ASN:H	1:207:A:ASN:HD21	1	0.15
(1,102)	1:191:A:LEU:H	1:191:A:LEU:HG	14	0.15
(1,865)	1:251:A:ASP:HB2	1:252:A:SER:H	17	0.14
(1,865)	1:251:A:ASP:HB3	1:252:A:SER:H	17	0.14
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG2	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG3	4	0.14
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG2	15	0.14
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG3	15	0.14
(1,234)	1:207:A:ASN:H	1:207:A:ASN:HD21	9	0.14
(1,861)	1:247:A:SER:H	1:248:A:TYR:HB2	4	0.13
(1,861)	1:247:A:SER:H	1:248:A:TYR:HB3	4	0.13
(1,728)	1:189:A:ILE:HG12	1:190:A:ARG:H	6	0.13
(1,728)	1:189:A:ILE:HG13	1:190:A:ARG:H	6	0.13
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG2	13	0.13
(1,685)	1:207:A:ASN:HD21	1:210:A:GLU:HG3	13	0.13
(1,234)	1:207:A:ASN:H	1:207:A:ASN:HD21	13	0.13
(1,234)	1:207:A:ASN:H	1:207:A:ASN:HD21	15	0.13
(1,90)	1:189:A:ILE:HD11	1:190:A:ARG:H	20	0.13
(1,90)	1:189:A:ILE:HD12	1:190:A:ARG:H	20	0.13
(1,90)	1:189:A:ILE:HD13	1:190:A:ARG:H	20	0.13
(1,860)	1:246:A:GLU:HG2	1:247:A:SER:H	14	0.12
(1,860)	1:246:A:GLU:HG3	1:247:A:SER:H	14	0.12
(1,728)	1:189:A:ILE:HG12	1:190:A:ARG:H	12	0.12
(1,728)	1:189:A:ILE:HG13	1:190:A:ARG:H	12	0.12
(1,728)	1:189:A:ILE:HG12	1:190:A:ARG:H	15	0.12
(1,728)	1:189:A:ILE:HG13	1:190:A:ARG:H	15	0.12
(1,726)	1:189:A:ILE:H	1:191:A:LEU:HD11	10	0.12
(1,726)	1:189:A:ILE:H	1:191:A:LEU:HD12	10	0.12
(1,726)	1:189:A:ILE:H	1:191:A:LEU:HD13	10	0.12
(1,726)	1:189:A:ILE:H	1:191:A:LEU:HD21	10	0.12
(1,726)	1:189:A:ILE:H	1:191:A:LEU:HD22	10	0.12
(1,726)	1:189:A:ILE:H	1:191:A:LEU:HD23	10	0.12
(1,612)	1:253:A:ILE:H	1:253:A:ILE:HB	13	0.12
(1,601)	1:193:A:MET:H	1:202:A:ASP:H	17	0.12
(1,580)	1:192:A:ASP:HA	1:202:A:ASP:H	11	0.12
(1,565)	1:249:A:PRO:HG2	1:250:A:THR:H	3	0.12
(1,565)	1:249:A:PRO:HG3	1:250:A:THR:H	3	0.12
(1,565)	1:249:A:PRO:HG2	1:250:A:THR:H	16	0.12
(1,565)	1:249:A:PRO:HG3	1:250:A:THR:H	16	0.12
(1,246)	1:185:A:VAL:H	1:209:A:ASN:H	20	0.12
(1,233)	1:207:A:ASN:H	1:210:A:GLU:HA	9	0.12
(1,233)	1:207:A:ASN:H	1:210:A:GLU:HA	10	0.12
(1,212)	1:188:A:PRO:HB2	1:204:A:PHE:H	19	0.12
(1,71)	1:187:A:VAL:H	1:206:A:TRP:HA	11	0.12
(1,737)	1:191:A:LEU:H	1:202:A:ASP:HB2	16	0.11
(1,737)	1:191:A:LEU:H	1:202:A:ASP:HB3	16	0.11
(1,699)	1:187:A:VAL:H	1:206:A:TRP:HE1	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,580)	1:192:A:ASP:HA	1:202:A:ASP:H	19	0.11
(1,565)	1:249:A:PRO:HG2	1:250:A:THR:H	7	0.11
(1,565)	1:249:A:PRO:HG3	1:250:A:THR:H	7	0.11
(1,565)	1:249:A:PRO:HG2	1:250:A:THR:H	13	0.11
(1,565)	1:249:A:PRO:HG3	1:250:A:THR:H	13	0.11
(1,565)	1:249:A:PRO:HG2	1:250:A:THR:H	14	0.11
(1,565)	1:249:A:PRO:HG3	1:250:A:THR:H	14	0.11
(1,565)	1:249:A:PRO:HG2	1:250:A:THR:H	15	0.11
(1,565)	1:249:A:PRO:HG3	1:250:A:THR:H	15	0.11
(1,565)	1:249:A:PRO:HG2	1:250:A:THR:H	17	0.11
(1,565)	1:249:A:PRO:HG3	1:250:A:THR:H	17	0.11
(1,516)	1:189:A:ILE:HD11	1:244:A:GLN:H	10	0.11
(1,516)	1:189:A:ILE:HD12	1:244:A:GLN:H	10	0.11
(1,516)	1:189:A:ILE:HD13	1:244:A:GLN:H	10	0.11
(1,425)	1:232:A:THR:HG21	1:233:A:PHE:H	13	0.11
(1,425)	1:232:A:THR:HG22	1:233:A:PHE:H	13	0.11
(1,425)	1:232:A:THR:HG23	1:233:A:PHE:H	13	0.11
(1,301)	1:217:A:MET:H	1:217:A:MET:HG2	18	0.11
(1,301)	1:217:A:MET:H	1:217:A:MET:HG3	18	0.11
(1,270)	1:211:A:LYS:HD2	1:212:A:LEU:H	10	0.11
(1,270)	1:211:A:LYS:HD3	1:212:A:LEU:H	10	0.11
(1,234)	1:207:A:ASN:H	1:207:A:ASN:HD21	8	0.11
(1,102)	1:191:A:LEU:H	1:191:A:LEU:HG	15	0.11
(1,102)	1:191:A:LEU:H	1:191:A:LEU:HG	16	0.11
(1,102)	1:191:A:LEU:H	1:191:A:LEU:HG	18	0.11
(1,866)	1:251:A:ASP:HB2	1:253:A:ILE:H	9	0.1
(1,866)	1:251:A:ASP:HB3	1:253:A:ILE:H	9	0.1
(1,860)	1:246:A:GLU:HG2	1:247:A:SER:H	5	0.1
(1,860)	1:246:A:GLU:HG3	1:247:A:SER:H	5	0.1
(1,850)	1:243:A:GLN:H	1:243:A:GLN:HG2	12	0.1
(1,850)	1:243:A:GLN:H	1:243:A:GLN:HG3	12	0.1
(1,728)	1:189:A:ILE:HG12	1:190:A:ARG:H	5	0.1
(1,728)	1:189:A:ILE:HG13	1:190:A:ARG:H	5	0.1

10 Dihedral-angle violation analysis [i](#)

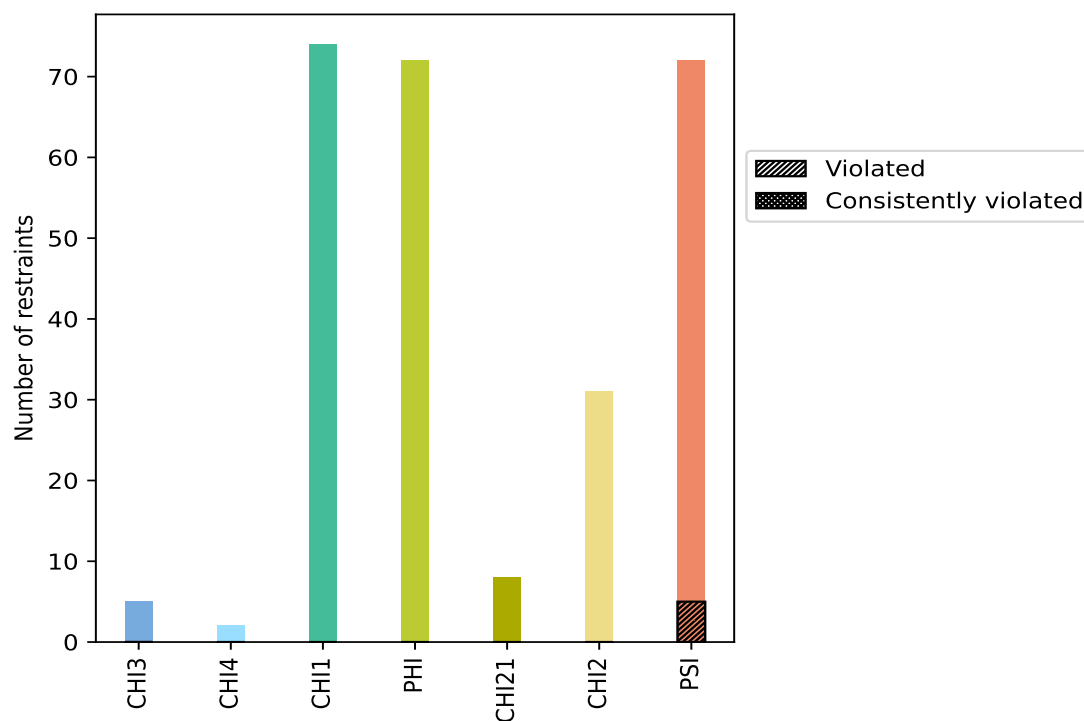
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
CHI3	5	1.9	0	0.0	0.0	0	0.0	0.0
CHI4	2	0.8	0	0.0	0.0	0	0.0	0.0
CHI1	74	28.0	0	0.0	0.0	0	0.0	0.0
PHI	72	27.3	0	0.0	0.0	0	0.0	0.0
CHI21	8	3.0	0	0.0	0.0	0	0.0	0.0
CHI2	31	11.7	0	0.0	0.0	0	0.0	0.0
PSI	72	27.3	5	6.9	1.9	0	0.0	0.0
Total	264	100.0	5	1.9	1.9	0	0.0	0.0

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



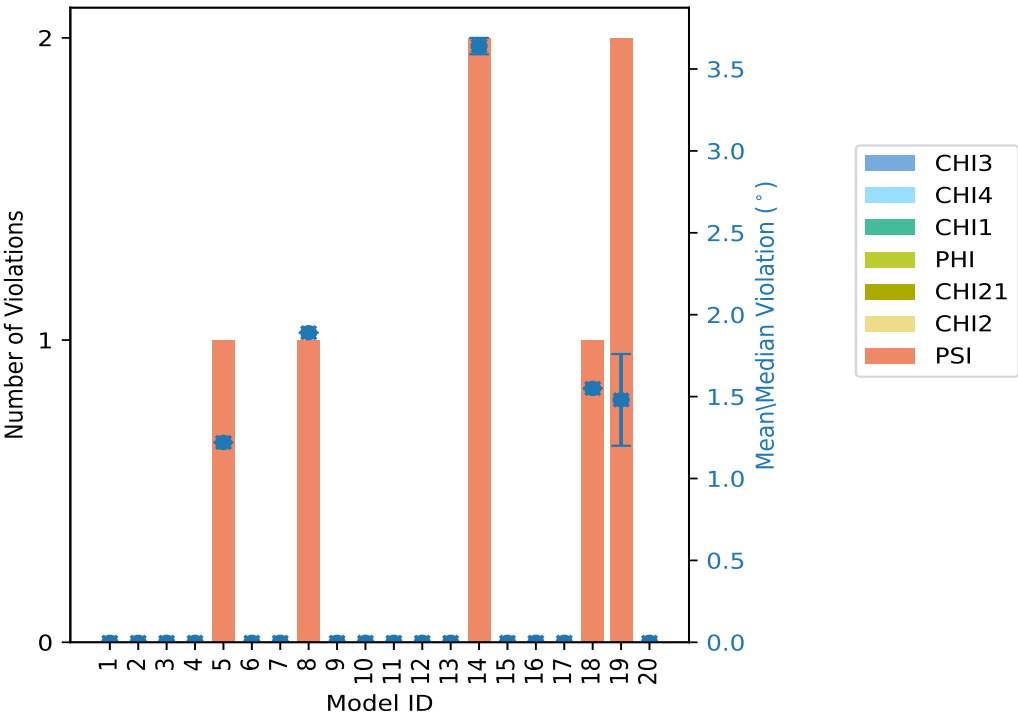
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations								Mean (°)	Max (°)	SD (°)	Median (°)
	CHI3	CHI4	CHI1	PHI	CHI21	CHI2	PSI	Total				
1	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	0	0	1	1	1.22	1.22	0.0	1.22
6	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0	0	0	1	1	1.89	1.89	0.0	1.89
9	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0	0	0	2	2	3.64	3.69	0.05	3.64
15	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0	0	0	1	1	1.55	1.55	0.0	1.55
19	0	0	0	0	0	0	2	2	1.48	1.75	0.28	1.48
20	0	0	0	0	0	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral 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

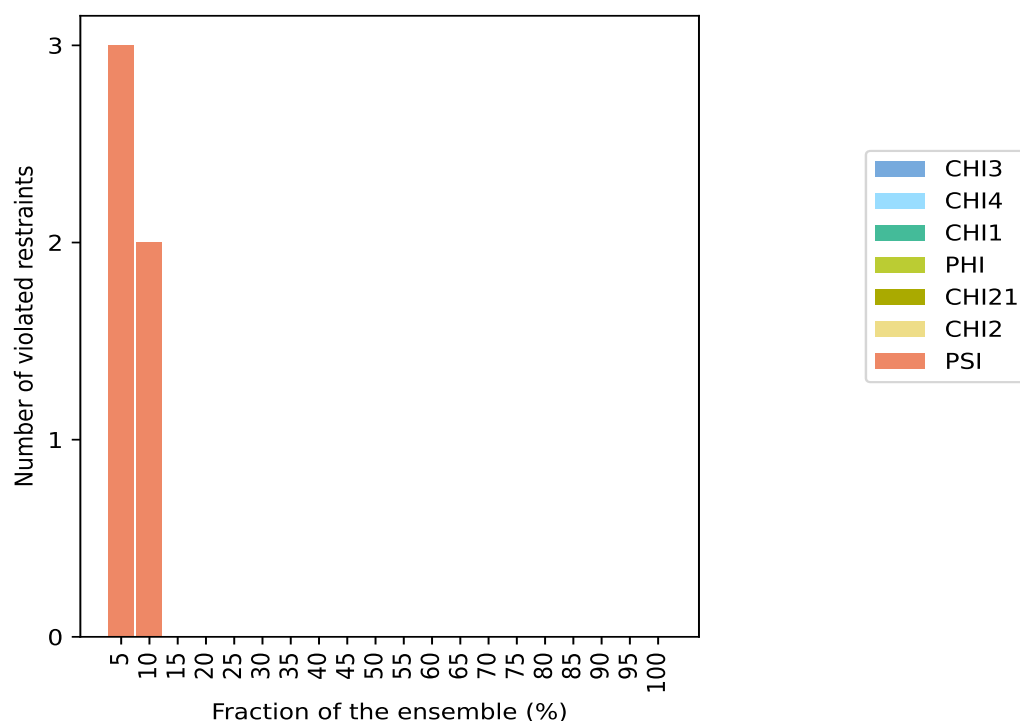
10.3 Dihedral-angle violation statistics for the ensemble

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints								Fraction of the ensemble	
CHI3	CHI4	CHI1	PHI	CHI21	CHI2	PSI	Total	Count ¹	%
0	0	0	0	0	0	3	3	1	5.0
0	0	0	0	0	0	2	2	2	10.0
0	0	0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	0	0	20	100.0

¹ Number of models with violations

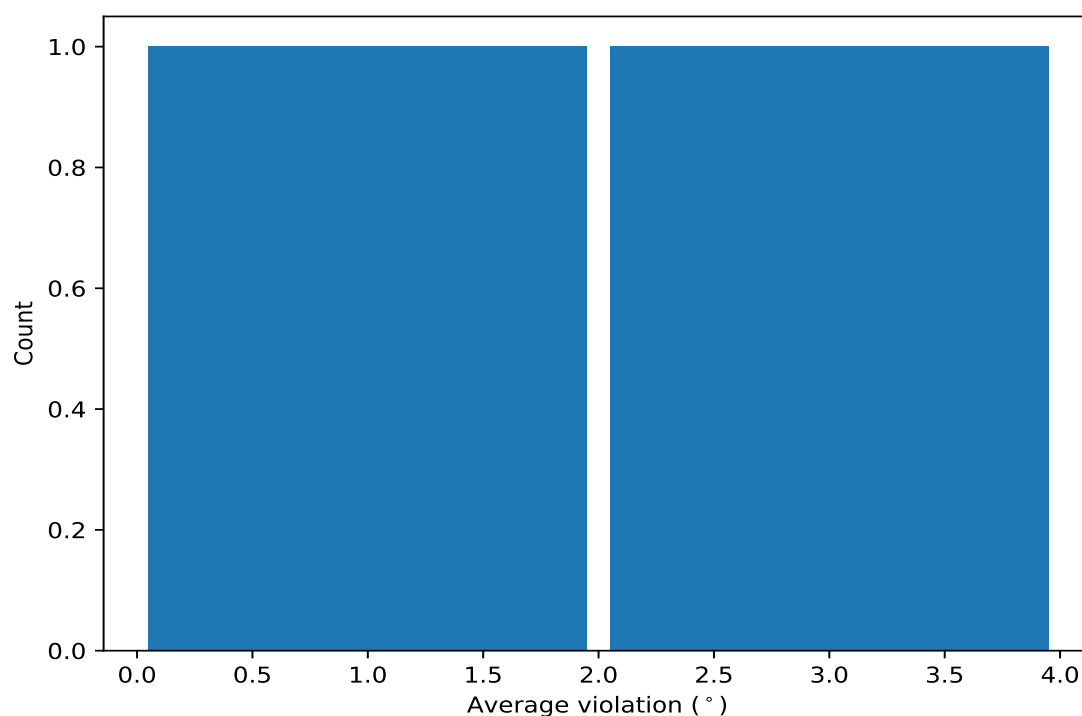
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

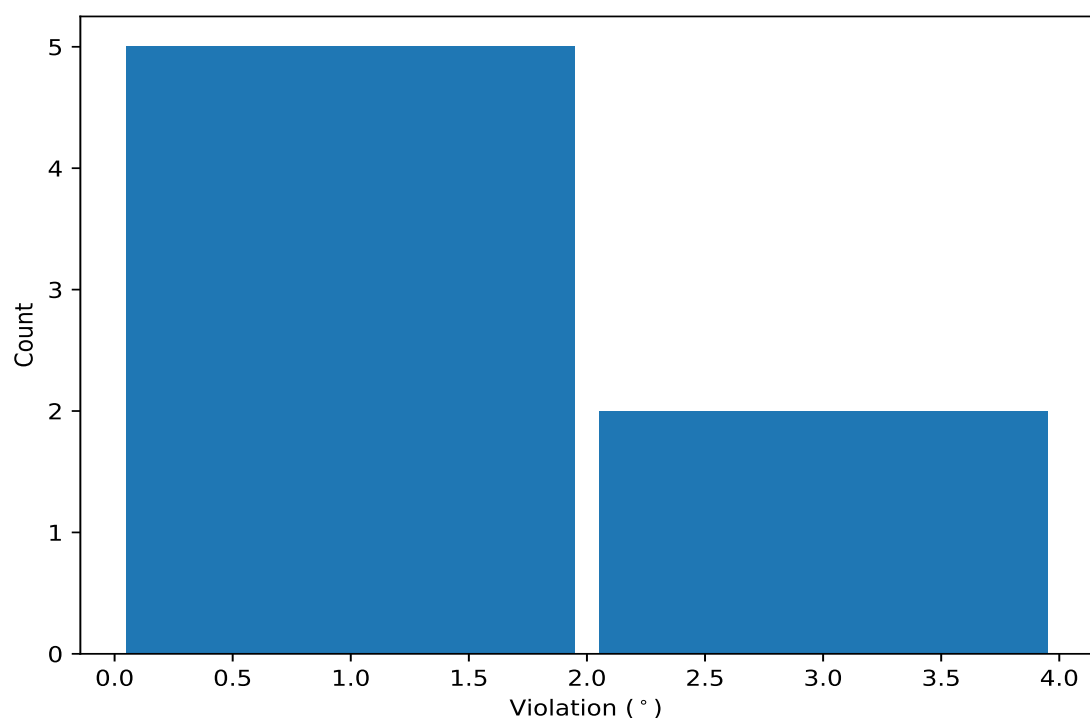
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,19)	1:184:A:GLU:N	1:184:A:GLU:CA	1:184:A:GLU:C	1:185:A:VAL:N	2	2.79	0.9	2.79
(1,137)	1:254:A:LEU:N	1:254:A:LEU:CA	1:254:A:LEU:C	1:255:A:GLU:N	2	1.38	0.17	1.38

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,19)	1:184:A:GLU:N	1:184:A:GLU:CA	1:184:A:GLU:C	1:185:A:VAL:N	14	3.69
(1,13)	1:179:A:ASN:N	1:179:A:ASN:CA	1:179:A:ASN:C	1:180:A:ALA:N	14	3.58
(1,19)	1:184:A:GLU:N	1:184:A:GLU:CA	1:184:A:GLU:C	1:185:A:VAL:N	8	1.89
(1,9)	1:177:A:HIS:N	1:177:A:HIS:CA	1:177:A:HIS:C	1:178:A:GLU:N	19	1.75
(1,137)	1:254:A:LEU:N	1:254:A:LEU:CA	1:254:A:LEU:C	1:255:A:GLU:N	18	1.55
(1,137)	1:254:A:LEU:N	1:254:A:LEU:CA	1:254:A:LEU:C	1:255:A:GLU:N	5	1.22
(1,131)	1:251:A:ASP:N	1:251:A:ASP:CA	1:251:A:ASP:C	1:252:A:SER:N	19	1.2