



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2NBU  
BMRB ID : 25825  
Title : Solution structure of the Rad23 ubiquitin-like (UBL) domain  
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Deposited on : 2016-03-12

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<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.40

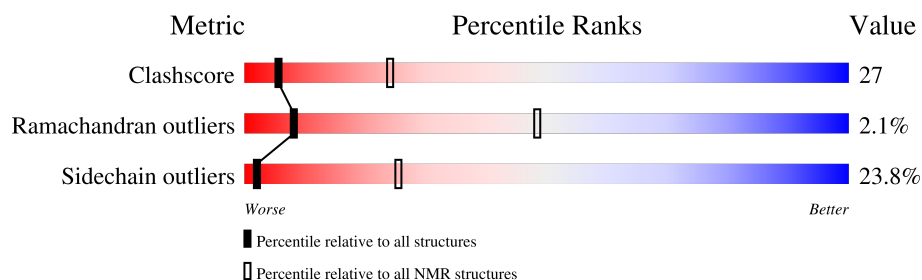
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 95%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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  $\geq 3$ , 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	99	<div> <div></div> <div>36%</div> <div>31%</div> <div>5%</div> <div>6%</div> <div>21%</div> </div>

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:2-A:73 (72)	0.25	2

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 3 clusters and 3 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1247 atoms, of which 641 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called UV excision repair protein RAD23.

Mol	Chain	Residues	Atoms						Trace
1	A	78	Total	C	H	N	O	S	0
			1247	383	641	97	122	4	

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ASP	-	expression tag	UNP P32628
A	80	PRO	-	expression tag	UNP P32628
A	81	ASN	-	expression tag	UNP P32628
A	82	SER	-	expression tag	UNP P32628
A	83	SER	-	expression tag	UNP P32628
A	84	SER	-	expression tag	UNP P32628
A	85	VAL	-	expression tag	UNP P32628
A	86	ASP	-	expression tag	UNP P32628
A	87	LYS	-	expression tag	UNP P32628
A	88	LEU	-	expression tag	UNP P32628
A	89	ALA	-	expression tag	UNP P32628
A	90	ALA	-	expression tag	UNP P32628
A	91	ALA	-	expression tag	UNP P32628
A	92	LEU	-	expression tag	UNP P32628
A	93	GLU	-	expression tag	UNP P32628
A	94	HIS	-	expression tag	UNP P32628
A	95	HIS	-	expression tag	UNP P32628
A	96	HIS	-	expression tag	UNP P32628
A	97	HIS	-	expression tag	UNP P32628
A	98	HIS	-	expression tag	UNP P32628
A	99	HIS	-	expression tag	UNP P32628



## 5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
TALOS	structure solution	
TALOS	refinement	
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	
ProcheckNMR	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	1177
Number of shifts mapped to atoms	1003
Number of unparsed shifts	0
Number of shifts with mapping errors	174
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	95%

## 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	558	584	584	31±3
All	All	11160	11680	11680	617

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 27.

5 of 124 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ALA:HB1	1:A:37:CYS:O	0.88	1.68	20	20
1:A:35:ILE:HD11	1:A:37:CYS:SG	0.86	2.11	3	2
1:A:45:ILE:N	1:A:45:ILE:HD13	0.73	1.99	5	20
1:A:25:LEU:C	1:A:25:LEU:HD13	0.71	2.06	14	14
1:A:6:PHE:CE2	1:A:44:LEU:HD11	0.71	2.19	17	9

### 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	72/99 (73%)	63±1 (87±1%)	8±1 (10±1%)	2±1 (2±1%)	8	48
All	All	1440/1980 (73%)	1259 (87%)	151 (10%)	30 (2%)	8	48

All 5 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	51	LEU	17
1	A	66	ASP	9
1	A	24	ILE	2
1	A	36	SER	1
1	A	11	LYS	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	68/92 (74%)	52±2 (76±3%)	16±2 (24±3%)	2	26
All	All	1360/1840 (74%)	1037 (76%)	323 (24%)	2	25

5 of 39 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	2	VAL	20
1	A	18	LEU	20
1	A	27	THR	20
1	A	42	ILE	20
1	A	45	ILE	20

### 6.3.3 RNA ⓘ

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

The completeness of assignment taking into account all chemical shift lists is 95% for the well-defined parts and 95% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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

Total number of shifts	1177
Number of shifts mapped to atoms	1003
Number of unparsed shifts	0
Number of shifts with mapping errors	174
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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 174) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	79	ASP	H	8.28	0	1
1	A	79	ASP	HA	4.878	0	1
1	A	79	ASP	HB2	2.774	0	2
1	A	79	ASP	HB3	2.574	0	2
1	A	79	ASP	C	175.013	0	1
1	A	79	ASP	CA	52.087	0	1
1	A	79	ASP	CB	41.205	0	1
1	A	79	ASP	N	124.382	0	1
1	A	80	PRO	HA	4.423	0	1
1	A	80	PRO	HB2	2.3	0	2
1	A	80	PRO	HB3	1.966	0	2
1	A	80	PRO	HG2	2.015	0	2
1	A	80	PRO	HG3	2.015	0	2
1	A	80	PRO	HD2	3.889	0	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	80	PRO	HD3	3.835	0	2
1	A	80	PRO	C	177.067	0	1
1	A	80	PRO	CA	63.802	0	1
1	A	80	PRO	CB	32.021	0	1
1	A	80	PRO	CG	26.959	0	1
1	A	80	PRO	CD	50.583	0	1
1	A	81	ASN	H	8.52	0	1
1	A	81	ASN	HA	4.736	0	1
1	A	81	ASN	HB2	2.863	0	2
1	A	81	ASN	HB3	2.789	0	2
1	A	81	ASN	HD21	6.95	0	2
1	A	81	ASN	HD22	7.756	0	2
1	A	81	ASN	C	175.519	0	1
1	A	81	ASN	CA	53.396	0	1
1	A	81	ASN	CB	38.771	0	1
1	A	81	ASN	N	117.478	0	1
1	A	81	ASN	ND2	113.877	0	1
1	A	82	SER	H	8.023	0	1
1	A	82	SER	HA	4.402	0	1
1	A	82	SER	HB2	3.875	0	2
1	A	82	SER	HB3	3.875	0	2
1	A	82	SER	C	174.653	0	1
1	A	82	SER	CA	58.739	0	1
1	A	82	SER	CB	63.802	0	1
1	A	82	SER	N	115.818	0	1
1	A	83	SER	H	8.331	0	1
1	A	83	SER	HA	4.491	0	1
1	A	83	SER	HB2	3.894	0	2
1	A	83	SER	HB3	3.894	0	2
1	A	83	SER	C	174.662	0	1
1	A	83	SER	CA	58.458	0	1
1	A	83	SER	CB	63.802	0	1
1	A	83	SER	N	117.494	0	1
1	A	84	SER	H	8.283	0	1
1	A	84	SER	C	174.886	0	1
1	A	84	SER	CA	58.461	0	1
1	A	84	SER	CB	63.523	0	1
1	A	84	SER	N	117.712	0	1
1	A	85	VAL	H	8.034	0	1
1	A	85	VAL	HA	4.062	0	1
1	A	85	VAL	HB	2.098	0	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	85	VAL	HG11	0.931	0	2
1	A	85	VAL	HG12	0.931	0	2
1	A	85	VAL	HG13	0.931	0	2
1	A	85	VAL	HG21	0.938	0	2
1	A	85	VAL	HG22	0.938	0	2
1	A	85	VAL	HG23	0.938	0	2
1	A	85	VAL	C	176.142	0	1
1	A	85	VAL	CA	62.889	0	1
1	A	85	VAL	CB	32.518	0	1
1	A	85	VAL	CG1	20.885	0	2
1	A	85	VAL	CG2	20.483	0	2
1	A	85	VAL	N	121.117	0	1
1	A	86	ASP	H	8.269	0	1
1	A	86	ASP	HA	4.565	0	1
1	A	86	ASP	HB2	2.713	0	2
1	A	86	ASP	HB3	2.612	0	2
1	A	86	ASP	C	176.766	0	1
1	A	86	ASP	CA	54.546	0	1
1	A	86	ASP	CB	40.752	0	1
1	A	86	ASP	N	123.029	0	1
1	A	87	LYS	H	8.172	0	1
1	A	87	LYS	HA	4.196	0	1
1	A	87	LYS	HB2	1.858	0	2
1	A	87	LYS	HB3	1.773	0	2
1	A	87	LYS	HG2	1.476	0	2
1	A	87	LYS	HG3	1.417	0	2
1	A	87	LYS	HD2	1.664	0	2
1	A	87	LYS	HD3	1.664	0	2
1	A	87	LYS	HE2	2.986	0	2
1	A	87	LYS	HE3	2.986	0	2
1	A	87	LYS	C	177.35	0	1
1	A	87	LYS	CA	57.052	0	1
1	A	87	LYS	CB	32.583	0	1
1	A	87	LYS	CG	24.709	0	1
1	A	87	LYS	CD	28.927	0	1
1	A	87	LYS	CE	41.865	0	1
1	A	87	LYS	N	121.906	0	1
1	A	88	LEU	H	8.101	0	1
1	A	88	LEU	HA	4.261	0	1
1	A	88	LEU	HB2	1.713	0	2
1	A	88	LEU	HB3	1.592	0	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	88	LEU	HG	1.62	0	1
1	A	88	LEU	HD11	0.909	0	2
1	A	88	LEU	HD12	0.909	0	2
1	A	88	LEU	HD13	0.909	0	2
1	A	88	LEU	HD21	0.851	0	2
1	A	88	LEU	HD22	0.851	0	2
1	A	88	LEU	HD23	0.851	0	2
1	A	88	LEU	C	177.798	0	1
1	A	88	LEU	CA	55.646	0	1
1	A	88	LEU	CB	41.583	0	1
1	A	88	LEU	CG	26.959	0	1
1	A	88	LEU	CD1	24.709	0	2
1	A	88	LEU	CD2	23.302	0	2
1	A	88	LEU	N	121.846	0	1
1	A	89	ALA	H	8.001	0	1
1	A	89	ALA	HA	4.189	0	1
1	A	89	ALA	HB1	1.395	0	1
1	A	89	ALA	HB2	1.395	0	1
1	A	89	ALA	HB3	1.395	0	1
1	A	89	ALA	C	178.382	0	1
1	A	89	ALA	CA	53.389	0	1
1	A	89	ALA	CB	18.521	0	1
1	A	89	ALA	N	123.573	0	1
1	A	90	ALA	H	8.023	0	1
1	A	90	ALA	HA	4.232	0	1
1	A	90	ALA	HB1	1.395	0	1
1	A	90	ALA	HB2	1.395	0	1
1	A	90	ALA	HB3	1.395	0	1
1	A	90	ALA	C	178.119	0	1
1	A	90	ALA	CA	52.833	0	1
1	A	90	ALA	CB	19.084	0	1
1	A	90	ALA	N	121.852	0	1
1	A	91	ALA	H	7.95	0	1
1	A	91	ALA	HA	4.232	0	1
1	A	91	ALA	HB1	1.394	0	1
1	A	91	ALA	HB2	1.394	0	1
1	A	91	ALA	HB3	1.394	0	1
1	A	91	ALA	C	178.1	0	1
1	A	91	ALA	CA	52.552	0	1
1	A	91	ALA	CB	18.802	0	1
1	A	91	ALA	N	121.781	0	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	92	LEU	H	7.928	0	1
1	A	92	LEU	HA	4.24	0	1
1	A	92	LEU	HB2	1.644	0	2
1	A	92	LEU	HB3	1.519	0	2
1	A	92	LEU	HG	1.641	0	1
1	A	92	LEU	HD11	0.889	0	2
1	A	92	LEU	HD12	0.889	0	2
1	A	92	LEU	HD13	0.889	0	2
1	A	92	LEU	HD21	0.835	0	2
1	A	92	LEU	HD22	0.835	0	2
1	A	92	LEU	HD23	0.835	0	2
1	A	92	LEU	C	177.584	0	1
1	A	92	LEU	CA	55.109	0	1
1	A	92	LEU	CB	42.159	0	1
1	A	92	LEU	CG	26.676	0	1
1	A	92	LEU	CD1	24.987	0	2
1	A	92	LEU	CD2	23.298	0	2
1	A	92	LEU	N	120.154	0	1
1	A	93	GLU	H	8.061	0	1
1	A	93	GLU	HA	4.16	0	1
1	A	93	GLU	HB2	1.897	0	2
1	A	93	GLU	HB3	1.897	0	2
1	A	93	GLU	HG2	2.205	0	2
1	A	93	GLU	HG3	2.121	0	2
1	A	93	GLU	C	176.308	0	1
1	A	93	GLU	CA	56.771	0	1
1	A	93	GLU	CB	30.052	0	1
1	A	93	GLU	CG	35.958	0	1
1	A	93	GLU	N	120.382	0	1
1	A	94	HIS	H	8.18	0	1
1	A	94	HIS	HA	4.565	0	1
1	A	94	HIS	HB2	3.057	0	2
1	A	94	HIS	HB3	2.98	0	2
1	A	94	HIS	C	174.955	0	1
1	A	94	HIS	CA	55.927	0	1
1	A	94	HIS	CB	30.333	0	1
1	A	94	HIS	N	119.338	0	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
$^{13}\text{C}_\alpha$	94	$-0.01 \pm 0.07$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	91	$0.12 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	94	$-0.05 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	90	$0.42 \pm 0.35$	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 95%, i.e. 923 atoms were assigned a chemical shift out of a possible 973. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	359/359 (100%)	145/145 (100%)	144/144 (100%)	70/70 (100%)
Sidechain	549/575 (95%)	373/373 (100%)	170/186 (91%)	6/16 (38%)
Aromatic	15/39 (38%)	15/19 (79%)	0/20 (0%)	0/0 (—%)
Overall	923/973 (95%)	533/537 (99%)	314/350 (90%)	76/86 (88%)

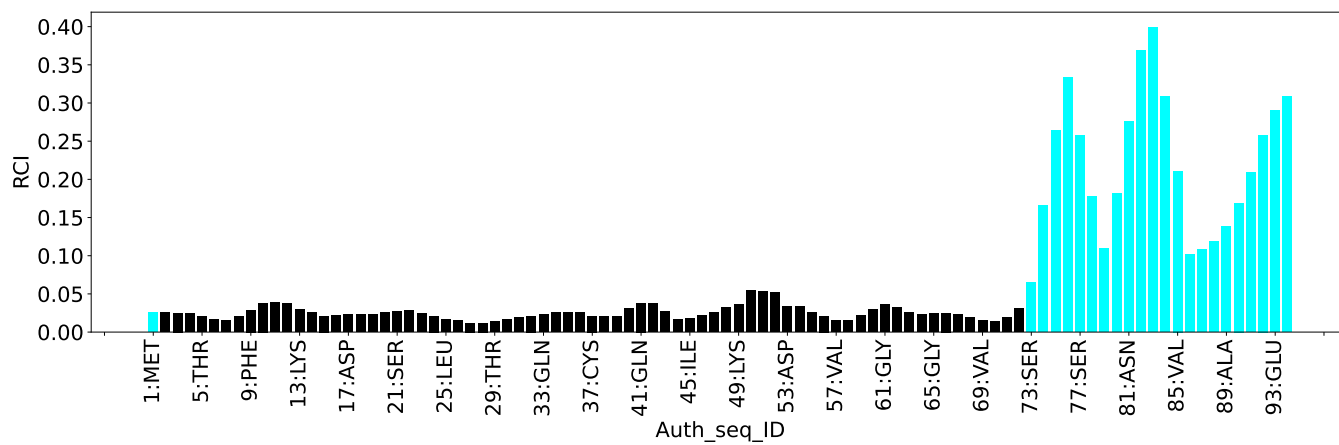
### 7.1.4 Statistically unusual chemical shifts [i](#)

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	1362
Intra-residue ( $ i-j =0$ )	556
Sequential ( $ i-j =1$ )	268
Medium range ( $ i-j >1$ and $ i-j <5$ )	197
Long range ( $ i-j \geq 5$ )	293
Inter-chain	0
Hydrogen bond restraints	48
Disulfide bond restraints	0
Total dihedral-angle restraints	137
Number of unmapped restraints	0
Number of restraints per residue	15.1
Number of long range restraints per residue <sup>1</sup>	3.3

<sup>1</sup>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)	30.9	0.2
0.2-0.5 (Medium)	2.8	0.35
>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)	9.6	3.26
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

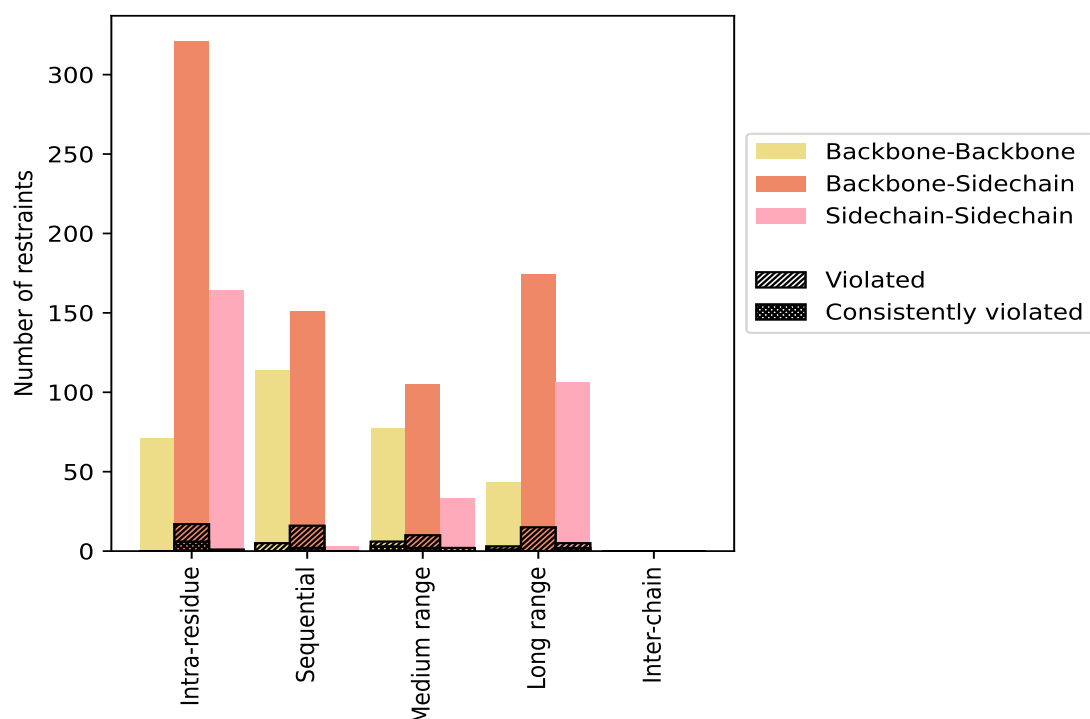
### 9.1 Summary of distance violations ⓘ

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	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>556</b>	<b>40.8</b>	<b>18</b>	<b>3.2</b>	<b>1.3</b>	<b>6</b>	<b>1.1</b>	<b>0.4</b>
Backbone-Backbone	71	5.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	321	23.6	17	5.3	1.2	6	1.9	0.4
Sidechain-Sidechain	164	12.0	1	0.6	0.1	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>268</b>	<b>19.7</b>	<b>21</b>	<b>7.8</b>	<b>1.5</b>	<b>2</b>	<b>0.7</b>	<b>0.1</b>
Backbone-Backbone	114	8.4	5	4.4	0.4	0	0.0	0.0
Backbone-Sidechain	151	11.1	16	10.6	1.2	2	1.3	0.1
Sidechain-Sidechain	3	0.2	0	0.0	0.0	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>197</b>	<b>14.5</b>	<b>16</b>	<b>8.1</b>	<b>1.2</b>	<b>5</b>	<b>2.5</b>	<b>0.4</b>
Backbone-Backbone	77	5.7	6	7.8	0.4	3	3.9	0.2
Backbone-Sidechain	87	6.4	8	9.2	0.6	2	2.3	0.1
Sidechain-Sidechain	33	2.4	2	6.1	0.1	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>293</b>	<b>21.5</b>	<b>22</b>	<b>7.5</b>	<b>1.6</b>	<b>3</b>	<b>1.0</b>	<b>0.2</b>
Backbone-Backbone	43	3.2	3	7.0	0.2	1	2.3	0.1
Backbone-Sidechain	144	10.6	14	9.7	1.0	0	0.0	0.0
Sidechain-Sidechain	106	7.8	5	4.7	0.4	2	1.9	0.1
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
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
<b>Hydrogen bond</b>	<b>48</b>	<b>3.5</b>	<b>3</b>	<b>6.2</b>	<b>0.2</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>1362</b>	<b>100.0</b>	<b>80</b>	<b>5.9</b>	<b>5.9</b>	<b>16</b>	<b>1.2</b>	<b>1.2</b>
Backbone-Backbone	305	22.4	14	4.6	1.0	4	1.3	0.3
Backbone-Sidechain	751	55.1	58	7.7	4.3	10	1.3	0.7
Sidechain-Sidechain	306	22.5	8	2.6	0.6	2	0.7	0.1

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> 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 <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	9	10	9	11	0	39	0.14	0.23	0.04	0.13
2	12	10	9	11	0	42	0.14	0.23	0.03	0.13
3	8	7	10	14	0	39	0.13	0.23	0.03	0.12
4	9	7	10	12	0	38	0.14	0.22	0.03	0.14
5	8	10	10	10	0	38	0.14	0.21	0.03	0.13
6	8	9	9	10	0	36	0.14	0.24	0.04	0.14
7	8	6	9	11	0	34	0.14	0.23	0.04	0.12
8	11	9	8	10	0	38	0.14	0.24	0.04	0.12
9	7	12	7	12	0	38	0.14	0.21	0.03	0.14
10	9	9	8	13	0	39	0.14	0.24	0.04	0.13

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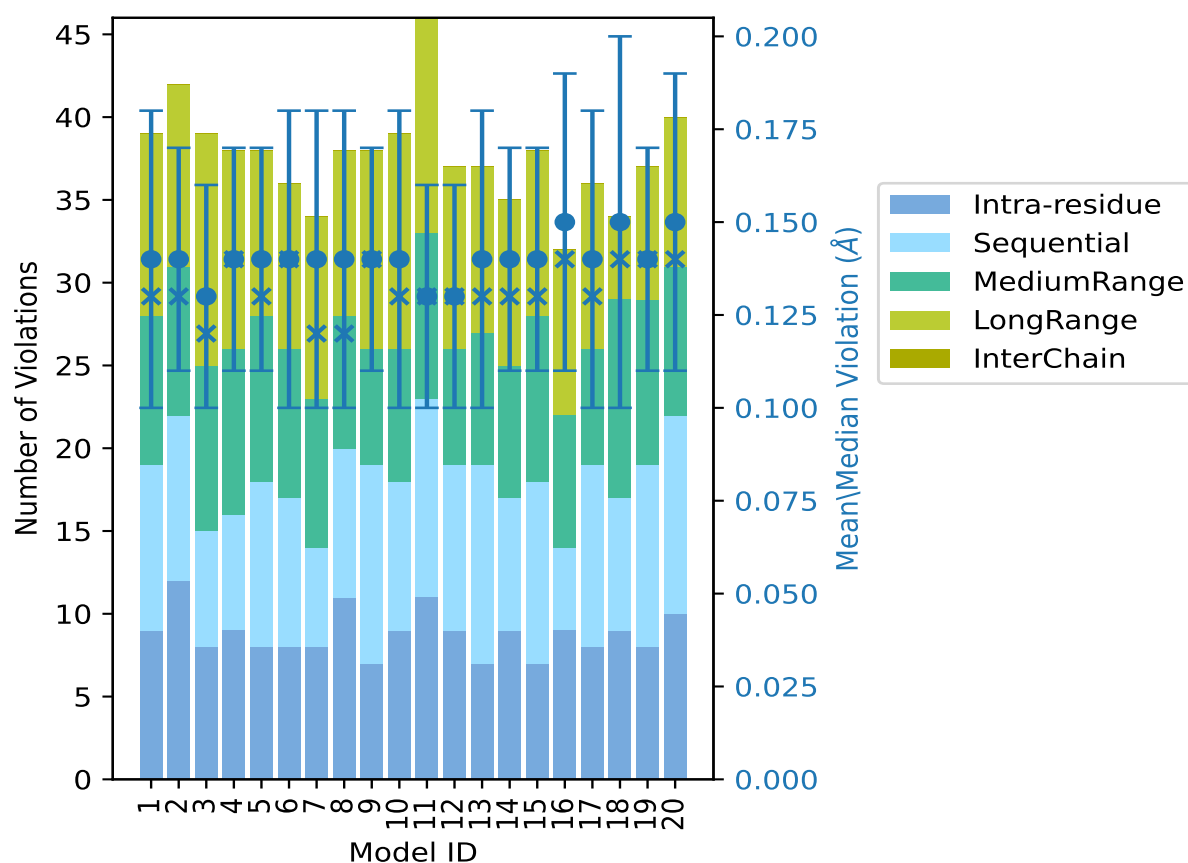
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	11	12	10	13	0	46	0.13	0.2	0.03	0.13
12	9	10	7	11	0	37	0.13	0.23	0.03	0.13
13	7	12	8	10	0	37	0.14	0.23	0.04	0.13
14	9	8	8	10	0	35	0.14	0.23	0.03	0.13
15	7	11	10	10	0	38	0.14	0.21	0.03	0.13
16	9	5	8	10	0	32	0.15	0.23	0.04	0.14
17	8	11	7	10	0	36	0.14	0.24	0.04	0.13
18	9	8	12	5	0	34	0.15	0.35	0.05	0.14
19	8	11	10	8	0	37	0.14	0.23	0.03	0.14
20	10	12	9	9	0	40	0.15	0.26	0.04	0.14

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup>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 ⓘ

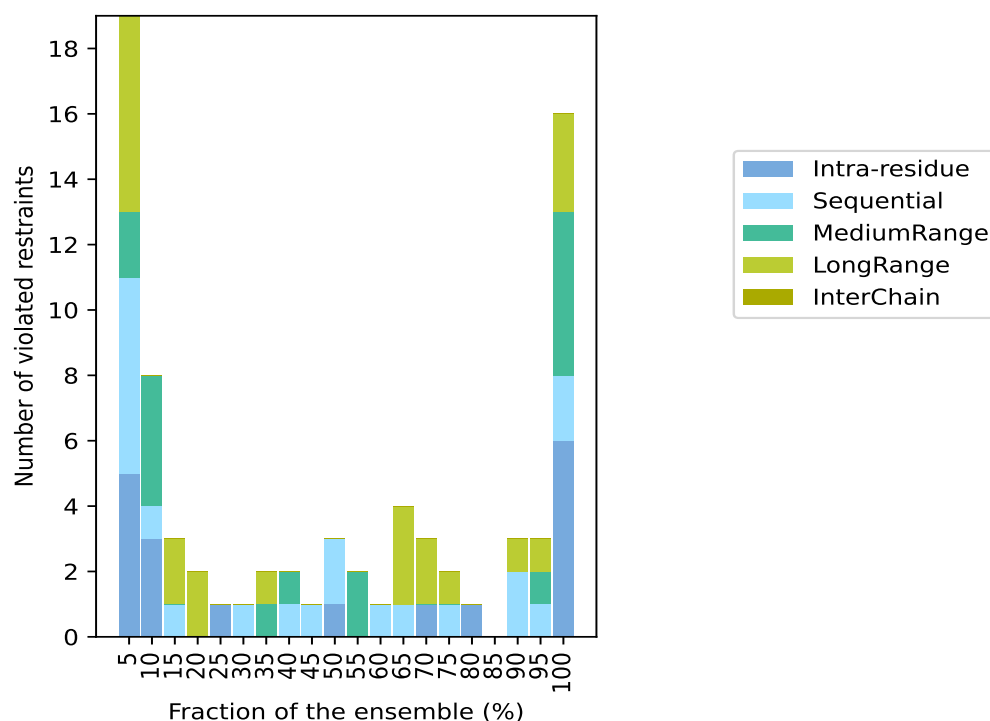
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1237(IR:538, SQ:247, MR:181, LR:271, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
5	6	2	6	0	19	1	5.0
3	1	4	0	0	8	2	10.0
0	1	0	2	0	3	3	15.0
0	0	0	2	0	2	4	20.0
1	0	0	0	0	1	5	25.0
0	1	0	0	0	1	6	30.0
0	0	1	1	0	2	7	35.0
0	1	1	0	0	2	8	40.0
0	1	0	0	0	1	9	45.0
1	2	0	0	0	3	10	50.0
0	0	2	0	0	2	11	55.0
0	1	0	0	0	1	12	60.0
0	1	0	3	0	4	13	65.0
1	0	0	2	0	3	14	70.0
0	1	0	1	0	2	15	75.0
1	0	0	0	0	1	16	80.0
0	0	0	0	0	0	17	85.0
0	2	0	1	0	3	18	90.0
0	1	1	1	0	3	19	95.0
6	2	5	3	0	16	20	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

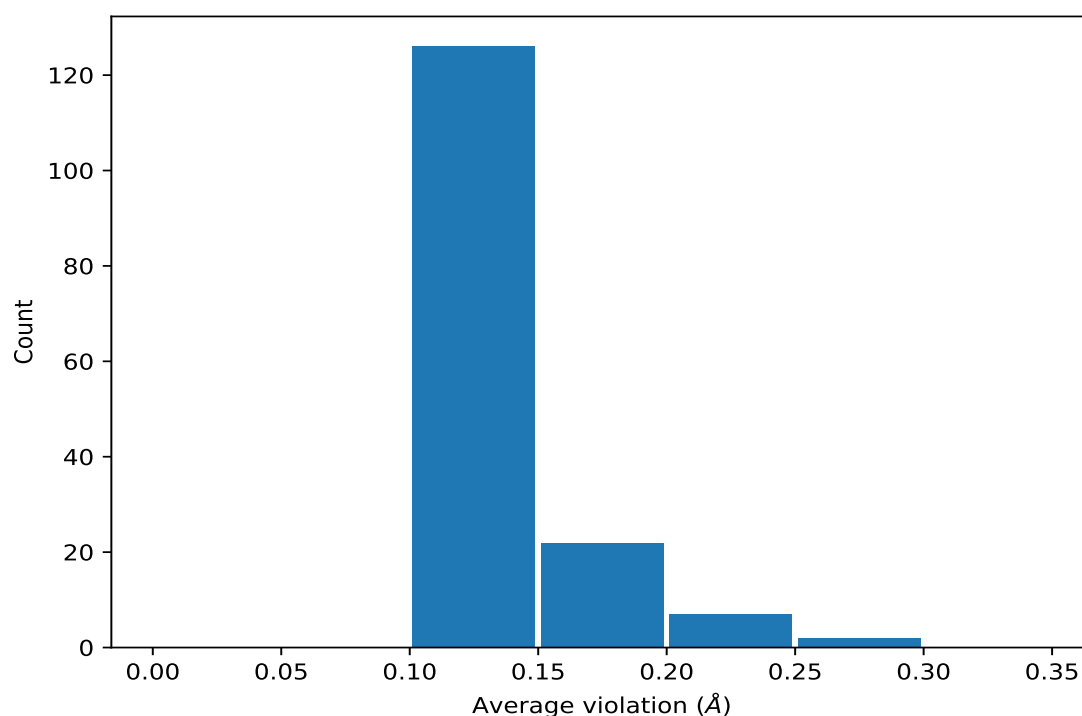
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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 <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,636)	1:45:A:ILE:HD11	1:49:A:LYS:H	20	0.21	0.01	0.21
(1,636)	1:45:A:ILE:HD12	1:49:A:LYS:H	20	0.21	0.01	0.21
(1,636)	1:45:A:ILE:HD13	1:49:A:LYS:H	20	0.21	0.01	0.21
(1,864)	1:28:A:LYS:HD2	1:28:A:LYS:HA	20	0.21	0.03	0.2
(1,864)	1:28:A:LYS:HD3	1:28:A:LYS:HA	20	0.21	0.03	0.2
(1,1139)	1:41:A:GLN:HA	1:41:A:GLN:HG2	20	0.2	0.04	0.21
(1,1139)	1:41:A:GLN:HA	1:41:A:GLN:HG3	20	0.2	0.04	0.21
(1,710)	1:56:A:THR:HG21	1:57:A:VAL:H	20	0.19	0.02	0.19
(1,710)	1:56:A:THR:HG22	1:57:A:VAL:H	20	0.19	0.02	0.19
(1,710)	1:56:A:THR:HG23	1:57:A:VAL:H	20	0.19	0.02	0.19
(1,627)	1:45:A:ILE:HG12	1:45:A:ILE:H	20	0.18	0.04	0.16
(1,627)	1:45:A:ILE:HG13	1:45:A:ILE:H	20	0.18	0.04	0.16
(1,1294)	1:62:A:LEU:HG	1:57:A:VAL:HG11	20	0.17	0.01	0.17
(1,1294)	1:62:A:LEU:HG	1:57:A:VAL:HG12	20	0.17	0.01	0.17
(1,1294)	1:62:A:LEU:HG	1:57:A:VAL:HG13	20	0.17	0.01	0.17
(1,1294)	1:62:A:LEU:HG	1:57:A:VAL:HG21	20	0.17	0.01	0.17

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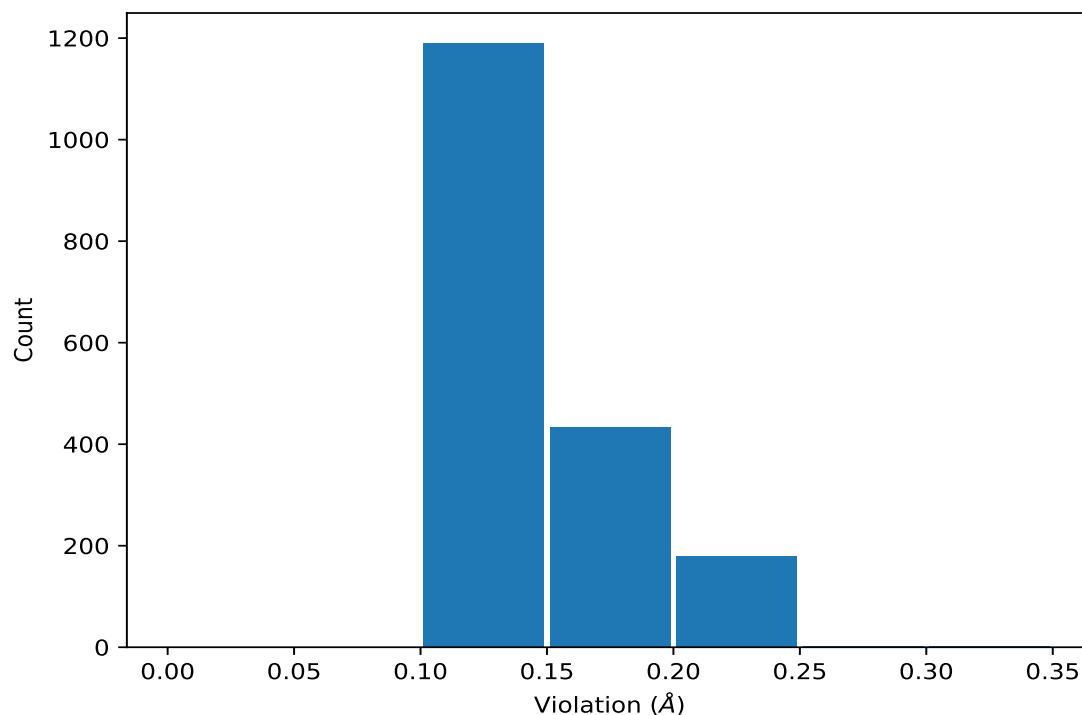
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1294)	1:62:A:LEU:HG	1:57:A:VAL:HG22	20	0.17	0.01	0.17
(1,1294)	1:62:A:LEU:HG	1:57:A:VAL:HG23	20	0.17	0.01	0.17
(1,732)	1:24:A:ILE:HG21	1:24:A:ILE:H	20	0.17	0.01	0.17
(1,732)	1:24:A:ILE:HG22	1:24:A:ILE:H	20	0.17	0.01	0.17
(1,732)	1:24:A:ILE:HG23	1:24:A:ILE:H	20	0.17	0.01	0.17
(1,1239)	1:23:A:THR:HB	1:56:A:THR:HB	20	0.17	0.02	0.17
(1,740)	1:24:A:ILE:HD11	1:28:A:LYS:H	20	0.17	0.02	0.17
(1,740)	1:24:A:ILE:HD12	1:28:A:LYS:H	20	0.17	0.02	0.17
(1,740)	1:24:A:ILE:HD13	1:28:A:LYS:H	20	0.17	0.02	0.17
(1,357)	1:36:A:SER:H	1:34:A:SER:H	20	0.17	0.01	0.17

<sup>1</sup>Number of violated models, <sup>2</sup>Standard 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 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)
(1,474)	1:8:A:ASN:H	1:8:A:ASN:HD21	18	0.35
(1,474)	1:8:A:ASN:H	1:8:A:ASN:HD22	18	0.35
(1,864)	1:28:A:LYS:HD2	1:28:A:LYS:HA	20	0.26
(1,864)	1:28:A:LYS:HD3	1:28:A:LYS:HA	20	0.26
(1,1139)	1:41:A:GLN:HA	1:41:A:GLN:HG2	20	0.24
(1,1139)	1:41:A:GLN:HA	1:41:A:GLN:HG3	20	0.24
(1,864)	1:28:A:LYS:HD2	1:28:A:LYS:HA	8	0.24
(1,864)	1:28:A:LYS:HD3	1:28:A:LYS:HA	8	0.24
(1,864)	1:28:A:LYS:HD2	1:28:A:LYS:HA	10	0.24
(1,864)	1:28:A:LYS:HD3	1:28:A:LYS:HA	10	0.24
(1,864)	1:28:A:LYS:HD2	1:28:A:LYS:HA	17	0.24
(1,864)	1:28:A:LYS:HD3	1:28:A:LYS:HA	17	0.24
(1,651)	1:5:A:THR:HG21	1:13:A:LYS:H	6	0.24
(1,651)	1:5:A:THR:HG22	1:13:A:LYS:H	6	0.24
(1,651)	1:5:A:THR:HG23	1:13:A:LYS:H	6	0.24
(1,1139)	1:41:A:GLN:HA	1:41:A:GLN:HG2	3	0.23
(1,1139)	1:41:A:GLN:HA	1:41:A:GLN:HG3	3	0.23
(1,1139)	1:41:A:GLN:HA	1:41:A:GLN:HG2	7	0.23
(1,1139)	1:41:A:GLN:HA	1:41:A:GLN:HG3	7	0.23
(1,1139)	1:41:A:GLN:HA	1:41:A:GLN:HG2	16	0.23

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

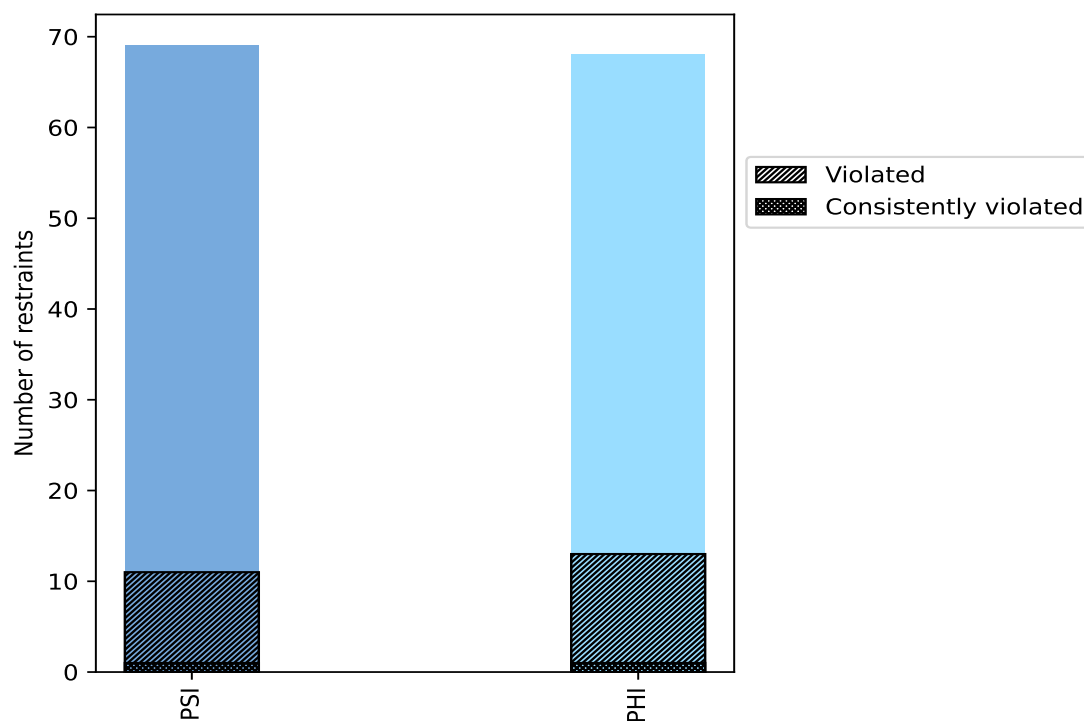
### 10.1 Summary of dihedral-angle violations [i](#)

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	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PSI	69	50.4	11	15.9	8.0	1	1.4	0.7
PHI	68	49.6	13	19.1	9.5	1	1.5	0.7
Total	137	100.0	24	17.5	17.5	2	1.5	1.5

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

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



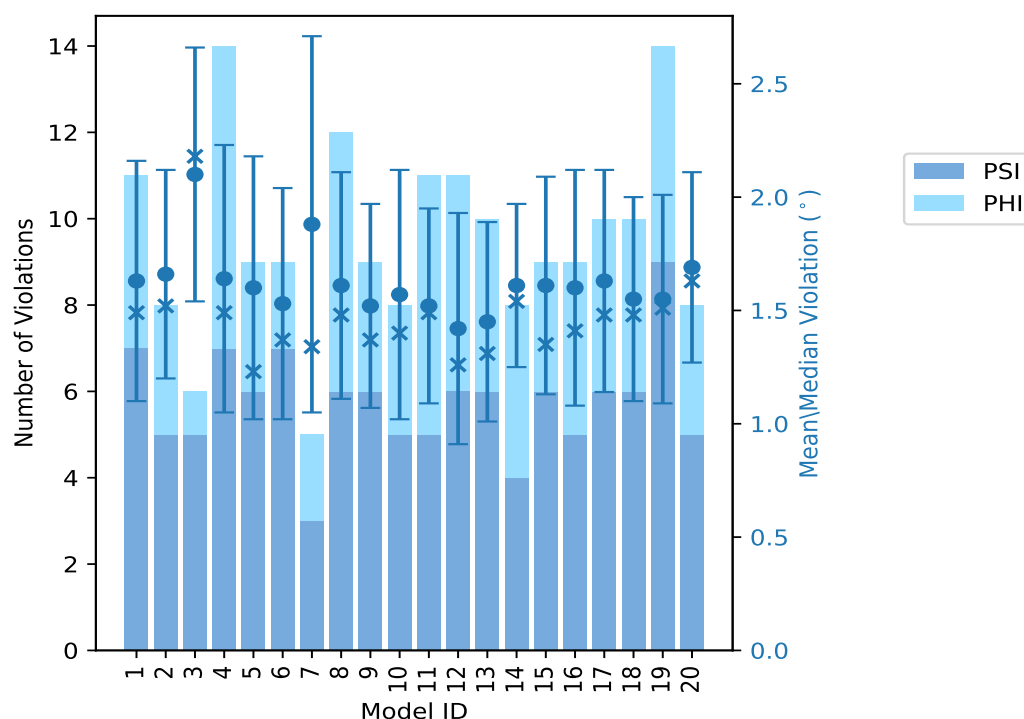
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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 (°)
	PSI	PHI	Total				
1	7	4	11	1.63	2.82	0.53	1.49
2	5	3	8	1.66	2.44	0.46	1.52
3	5	1	6	2.1	2.96	0.56	2.18
4	7	7	14	1.64	3.26	0.59	1.49
5	6	3	9	1.6	2.59	0.58	1.23
6	7	2	9	1.53	2.41	0.51	1.37
7	3	2	5	1.88	3.21	0.83	1.34
8	6	6	12	1.61	2.74	0.5	1.48
9	6	3	9	1.52	2.38	0.45	1.37
10	5	3	8	1.57	2.58	0.55	1.4
11	5	6	11	1.52	2.52	0.43	1.49
12	6	5	11	1.42	2.57	0.51	1.26
13	6	4	10	1.45	2.38	0.44	1.31
14	4	4	8	1.61	2.44	0.36	1.54
15	6	3	9	1.61	2.48	0.48	1.35
16	5	4	9	1.6	2.58	0.52	1.41
17	6	4	10	1.63	2.74	0.49	1.48
18	6	4	10	1.55	2.38	0.45	1.48
19	9	5	14	1.55	2.72	0.46	1.51
20	5	3	8	1.69	2.52	0.42	1.63

### 10.2.1 Bar graph : Dihedral 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

### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	
PSI	PHI	Total	Count <sup>1</sup>	%
2	4	6	1	5.0
0	1	1	2	10.0
0	2	2	3	15.0
1	1	2	4	20.0
1	0	1	5	25.0
0	0	0	6	30.0
0	1	1	7	35.0
2	1	3	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

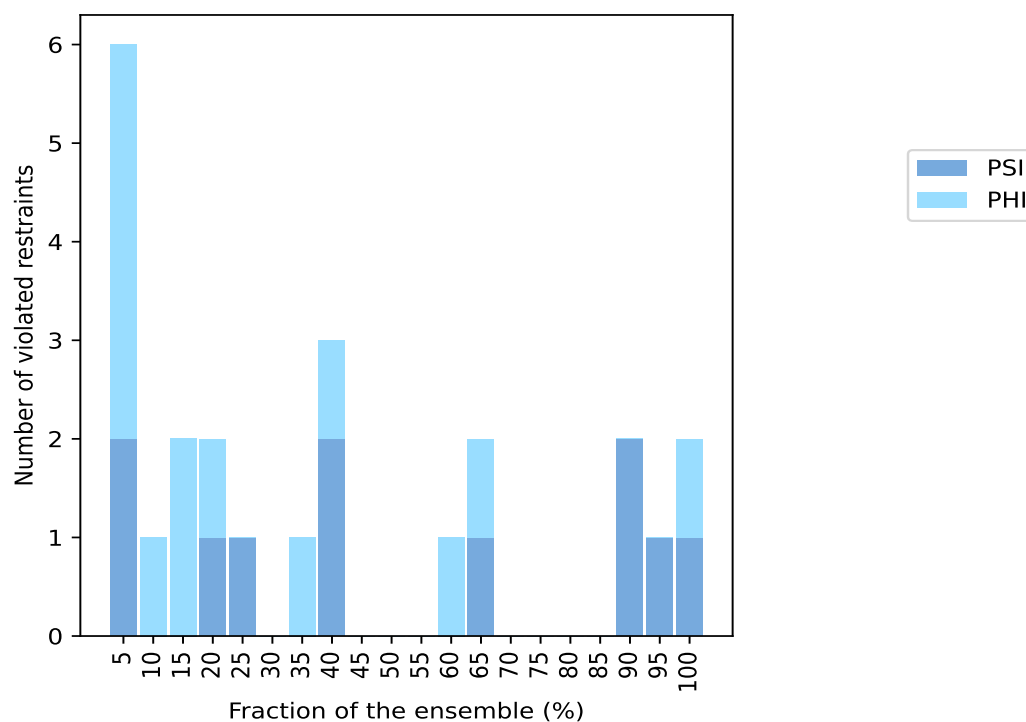
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
0	1	1	12	60.0
1	1	2	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
2	0	2	18	90.0
1	0	1	19	95.0
1	1	2	20	100.0

<sup>1</sup> Number of models with violations

### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

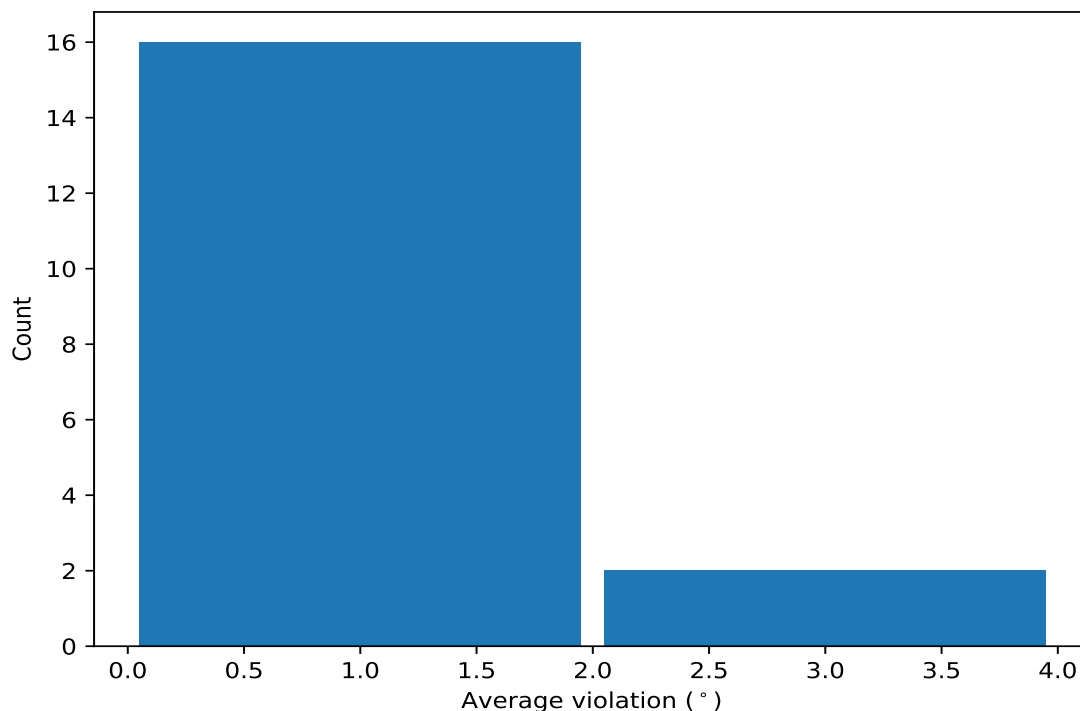


## 10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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 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.

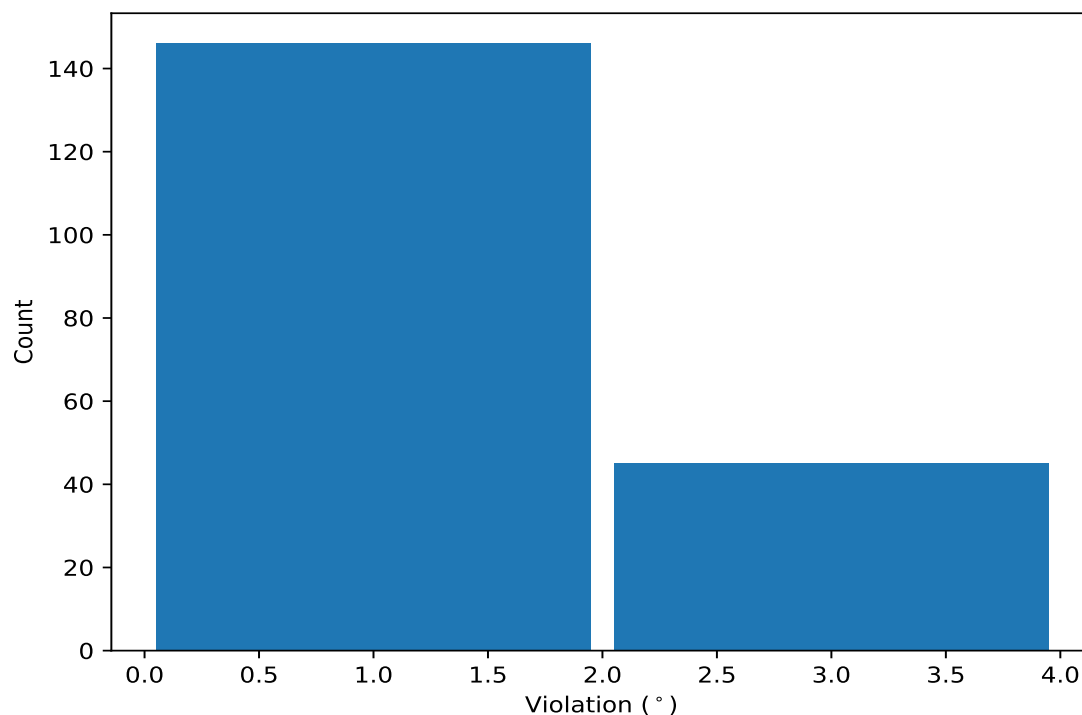
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,84)	1:44:A:LEU:C	1:45:A:ILE:N	1:45:A:ILE:CA	1:45:A:ILE:C	20	2.42	0.24	2.42
(1,61)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:SER:N	20	2.41	0.29	2.36
(1,87)	1:46:A:TYR:N	1:46:A:TYR:CA	1:46:A:TYR:C	1:47:A:SER:N	19	1.65	0.2	1.62
(1,89)	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	1:49:A:LYS:N	18	1.54	0.31	1.56
(1,73)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:SER:N	18	1.32	0.14	1.3
(1,72)	1:38:A:GLU:C	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	13	1.4	0.15	1.41
(1,39)	1:21:A:SER:N	1:21:A:SER:CA	1:21:A:SER:C	1:22:A:ASN:N	13	1.14	0.1	1.1
(1,34)	1:18:A:LEU:C	1:19:A:GLU:N	1:19:A:GLU:CA	1:19:A:GLU:C	12	1.16	0.12	1.1
(1,110)	1:58:A:SER:C	1:59:A:GLU:N	1:59:A:GLU:CA	1:59:A:GLU:C	8	1.55	0.3	1.44
(1,69)	1:37:A:CYS:N	1:37:A:CYS:CA	1:37:A:CYS:C	1:38:A:GLU:N	8	1.52	0.33	1.42

<sup>1</sup> Number of violated models, <sup>2</sup>Standard 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 provides the list of violations for 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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,105)	1:56:A:THR:N	1:56:A:THR:CA	1:56:A:THR:C	1:57:A:VAL:N	4	3.26
(1,61)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:SER:N	7	3.21
(1,61)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:SER:N	3	2.96
(1,84)	1:44:A:LEU:C	1:45:A:ILE:N	1:45:A:ILE:CA	1:45:A:ILE:C	1	2.82
(1,84)	1:44:A:LEU:C	1:45:A:ILE:N	1:45:A:ILE:CA	1:45:A:ILE:C	8	2.74
(1,61)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:SER:N	17	2.74
(1,84)	1:44:A:LEU:C	1:45:A:ILE:N	1:45:A:ILE:CA	1:45:A:ILE:C	19	2.72
(1,61)	1:33:A:GLN:N	1:33:A:GLN:CA	1:33:A:GLN:C	1:34:A:SER:N	5	2.59
(1,84)	1:44:A:LEU:C	1:45:A:ILE:N	1:45:A:ILE:CA	1:45:A:ILE:C	10	2.58
(1,84)	1:44:A:LEU:C	1:45:A:ILE:N	1:45:A:ILE:CA	1:45:A:ILE:C	16	2.58