



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2NBQ
BMRB ID : 25985
Title : NMR Structure of the C-Terminal Domain of human APOBEC3B
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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 : 4.02b-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

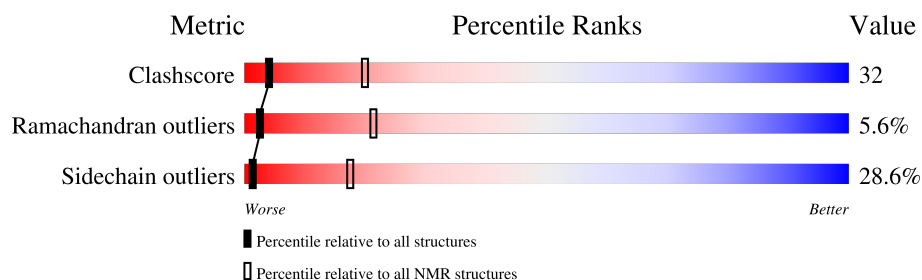
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 67%.

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 ≥ 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	205	

2 Ensemble composition and analysis

This entry contains 30 models. Model 11 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:191-A:202, A:214-A:240, A:252-A:377 (165)	0.78	11

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 5 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3208 atoms, of which 1563 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA dC->dU-editing enzyme APOBEC-3B.

Mol	Chain	Residues	Atoms						Trace
1	A	197	Total	C	H	N	O	S	0
			3207	1055	1563	282	294	13	

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	MET	-	expression tag	UNP Q9UH17
A	383	LEU	-	expression tag	UNP Q9UH17
A	384	GLU	-	expression tag	UNP Q9UH17
A	385	HIS	-	expression tag	UNP Q9UH17
A	386	HIS	-	expression tag	UNP Q9UH17
A	387	HIS	-	expression tag	UNP Q9UH17
A	388	HIS	-	expression tag	UNP Q9UH17
A	389	HIS	-	expression tag	UNP Q9UH17
A	390	HIS	-	expression tag	UNP Q9UH17

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

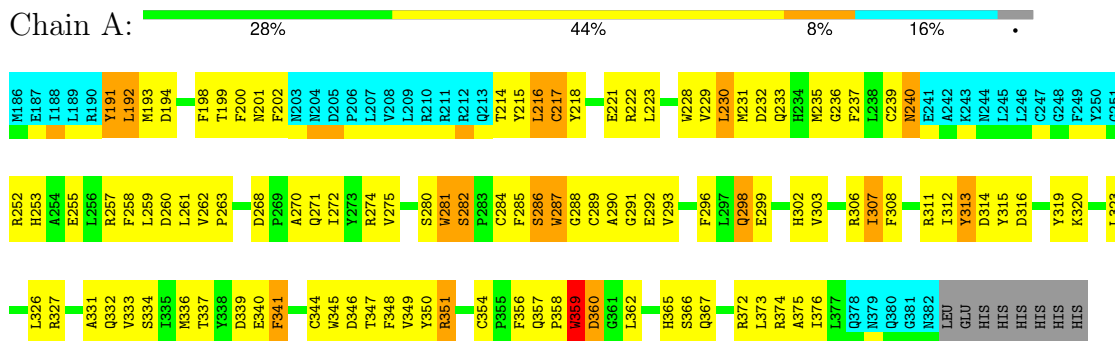
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

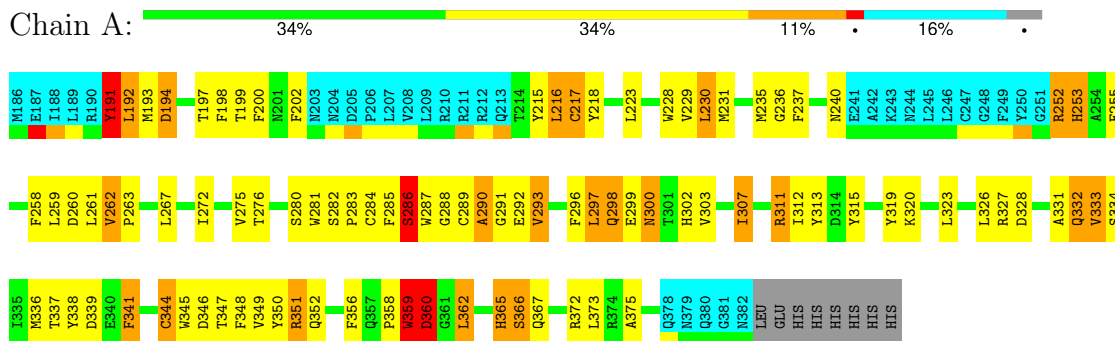
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



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

The representative model is number 11. Colouring as in section 4.1 above.

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3B



5 Refinement protocol and experimental data overview

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

Of the 256 calculated structures, 30 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
XPLOR-NIH	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	2
Total number of shifts	2228
Number of shifts mapped to atoms	2166
Number of unparsed shifts	0
Number of shifts with mapping errors	62
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	67%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1382	1298	1298	87±10
All	All	41490	38940	38940	2604

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 32.

5 of 717 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:335:ILE:HD11	1:A:369:LEU:HD23	0.85	1.46	16	4
1:A:327:ARG:CZ	1:A:377:LEU:HD11	0.81	2.06	13	2
1:A:312:ILE:HD12	1:A:312:ILE:H	0.80	1.36	3	2
1:A:307:ILE:N	1:A:307:ILE:HD12	0.79	1.92	11	5
1:A:238:LEU:N	1:A:238:LEU:HD23	0.79	1.91	6	2

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	165/205 (80%)	131±4 (80±2%)	25±3 (15±2%)	9±2 (6±1%)	2	21
All	All	4950/6150 (80%)	3936 (80%)	738 (15%)	276 (6%)	2	21

5 of 34 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	287	TRP	28
1	A	359	TRP	27
1	A	360	ASP	26
1	A	192	LEU	22
1	A	281	TRP	20

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	146/182 (80%)	104±4 (71±3%)	42±4 (29±3%)	1	17
All	All	4380/5460 (80%)	3129 (71%)	1251 (29%)	1	17

5 of 118 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	275	VAL	30
1	A	302	HIS	30
1	A	303	VAL	30
1	A	334	SER	30
1	A	337	THR	30

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 67% for the well-defined parts and 64% 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	1840
Number of shifts mapped to atoms	1788
Number of unparsed shifts	0
Number of shifts with mapping errors	52
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

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 52) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	383	LEU	H	8.259	0.005	1
1	A	383	LEU	HA	4.265	0.006	1
1	A	383	LEU	HB2	1.568	0.001	2
1	A	383	LEU	HB3	1.524	0.013	2
1	A	383	LEU	HG	1.573	0.004	1
1	A	383	LEU	HD11	0.799	0.005	2
1	A	383	LEU	HD12	0.799	0.005	2
1	A	383	LEU	HD13	0.799	0.005	2
1	A	383	LEU	HD21	0.877	0.003	2
1	A	383	LEU	HD22	0.877	0.003	2
1	A	383	LEU	HD23	0.877	0.003	2
1	A	383	LEU	CA	55.309	0.147	1
1	A	383	LEU	CB	41.701	0.158	1
1	A	383	LEU	CG	26.914	0.001	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	383	LEU	CD1	23.411	0.018	2
1	A	383	LEU	CD2	24.897	0.003	2
1	A	383	LEU	N	122.433	0.072	1
1	A	384	GLU	H	8.306	0.004	1
1	A	384	GLU	HA	4.17	0.01	1
1	A	384	GLU	HB2	1.832	0.005	2
1	A	384	GLU	HB3	1.88	0.006	2
1	A	384	GLU	HG2	2.18	0.005	2
1	A	384	GLU	HG3	2.116	0.004	2
1	A	384	GLU	CA	56.607	0.053	1
1	A	384	GLU	CB	30.129	0.112	1
1	A	384	GLU	CG	36.22	0.031	1
1	A	384	GLU	N	121.077	0.053	1
1	A	385	HIS	H	8.331	0.006	1
1	A	385	HIS	N	119.501	0.034	1
1	A	387	HIS	HA	4.567	0.001	1
1	A	387	HIS	HB2	2.95	.	2
1	A	387	HIS	HB3	3.019	.	2
1	A	387	HIS	CA	55.998	.	1
1	A	388	HIS	HA	4.491	0.001	1
1	A	388	HIS	HB2	2.902	.	2
1	A	388	HIS	HB3	2.983	.	2
1	A	388	HIS	CA	56.626	0.032	1
1	A	388	HIS	CB	29.649	.	1
1	A	389	HIS	H	8.233	0.007	1
1	A	389	HIS	HA	4.579	0.01	1
1	A	389	HIS	HB2	3.1	.	2
1	A	389	HIS	HB3	3.042	.	2
1	A	389	HIS	CA	56.122	0.16	1
1	A	389	HIS	CB	30.045	0.067	1
1	A	389	HIS	N	120.159	0.059	1
1	A	390	HIS	H	8.044	0.008	1
1	A	390	HIS	HA	4.395	0.005	1
1	A	390	HIS	HB2	3.154	0.003	2
1	A	390	HIS	HB3	3.029	0.007	2
1	A	390	HIS	CA	57.459	0.029	1
1	A	390	HIS	CB	30.415	0.142	1
1	A	390	HIS	N	125.601	0.022	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
$^{13}\text{C}_\alpha$	187	-0.41 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	171	0.57 ± 0.10	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	180	-0.12 ± 0.25	None needed (< 0.5 ppm)

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 67%, i.e. 1557 atoms were assigned a chemical shift out of a possible 2339. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	621/819 (76%)	312/331 (94%)	156/330 (47%)	153/158 (97%)
Sidechain	819/1210 (68%)	567/787 (72%)	243/373 (65%)	9/50 (18%)
Aromatic	117/310 (38%)	111/152 (73%)	0/148 (0%)	6/10 (60%)
Overall	1557/2339 (67%)	990/1270 (78%)	399/851 (47%)	168/218 (77%)

7.1.4 Statistically unusual chemical shifts ⓘ

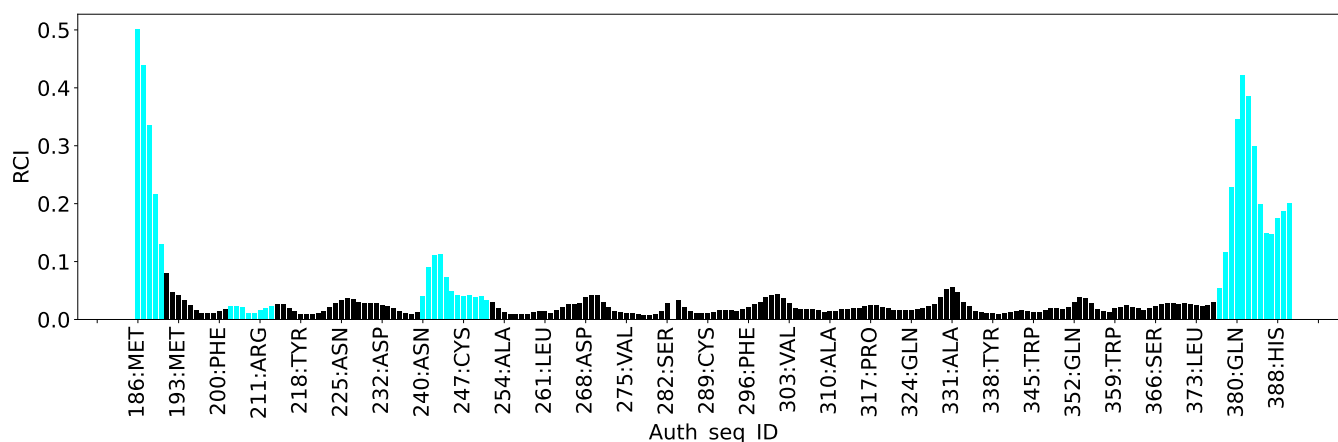
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	351	ARG	HD3	0.32	1.81 – 4.39	-10.8
1	A	277	TRP	HE1	5.50	6.88 – 13.28	-7.2
1	A	255	GLU	H	12.41	5.45 – 11.20	7.1
1	A	223	LEU	HD21	-0.84	-0.65 – 2.13	-5.7
1	A	223	LEU	HD22	-0.84	-0.65 – 2.13	-5.7
1	A	223	LEU	HD23	-0.84	-0.65 – 2.13	-5.7
1	A	351	ARG	HD2	1.85	1.97 – 4.26	-5.5
1	A	347	THR	HG21	-0.03	0.08 – 2.19	-5.5
1	A	347	THR	HG22	-0.03	0.08 – 2.19	-5.5
1	A	347	THR	HG23	-0.03	0.08 – 2.19	-5.5

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1_dup*

7.2.1 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	388
Number of shifts mapped to atoms	378
Number of unparsed shifts	0
Number of shifts with mapping errors	10
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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 10) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	383	LEU	H	8.261	.	1
2	A	383	LEU	N	122.451	.	1
2	A	384	GLU	H	8.314	.	1
2	A	384	GLU	N	121.075	.	1
2	A	385	HIS	H	8.458	.	1
2	A	385	HIS	N	119.293	.	1
2	A	389	HIS	H	8.219	.	1
2	A	389	HIS	N	119.965	.	1
2	A	390	HIS	H	8.035	.	1
2	A	390	HIS	N	125.611	.	1

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	170	0.26 ± 0.51	None needed (< 0.5 ppm)

7.2.3 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 14%, i.e. 329 atoms were assigned a chemical shift out of a possible 2339. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	291/819 (36%)	145/331 (44%)	0/330 (0%)	146/158 (92%)
Sidechain	26/1210 (2%)	17/787 (2%)	0/373 (0%)	9/50 (18%)
Aromatic	12/310 (4%)	6/152 (4%)	0/148 (0%)	6/10 (60%)
Overall	329/2339 (14%)	168/1270 (13%)	0/851 (0%)	161/218 (74%)

7.2.4 Statistically unusual chemical shifts [i](#)

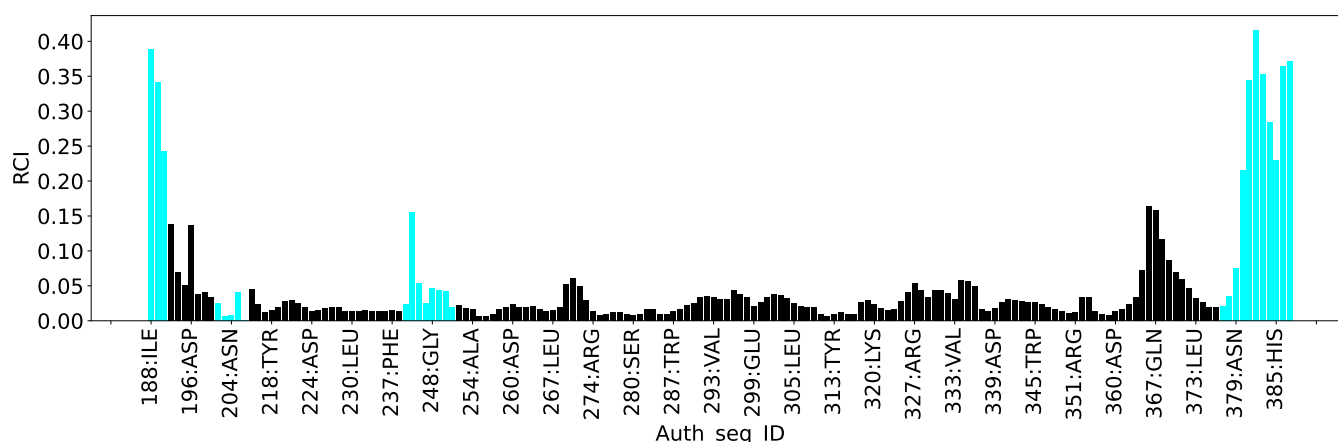
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	255	GLU	H	12.56	5.45 – 11.20	7.4
2	A	277	TRP	HE1	5.52	6.88 – 13.28	-7.1

7.2.5 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	3239
Intra-residue ($ i-j =0$)	1270
Sequential ($ i-j =1$)	639
Medium range ($ i-j >1$ and $ i-j <5$)	338
Long range ($ i-j \geq 5$)	824
Inter-chain	0
Hydrogen bond restraints	166
Disulfide bond restraints	0
Total dihedral-angle restraints	309
Number of unmapped restraints	0
Number of restraints per residue	17.2
Number of long range restraints per residue ¹	4.3

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)	53.2	0.2
0.2-0.5 (Medium)	18.5	0.46
>0.5 (Large)	0.2	1.26

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)	11.2	5.58
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

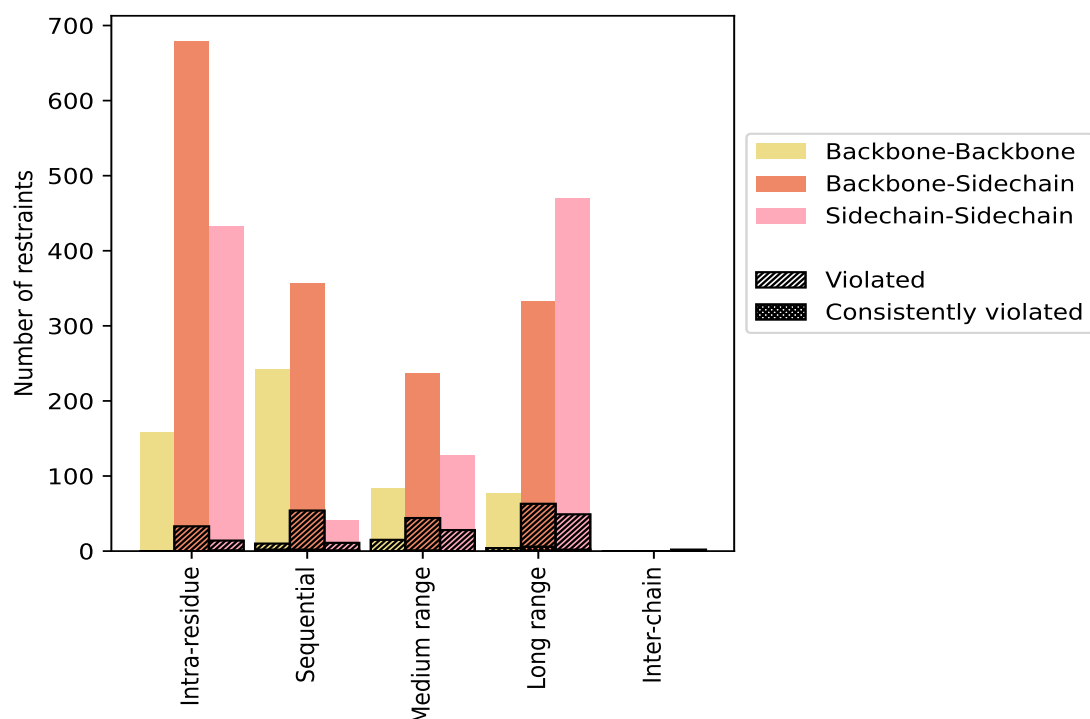
9.1 Summary of distance violations ⓘ

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)	1270	39.2	47	3.7	1.5	1	0.1	0.0
Backbone-Backbone	158	4.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	679	21.0	33	4.9	1.0	0	0.0	0.0
Sidechain-Sidechain	433	13.4	14	3.2	0.4	1	0.2	0.0
Sequential (i-j =1)	639	19.7	75	11.7	2.3	5	0.8	0.2
Backbone-Backbone	242	7.5	10	4.1	0.3	2	0.8	0.1
Backbone-Sidechain	356	11.0	54	15.2	1.7	2	0.6	0.1
Sidechain-Sidechain	41	1.3	11	26.8	0.3	1	2.4	0.0
Medium range (i-j >1 & i-j <5)	338	10.4	67	19.8	2.1	1	0.3	0.0
Backbone-Backbone	83	2.6	15	18.1	0.5	0	0.0	0.0
Backbone-Sidechain	127	3.9	24	18.9	0.7	1	0.8	0.0
Sidechain-Sidechain	128	4.0	28	21.9	0.9	0	0.0	0.0
Long range (i-j ≥5)	824	25.4	100	12.1	3.1	6	0.7	0.2
Backbone-Backbone	77	2.4	4	5.2	0.1	0	0.0	0.0
Backbone-Sidechain	277	8.6	47	17.0	1.5	4	1.4	0.1
Sidechain-Sidechain	470	14.5	49	10.4	1.5	2	0.4	0.1
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	166	5.1	36	21.7	1.1	2	1.2	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3239	100.0	327	10.1	10.1	15	0.5	0.5
Backbone-Backbone	560	17.3	29	5.2	0.9	2	0.4	0.1
Backbone-Sidechain	1605	49.6	194	12.1	6.0	9	0.6	0.3
Sidechain-Sidechain	1074	33.2	104	9.7	3.2	4	0.4	0.1

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	9	21	9	36	0	75	0.16	0.34	0.05	0.15
2	3	17	6	31	0	57	0.17	0.34	0.06	0.15
3	7	15	13	30	0	65	0.16	0.3	0.05	0.14
4	6	21	16	38	0	81	0.17	0.36	0.06	0.16
5	7	21	10	30	0	68	0.18	0.37	0.06	0.16
6	12	19	13	29	1	74	0.17	0.38	0.06	0.16
7	6	20	21	33	0	80	0.17	0.34	0.06	0.15
8	5	19	12	31	1	68	0.18	0.37	0.06	0.16
9	7	15	18	37	0	77	0.17	0.35	0.06	0.16
10	8	19	13	33	0	73	0.18	0.34	0.06	0.17

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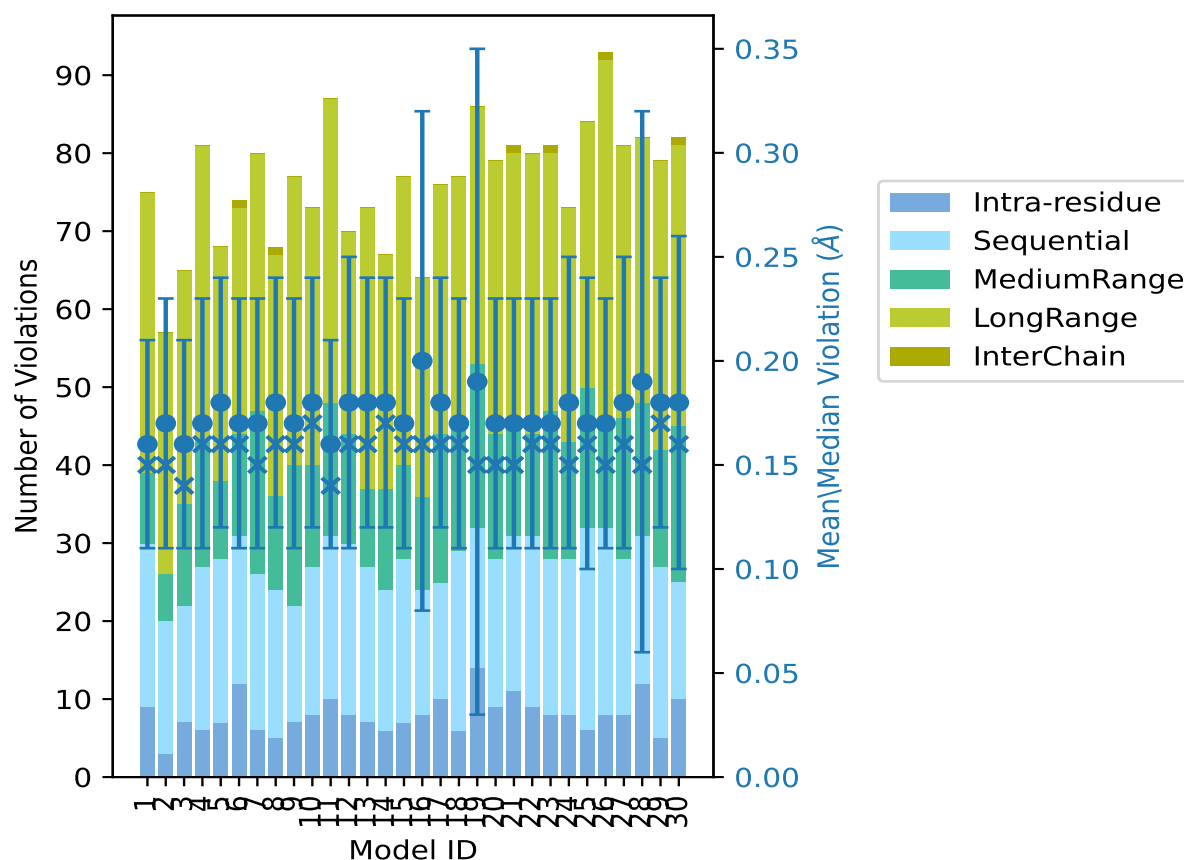
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	10	21	17	39	0	87	0.16	0.32	0.05	0.14
12	8	22	14	26	0	70	0.18	0.45	0.07	0.16
13	7	20	10	36	0	73	0.18	0.37	0.06	0.16
14	6	18	13	30	0	67	0.18	0.39	0.06	0.17
15	7	21	12	37	0	77	0.17	0.38	0.06	0.16
16	8	16	12	28	0	64	0.2	0.9	0.12	0.16
17	10	15	19	32	0	76	0.18	0.38	0.06	0.16
18	6	23	16	32	0	77	0.17	0.34	0.06	0.16
19	14	18	21	33	0	86	0.19	1.26	0.16	0.15
20	9	19	16	35	0	79	0.17	0.38	0.06	0.15
21	11	20	14	35	1	81	0.17	0.36	0.06	0.15
22	9	22	13	36	0	80	0.17	0.42	0.06	0.16
23	8	20	19	33	1	81	0.17	0.35	0.06	0.16
24	8	20	15	30	0	73	0.18	0.39	0.07	0.15
25	6	26	18	34	0	84	0.17	0.44	0.07	0.16
26	8	24	14	46	1	93	0.17	0.34	0.06	0.15
27	8	20	18	35	0	81	0.18	0.44	0.07	0.16
28	12	19	17	34	0	82	0.19	0.94	0.13	0.15
29	5	22	15	37	0	79	0.18	0.38	0.06	0.17
30	10	15	20	36	1	82	0.18	0.43	0.08	0.16

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2782(IR:1223, SQ:564, MR:271, LR:724, 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	%
15	19	19	32	0	85	1	3.3
3	6	15	8	0	32	2	6.7
5	9	5	4	0	23	3	10.0
6	7	5	8	0	26	4	13.3
2	7	4	3	0	16	5	16.7
5	2	3	0	0	10	6	20.0

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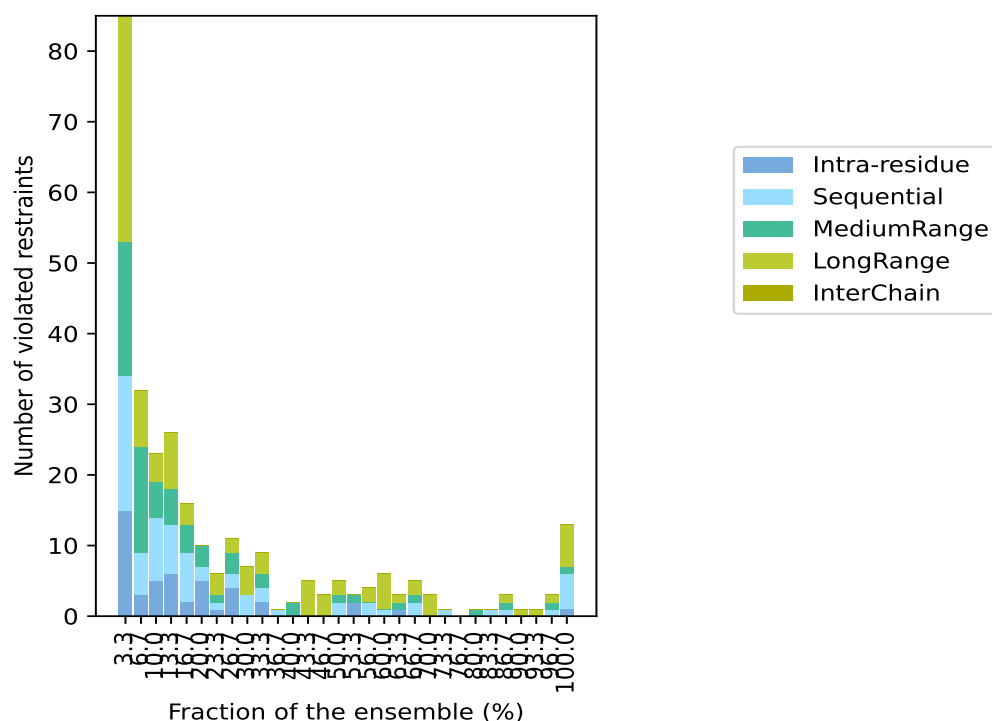
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	1	1	3	0	6	7	23.3
4	2	3	2	0	11	8	26.7
0	3	0	4	0	7	9	30.0
2	2	2	3	0	9	10	33.3
0	1	0	0	0	1	11	36.7
0	0	2	0	0	2	12	40.0
0	0	0	5	0	5	13	43.3
0	0	0	3	0	3	14	46.7
0	2	1	2	0	5	15	50.0
2	0	1	0	0	3	16	53.3
0	2	0	2	0	4	17	56.7
0	1	0	5	0	6	18	60.0
1	0	1	1	0	3	19	63.3
0	2	1	2	0	5	20	66.7
0	0	0	3	0	3	21	70.0
0	1	0	0	0	1	22	73.3
0	0	0	0	0	0	23	76.7
0	0	1	0	0	1	24	80.0
0	1	0	0	0	1	25	83.3
0	1	1	1	0	3	26	86.7
0	0	0	1	0	1	27	90.0
0	0	0	1	0	1	28	93.3
0	1	1	1	0	3	29	96.7
1	5	1	6	0	13	30	100.0

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

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

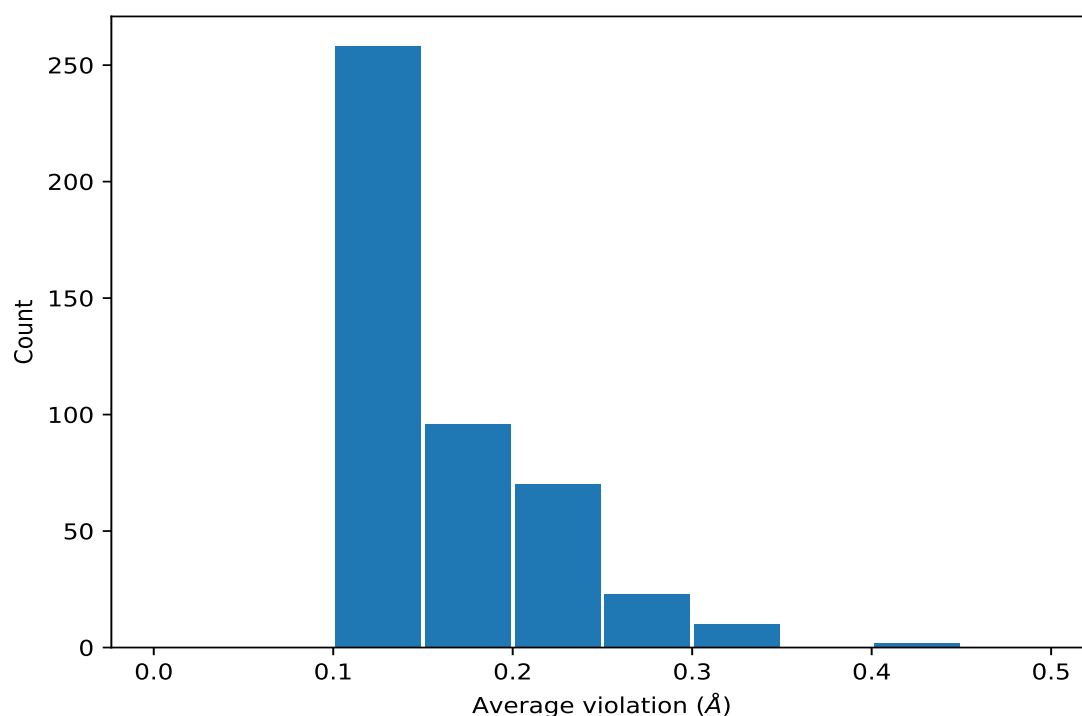
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

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



9.4.2 Table: Most violated distance restraints [i](#)

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,484)	1:223:A:LEU:HG	1:228:A:TRP:HE3	30	0.35	0.04	0.34
(1,480)	1:223:A:LEU:HD11	1:224:A:ASP:HB3	30	0.31	0.04	0.31
(1,480)	1:223:A:LEU:HD12	1:224:A:ASP:HB3	30	0.31	0.04	0.31
(1,480)	1:223:A:LEU:HD13	1:224:A:ASP:HB3	30	0.31	0.04	0.31
(1,1892)	1:303:A:VAL:HG11	1:273:A:TYR:HA	30	0.28	0.06	0.28
(1,1892)	1:303:A:VAL:HG12	1:273:A:TYR:HA	30	0.28	0.06	0.28
(1,1892)	1:303:A:VAL:HG13	1:273:A:TYR:HA	30	0.28	0.06	0.28
(1,1524)	1:277:A:TRP:HH2	1:258:A:PHE:HA	30	0.26	0.06	0.27
(1,580)	1:228:A:TRP:HA	1:223:A:LEU:HD21	30	0.26	0.04	0.26
(1,580)	1:228:A:TRP:HA	1:223:A:LEU:HD22	30	0.26	0.04	0.26
(1,580)	1:228:A:TRP:HA	1:223:A:LEU:HD23	30	0.26	0.04	0.26
(1,499)	1:224:A:ASP:H	1:229:A:VAL:HB	30	0.24	0.01	0.24
(1,1154)	1:262:A:VAL:HG11	1:260:A:ASP:H	30	0.24	0.06	0.24
(1,1154)	1:262:A:VAL:HG12	1:260:A:ASP:H	30	0.24	0.06	0.24
(1,1154)	1:262:A:VAL:HG13	1:260:A:ASP:H	30	0.24	0.06	0.24
(1,1317)	1:270:A:ALA:H	1:269:A:PRO:HA	30	0.22	0.02	0.21

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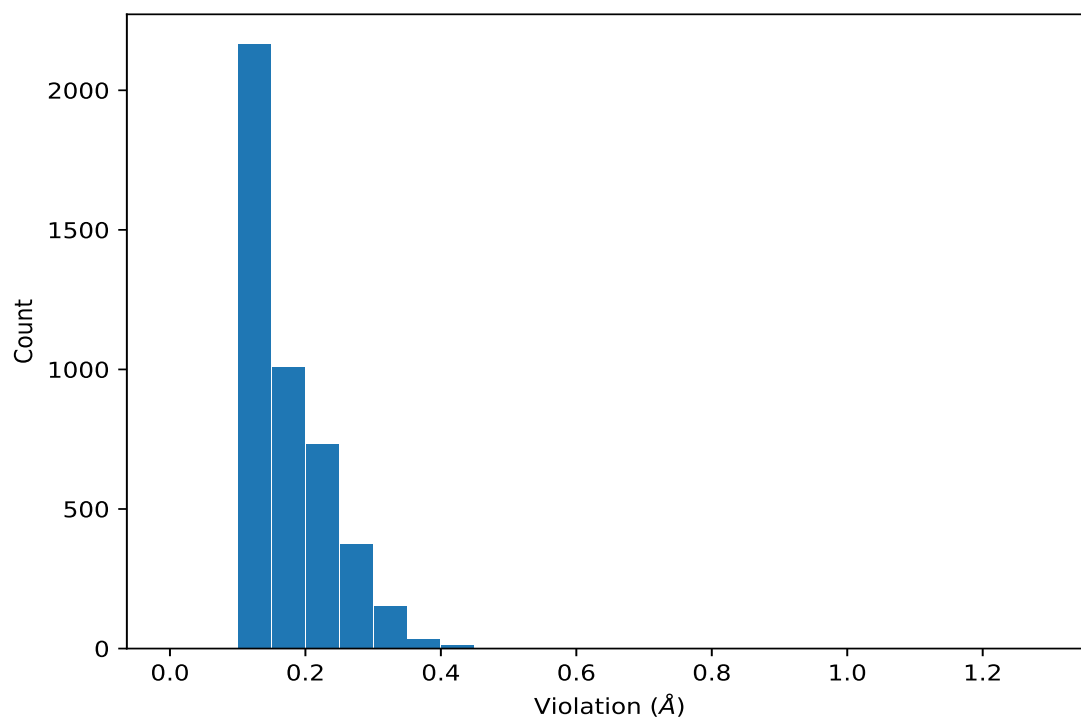
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,501)	1:224:A:ASP:HB3	1:229:A:VAL:HB	30	0.2	0.03	0.2
(1,3061)	1:380:A:GLN:HE22	1:380:A:GLN:HG3	30	0.18	0.0	0.18

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

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



9.5.2 Table : All distance violations [i](#)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3070)	1:255:A:GLU:H	1:255:A:GLU:OE1	19	1.26
(1,3071)	1:255:A:GLU:N	1:255:A:GLU:OE1	19	0.96
(1,3070)	1:255:A:GLU:H	1:255:A:GLU:OE1	28	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3070)	1:255:A:GLU:H	1:255:A:GLU:OE1	16	0.9
(1,3071)	1:255:A:GLU:N	1:255:A:GLU:OE1	28	0.7
(1,3071)	1:255:A:GLU:N	1:255:A:GLU:OE1	16	0.66
(1,2758)	1:359:A:TRP:HE3	1:360:A:ASP:H	28	0.46
(1,2862)	1:367:A:GLN:HG2	1:364:A:GLU:HA	12	0.45
(1,2862)	1:367:A:GLN:HG2	1:364:A:GLU:HA	27	0.44
(1,638)	1:230:A:LEU:HD11	1:222:A:ARG:H	25	0.44

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

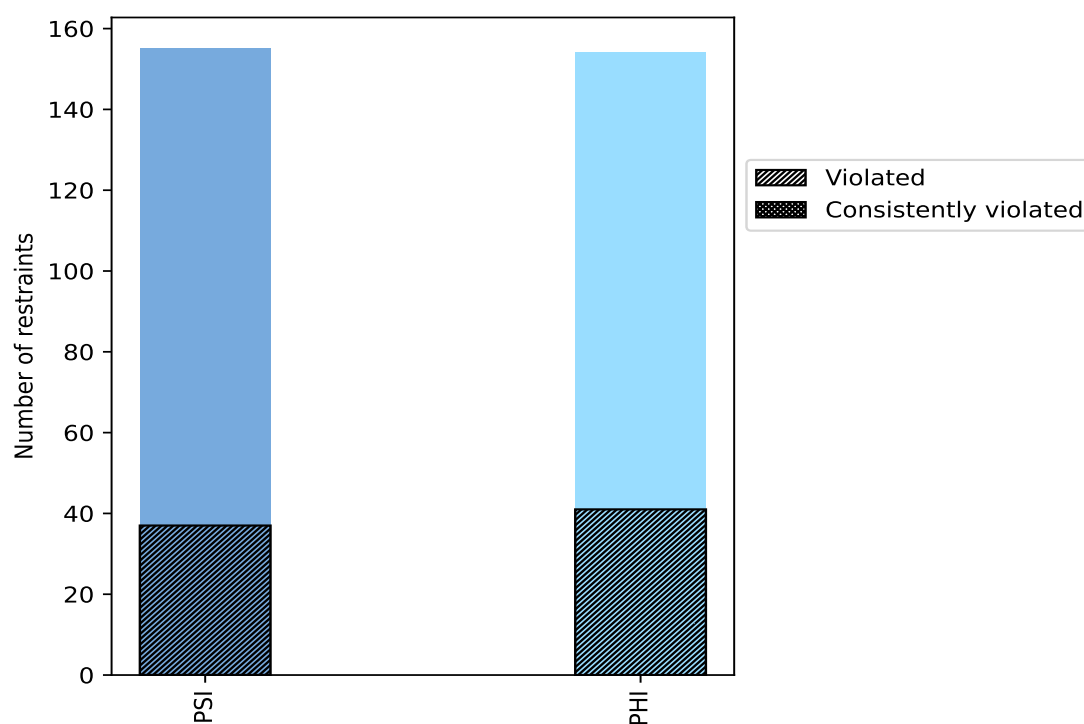
10.1 Summary of dihedral-angle violations [i](#)

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
PSI	155	50.2	37	23.9	12.0	0	0.0	0.0
PHI	154	49.8	41	26.6	13.3	0	0.0	0.0
Total	309	100.0	78	25.2	25.2	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](#)



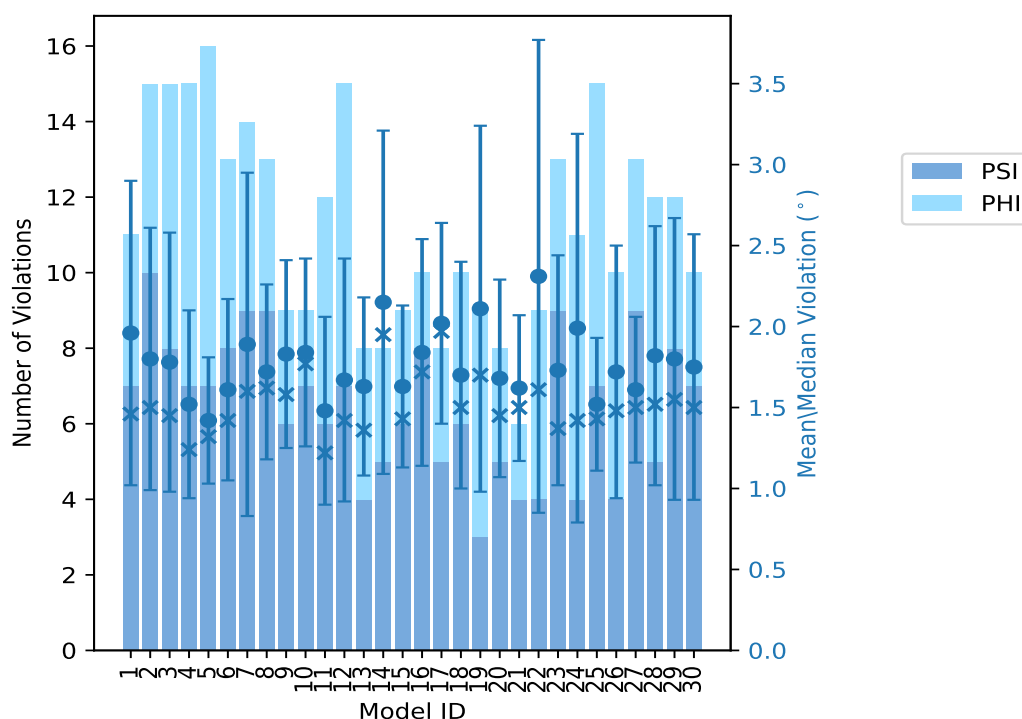
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PSI	PHI	Total				
1	7	4	11	1.96	3.72	0.94	1.46
2	10	5	15	1.8	4.09	0.81	1.5
3	8	7	15	1.78	4.11	0.8	1.45
4	7	8	15	1.52	3.03	0.58	1.24
5	7	9	16	1.42	2.46	0.39	1.32
6	8	5	13	1.61	2.74	0.56	1.42
7	9	5	14	1.89	4.79	1.06	1.6
8	9	4	13	1.72	2.71	0.54	1.62
9	6	3	9	1.83	2.97	0.58	1.58
10	7	2	9	1.84	2.85	0.58	1.77
11	6	6	12	1.48	2.83	0.58	1.22
12	7	8	15	1.67	3.18	0.75	1.42
13	4	4	8	1.63	2.68	0.55	1.36
14	5	3	8	2.15	4.43	1.06	1.95
15	6	3	9	1.63	2.84	0.5	1.43
16	8	2	10	1.84	3.34	0.7	1.72
17	5	3	8	2.02	2.79	0.62	1.97
18	6	4	10	1.7	3.51	0.7	1.5
19	3	6	9	2.11	4.89	1.13	1.7
20	5	3	8	1.68	3.18	0.61	1.45
21	4	2	6	1.62	2.51	0.45	1.5
22	4	5	9	2.31	5.58	1.46	1.61
23	9	4	13	1.73	3.02	0.71	1.37
24	4	7	11	1.99	5.14	1.2	1.42
25	7	8	15	1.52	2.39	0.41	1.43
26	4	6	10	1.72	3.59	0.78	1.48
27	9	4	13	1.61	2.79	0.45	1.5
28	5	7	12	1.82	4.16	0.8	1.52
29	8	4	12	1.8	4.09	0.87	1.55
30	7	3	10	1.75	4.04	0.82	1.5

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 ¹	%
13	19	32	1	3.3
2	6	8	2	6.7
1	4	5	3	10.0
6	3	9	4	13.3
2	1	3	5	16.7
4	3	7	6	20.0
0	0	0	7	23.3
2	1	3	8	26.7
0	2	2	9	30.0
2	0	2	10	33.3
0	0	0	11	36.7

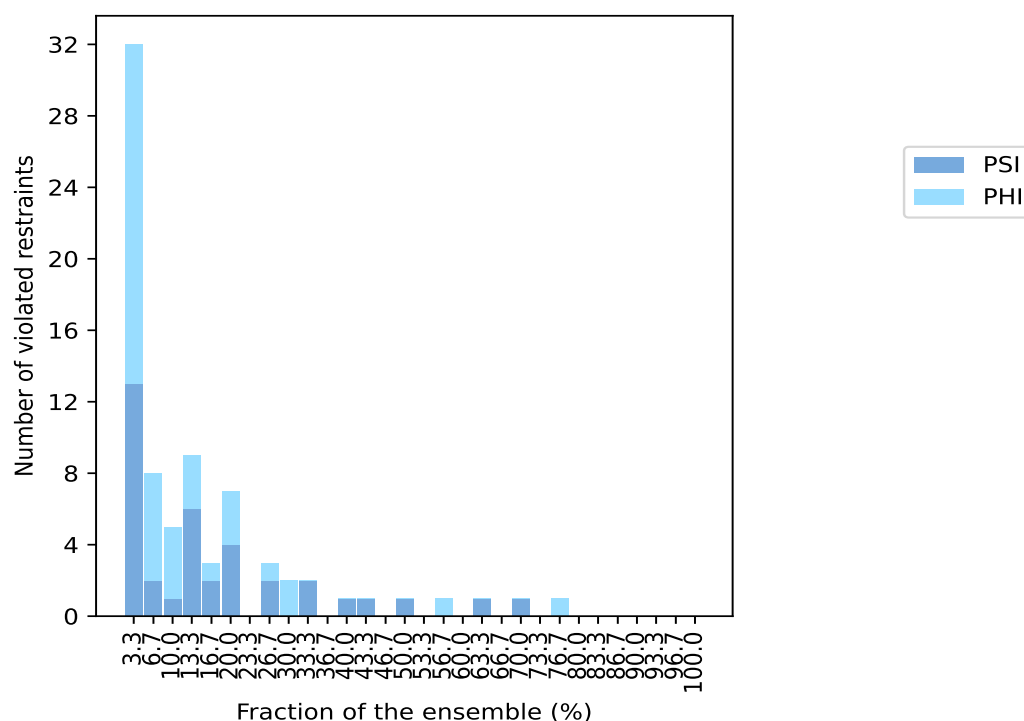
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
1	0	1	12	40.0
1	0	1	13	43.3
0	0	0	14	46.7
1	0	1	15	50.0
0	0	0	16	53.3
0	1	1	17	56.7
0	0	0	18	60.0
1	0	1	19	63.3
0	0	0	20	66.7
1	0	1	21	70.0
0	0	0	22	73.3
0	1	1	23	76.7
0	0	0	24	80.0
0	0	0	25	83.3
0	0	0	26	86.7
0	0	0	27	90.0
0	0	0	28	93.3
0	0	0	29	96.7
0	0	0	30	100.0

¹ Number of models with violations

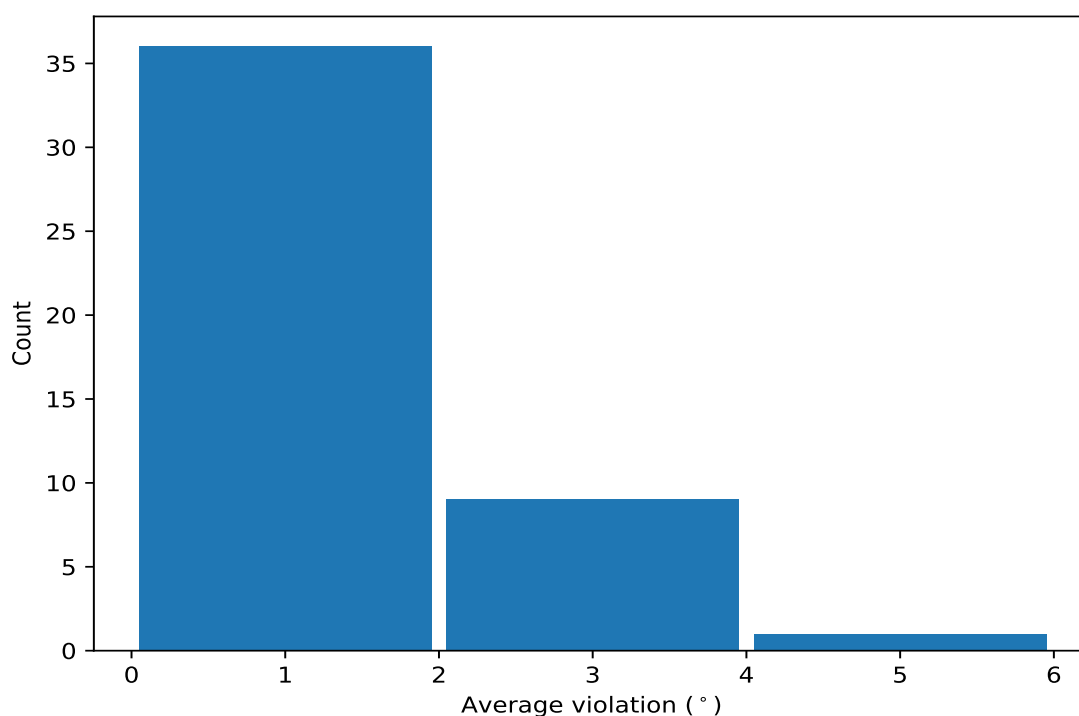
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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 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.

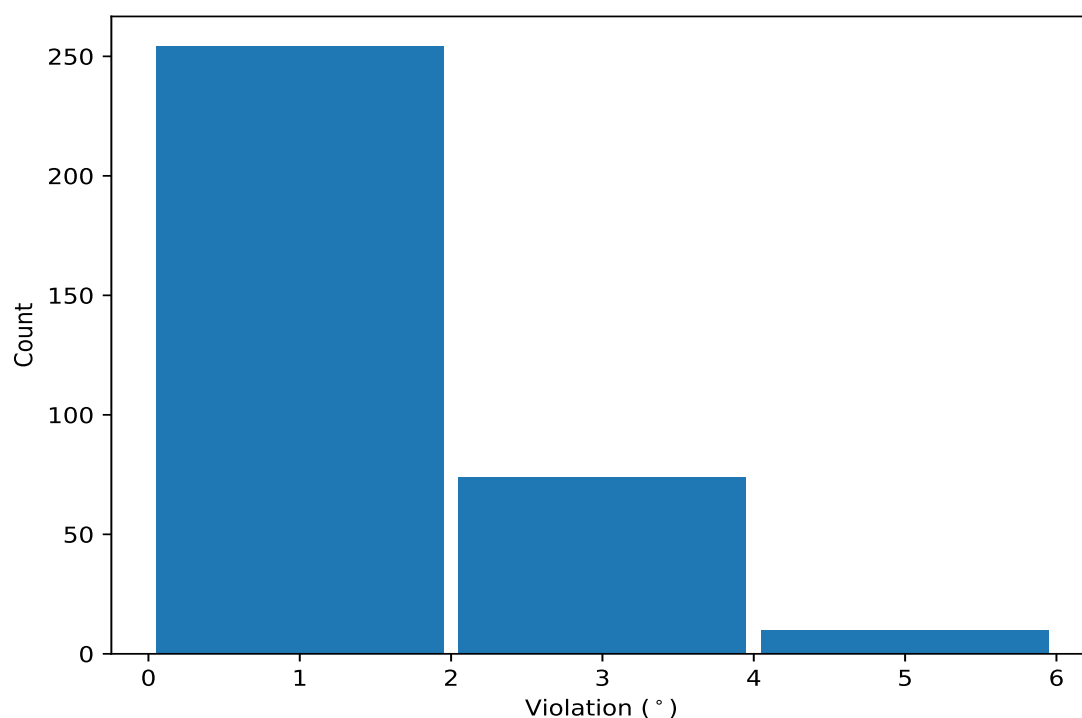
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,150)	1:288:A:GLY:C	1:289:A:CYS:N	1:289:A:CYS:CA	1:289:A:CYS:C	23	1.84	0.61	1.65
(1,271)	1:356:A:PHE:N	1:356:A:PHE:CA	1:356:A:PHE:C	1:357:A:GLN:N	21	2.46	0.42	2.49
(1,185)	1:308:A:PHE:N	1:308:A:PHE:CA	1:308:A:PHE:C	1:309:A:ALA:N	19	2.03	0.79	1.89
(1,104)	1:259:A:LEU:C	1:260:A:ASP:N	1:260:A:ASP:CA	1:260:A:ASP:C	17	2.72	1.17	2.83
(1,261)	1:350:A:TYR:N	1:350:A:TYR:CA	1:350:A:TYR:C	1:351:A:ARG:N	15	2.16	0.72	2.0
(1,231)	1:334:A:SER:N	1:334:A:SER:CA	1:334:A:SER:C	1:335:A:ILE:N	13	1.4	0.22	1.34
(1,134)	1:277:A:TRP:N	1:277:A:TRP:CA	1:277:A:TRP:C	1:278:A:PHE:N	12	1.41	0.21	1.43
(1,279)	1:362:A:LEU:N	1:362:A:LEU:CA	1:362:A:LEU:C	1:363:A:GLU:N	10	1.45	0.1	1.42
(1,171)	1:299:A:GLU:N	1:299:A:GLU:CA	1:299:A:GLU:C	1:300:A:ASN:N	10	1.15	0.1	1.17
(1,106)	1:260:A:ASP:C	1:261:A:LEU:N	1:261:A:LEU:CA	1:261:A:LEU:C	9	1.67	0.47	1.58

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 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 (°)
(1,275)	1:358:A:PRO:N	1:358:A:PRO:CA	1:358:A:PRO:C	1:359:A:TRP:N	22	5.58
(1,275)	1:358:A:PRO:N	1:358:A:PRO:CA	1:358:A:PRO:C	1:359:A:TRP:N	24	5.14
(1,104)	1:259:A:LEU:C	1:260:A:ASP:N	1:260:A:ASP:CA	1:260:A:ASP:C	19	4.89
(1,64)	1:232:A:ASP:C	1:233:A:GLN:N	1:233:A:GLN:CA	1:233:A:GLN:C	7	4.79
(1,275)	1:358:A:PRO:N	1:358:A:PRO:CA	1:358:A:PRO:C	1:359:A:TRP:N	14	4.43
(1,275)	1:358:A:PRO:N	1:358:A:PRO:CA	1:358:A:PRO:C	1:359:A:TRP:N	28	4.16
(1,104)	1:259:A:LEU:C	1:260:A:ASP:N	1:260:A:ASP:CA	1:260:A:ASP:C	3	4.11
(1,150)	1:288:A:GLY:C	1:289:A:CYS:N	1:289:A:CYS:CA	1:289:A:CYS:C	29	4.09
(1,104)	1:259:A:LEU:C	1:260:A:ASP:N	1:260:A:ASP:CA	1:260:A:ASP:C	2	4.09
(1,185)	1:308:A:PHE:N	1:308:A:PHE:CA	1:308:A:PHE:C	1:309:A:ALA:N	30	4.04