



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 6SDW / pdb_00006sdw
BMRB ID : 34421
Title : Solution structure of Staufen1 dsRBD3+4 - hARF1 SBS dsRNA complex.
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Deposited on : 2019-07-29

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

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<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

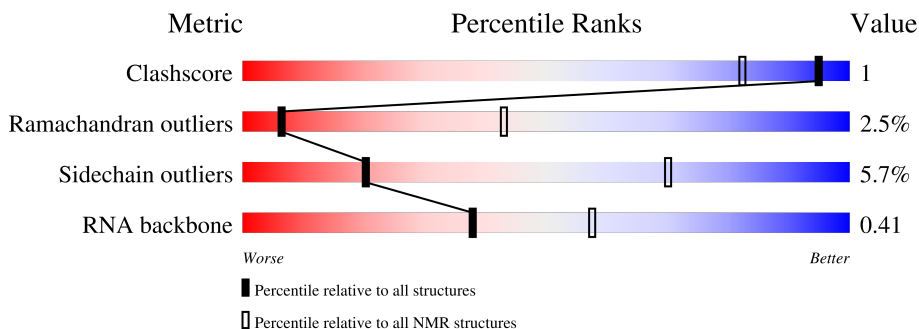
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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
RNA backbone	8273	777

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	177	
2	B	34	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:103-A:121, A:137-A:148, A:157-A:169, A:204-A:274 (115)	1.24	1

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 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3949 atoms, of which 1842 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Double-stranded RNA-binding protein Staufen homolog 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	177	2863	879	1476	254	250	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	GLY	-	expression tag	UNP O95793
A	99	SER	-	expression tag	UNP O95793
A	100	HIS	-	expression tag	UNP O95793
A	101	MET	-	expression tag	UNP O95793

- Molecule 2 is a RNA chain called hARF1 SBS dsRNA.

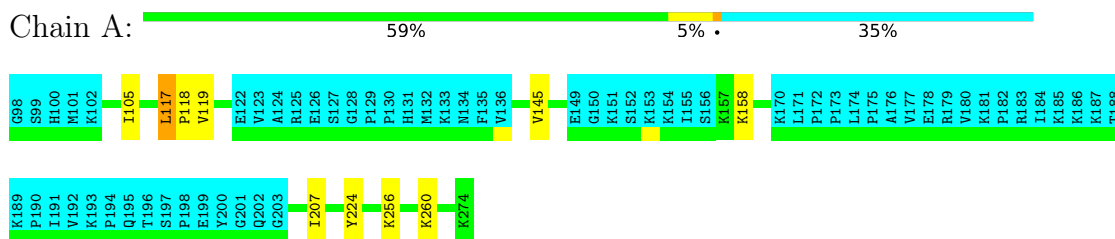
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	34	1086	322	366	126	239	33	0

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: Double-stranded RNA-binding protein Staufen homolog 1



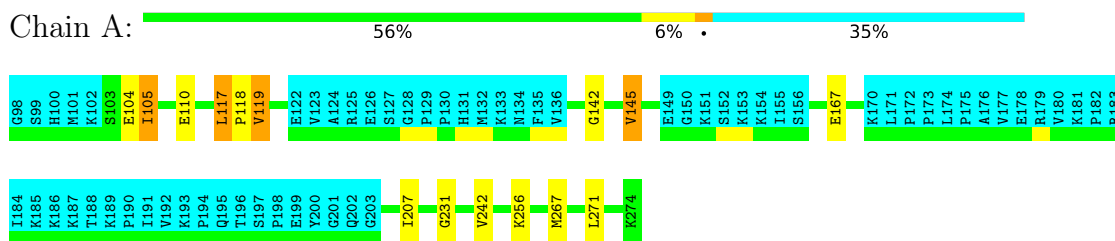
- Molecule 2: hARF1 SBS dsRNA



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

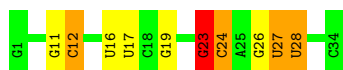
The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Double-stranded RNA-binding protein Staufen homolog 1



- Molecule 2: hARF1 SBS dsRNA





5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
Amber	refinement	AMBER14
CYANA	structure calculation	cyana-3.98.5
ATNOS-CANDID	structure calculation	UNIO 2.0.3
PROCHECK / PROCHECK-NMR	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	2385
Number of shifts mapped to atoms	2385
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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.90±0.01	0±0/914 (0.0± 0.0%)	1.50±0.03	4±2/1224 (0.3± 0.2%)
2	B	0.84±0.01	0±0/803 (0.0± 0.0%)	1.38±0.03	8±2/1250 (0.6± 0.2%)
All	All	0.87	0/34340 (0.0%)	1.44	235/49480 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
2	B	0.0±0.0	9.1±1.9
All	All	0	182

There are no bond-length outliers.

5 of 58 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	28	U	C3'-C2'-C1'	9.87	111.17	101.30	18	16
1	A	266	ASN	CA-CB-CG	9.46	122.06	112.60	4	1
2	B	28	U	O4'-C4'-C3'	7.46	111.46	104.00	14	16
2	B	28	U	O4'-C1'-N1	7.33	119.49	108.50	19	11
1	A	206	PRO	CA-C-N	7.31	129.83	120.70	12	9

There are no chirality outliers.

5 of 27 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	B	23	G	Sidechain	19
2	B	26	G	Sidechain	16

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Mol	Chain	Res	Type	Group	Models (Total)
2	B	21	A	Sidechain	16
2	B	20	G	Sidechain	13
2	B	9	C	Sidechain	12

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	904	952	952	3±1
2	B	720	366	366	1±1
All	All	32480	26360	26372	63

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 1.

5 of 18 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:224:TYR:CZ	1:A:260:LYS:HE3	0.51	2.40	20	15
1:A:117:LEU:H	1:A:118:PRO:CD	0.49	2.21	11	15
1:A:256:LYS:HE3	2:B:23:G:H5''	0.48	1.85	1	11
1:A:158:LYS:HA	1:A:158:LYS:HE3	0.48	1.85	9	3
1:A:207:ILE:HG21	2:B:7:A:H5'	0.48	1.83	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	114/177 (64%)	97±3 (85±3%)	14±3 (12±3%)	3±1 (2±1%)	6	43
All	All	2280/3540 (64%)	1944 (85%)	280 (12%)	56 (2%)	6	43

5 of 17 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	117	LEU	20
1	A	119	VAL	10
1	A	142	GLY	5
1	A	118	PRO	4
1	A	231	GLY	3

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	97/152 (64%)	92±2 (94±2%)	6±2 (6±2%)	20 70
All	All	1940/3040 (64%)	1830 (94%)	110 (6%)	20 70

5 of 29 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	207	ILE	16
1	A	145	VAL	10
1	A	105	ILE	8
1	A	165	LEU	8
1	A	119	VAL	6

6.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	B	33/34 (97%)	2±0 (6±0%)	2±1 (6±2%)	0.48±0.00
All	All	660/680 (97%)	40 (6%)	38 (6%)	0.48

The overall RNA backbone suiteness is 0.41.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	23	G	20

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Mol	Chain	Res	Type	Models (Total)
2	B	24	C	20

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	23	G	19
2	B	28	U	16
2	B	33	C	2
2	B	2	G	1

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 76% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: starch_output_prot_RBD3

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	1942
Number of shifts mapped to atoms	1942
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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
$^{13}\text{C}_\alpha$	151	-0.35 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	140	-0.03 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	132	0.05 ± 0.14	None needed (< 0.5 ppm)
^{15}N	139	0.04 ± 0.24	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 65%, i.e. 1476 atoms were assigned a chemical shift out of a possible 2267. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	559/575 (97%)	230/234 (98%)	221/230 (96%)	108/111 (97%)
Sidechain	867/985 (88%)	590/636 (93%)	262/302 (87%)	15/47 (32%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	50/66 (76%)	31/33 (94%)	19/32 (59%)	0/1 (0%)
Sugar	0/374 (0%)	0/204 (0%)	0/170 (0%)	0/0 (—%)
Base	0/267 (0%)	0/165 (0%)	0/57 (0%)	0/45 (0%)
Overall	1476/2267 (65%)	851/1272 (67%)	502/791 (63%)	123/204 (60%)

7.1.4 Statistically unusual chemical shifts [i](#)

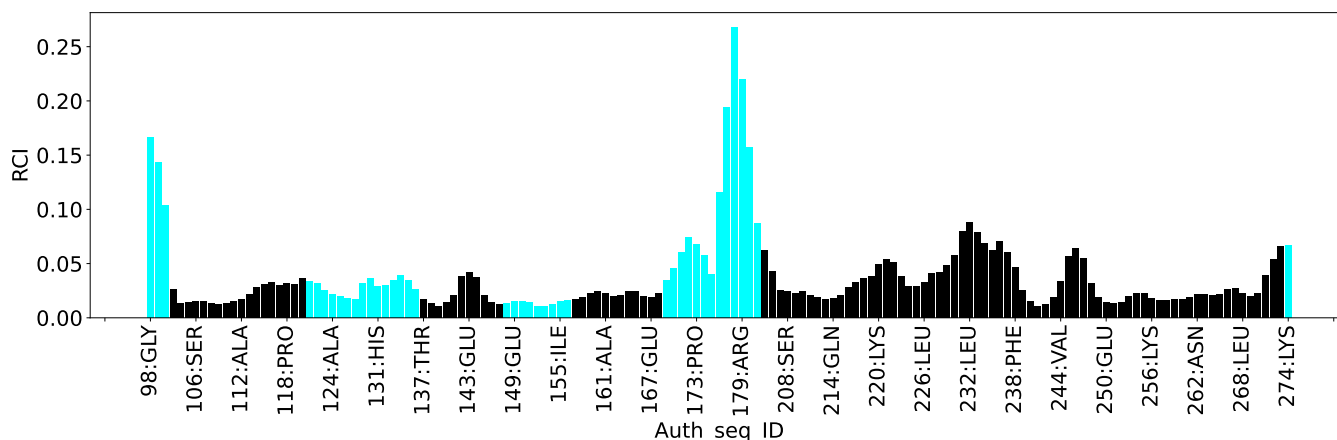
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	260	LYS	HE3	1.51	1.92 – 3.89	-7.1
1	A	175	PRO	CA	54.92	55.85 – 70.84	-5.6
1	A	260	LYS	HE2	1.87	1.95 – 3.88	-5.4

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: starch_output_dsRNA-hARF1

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	443
Number of shifts mapped to atoms	443
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

7.2.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

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 19%, i.e. 427 atoms were assigned a chemical shift out of a possible 2267. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/575 (0%)	0/234 (0%)	0/230 (0%)	0/111 (0%)
Sidechain	0/985 (0%)	0/636 (0%)	0/302 (0%)	0/47 (0%)
Aromatic	0/66 (0%)	0/33 (0%)	0/32 (0%)	0/1 (0%)
Sugar	368/374 (98%)	200/204 (98%)	168/170 (99%)	0/0 (—%)
Base	59/267 (22%)	49/165 (30%)	10/57 (18%)	0/45 (0%)
Overall	427/2267 (19%)	249/1272 (20%)	178/791 (23%)	0/204 (0%)

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins

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	3249
Intra-residue ($ i-j =0$)	976
Sequential ($ i-j =1$)	877
Medium range ($ i-j >1$ and $ i-j <5$)	434
Long range ($ i-j \geq 5$)	697
Inter-chain	156
Hydrogen bond restraints	109
Disulfide bond restraints	0
Total dihedral-angle restraints	846
Number of unmapped restraints	0
Number of restraints per residue	19.4
Number of long range restraints per residue ¹	3.7

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)	8.9	0.2
0.2-0.5 (Medium)	1.1	0.44
>0.5 (Large)	1.1	1.78

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)	2.0	3.3
10.0-20.0 (Medium)	None	None
>20.0 (Large)	145.0	170.0

9 Distance violation analysis [i](#)

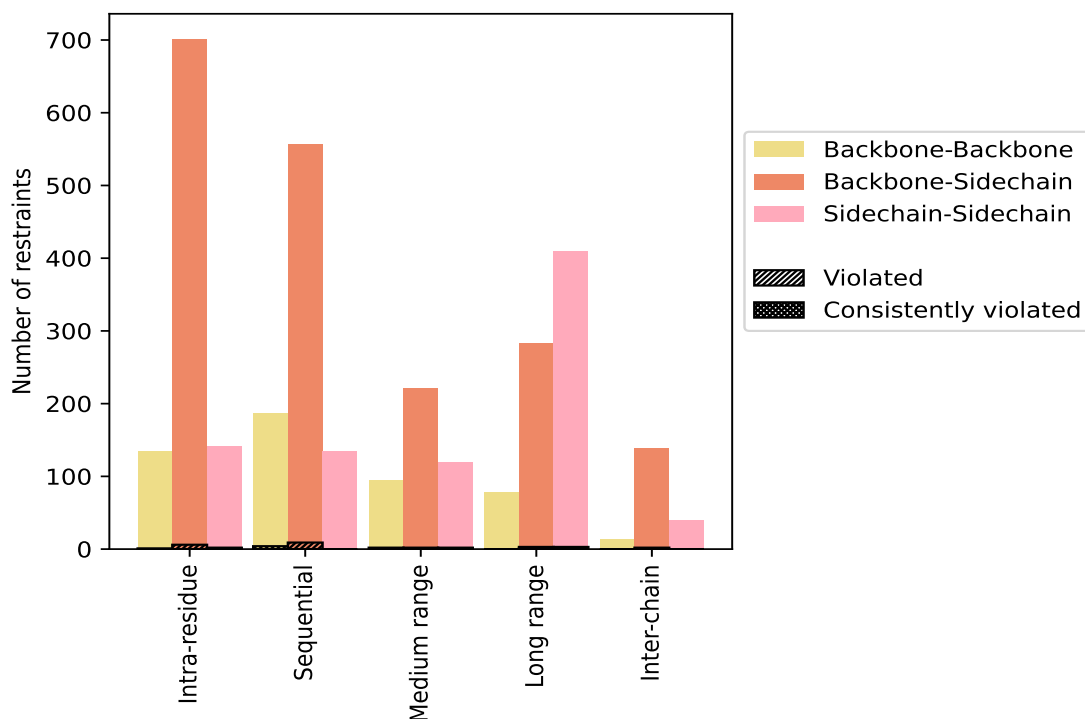
9.1 Summary of distance violations [i](#)

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 ($i-j =0$)	976	30.0	9	0.9	0.3	1	0.1	0.0
Backbone-Backbone	134	4.1	1	0.7	0.0	0	0.0	0.0
Backbone-Sidechain	701	21.6	6	0.9	0.2	0	0.0	0.0
Sidechain-Sidechain	141	4.3	2	1.4	0.1	1	0.7	0.0
Sequential ($i-j =1$)	877	27.0	13	1.5	0.4	0	0.0	0.0
Backbone-Backbone	186	5.7	4	2.2	0.1	0	0.0	0.0
Backbone-Sidechain	557	17.1	9	1.6	0.3	0	0.0	0.0
Sidechain-Sidechain	134	4.1	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	434	13.4	6	1.4	0.2	0	0.0	0.0
Backbone-Backbone	94	2.9	2	2.1	0.1	0	0.0	0.0
Backbone-Sidechain	221	6.8	2	0.9	0.1	0	0.0	0.0
Sidechain-Sidechain	119	3.7	2	1.7	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	697	21.5	6	0.9	0.2	1	0.1	0.0
Backbone-Backbone	78	2.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	283	8.7	3	1.1	0.1	1	0.4	0.0
Sidechain-Sidechain	336	10.3	3	0.9	0.1	0	0.0	0.0
Inter-chain	156	4.8	2	1.3	0.1	0	0.0	0.0
Backbone-Backbone	13	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	134	4.1	2	1.5	0.1	0	0.0	0.0
Sidechain-Sidechain	9	0.3	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	109	3.4	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	3249	100.0	36	1.1	1.1	2	0.1	0.1
Backbone-Backbone	505	15.5	7	1.4	0.2	0	0.0	0.0
Backbone-Sidechain	1901	58.5	22	1.2	0.7	1	0.1	0.0
Sidechain-Sidechain	843	25.9	7	0.8	0.2	1	0.1	0.0

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfid 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	4	0	1	3	2	10	0.4	1.77	0.51	0.18
2	2	1	2	6	1	12	0.19	0.84	0.2	0.12
3	5	3	2	2	2	14	0.22	1.12	0.25	0.15
4	4	2	1	2	1	10	0.15	0.28	0.05	0.14
5	5	1	3	5	2	16	0.31	1.77	0.43	0.14
6	3	2	3	3	2	13	0.32	1.7	0.46	0.13
7	1	2	2	4	2	11	0.19	0.75	0.18	0.13
8	2	0	2	2	2	8	0.45	1.75	0.55	0.15
9	3	2	2	2	1	10	0.32	1.19	0.38	0.14
10	3	5	2	1	1	12	0.16	0.34	0.07	0.15

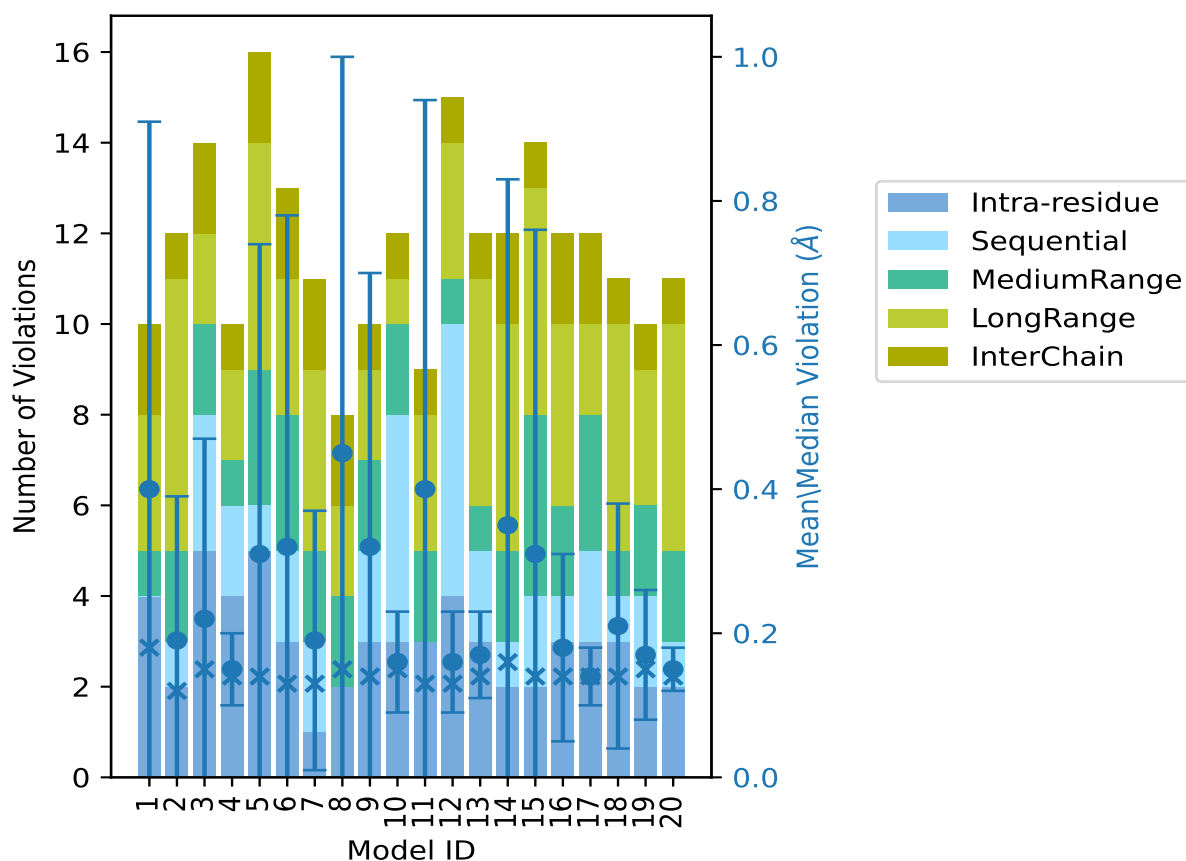
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	3	0	2	3	1	9	0.4	1.74	0.54	0.13
12	4	6	1	3	1	15	0.16	0.38	0.07	0.13
13	3	2	1	5	1	12	0.17	0.31	0.06	0.14
14	2	1	2	5	2	12	0.35	1.78	0.48	0.16
15	2	2	4	5	1	14	0.31	1.72	0.45	0.14
16	3	1	2	4	2	12	0.18	0.61	0.13	0.14
17	3	2	3	2	2	12	0.14	0.24	0.04	0.14
18	3	1	1	5	1	11	0.21	0.72	0.17	0.14
19	2	2	2	3	1	10	0.17	0.44	0.09	0.15
20	2	1	2	5	1	11	0.15	0.23	0.03	0.14

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

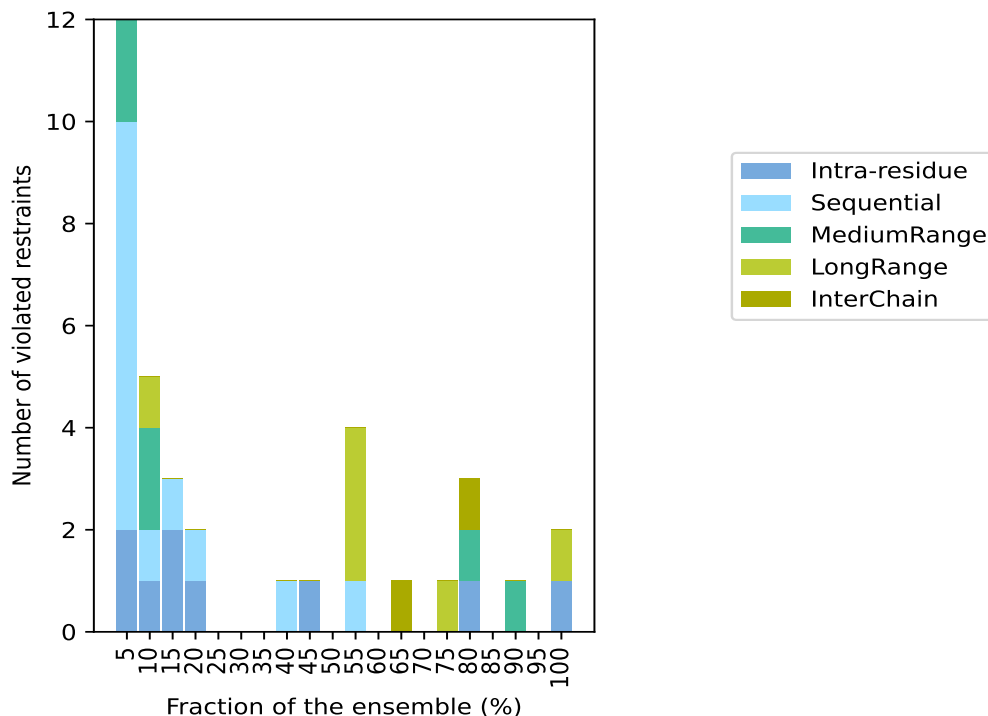
9.3 Distance violation statistics for the ensemble

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, 3104(IR:967, SQ:864, MR:428, LR:691, IC:154) 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	%
2	8	2	0	0	12	1	5.0
1	1	2	1	0	5	2	10.0
2	1	0	0	0	3	3	15.0
1	1	0	0	0	2	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	1	0	0	0	1	8	40.0
1	0	0	0	0	1	9	45.0
0	0	0	0	0	0	10	50.0
0	1	0	3	0	4	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	1	1	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	1	0	1	15	75.0
1	0	1	0	1	3	16	80.0
0	0	0	0	0	0	17	85.0
0	0	1	0	0	1	18	90.0
0	0	0	0	0	0	19	95.0
1	0	0	1	0	2	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶ Number of models with violations

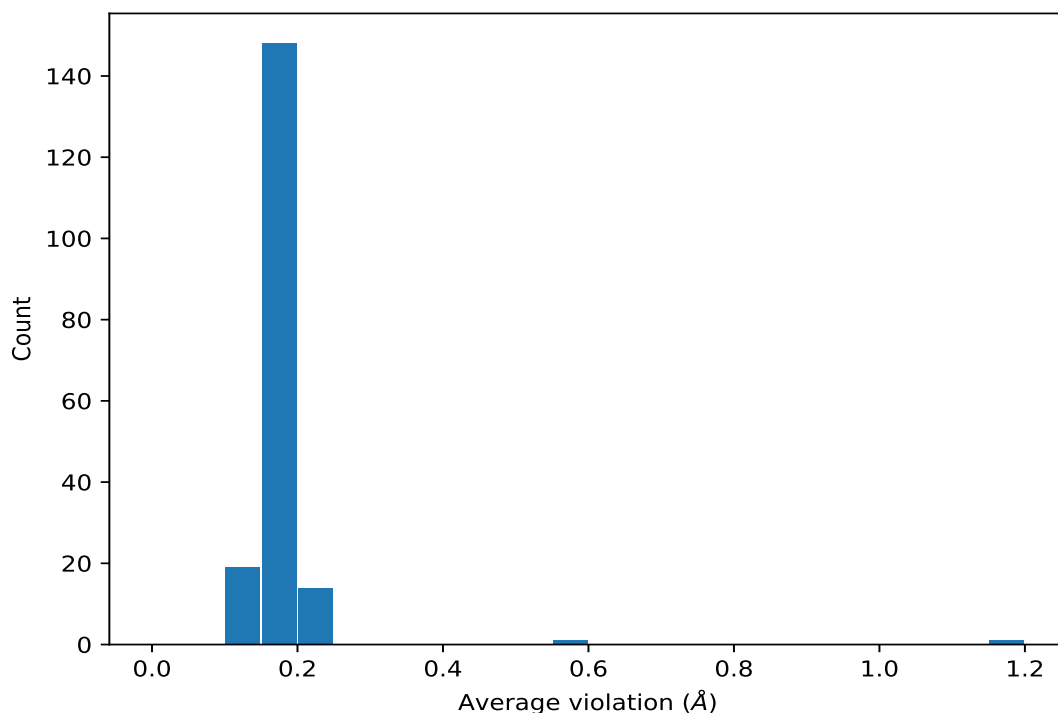
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 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)
(1,2430)	2:5:B:G:H1'	2:31:B:U:H3	20	0.14	0.02	0.15
(1,1016)	1:113:A:LEU:HB2	1:113:A:LEU:HG	20	0.12	0.0	0.12
(1,2875)	2:16:B:U:H5''	2:19:B:G:H1	18	0.13	0.01	0.13
(1,829)	1:104:A:GLU:HG2	1:107:A:GLN:HE22	16	1.15	0.58	1.16
(1,881)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	16	0.59	0.37	0.64
(1,3102)	1:256:A:LYS:HE3	2:23:B:G:H5'	16	0.13	0.02	0.14
(1,2469)	2:26:B:G:H1'	2:10:B:U:H3	15	0.11	0.01	0.11
(1,3124)	1:215:A:GLN:HE22	2:31:B:U:H1'	13	0.23	0.07	0.25
(1,151)	1:139:A:VAL:HG22	1:164:A:VAL:HG11	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG22	1:164:A:VAL:HG12	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG22	1:164:A:VAL:HG13	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG22	1:164:A:VAL:HG21	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG22	1:164:A:VAL:HG22	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG22	1:164:A:VAL:HG23	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG23	1:164:A:VAL:HG11	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG23	1:164:A:VAL:HG12	11	0.17	0.02	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,151)	1:139:A:VAL:HG23	1:164:A:VAL:HG13	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG23	1:164:A:VAL:HG21	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG23	1:164:A:VAL:HG22	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG23	1:164:A:VAL:HG23	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG11	1:164:A:VAL:HG11	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG11	1:164:A:VAL:HG12	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG11	1:164:A:VAL:HG13	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG11	1:164:A:VAL:HG21	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG11	1:164:A:VAL:HG22	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG11	1:164:A:VAL:HG23	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG12	1:164:A:VAL:HG11	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG12	1:164:A:VAL:HG12	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG12	1:164:A:VAL:HG13	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG12	1:164:A:VAL:HG21	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG12	1:164:A:VAL:HG22	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG12	1:164:A:VAL:HG23	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG13	1:164:A:VAL:HG11	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG13	1:164:A:VAL:HG12	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG13	1:164:A:VAL:HG13	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG13	1:164:A:VAL:HG21	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG13	1:164:A:VAL:HG22	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG13	1:164:A:VAL:HG23	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG21	1:164:A:VAL:HG11	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG21	1:164:A:VAL:HG12	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG21	1:164:A:VAL:HG13	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG21	1:164:A:VAL:HG21	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG21	1:164:A:VAL:HG22	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG21	1:164:A:VAL:HG23	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG22	1:164:A:VAL:HG11	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG22	1:164:A:VAL:HG12	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG22	1:164:A:VAL:HG13	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG22	1:164:A:VAL:HG21	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG22	1:164:A:VAL:HG22	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG22	1:164:A:VAL:HG23	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG23	1:164:A:VAL:HG11	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG23	1:164:A:VAL:HG12	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG23	1:164:A:VAL:HG13	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG23	1:164:A:VAL:HG21	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG23	1:164:A:VAL:HG22	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG23	1:164:A:VAL:HG23	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG11	1:164:A:VAL:HG11	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG11	1:164:A:VAL:HG12	11	0.17	0.02	0.18

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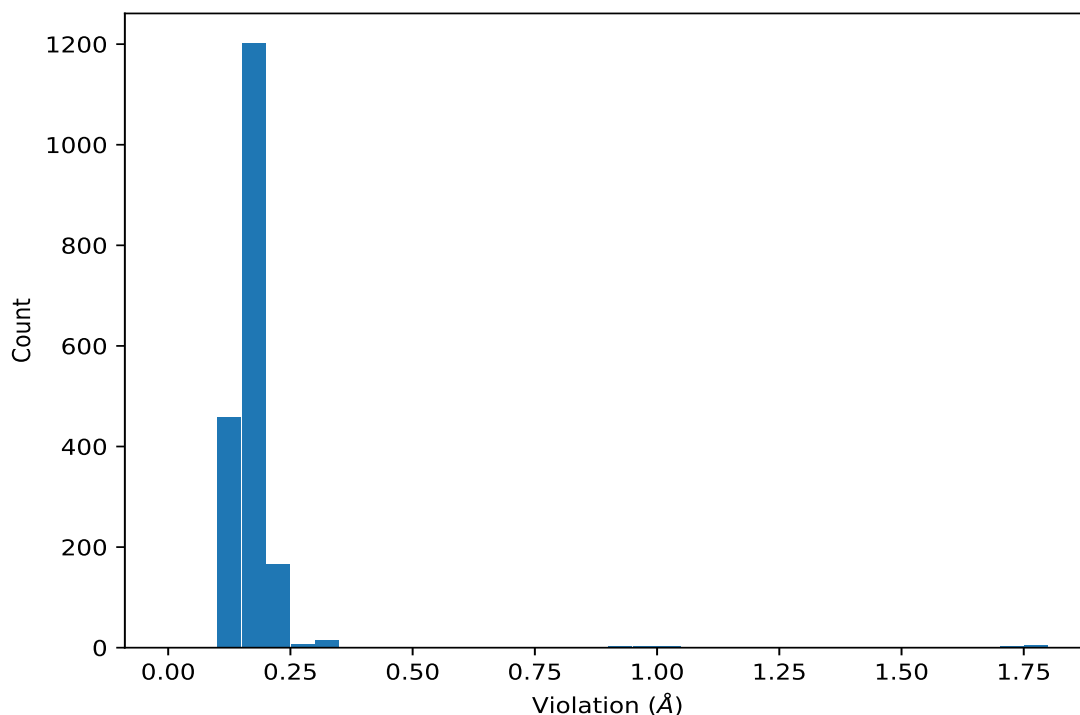
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,151)	1:139:A:VAL:HG11	1:164:A:VAL:HG13	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG11	1:164:A:VAL:HG21	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG11	1:164:A:VAL:HG22	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG11	1:164:A:VAL:HG23	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG12	1:164:A:VAL:HG11	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG12	1:164:A:VAL:HG12	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG12	1:164:A:VAL:HG13	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG12	1:164:A:VAL:HG21	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG12	1:164:A:VAL:HG22	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG12	1:164:A:VAL:HG23	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG13	1:164:A:VAL:HG11	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG13	1:164:A:VAL:HG12	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG13	1:164:A:VAL:HG13	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG13	1:164:A:VAL:HG21	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG13	1:164:A:VAL:HG22	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG13	1:164:A:VAL:HG23	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG21	1:164:A:VAL:HG11	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG21	1:164:A:VAL:HG12	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG21	1:164:A:VAL:HG13	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG21	1:164:A:VAL:HG21	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG21	1:164:A:VAL:HG22	11	0.17	0.02	0.18
(1,151)	1:139:A:VAL:HG21	1:164:A:VAL:HG23	11	0.17	0.02	0.18
(1,181)	1:139:A:VAL:HG22	1:164:A:VAL:HG11	11	0.17	0.02	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)
(1,829)	1:104:A:GLU:HG2	1:107:A:GLN:HE22	14	1.78
(1,829)	1:104:A:GLU:HG2	1:107:A:GLN:HE22	1	1.77
(1,829)	1:104:A:GLU:HG2	1:107:A:GLN:HE22	5	1.77
(1,829)	1:104:A:GLU:HG2	1:107:A:GLN:HE22	8	1.75
(1,829)	1:104:A:GLU:HG2	1:107:A:GLN:HE22	11	1.74
(1,829)	1:104:A:GLU:HG2	1:107:A:GLN:HE22	15	1.72
(1,829)	1:104:A:GLU:HG2	1:107:A:GLN:HE22	6	1.7
(1,829)	1:104:A:GLU:HG2	1:107:A:GLN:HE22	9	1.19
(1,829)	1:104:A:GLU:HG2	1:107:A:GLN:HE22	3	1.12
(1,881)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	6	1.01

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

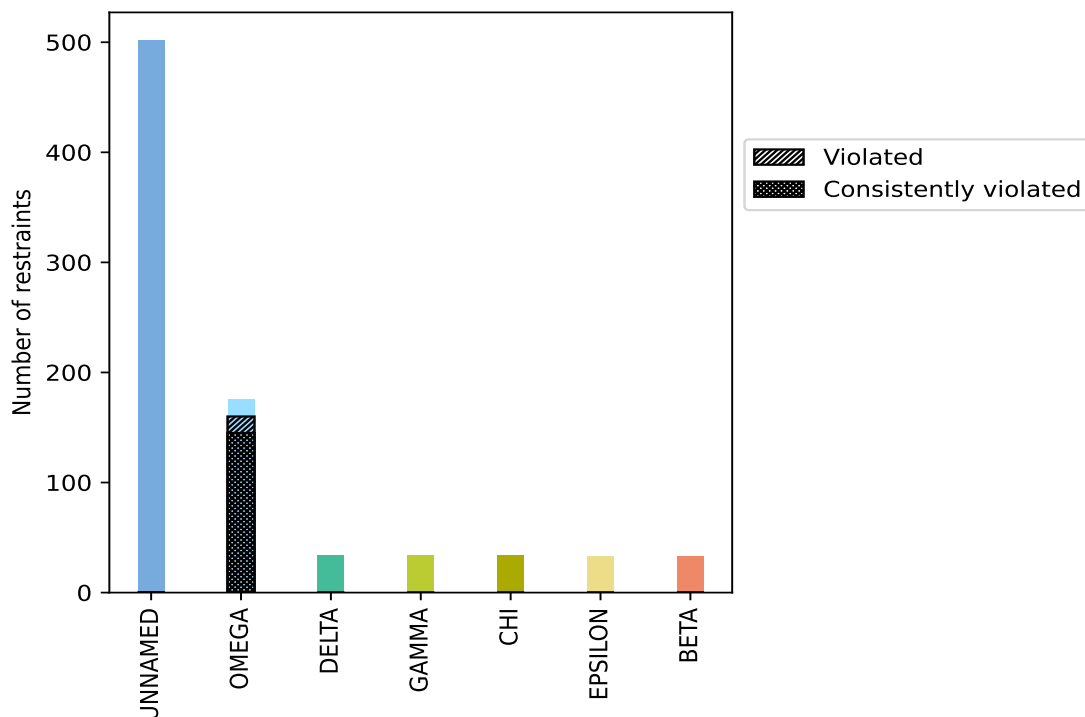
10.1 Summary of dihedral-angle violations [i](#)

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
UNNAMED	502	59.3	0	0.0	0.0	0	0.0	0.0
OMEGA	176	20.8	160	90.9	18.9	145	82.4	17.1
DELTA	34	4.0	0	0.0	0.0	0	0.0	0.0
GAMMA	34	4.0	0	0.0	0.0	0	0.0	0.0
CHI	34	4.0	0	0.0	0.0	0	0.0	0.0
EPSILON	33	3.9	0	0.0	0.0	0	0.0	0.0
BETA	33	3.9	0	0.0	0.0	0	0.0	0.0
Total	846	100.0	160	18.9	18.9	145	17.1	17.1

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](#)



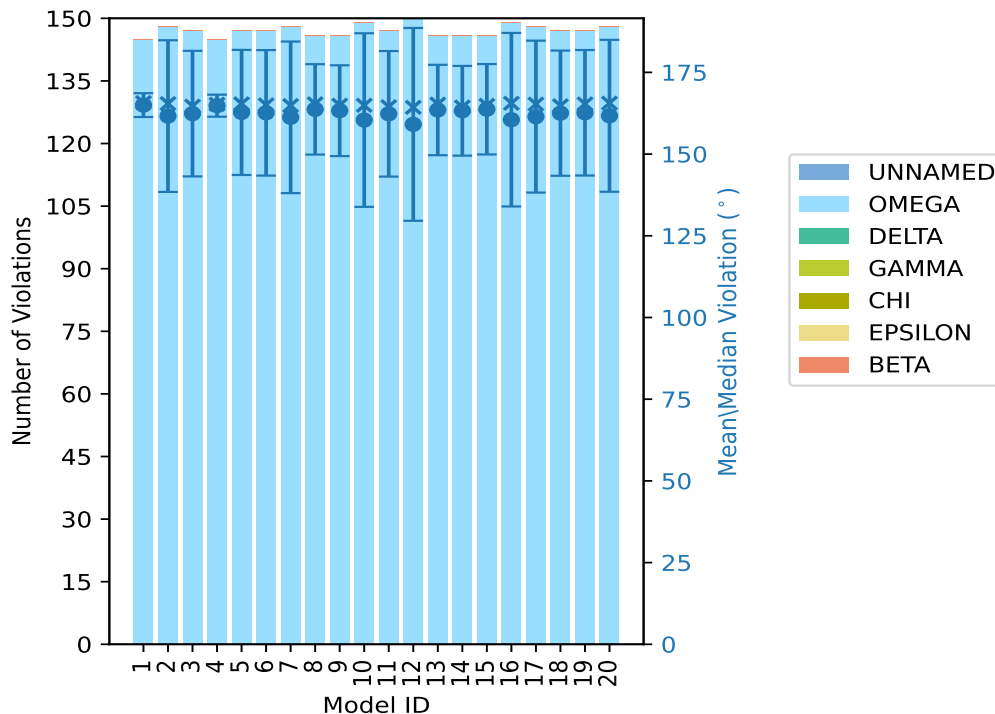
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model [i](#)

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							Total	Mean (°)	Max (°)	SD (°)	Median (°)
	UNNAMED	OMEGA	DELTA	GAMMA	CHI	EPSILON	BETA					
1	0	145	0	0	0	0	0	145	164.99	169.99	3.65	165.75
2	0	148	0	0	0	0	0	148	161.63	169.97	23.2	165.45
3	0	147	0	0	0	0	0	147	162.38	169.91	19.21	164.67
4	0	145	0	0	0	0	0	145	164.81	169.93	3.37	165.25
5	0	147	0	0	0	0	0	147	162.75	169.98	19.14	165.4
6	0	147	0	0	0	0	0	147	162.62	169.93	19.2	165.06
7	0	148	0	0	0	0	0	148	161.25	169.97	23.19	164.86
8	0	146	0	0	0	0	0	146	163.68	169.99	13.83	165.39
9	0	146	0	0	0	0	0	146	163.28	169.95	13.89	164.96
10	0	149	0	0	0	0	0	149	160.41	169.98	26.56	164.93
11	0	147	0	0	0	0	0	147	162.32	169.97	19.21	164.5
12	0	150	0	0	0	0	0	150	159.09	169.98	29.5	164.3
13	0	146	0	0	0	0	0	146	163.49	169.98	13.83	165.31
14	0	146	0	0	0	0	0	146	163.25	169.84	13.73	164.4
15	0	146	0	0	0	0	0	146	163.72	170.0	13.83	164.92
16	0	149	0	0	0	0	0	149	160.52	169.85	26.55	165.55
17	0	148	0	0	0	0	0	148	161.46	169.95	23.24	165.3
18	0	147	0	0	0	0	0	147	162.52	169.99	19.16	164.79
19	0	147	0	0	0	0	0	147	162.64	169.9	19.2	165.36
20	0	148	0	0	0	0	0	148	161.72	169.72	23.24	165.59

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

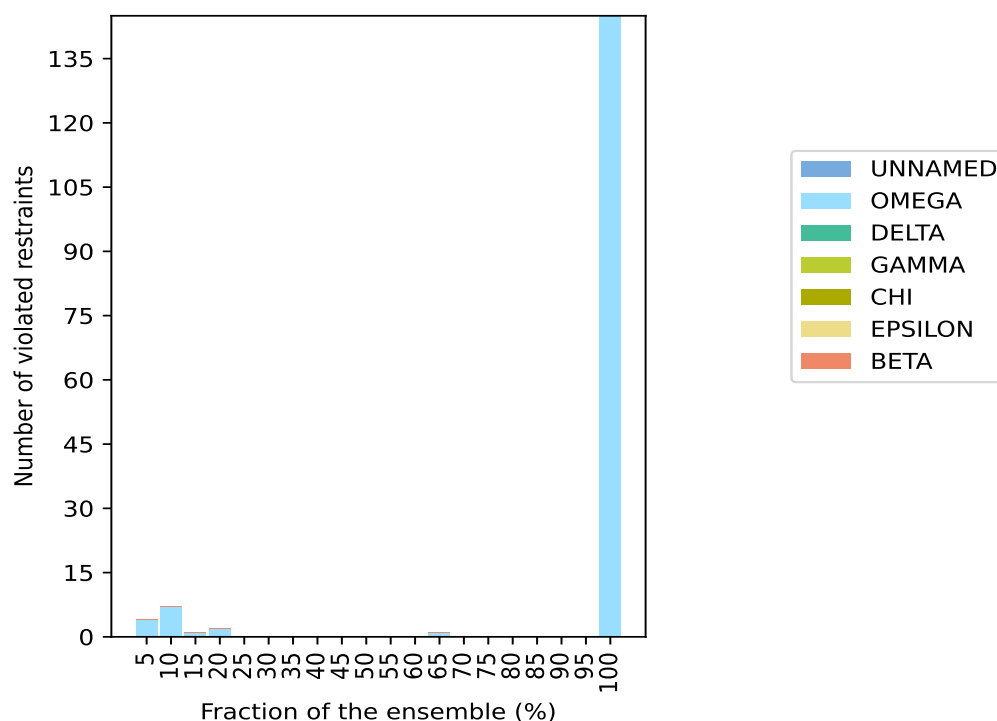
10.3 Dihedral-angle violation statistics for the ensemble

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.

UNNAMED	Number of violated restraints							Fraction of the ensemble	
	OMEGA	DELTA	GAMMA	CHI	EPSILON	BETA	Total	Count ¹	%
0	4	0	0	0	0	0	4	1	5.0
0	7	0	0	0	0	0	7	2	10.0
0	1	0	0	0	0	0	1	3	15.0
0	2	0	0	0	0	0	2	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	1	0	0	0	0	0	1	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	145	0	0	0	0	0	145	20	100.0

¹ Number of models with violations

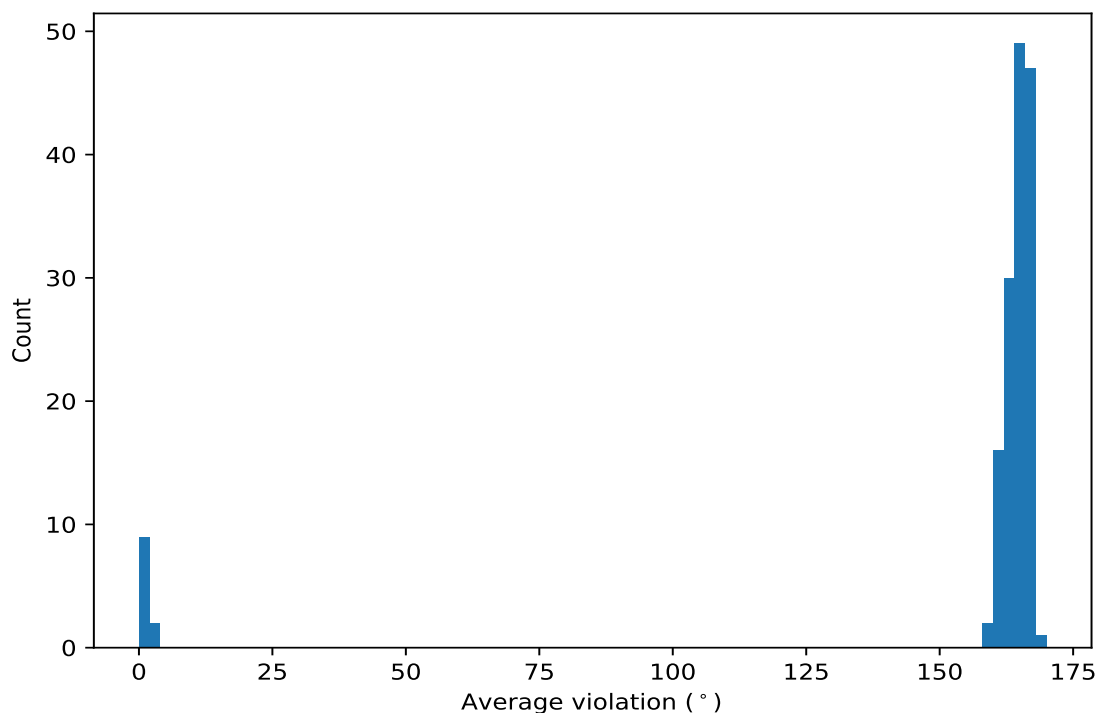
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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 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.

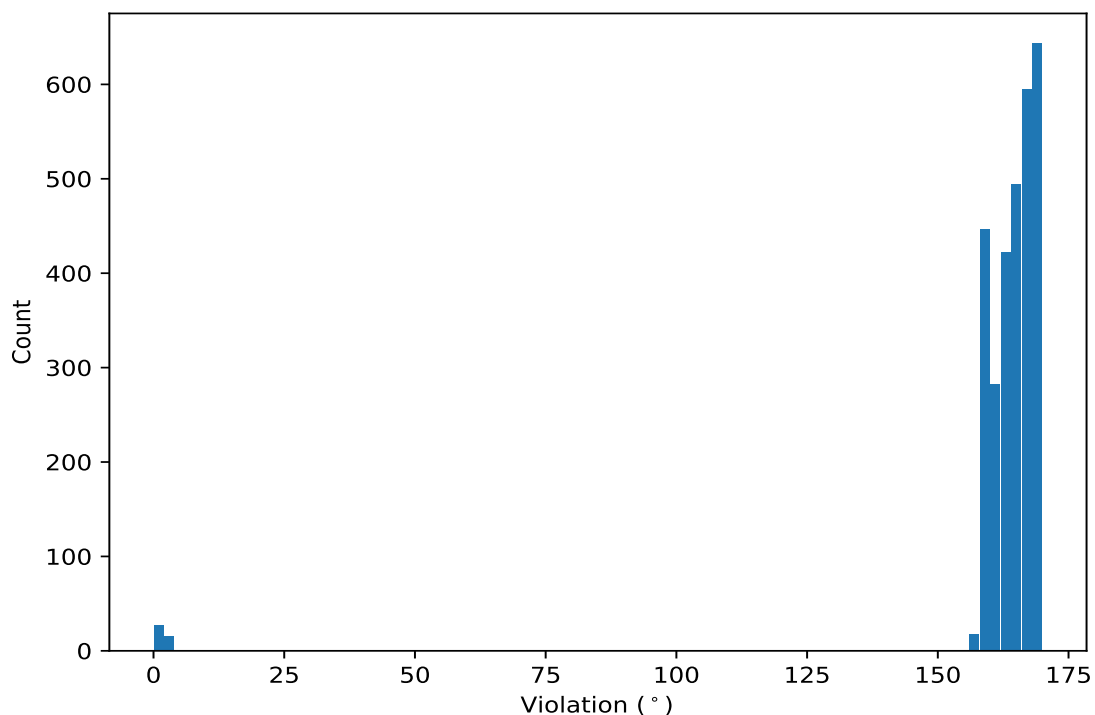
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,823)	1:251:A:GLY:CA	1:251:A:GLY:N	1:250:A:GLU:C	1:250:A:GLU:CA	20	168.61	1.12	169.02
(1,786)	1:214:A:GLN:CA	1:214:A:GLN:N	1:213:A:ILE:C	1:213:A:ILE:CA	20	167.78	1.4	167.62
(1,784)	1:212:A:GLN:CA	1:212:A:GLN:N	1:211:A:ALA:C	1:211:A:ALA:CA	20	167.67	1.6	167.56
(1,718)	1:146:A:GLY:CA	1:146:A:GLY:N	1:145:A:VAL:C	1:145:A:VAL:CA	20	167.52	2.51	168.65
(1,757)	1:185:A:LYS:CA	1:185:A:LYS:N	1:184:A:ILE:C	1:184:A:ILE:CA	20	167.42	1.64	167.32
(1,765)	1:193:A:LYS:CA	1:193:A:LYS:N	1:192:A:VAL:C	1:192:A:VAL:CA	20	167.41	2.04	167.82
(1,818)	1:246:A:ASN:CA	1:246:A:ASN:N	1:245:A:GLY:C	1:245:A:GLY:CA	20	167.34	2.21	167.62
(1,841)	1:269:A:GLU:CA	1:269:A:GLU:N	1:268:A:LEU:C	1:268:A:LEU:CA	20	167.34	1.61	166.97
(1,828)	1:256:A:LYS:CA	1:256:A:LYS:N	1:255:A:ASN:C	1:255:A:ASN:CA	20	167.34	1.28	167.85
(1,822)	1:250:A:GLU:CA	1:250:A:GLU:N	1:249:A:ALA:C	1:249:A:ALA:CA	20	167.31	2.22	167.68

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 (°)
(1,748)	1:176:A:ALA:CA	1:176:A:ALA:N	1:175:A:PRO:C	1:175:A:PRO:CA	15	170.0
(1,786)	1:214:A:GLN:CA	1:214:A:GLN:N	1:213:A:ILE:C	1:213:A:ILE:CA	1	169.99
(1,773)	1:201:A:GLY:CA	1:201:A:GLY:N	1:200:A:TYR:C	1:200:A:TYR:CA	1	169.99
(1,759)	1:187:A:LYS:CA	1:187:A:LYS:N	1:186:A:LYS:C	1:186:A:LYS:CA	18	169.99
(1,743)	1:171:A:LEU:CA	1:171:A:LEU:N	1:170:A:LYS:C	1:170:A:LYS:CA	8	169.99
(1,834)	1:262:A:ASN:CA	1:262:A:ASN:N	1:261:A:ARG:C	1:261:A:ARG:CA	10	169.98
(1,802)	1:230:A:ARG:CA	1:230:A:ARG:N	1:229:A:GLU:C	1:229:A:GLU:CA	5	169.98
(1,768)	1:196:A:THR:CA	1:196:A:THR:N	1:195:A:GLN:C	1:195:A:GLN:CA	1	169.98
(1,760)	1:188:A:THR:CA	1:188:A:THR:N	1:187:A:LYS:C	1:187:A:LYS:CA	13	169.98
(1,718)	1:146:A:GLY:CA	1:146:A:GLY:N	1:145:A:VAL:C	1:145:A:VAL:CA	12	169.98