



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 15, 2026 – 10:40 AM UTC

PDB ID : 6N2M / pdb_00006n2m
BMRB ID : 30543
Title : NMR solution structure of the homodimeric, autoinhibited state of the CARD9 CARD and first coiled-coil
Authors : Holliday, M.J.; Fairbrother, W.J.; Dueber, E.C.
Deposited on : 2018-11-13

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 : **FAILED**
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 45%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 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:8-A:50, A:56-A:140, B:7-B:50, B:56-B:140 (257)	1.16	6

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 2 clusters. No single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4566 atoms, of which 2304 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Caspase recruitment domain-containing protein 9.

Mol	Chain	Residues	Atoms						Trace
1	A	142	Total	C	H	N	O	S	0
			2282	716	1152	187	222	5	
1	B	142	Total	C	H	N	O	S	0
			2282	716	1152	187	222	5	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9H257
B	1	GLY	-	expression tag	UNP Q9H257

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

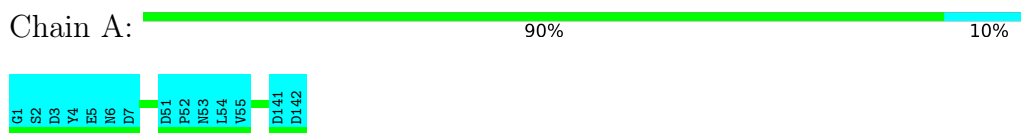
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1
2	B	1	Total	Zn
			1	1

4 Residue-property plots [i](#)

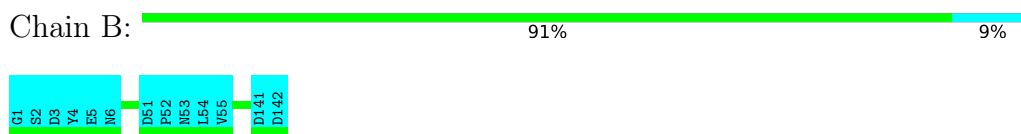
4.1 Average score per residue in the NMR ensemble

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: Caspase recruitment domain-containing protein 9



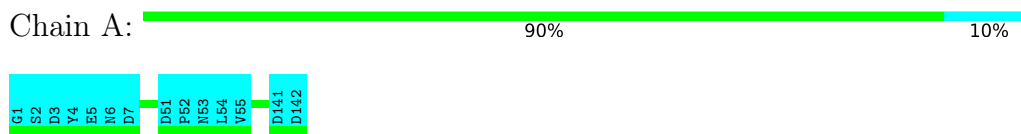
- Molecule 1: Caspase recruitment domain-containing protein 9



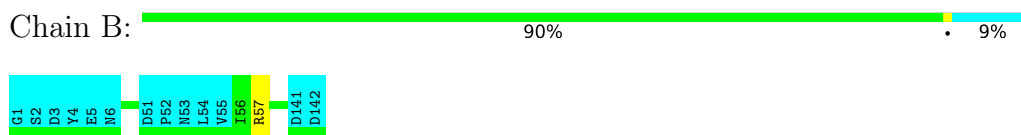
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 6. Colouring as in section 4.1 above.

- Molecule 1: Caspase recruitment domain-containing protein 9



- Molecule 1: Caspase recruitment domain-containing protein 9



5 Refinement protocol and experimental data overview

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

Of the 100 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
CNS	refinement	1.2
CYANA	refinement	3.97
CYANA	structure calculation	3.97

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	2461
Number of shifts mapped to atoms	2461
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

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6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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6.3.2 Protein sidechains [i](#)

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6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

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

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6.5 Carbohydrates [i](#)

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6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 45% for the well-defined parts and 45% 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	697
Number of shifts mapped to atoms	697
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	136	-0.23 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	122	0.97 ± 0.08	Should be checked
$^{13}\text{C}'$	133	-0.49 ± 0.14	None needed (< 0.5 ppm)
^{15}N	129	0.89 ± 0.37	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 17%, i.e. 637 atoms were assigned a chemical shift out of a possible 3645. 0 out of 62 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	483/1279 (38%)	120/518 (23%)	244/514 (47%)	119/247 (48%)
Sidechain	124/2178 (6%)	12/1420 (1%)	112/678 (17%)	0/80 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	30/188 (16%)	17/90 (19%)	12/94 (13%)	1/4 (25%)
Overall	637/3645 (17%)	149/2028 (7%)	368/1286 (29%)	120/331 (36%)

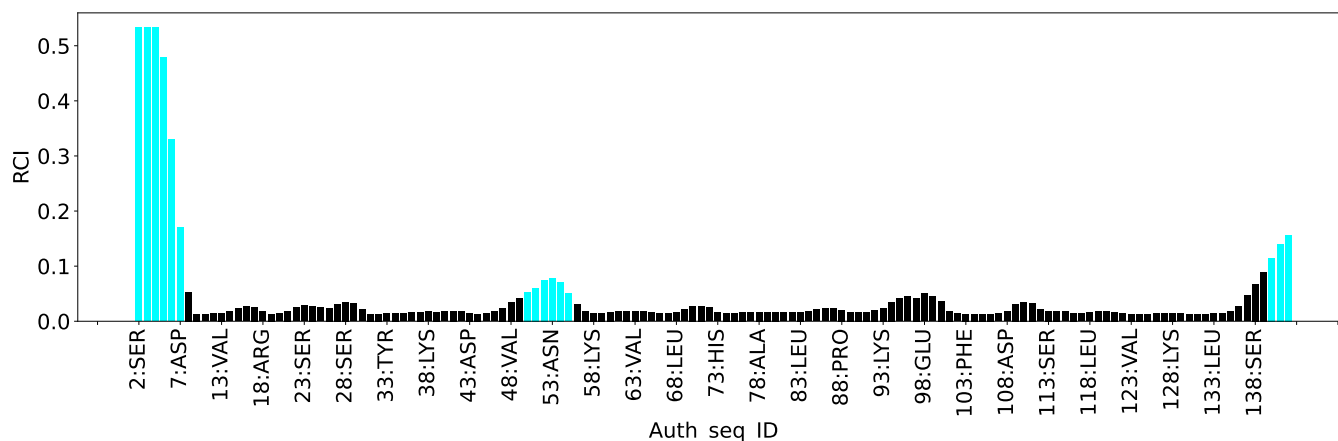
7.1.4 Statistically unusual chemical shifts [i](#)

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1_2*

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	1764
Number of shifts mapped to atoms	1764
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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
$^{13}\text{C}_\alpha$	142	-0.78 ± 0.08	Should be checked
$^{13}\text{C}_\beta$	130	0.04 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	132	-0.53 ± 0.18	Should be applied
^{15}N	129	0.78 ± 0.20	Should be applied

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 45%, i.e. 1625 atoms were assigned a chemical shift out of a possible 3645. 0 out of 62 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	611/1279 (48%)	244/518 (47%)	248/514 (48%)	119/247 (48%)
Sidechain	928/2178 (43%)	627/1420 (44%)	293/678 (43%)	8/80 (10%)
Aromatic	86/188 (46%)	43/90 (48%)	42/94 (45%)	1/4 (25%)
Overall	1625/3645 (45%)	914/2028 (45%)	583/1286 (45%)	128/331 (39%)

7.2.4 Statistically unusual chemical shifts [i](#)

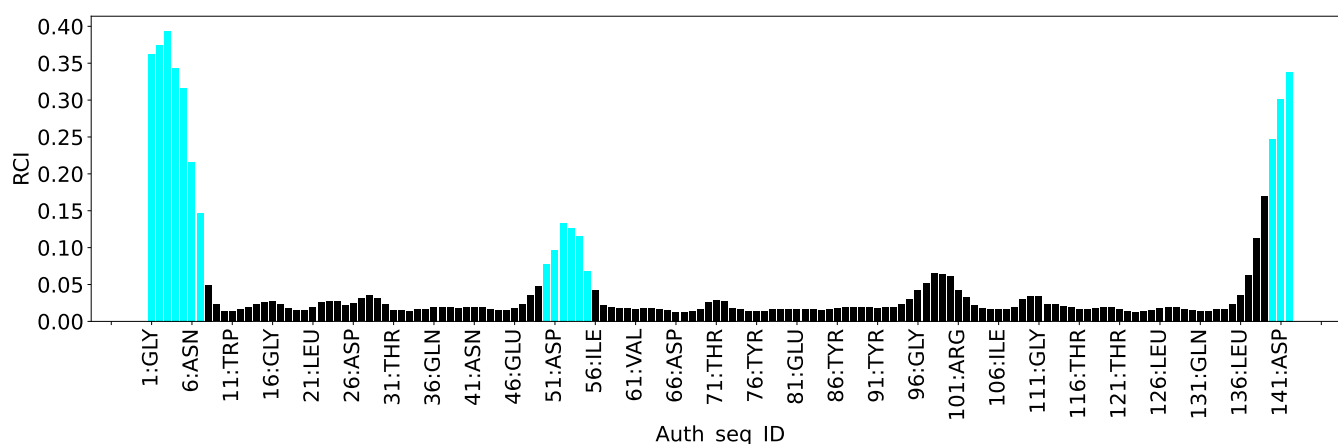
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	88	PRO	CB	50.08	26.06 – 37.61	15.8
2	A	84	GLU	HG2	0.40	1.24 – 3.30	-9.1

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 [i](#)

8.1 Conformationally restricting restraints [i](#)

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	4103
Intra-residue ($ i-j =0$)	1102
Sequential ($ i-j =1$)	997
Medium range ($ i-j >1$ and $ i-j <5$)	770
Long range ($ i-j \geq 5$)	766
Inter-chain	282
Hydrogen bond restraints	180
Disulfide bond restraints	0
Total dihedral-angle restraints	428
Number of unmapped restraints	0
Number of restraints per residue	15.8
Number of long range restraints per residue ¹	2.7

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 [i](#)

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 [i](#)

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)	45.4	0.2
0.2-0.5 (Medium)	9.8	0.45
>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)	17.3	9.74
10.0-20.0 (Medium)	0.3	11.2
>20.0 (Large)	None	None

9 Distance violation analysis

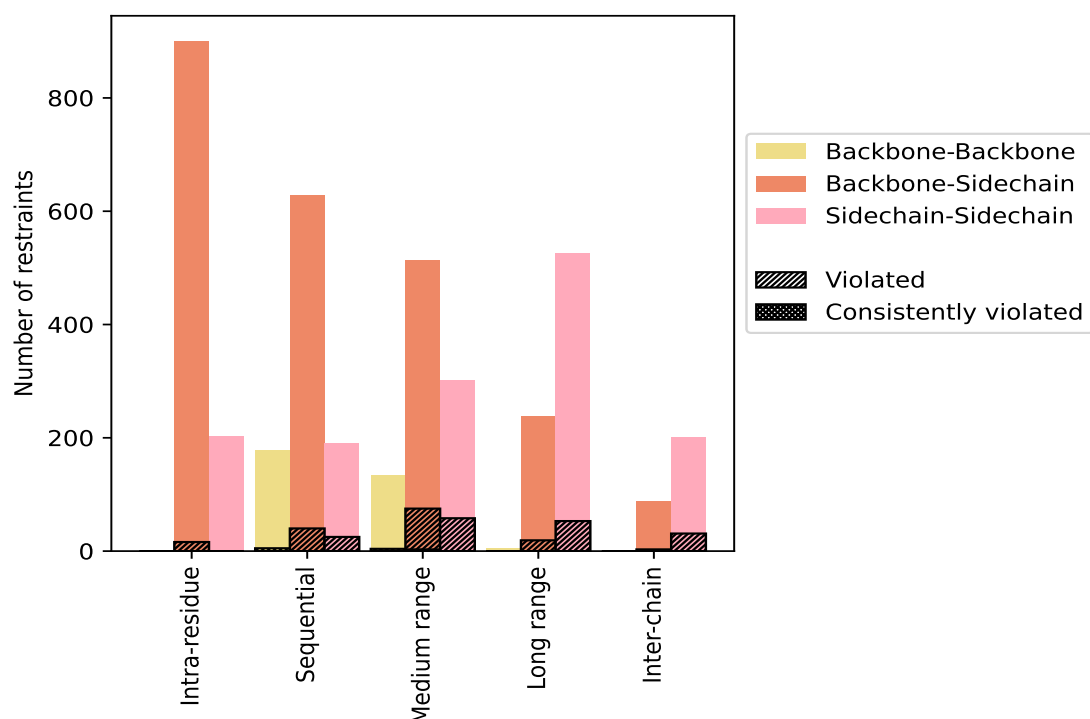
9.1 Summary of distance violations

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 ($i-j =0$)	1102	26.9	16	1.5	0.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	900	21.9	16	1.8	0.4	0	0.0	0.0
Sidechain-Sidechain	202	4.9	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	997	24.3	70	7.0	1.7	0	0.0	0.0
Backbone-Backbone	178	4.3	5	2.8	0.1	0	0.0	0.0
Backbone-Sidechain	628	15.3	40	6.4	1.0	0	0.0	0.0
Sidechain-Sidechain	191	4.7	25	13.1	0.6	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	770	18.8	99	12.9	2.4	0	0.0	0.0
Backbone-Backbone	134	3.3	4	3.0	0.1	0	0.0	0.0
Backbone-Sidechain	334	8.1	37	11.1	0.9	0	0.0	0.0
Sidechain-Sidechain	302	7.4	58	19.2	1.4	0	0.0	0.0
Long range ($i-j \geq 5$)	766	18.7	72	9.4	1.8	0	0.0	0.0
Backbone-Backbone	4	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	237	5.8	19	8.0	0.5	0	0.0	0.0
Sidechain-Sidechain	525	12.8	53	10.1	1.3	0	0.0	0.0
Inter-chain	282	6.9	29	10.3	0.7	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	88	2.1	3	3.4	0.1	0	0.0	0.0
Sidechain-Sidechain	194	4.7	26	13.4	0.6	0	0.0	0.0
Hydrogen bond	180	4.4	38	21.1	0.9	3	1.7	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	4103	100.0	329	8.0	8.0	3	0.1	0.1
Backbone-Backbone	316	7.7	9	2.8	0.2	0	0.0	0.0
Backbone-Sidechain	2367	57.7	153	6.5	3.7	3	0.1	0.1
Sidechain-Sidechain	1420	34.6	167	11.8	4.1	0	0.0	0.0

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

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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	3	13	24	8	7	55	0.16	0.4	0.07	0.14
2	2	12	30	8	7	59	0.15	0.28	0.04	0.14
3	2	14	28	12	7	63	0.16	0.42	0.05	0.14
4	3	10	30	15	5	63	0.16	0.37	0.06	0.14
5	4	11	27	8	4	54	0.16	0.33	0.06	0.14
6	3	9	28	6	1	47	0.15	0.31	0.05	0.13
7	6	10	27	10	5	58	0.16	0.39	0.06	0.15
8	5	14	34	6	9	68	0.17	0.45	0.07	0.15
9	2	14	26	10	5	57	0.15	0.29	0.04	0.14
10	1	9	33	14	7	64	0.16	0.4	0.06	0.14

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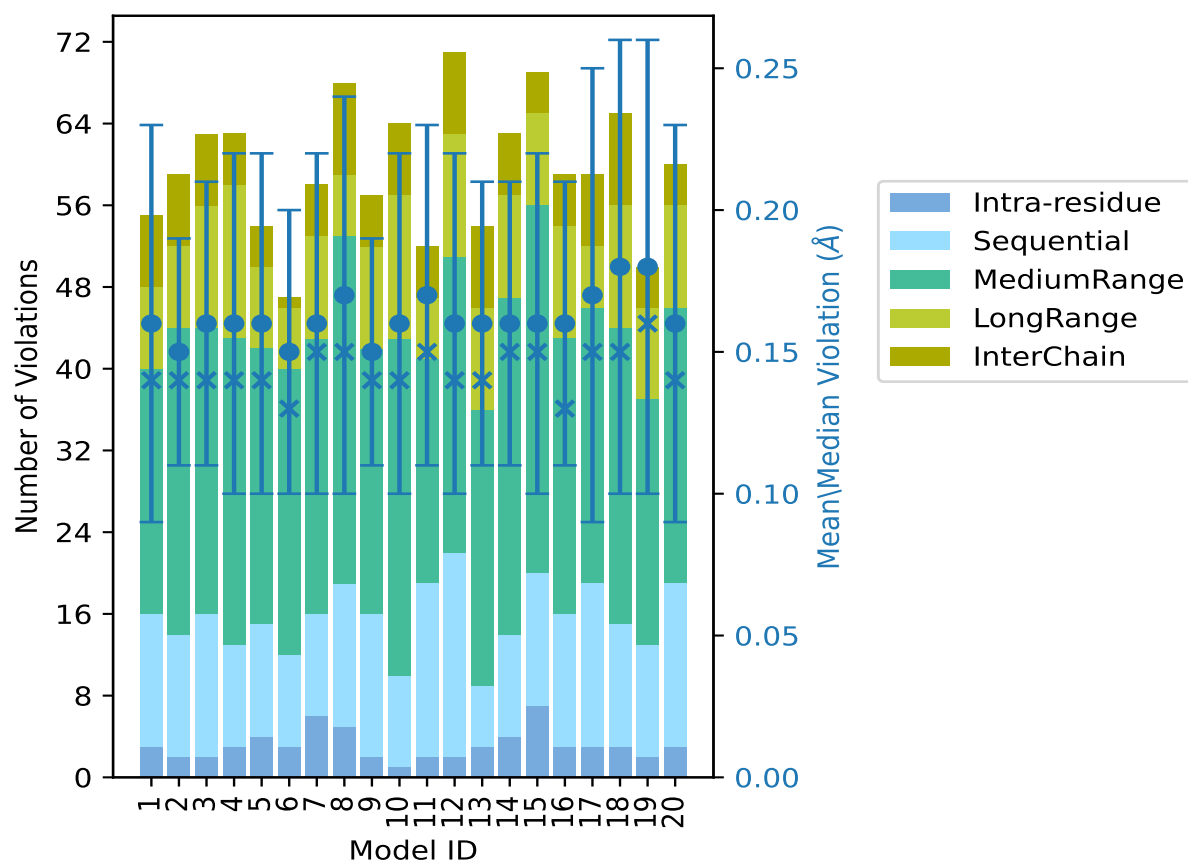
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	2	17	22	6	5	52	0.17	0.38	0.06	0.15
12	2	20	29	12	8	71	0.16	0.42	0.06	0.14
13	3	6	27	10	8	54	0.16	0.41	0.05	0.14
14	4	10	33	10	6	63	0.16	0.35	0.05	0.15
15	7	13	36	9	4	69	0.16	0.38	0.06	0.15
16	3	13	27	11	5	59	0.16	0.31	0.05	0.13
17	3	16	27	6	7	59	0.17	0.43	0.08	0.15
18	3	12	29	12	9	65	0.18	0.44	0.08	0.15
19	2	11	24	9	4	50	0.18	0.42	0.08	0.16
20	3	16	27	10	4	60	0.16	0.41	0.07	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 ⓘ



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

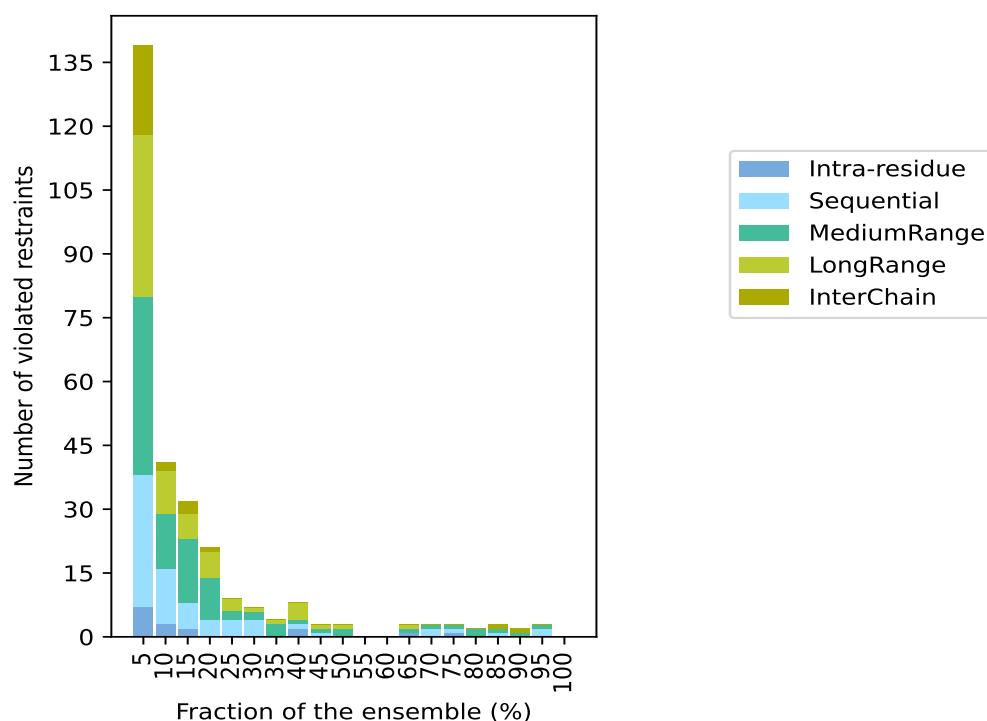
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3631(IR:1086, SQ:927, MR:671, LR:694, IC:253) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
7	31	42	38	21	139	1	5.0
3	13	13	10	2	41	2	10.0
2	6	15	6	3	32	3	15.0
0	4	10	6	1	21	4	20.0
0	4	2	3	0	9	5	25.0
0	4	2	1	0	7	6	30.0
0	0	3	1	0	4	7	35.0
2	1	1	4	0	8	8	40.0
0	1	1	1	0	3	9	45.0
0	0	2	1	0	3	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
1	0	1	1	0	3	13	65.0
0	2	1	0	0	3	14	70.0
1	1	1	0	0	3	15	75.0
0	0	2	0	0	2	16	80.0
0	1	1	0	1	3	17	85.0
0	0	1	0	1	2	18	90.0
0	2	1	0	0	3	19	95.0
0	0	0	0	0	0	20	100.0

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

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

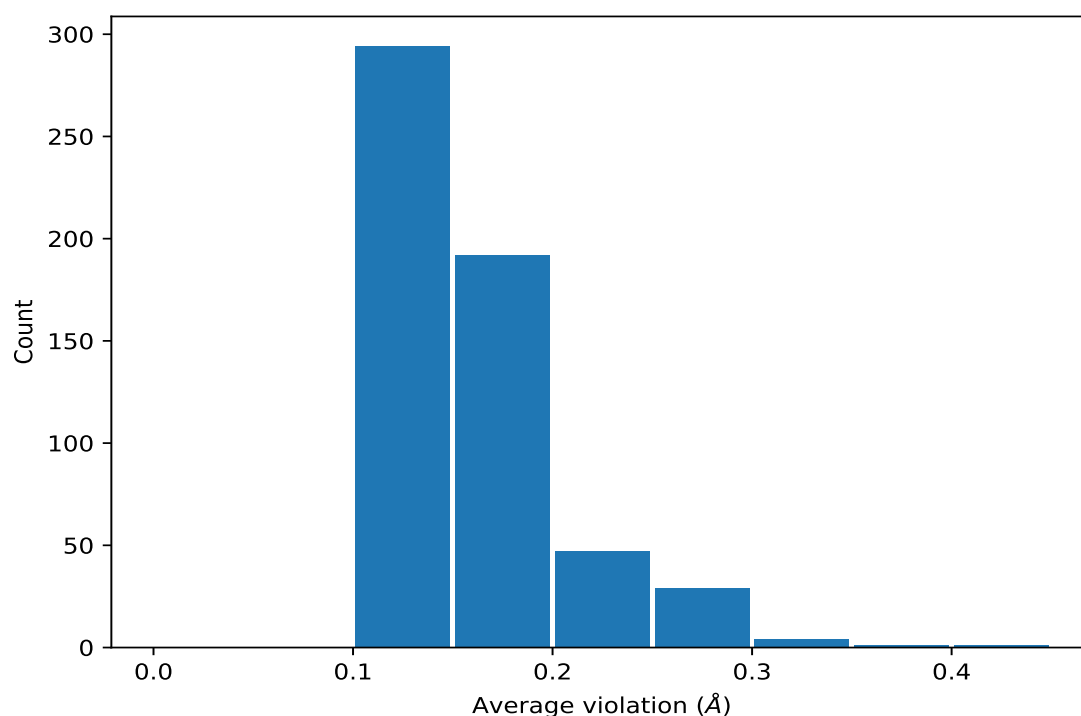
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

The following table provides the mean and the standard deviation of the 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)
(1,161)	1:121:B:THR:O	1:124:B:MET:H	20	0.15	0.01	0.15
(1,11)	1:26:A:ASP:O	1:29:A:ARG:H	20	0.15	0.02	0.15
(1,71)	1:121:A:THR:O	1:124:A:MET:H	20	0.15	0.02	0.15
(2,2728)	1:83:A:LEU:HD21	1:87:A:TYR:H	19	0.22	0.07	0.19
(2,2728)	1:83:A:LEU:HD22	1:87:A:TYR:H	19	0.22	0.07	0.19
(2,2728)	1:83:A:LEU:HD23	1:87:A:TYR:H	19	0.22	0.07	0.19
(2,791)	1:132:B:ASP:H	1:133:B:LEU:HD21	19	0.17	0.04	0.18
(2,791)	1:132:B:ASP:H	1:133:B:LEU:HD22	19	0.17	0.04	0.18
(2,791)	1:132:B:ASP:H	1:133:B:LEU:HD23	19	0.17	0.04	0.18
(2,790)	1:132:A:ASP:H	1:133:A:LEU:HD21	19	0.16	0.05	0.14
(2,790)	1:132:A:ASP:H	1:133:A:LEU:HD22	19	0.16	0.05	0.14
(2,790)	1:132:A:ASP:H	1:133:A:LEU:HD23	19	0.16	0.05	0.14
(2,2729)	1:83:B:LEU:HD21	1:87:B:TYR:H	18	0.25	0.08	0.23
(2,2729)	1:83:B:LEU:HD22	1:87:B:TYR:H	18	0.25	0.08	0.23
(2,2729)	1:83:B:LEU:HD23	1:87:B:TYR:H	18	0.25	0.08	0.23
(2,3071)	1:126:A:LEU:HG	1:126:B:LEU:HD21	18	0.15	0.04	0.14

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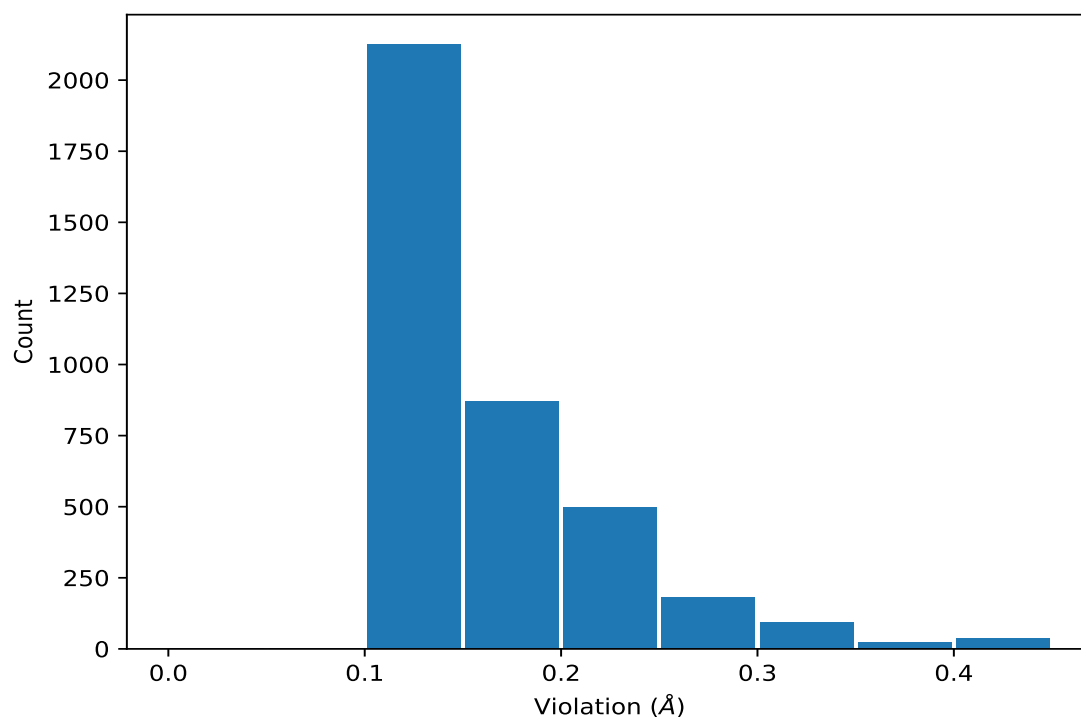
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3071)	1:126:A:LEU:HG	1:126:B:LEU:HD22	18	0.15	0.04	0.14
(2,3071)	1:126:A:LEU:HG	1:126:B:LEU:HD23	18	0.15	0.04	0.14
(2,2272)	1:131:B:GLN:HG2	1:135:B:ALA:HB1	17	0.16	0.04	0.15
(2,2272)	1:131:B:GLN:HG2	1:135:B:ALA:HB2	17	0.16	0.04	0.15
(2,2272)	1:131:B:GLN:HG2	1:135:B:ALA:HB3	17	0.16	0.04	0.15
(2,3072)	1:126:A:LEU:HD21	1:126:B:LEU:HG	17	0.16	0.04	0.15

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)
(2,2193)	1:125:A:LYS:HA	1:125:A:LYS:HE2	8	0.45
(2,2193)	1:125:A:LYS:HA	1:125:A:LYS:HE3	8	0.45
(2,2725)	1:79:B:PHE:HE1	1:83:B:LEU:HD21	18	0.44
(2,2725)	1:79:B:PHE:HE1	1:83:B:LEU:HD22	18	0.44
(2,2725)	1:79:B:PHE:HE1	1:83:B:LEU:HD23	18	0.44
(2,2725)	1:79:B:PHE:HE2	1:83:B:LEU:HD21	18	0.44
(2,2725)	1:79:B:PHE:HE2	1:83:B:LEU:HD22	18	0.44
(2,2725)	1:79:B:PHE:HE2	1:83:B:LEU:HD23	18	0.44
(2,374)	1:62:A:GLY:H	1:63:A:VAL:HG11	17	0.43
(2,374)	1:62:A:GLY:H	1:63:A:VAL:HG12	17	0.43
(2,374)	1:62:A:GLY:H	1:63:A:VAL:HG13	17	0.43
(2,2729)	1:83:B:LEU:HD21	1:87:B:TYR:H	19	0.42
(2,2729)	1:83:B:LEU:HD22	1:87:B:TYR:H	19	0.42
(2,2729)	1:83:B:LEU:HD23	1:87:B:TYR:H	19	0.42
(2,2193)	1:125:A:LYS:HA	1:125:A:LYS:HE2	19	0.42
(2,2193)	1:125:A:LYS:HA	1:125:A:LYS:HE3	19	0.42
(2,1998)	1:106:B:ILE:HD11	1:109:B:ALA:HB1	17	0.42
(2,1998)	1:106:B:ILE:HD11	1:109:B:ALA:HB2	17	0.42
(2,1998)	1:106:B:ILE:HD11	1:109:B:ALA:HB3	17	0.42
(2,1998)	1:106:B:ILE:HD12	1:109:B:ALA:HB1	17	0.42
(2,1998)	1:106:B:ILE:HD12	1:109:B:ALA:HB2	17	0.42
(2,1998)	1:106:B:ILE:HD12	1:109:B:ALA:HB3	17	0.42
(2,1998)	1:106:B:ILE:HD13	1:109:B:ALA:HB1	17	0.42
(2,1998)	1:106:B:ILE:HD13	1:109:B:ALA:HB2	17	0.42
(2,1998)	1:106:B:ILE:HD13	1:109:B:ALA:HB3	17	0.42
(2,1465)	1:129:A:LYS:HE3	1:130:B:VAL:HB	3	0.42
(2,773)	1:131:B:GLN:H	1:131:B:GLN:HG2	12	0.42
(2,2194)	1:125:B:LYS:HA	1:125:B:LYS:HE2	20	0.41
(2,2194)	1:125:B:LYS:HA	1:125:B:LYS:HE3	20	0.41
(2,20)	1:140:B:LYS:HA	1:141:B:ASP:H	12	0.41

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

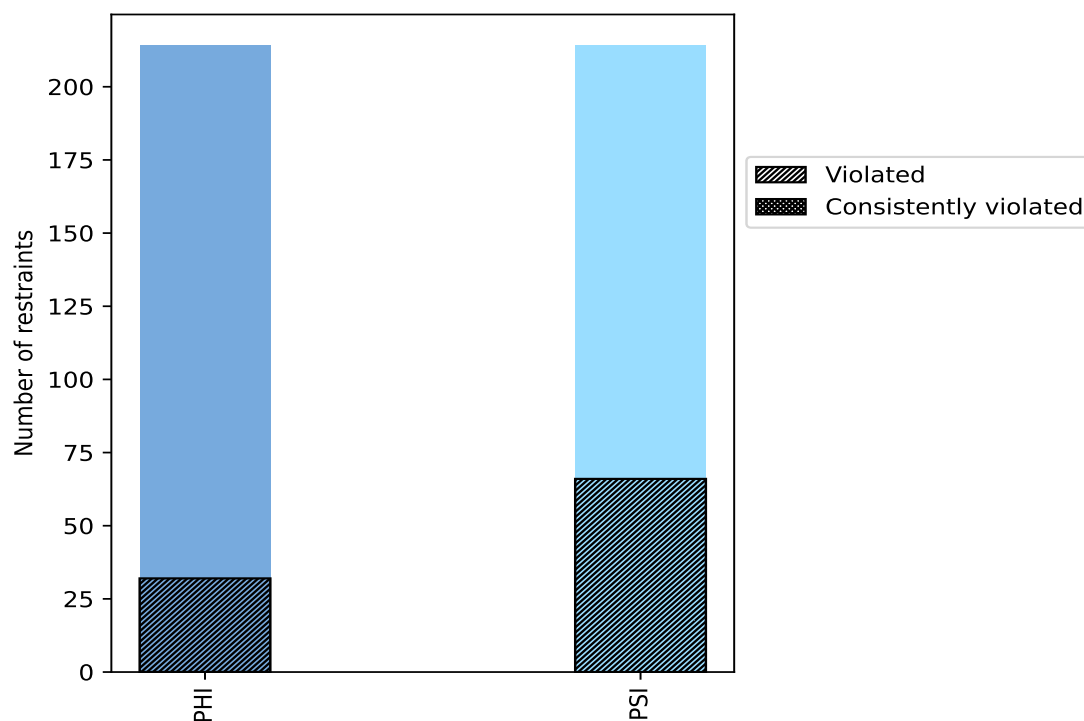
10.1 Summary of dihedral-angle violations [i](#)

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
PHI	214	50.0	32	15.0	7.5	0	0.0	0.0
PSI	214	50.0	66	30.8	15.4	0	0.0	0.0
Total	428	100.0	98	22.9	22.9	0	0.0	0.0

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

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



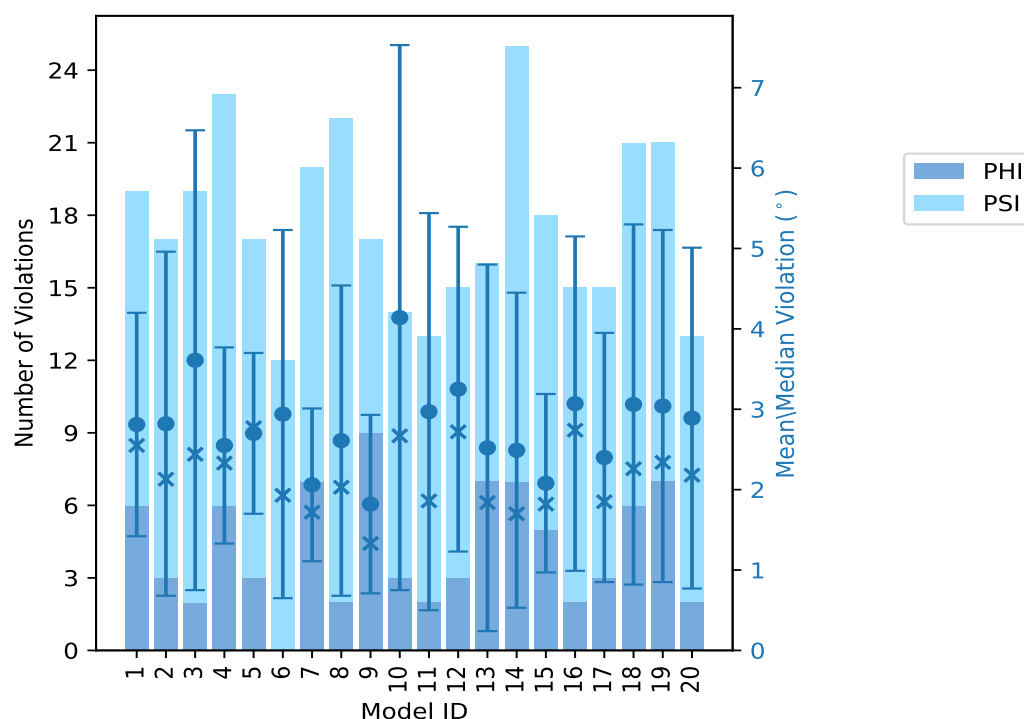
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	6	13	19	2.81	5.8	1.39	2.55
2	3	14	17	2.82	10.41	2.14	2.13
3	2	17	19	3.61	9.74	2.86	2.44
4	6	17	23	2.55	6.79	1.22	2.33
5	3	14	17	2.7	4.85	1.0	2.77
6	0	12	12	2.94	9.21	2.29	1.93
7	7	13	20	2.06	4.6	0.95	1.72
8	2	20	22	2.61	9.21	1.93	2.03
9	9	8	17	1.82	4.71	1.11	1.33
10	3	11	14	4.14	11.2	3.39	2.67
11	2	11	13	2.97	10.01	2.47	1.86
12	3	12	15	3.25	7.78	2.02	2.72
13	7	9	16	2.52	10.92	2.28	1.84
14	7	18	25	2.49	7.99	1.96	1.7
15	5	13	18	2.08	4.81	1.11	1.82
16	2	13	15	3.07	7.58	2.08	2.74
17	3	12	15	2.4	7.52	1.55	1.85
18	6	15	21	3.06	10.6	2.24	2.26
19	7	14	21	3.04	10.62	2.19	2.34
20	2	11	13	2.89	8.23	2.12	2.18

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	
PHI	PSI	Total	Count ¹	%
15	25	40	1	5.0
6	9	15	2	10.0
2	7	9	3	15.0
4	5	9	4	20.0
1	2	3	5	25.0
1	4	5	6	30.0
1	2	3	7	35.0
1	3	4	8	40.0
0	3	3	9	45.0
1	1	2	10	50.0
0	1	1	11	55.0

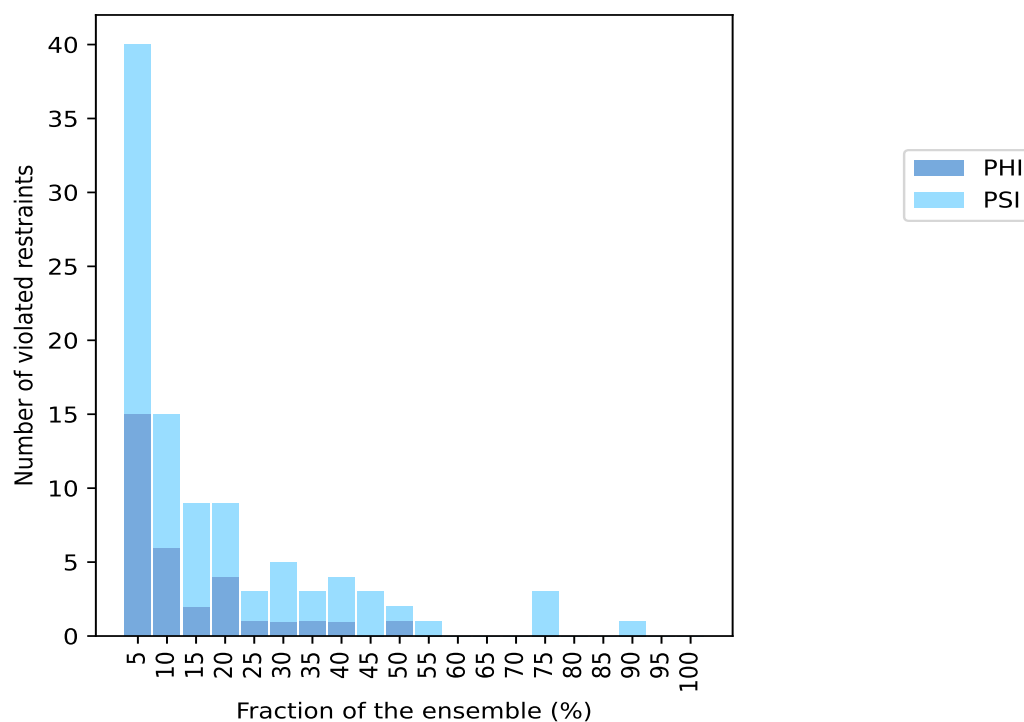
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	3	3	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	1	1	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

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

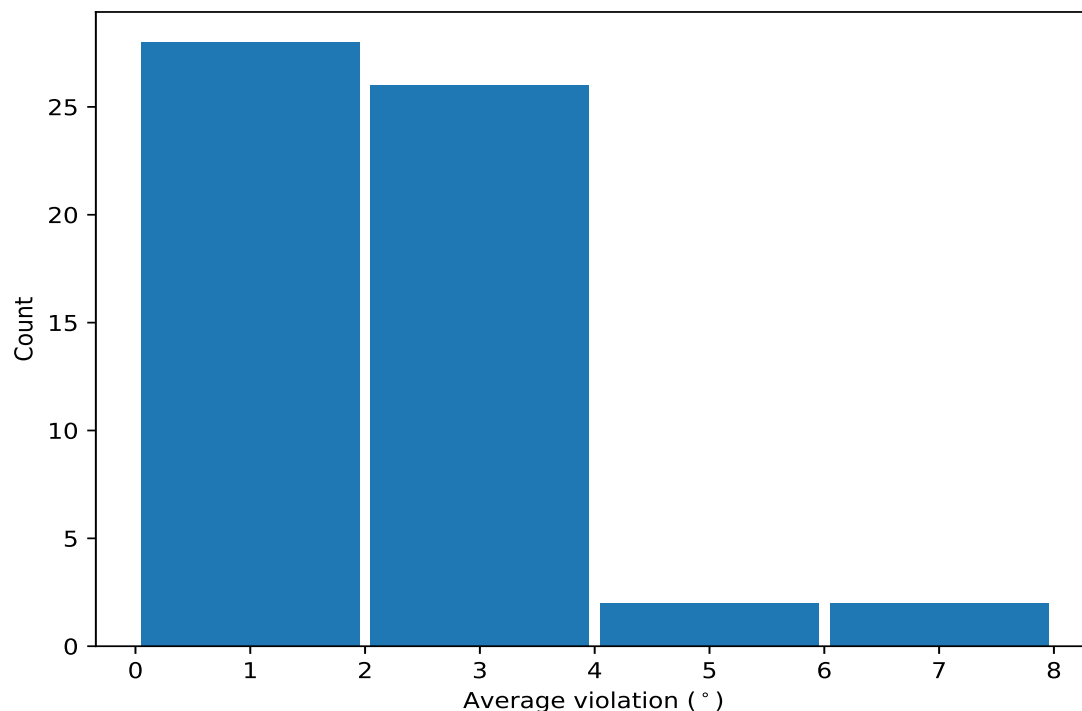


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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

in the ensemble



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

The following table provides the mean and the standard deviation of the 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.

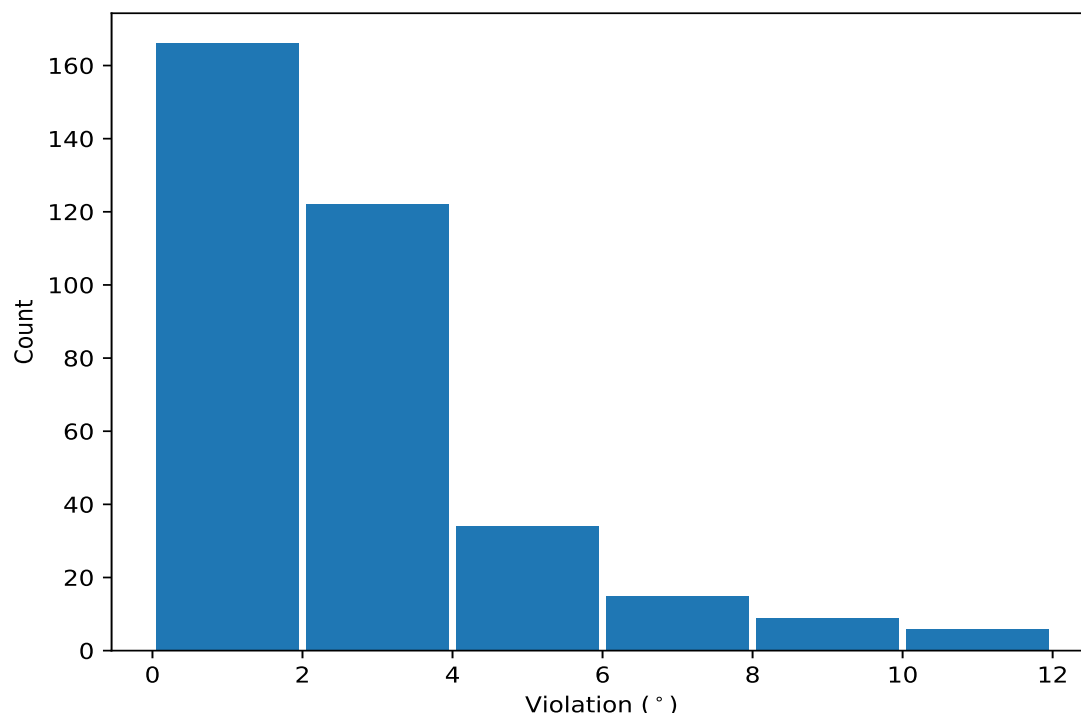
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,360)	1:102:B:VAL:N	1:102:B:VAL:CA	1:102:B:VAL:C	1:103:B:PHE:N	18	6.53	2.69	6.99
(1,146)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1:103:A:PHE:N	15	6.3	2.42	5.8
(1,68)	1:56:A:ILE:N	1:56:A:ILE:CA	1:56:A:ILE:C	1:57:A:ARG:N	15	3.31	1.7	2.86
(1,282)	1:56:B:ILE:N	1:56:B:ILE:CA	1:56:B:ILE:C	1:57:B:ARG:N	15	3.24	1.98	2.57
(1,144)	1:101:A:ARG:N	1:101:A:ARG:CA	1:101:A:ARG:C	1:102:A:VAL:N	11	3.89	2.71	2.32
(1,1)	1:7:A:ASP:C	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	10	2.72	2.28	1.94
(1,152)	1:105:A:MET:N	1:105:A:MET:CA	1:105:A:MET:C	1:106:A:ILE:N	10	1.97	1.1	1.48
(1,358)	1:101:B:ARG:N	1:101:B:ARG:CA	1:101:B:ARG:C	1:102:B:VAL:N	9	5.37	3.31	4.4
(1,222)	1:11:B:TRP:N	1:11:B:TRP:CA	1:11:B:TRP:C	1:12:B:SER:N	9	2.53	1.28	1.77
(1,64)	1:50:A:SER:N	1:50:A:SER:CA	1:50:A:SER:C	1:51:A:ASP:N	9	2.04	0.93	1.5

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 (°)
(1,360)	1:102:B:VAL:N	1:102:B:VAL:CA	1:102:B:VAL:C	1:103:B:PHE:N	10	11.2
(1,146)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1:103:A:PHE:N	13	10.92
(1,358)	1:101:B:ARG:N	1:101:B:ARG:CA	1:101:B:ARG:C	1:102:B:VAL:N	19	10.62
(1,358)	1:101:B:ARG:N	1:101:B:ARG:CA	1:101:B:ARG:C	1:102:B:VAL:N	18	10.6
(1,360)	1:102:B:VAL:N	1:102:B:VAL:CA	1:102:B:VAL:C	1:103:B:PHE:N	2	10.41
(1,360)	1:102:B:VAL:N	1:102:B:VAL:CA	1:102:B:VAL:C	1:103:B:PHE:N	11	10.01
(1,360)	1:102:B:VAL:N	1:102:B:VAL:CA	1:102:B:VAL:C	1:103:B:PHE:N	3	9.74
(1,1)	1:7:A:ASP:C	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	3	9.33
(1,146)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1:103:A:PHE:N	6	9.21
(1,146)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1:103:A:PHE:N	8	9.21