



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2N4B / pdb_00002n4b
BMRB ID : 17611
Title : EC-NMR Structure of *Ralstonia metallidurans* Rmet_5065 Determined by Combining Evolutionary Couplings (EC) and Sparse NMR Data. Northeast Structural Genomics Consortium target CrR115
Authors : Tang, Y.; Huang, Y.J.; Hopf, T.A.; Sander, C.; Marks, D.; Montelione, G.T.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2015-06-17

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

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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

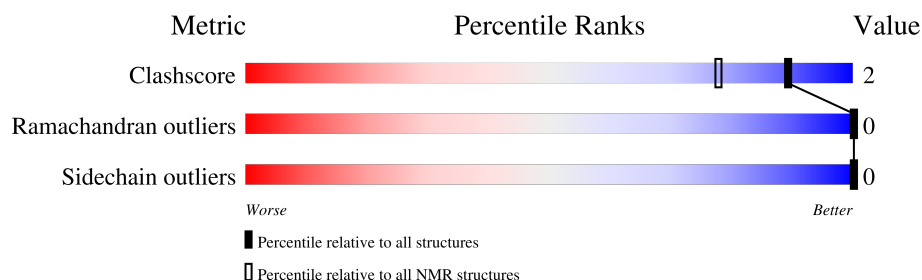
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 95%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	142	

2 Ensemble composition and analysis

This entry contains 20 models. Model 16 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:1-A:26, A:40-A:54, A:66-A:134 (110)	0.79	16

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 4 clusters and 5 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2136 atoms, of which 1037 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
1	A	138	Total	C	H	N	O	S	0
			2136	691	1037	192	213	3	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	LEU	-	expression tag	UNP Q1LD49
A	136	GLU	-	expression tag	UNP Q1LD49
A	137	HIS	-	expression tag	UNP Q1LD49
A	138	HIS	-	expression tag	UNP Q1LD49
A	139	HIS	-	expression tag	UNP Q1LD49
A	140	HIS	-	expression tag	UNP Q1LD49
A	141	HIS	-	expression tag	UNP Q1LD49
A	142	HIS	-	expression tag	UNP Q1LD49

5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *lowest energy*.

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

Software name	Classification	Version
Rosetta	refinement	
Reduce	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1741
Number of shifts mapped to atoms	1741
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	95%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	872	848	850	3±1
All	All	17440	16960	17000	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 2.

5 of 20 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:PHE:O	1:A:83:PHE:CD1	0.66	2.49	1	1
1:A:68:GLY:HA3	1:A:82:ALA:O	0.61	1.95	14	5
1:A:16:VAL:HG21	1:A:99:VAL:HG11	0.59	1.74	17	1
1:A:23:PRO:HB3	1:A:41:ALA:HB3	0.55	1.78	7	6
1:A:127:PHE:O	1:A:127:PHE:CD1	0.55	2.59	13	3

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	109/142 (77%)	107±1 (98±1%)	2±1 (2±1%)	0±0 (0±0%)	100	100
All	All	2180/2840 (77%)	2147 (98%)	33 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	91/118 (77%)	91±0 (100±0%)	0±0 (0±0%)	100	100
All	All	1820/2360 (77%)	1820 (100%)	0 (0%)	100	100

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 95% for the well-defined parts and 94% 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	1741
Number of shifts mapped to atoms	1741
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	137	-0.36 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	128	0.06 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	133	0.21 ± 0.12	None needed (< 0.5 ppm)
^{15}N	133	-0.52 ± 0.21	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 95%, i.e. 1417 atoms were assigned a chemical shift out of a possible 1496. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	543/549 (99%)	222/223 (100%)	216/220 (98%)	105/106 (99%)
Sidechain	751/813 (92%)	499/527 (95%)	235/250 (94%)	17/36 (47%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	123/134 (92%)	61/66 (92%)	58/64 (91%)	4/4 (100%)
Overall	1417/1496 (95%)	782/816 (96%)	509/534 (95%)	126/146 (86%)

7.1.4 Statistically unusual chemical shifts [i](#)

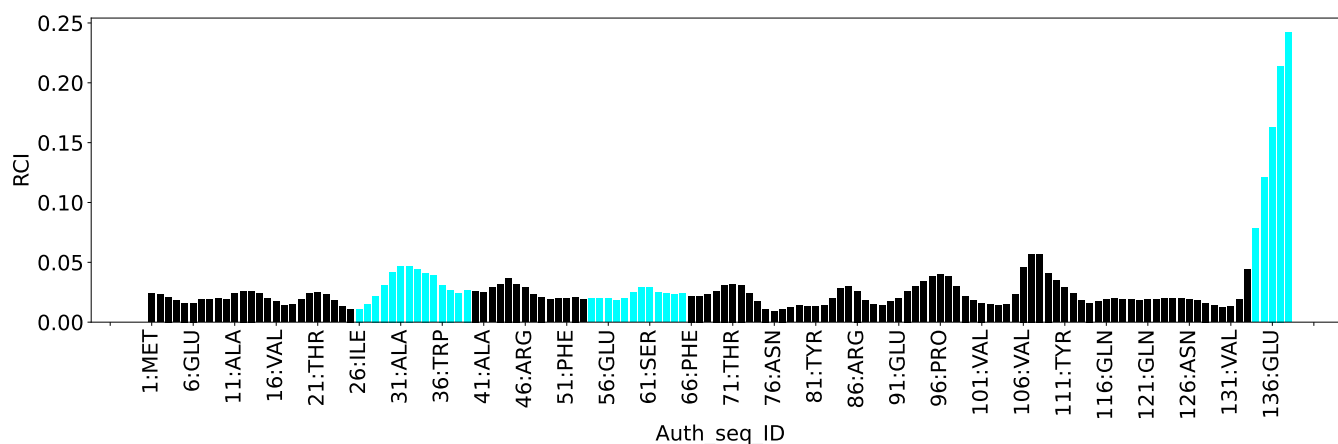
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	22	THR	HG1	6.39	0.08 – 2.19	24.9
1	A	38	THR	HG1	5.70	0.08 – 2.19	21.6
1	A	7	THR	HG1	5.54	0.08 – 2.19	20.9
1	A	86	ARG	NE	112.80	76.53 – 92.65	17.5
1	A	129	ARG	NE	110.60	76.53 – 92.65	16.1
1	A	76	ASN	H	3.39	5.28 – 11.36	-8.1
1	A	30	ASN	HB3	0.75	1.12 – 4.38	-6.1
1	A	3	ILE	HB	0.23	0.35 – 3.22	-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:



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	172
Intra-residue ($ i-j =0$)	3
Sequential ($ i-j =1$)	93
Medium range ($ i-j >1$ and $ i-j <5$)	27
Long range ($ i-j \geq 5$)	49
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	242
Number of unmapped restraints	0
Number of restraints per residue	2.9
Number of long range restraints per residue ¹	0.3

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 [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. There are no distance violations

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)	4.2	9.8

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Bins (°)	Average number of violations per model	Max (°)
10.0-20.0 (Medium)	4.7	19.88
>20.0 (Large)	232.4	178.94

9 Distance violation analysis ⓘ

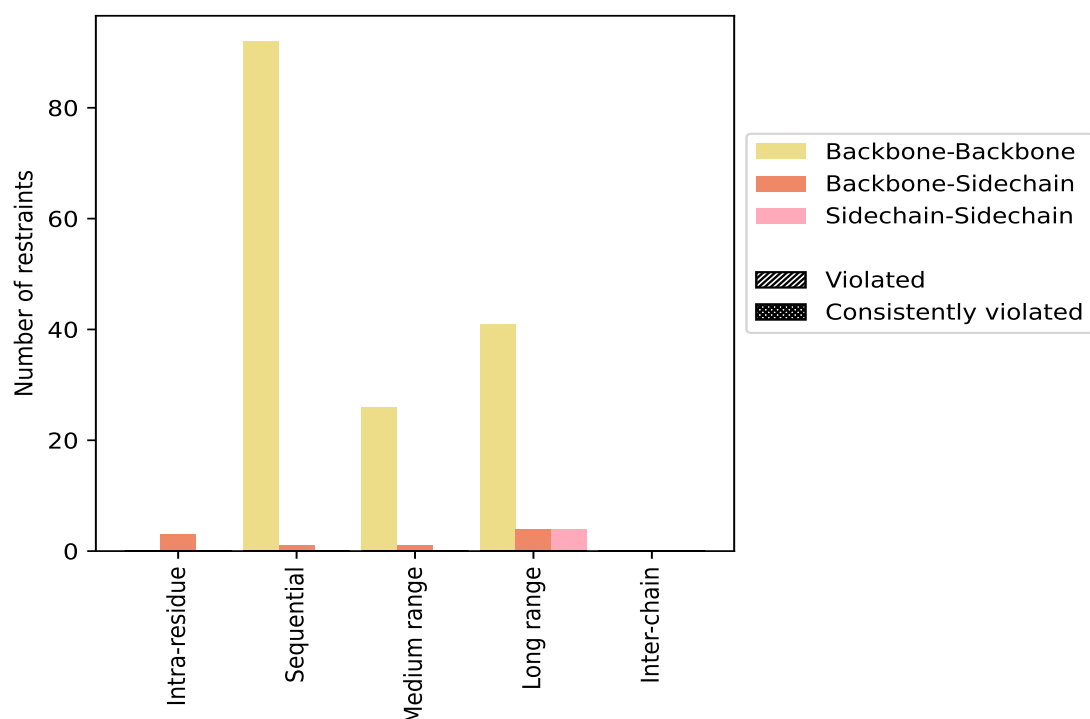
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	3	1.7	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	3	1.7	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
Sequential ($i-j =1$)	93	54.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	92	53.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1	0.6	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
Medium range ($i-j >1$ & $i-j <5$)	27	15.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	26	15.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1	0.6	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
Long range ($i-j \geq 5$)	49	28.5	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	41	23.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	4	2.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	4	2.3	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	172	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	159	92.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	9	5.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	4	2.3	0	0.0	0.0	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](#)

No violations found

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

No violations found

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

No violations found

9.5 All violated distance restraints [i](#)

No violations found

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

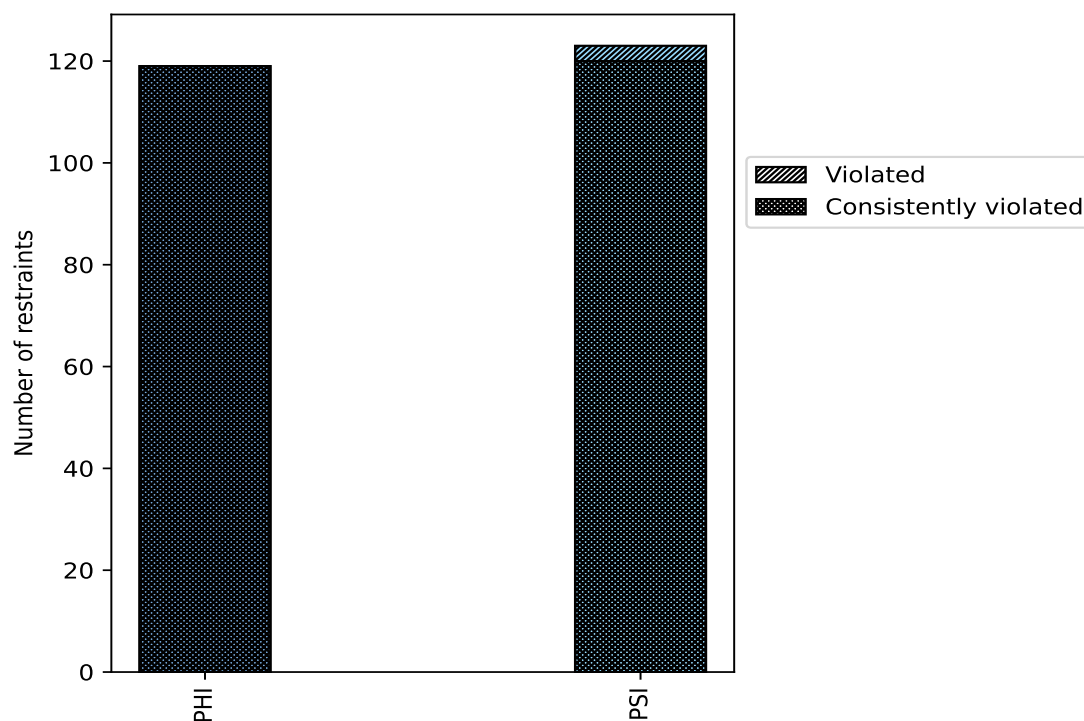
10.1 Summary of dihedral-angle violations [i](#)

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	119	49.2	119	100.0	49.2	119	100.0	49.2
PSI	123	50.8	123	100.0	50.8	120	97.6	49.6
Total	242	100.0	242	100.0	100.0	239	98.8	98.8

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](#)



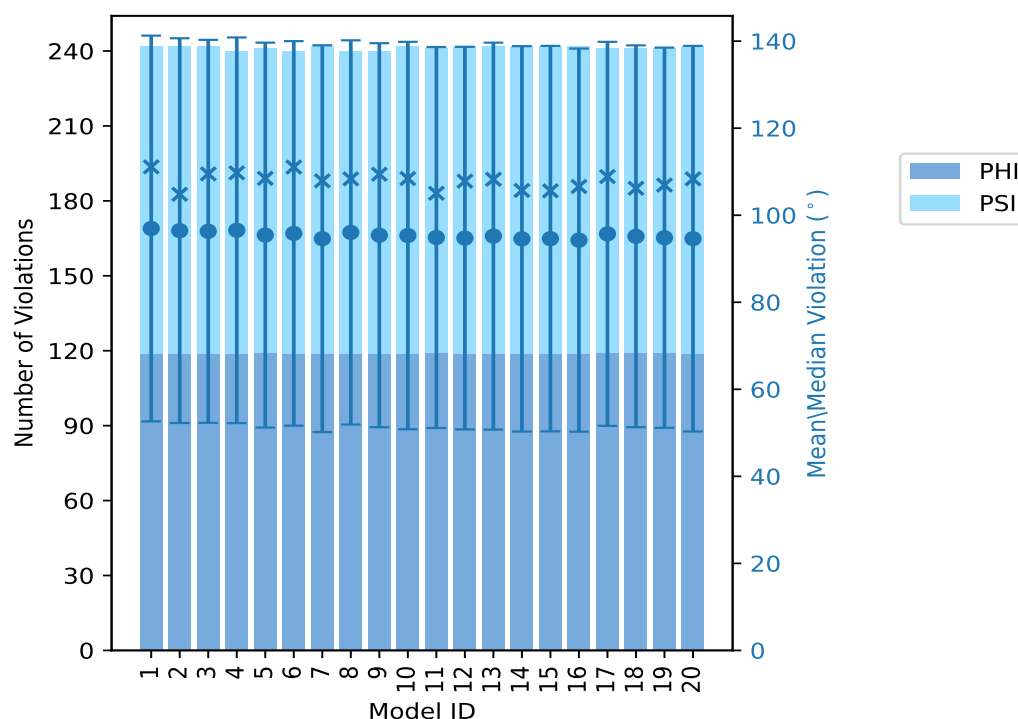
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	119	123	242	96.95	174.08	44.32	111.11
2	119	123	242	96.46	178.94	44.2	104.81
3	119	123	242	96.3	175.6	44.0	109.5
4	119	121	240	96.54	178.56	44.31	109.74
5	119	122	241	95.43	178.6	44.22	108.47
6	119	121	240	95.82	174.19	44.18	111.06
7	119	123	242	94.61	176.69	44.44	107.9
8	119	121	240	96.05	178.13	44.14	108.36
9	119	121	240	95.41	177.1	44.12	109.42
10	119	123	242	95.33	178.71	44.51	108.44
11	119	122	241	94.88	172.85	43.77	105.05
12	119	123	242	94.74	175.19	43.96	107.82
13	119	123	242	95.2	178.43	44.45	108.26
14	119	123	242	94.57	175.22	44.28	105.7
15	119	123	242	94.62	171.7	44.29	105.61
16	119	123	242	94.28	176.6	44.02	106.6
17	119	122	241	95.72	177.74	44.12	108.88
18	119	122	241	95.16	175.41	43.87	106.19
19	119	122	241	94.83	175.4	43.68	106.93
20	119	123	242	94.61	175.67	44.3	108.36

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	%
0	0	0	1	5.0
0	0	0	2	10.0
0	0	0	3	15.0
0	0	0	4	20.0
0	0	0	5	25.0
0	0	0	6	30.0
0	0	0	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

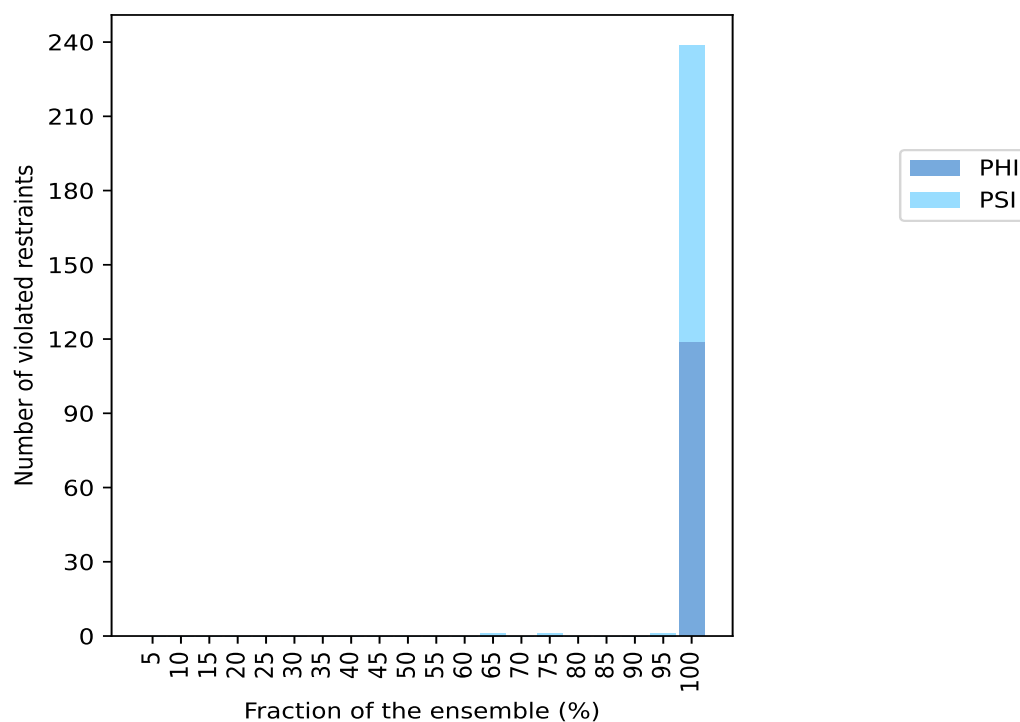
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
0	1	1	13	65.0
0	0	0	14	70.0
0	1	1	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	1	1	19	95.0
119	120	239	20	100.0

¹ Number of models with violations

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

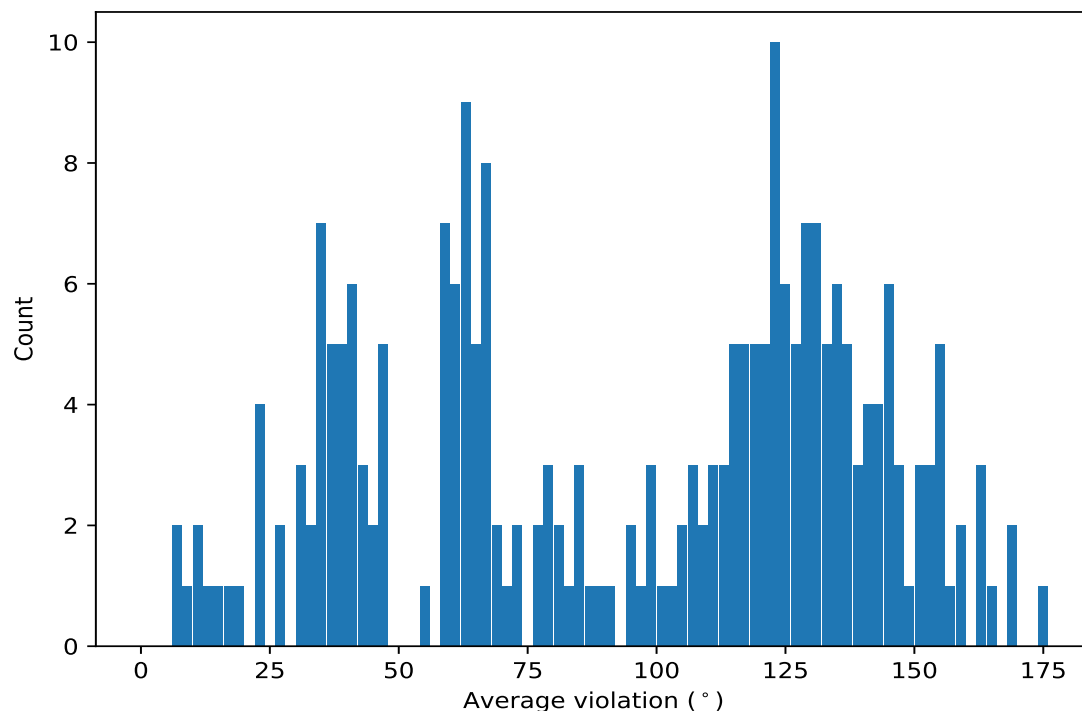


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

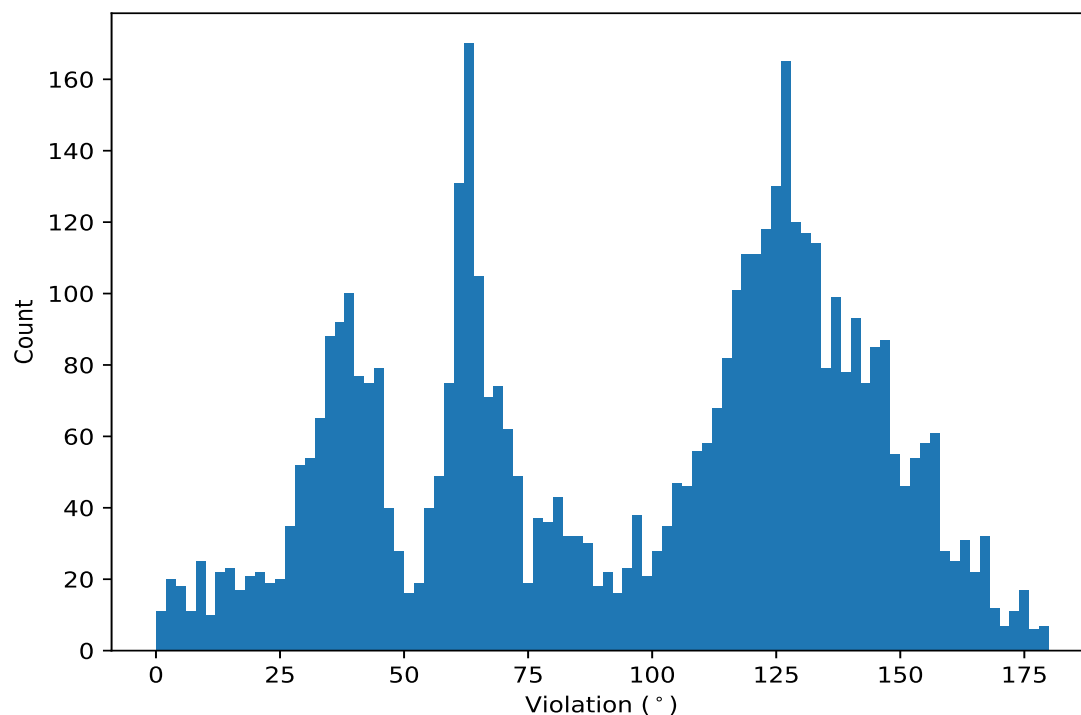
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,172)	1:97:A:GLN:C	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	20	175.66	2.06	175.4
(1,173)	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1:99:A:VAL:N	20	168.39	3.22	167.1
(1,118)	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	1:69:A:THR:N	20	168.25	4.5	167.46
(1,107)	1:62:A:MET:C	1:63:A:GLY:N	1:63:A:GLY:CA	1:63:A:GLY:C	20	164.96	11.74	168.42
(1,150)	1:86:A:ARG:N	1:86:A:ARG:CA	1:86:A:ARG:C	1:87:A:THR:N	20	163.97	3.83	163.72
(1,73)	1:45:A:LEU:C	1:46:A:ARG:N	1:46:A:ARG:CA	1:46:A:ARG:C	20	163.4	3.17	163.46
(1,108)	1:63:A:GLY:N	1:63:A:GLY:CA	1:63:A:GLY:C	1:64:A:PHE:N	20	162.78	7.66	161.87
(1,117)	1:67:A:ALA:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	20	159.7	6.49	158.5
(1,106)	1:62:A:MET:N	1:62:A:MET:CA	1:62:A:MET:C	1:63:A:GLY:N	20	158.65	2.3	158.27
(1,105)	1:61:A:SER:C	1:62:A:MET:N	1:62:A:MET:CA	1:62:A:MET:C	20	156.34	3.54	156.68

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 (°)
(1,117)	1:67:A:ALA:C	1:68:A:GLY:N	1:68:A:GLY:CA	1:68:A:GLY:C	2	178.94
(1,108)	1:63:A:GLY:N	1:63:A:GLY:CA	1:63:A:GLY:C	1:64:A:PHE:N	10	178.71
(1,172)	1:97:A:GLN:C	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	5	178.6
(1,172)	1:97:A:GLN:C	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	4	178.56
(1,172)	1:97:A:GLN:C	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	13	178.43
(1,172)	1:97:A:GLN:C	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	8	178.13
(1,107)	1:62:A:MET:C	1:63:A:GLY:N	1:63:A:GLY:CA	1:63:A:GLY:C	2	178.08
(1,172)	1:97:A:GLN:C	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	17	177.74
(1,107)	1:62:A:MET:C	1:63:A:GLY:N	1:63:A:GLY:CA	1:63:A:GLY:C	17	177.51
(1,172)	1:97:A:GLN:C	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	9	177.1