



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 10:32 AM UTC

PDB ID : 5LCB / pdb_00005lcb
EMDB ID : EMD-4033
BMRB ID : 34012
Title : In situ atomic-resolution structure of the baseplate antenna complex in Chlorobaculum tepidum obtained combining solid-state NMR spectroscopy, cryo electron microscopy and polarization spectroscopy
Authors : Nielsen, J.T.; Kulminskaya, N.V.; Bjerring, M.; Linnanto, J.M.; Ratsep, M.; Pedersen, M.; Lambrev, P.H.; Dorogi, M.; Garab, G.; Thomsen, K.; Jegerschold, C.; Frigaard, N.U.; Lindahl, M.; Nielsen, N.C.
Deposited on : 2016-06-20

This is a Full wwPDB NMR Structure Validation 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:

EMDB validation analysis : **NOT EXECUTED**
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY, SOLID-STATE NMR

The reported resolution of this entry is 26.50 Å.

The overall completeness of chemical shifts assignment is 2%.

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

The sequence quality summary graphics cannot be shown.

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13860 atoms, of which 6930 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Bacteriochlorophyll c-binding protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	59	Total	C	H	N	O	S	0	
			850	266	421	77	81	5		
1	B	59	Total	C	H	N	O	S	0	
			850	266	421	77	81	5		
1	C	59	Total	C	H	N	O	S	0	
			850	266	421	77	81	5		
1	D	59	Total	C	H	N	O	S	0	
			850	266	421	77	81	5		
1	E	59	Total	C	H	N	O	S	0	
			850	266	421	77	81	5		
1	F	59	Total	C	H	N	O	S	0	
			850	266	421	77	81	5		
1	G	59	Total	C	H	N	O	S	0	
			850	266	421	77	81	5		
1	H	59	Total	C	H	N	O	S	0	
			850	266	421	77	81	5		
1	I	59	Total	C	H	N	O	S	0	
			850	266	421	77	81	5		
1	J	59	Total	C	H	N	O	S	0	
			850	266	421	77	81	5		
1	K	59	Total	C	H	N	O	S	0	
			850	266	421	77	81	5		
1	L	59	Total	C	H	N	O	S	0	
			850	266	421	77	81	5		
1	M	59	Total	C	H	N	O	S	0	
			850	266	421	77	81	5		
1	N	59	Total	C	H	N	O	S	0	
			850	266	421	77	81	5		

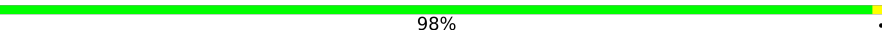
- Molecule 2 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).

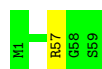


4 Residue-property plots

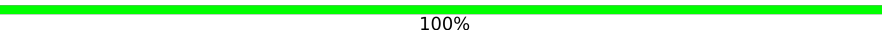
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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: Bacteriochlorophyll c-binding protein

Chain A:  98%

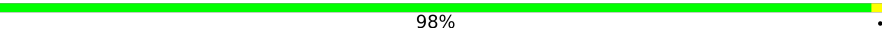


- Molecule 1: Bacteriochlorophyll c-binding protein

Chain B:  100%

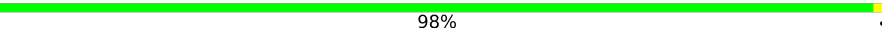
There are no outlier residues in this chain.

- Molecule 1: Bacteriochlorophyll c-binding protein

Chain C:  98%



- Molecule 1: Bacteriochlorophyll c-binding protein

Chain D:  98%



- Molecule 1: Bacteriochlorophyll c-binding protein

Chain E:  100%

There are no outlier residues in this chain.

- Molecule 1: Bacteriochlorophyll c-binding protein

Chain F:  100%

There are no outlier residues in this chain.

- Molecule 1: Bacteriochlorophyll c-binding protein

Chain G:  98%



- Molecule 1: Bacteriochlorophyll c-binding protein

Chain H:  98%



- Molecule 1: Bacteriochlorophyll c-binding protein

Chain I:  98%



- Molecule 1: Bacteriochlorophyll c-binding protein

Chain J:  100%

There are no outlier residues in this chain.

- Molecule 1: Bacteriochlorophyll c-binding protein

Chain K:  100%

There are no outlier residues in this chain.

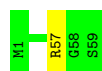
- Molecule 1: Bacteriochlorophyll c-binding protein

Chain L:  100%

There are no outlier residues in this chain.

- Molecule 1: Bacteriochlorophyll c-binding protein

Chain M:  98%



- Molecule 1: Bacteriochlorophyll c-binding protein

Chain N:  98%



5 Refinement protocol and experimental data overview

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

Of the 80 calculated structures, 1 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Xplor-NIH	refinement	2.33
GASyCS	structure calculation	

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	207
Number of shifts mapped to atoms	207
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	2%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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](#)

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

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

6.3.2 Protein sidechains [i](#)

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

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](#)

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

6.5 Carbohydrates [i](#)

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

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 2% for the well-defined parts and 2% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *csmanewer31.str*

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	207
Number of shifts mapped to atoms	207
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
$^{13}\text{C}_\alpha$	44	-1.09 ± 0.44	Should be checked
$^{13}\text{C}_\beta$	34	0.85 ± 0.37	Should be checked
$^{13}\text{C}'$	43	-0.61 ± 0.35	None needed (imprecise)
^{15}N	44	1.97 ± 0.85	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 2%, i.e. 204 atoms were assigned a chemical shift out of a possible 10388. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	131/4312 (3%)	0/1834 (0%)	87/1652 (5%)	44/826 (5%)
Sidechain	73/5264 (1%)	0/3472 (0%)	73/1582 (5%)	0/210 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/812 (0%)	0/406 (0%)	0/378 (0%)	0/28 (0%)
Overall	204/10388 (2%)	0/5712 (0%)	160/3612 (4%)	44/1064 (4%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 204 atoms were assigned a chemical shift out of a possible 10388. 0 out of 112 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	131/4312 (3%)	0/1834 (0%)	87/1652 (5%)	44/826 (5%)
Sidechain	73/5264 (1%)	0/3472 (0%)	73/1582 (5%)	0/210 (0%)
Aromatic	0/812 (0%)	0/406 (0%)	0/378 (0%)	0/28 (0%)
Overall	204/10388 (2%)	0/5712 (0%)	160/3612 (4%)	44/1064 (4%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

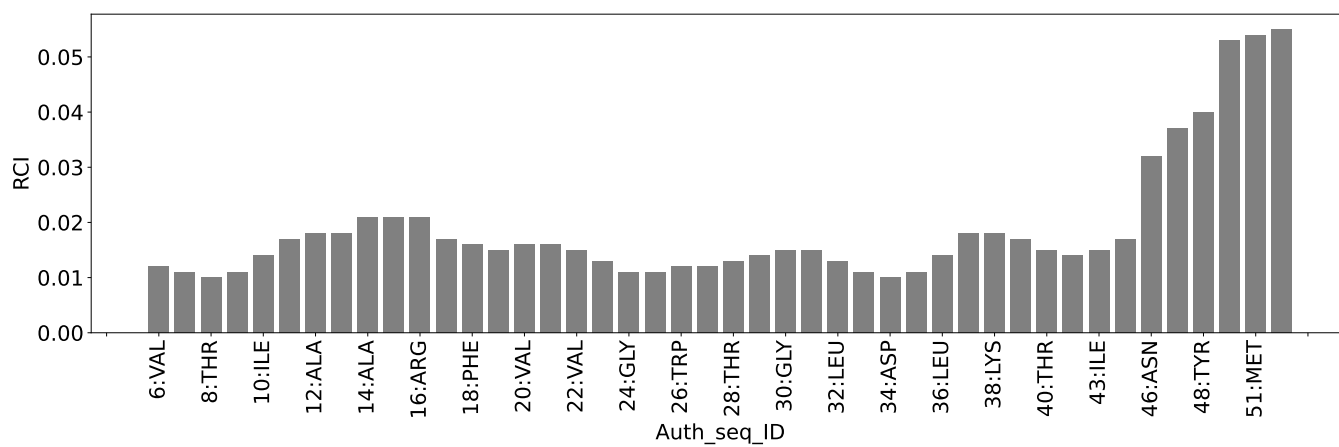
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	54
Intra-residue ($ i-j =0$)	1
Sequential ($ i-j =1$)	15
Medium range ($ i-j >1$ and $ i-j <5$)	19
Long range ($ i-j \geq 5$)	9
Inter-chain	10
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.1
Number of long range restraints per residue ¹	0.0

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)	None	None
0.2-0.5 (Medium)	None	None
>0.5 (Large)	6.0	2.39

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

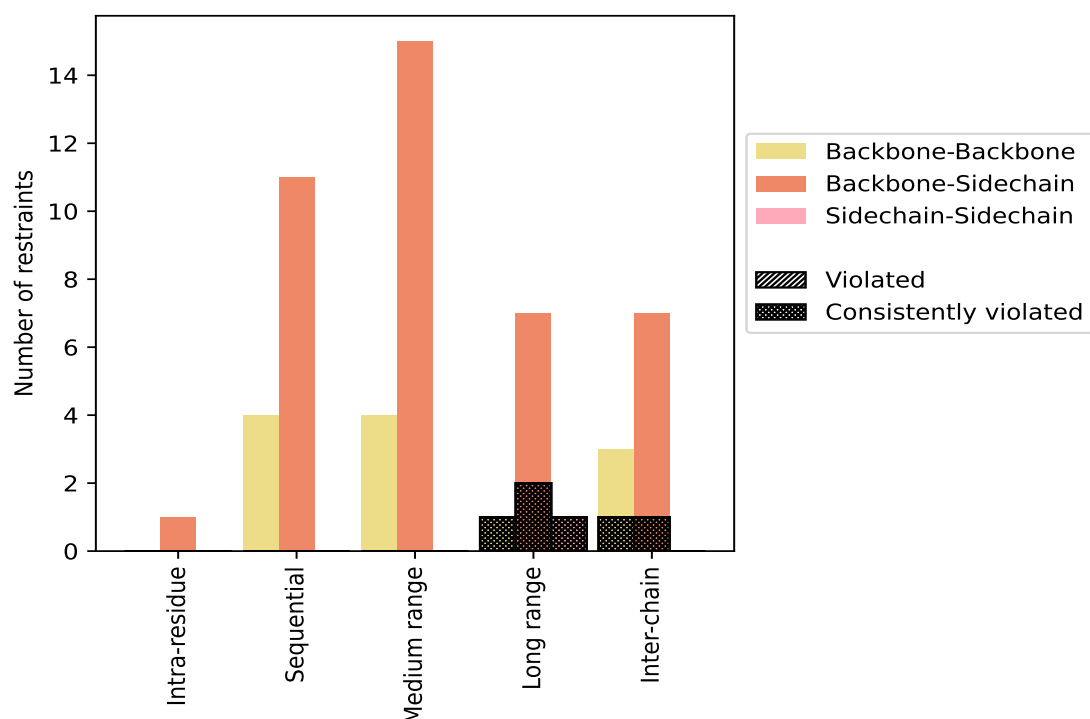
9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1	1.9	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	1	1.9	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 ($i-j =1$)	15	27.8	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	4	7.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	11	20.4	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 ($i-j >1$ & $i-j <5$)	19	35.2	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	4	7.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	15	27.8	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 ($i-j \geq 5$)	9	16.7	4	44.4	7.4	4	44.4	7.4
Backbone-Backbone	1	1.9	1	100.0	1.9	1	100.0	1.9
Backbone-Sidechain	7	13.0	2	28.6	3.7	2	28.6	3.7
Sidechain-Sidechain	1	1.9	1	100.0	1.9	1	100.0	1.9
Inter-chain	10	18.5	2	20.0	3.7	2	20.0	3.7
Backbone-Backbone	3	5.6	1	33.3	1.9	1	33.3	1.9
Backbone-Sidechain	7	13.0	1	14.3	1.9	1	14.3	1.9
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	54	100.0	6	11.1	11.1	6	11.1	11.1
Backbone-Backbone	12	22.2	2	16.7	3.7	2	16.7	3.7
Backbone-Sidechain	41	75.9	3	7.3	5.6	3	7.3	5.6
Sidechain-Sidechain	1	1.9	1	100.0	1.9	1	100.0	1.9

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](#)

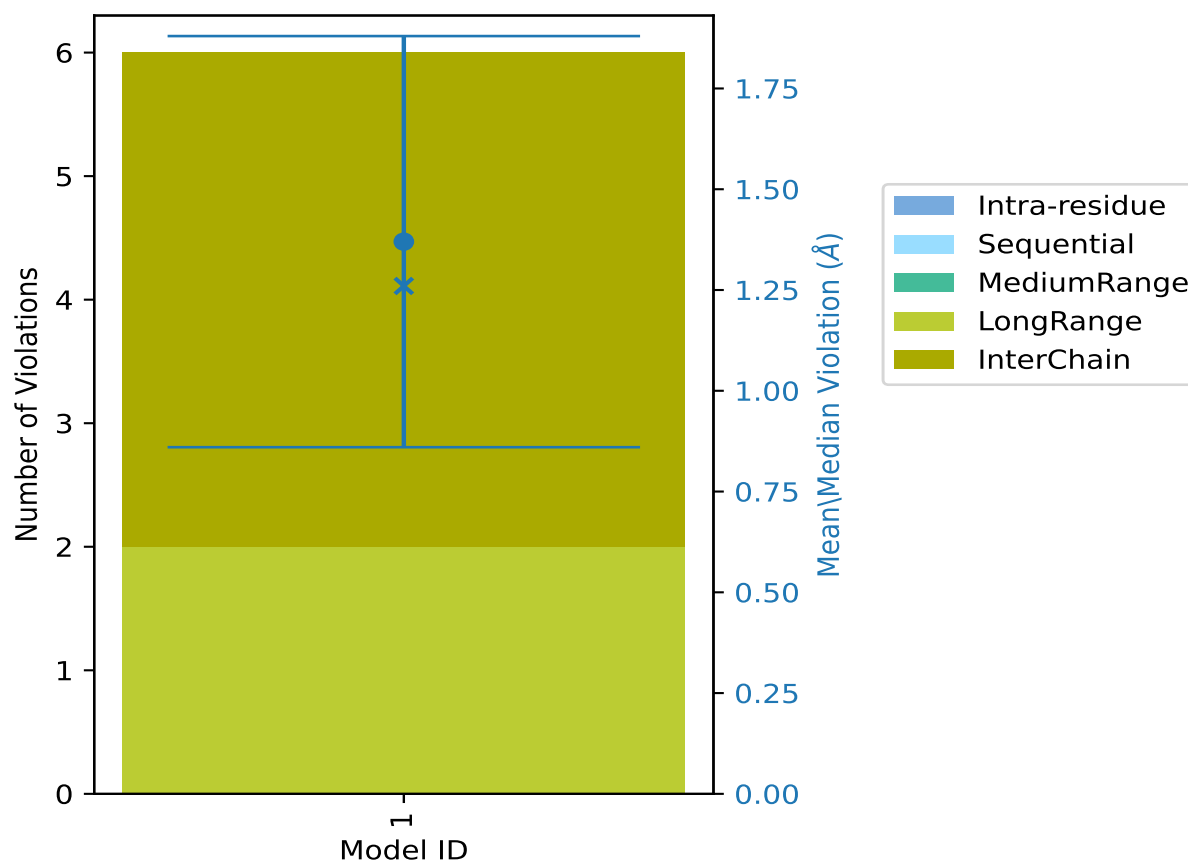
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

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	0	0	0	2	4	6	1.37	2.39	0.51	1.26

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

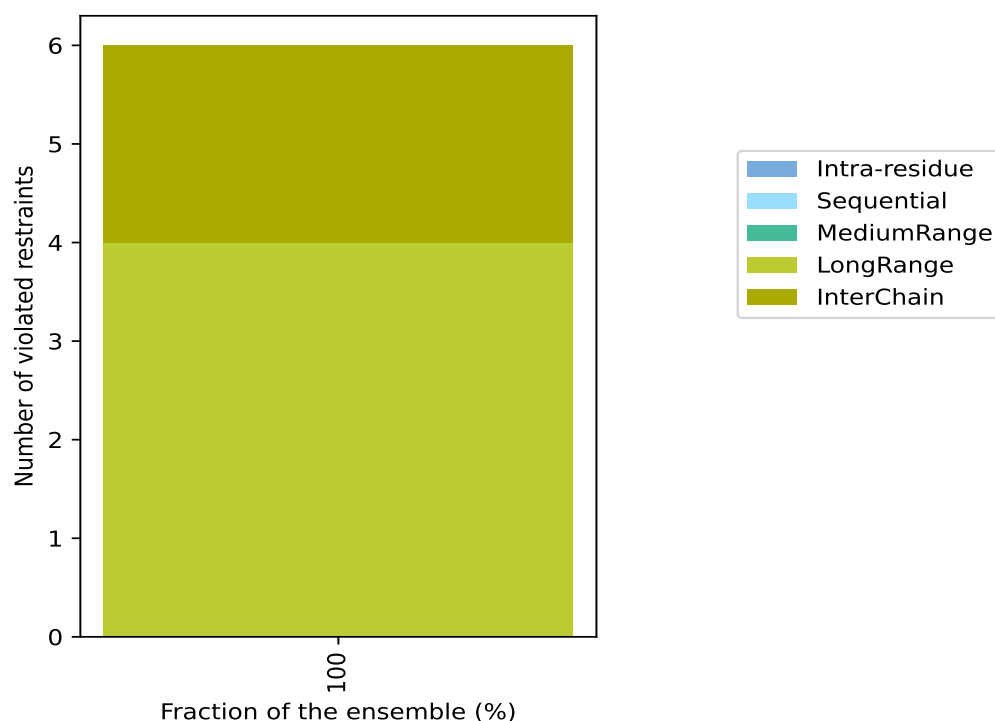
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 48(IR:1, SQ:15, MR:19, LR:5, IC:8) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	4	2	6	1	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](#)



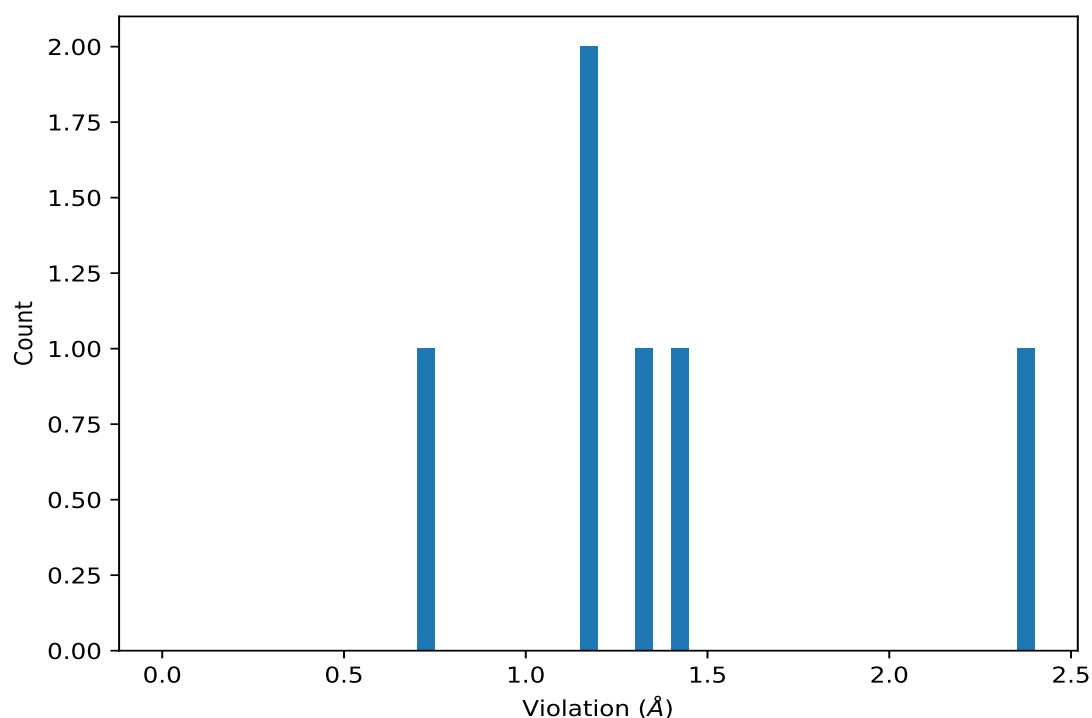
9.4 Most violated distance restraints in the ensemble [i](#)

No violations found

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 lists the absolute value of the violation for each restraint in the ensemble sorted by its 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)
(1,48)	1:39:B:GLY:CA	1:14:J:ALA:CA	1	2.39
(1,13)	1:11:J:LEU:CG	1:28:A:THR:CA	1	1.4
(1,7)	1:34:B:ASP:CB	1:8:J:THR:CA	1	1.33
(1,24)	1:29:E:VAL:CG2	1:24:E:GLY:CA	1	1.19
(1,2)	1:29:E:VAL:CG2	1:24:E:GLY:CA	1	1.19
(1,41)	1:47:H:ALA:CA	1:40:A:THR:C	1	0.71

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found