



# Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2BW2  
BMRB ID : 6731  
Title : BofC from Bacillus subtilis  
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Deposited on : 2005-07-08

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

Cyrange : NOT EXECUTED  
NmrClust : NOT EXECUTED  
MolProbity : FAILED  
Percentile statistics : NOT EXECUTED  
wwPDB-RCI : NOT EXECUTED  
PANAV : NOT EXECUTED  
wwPDB-ShiftChecker : NOT EXECUTED  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

## 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 was not calculated.

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 25 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores.

Cyrange was unable to find well-defined residues.

Error message: Cyrange did not run

NmrClust was unable to cluster the ensemble.

Error message: NmrClust did not run

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2248 atoms, of which 1105 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BYPASS OF FORESPORE C.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	140	2248	733	1105	189	217	4	0

SEQUENCE-PLOTS INFOmissingINFO

## 4 Refinement protocol and experimental data overview

The models were refined using the following method: *CANDID AND CNS*.

Of the 100 calculated structures, 25 were deposited, based on the following criterion: *ENERGY*.

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

Software name	Classification	Version
CNS	refinement	
Sparky	structure solution	

No chemical shift data was provided.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

### 5.2 Too-close contacts [i](#)

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

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

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

#### 5.3.2 Protein sidechains [i](#)

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

#### 5.3.3 RNA [i](#)

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

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

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

### 5.5 Carbohydrates [i](#)

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

### 5.6 Ligand geometry [i](#)

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

### 5.7 Other polymers [i](#)

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

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.