Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2BW2
BMRB ID	:	6731
Title	:	BofC from Bacillus subtilis
Authors	:	Patterson, H.M.; Brannigan, J.A.; Cutting, S.M.; Wilson, K.S.; Wilkinson, A.J.; Ab, E.; Diercks, T.; Folkers, G.E.; de Jong, R.N.; Truffault, V.; Kaptein, R.
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) 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 (i)

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 (i)

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 (i)

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 (i)

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 (i)

There are no chain breaks in this entry.