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online data

SUPPLEMENTARY ONLINE DATA

The HicA toxin from *Burkholderia pseudomallei* has a role in persister cell formation

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Table S1 NMR assignment, structure calculation and validation statistics

Parameter	Values
Degree of assignment*	
Backbone (Cα, C', N and H^N) (%)	91.2
Side-chain H (%)	79.4
Side-chain non-H (%)	39.7
Number of restraints	
Distance restraints	
Intra-residue ($\|i-j\|=0$)	515
Sequential ($\|i-j\|=1$)	216
Medium range ($2\leqslant\|i-j\|<5$)	109
Long range ($\|i-j\|\geqslant 5$)	172
Ambiguous	59
Total	1012
Dihedral angle restraints (Φ/Ψ)	94 (47/47)
Restraint statistics†	
RMSD of distance violations (Å)	0.019 ± 0.003
RMSD of dihedral violations (°)	0.27
Violations>0.5 Å	0
Violations>0.3 Å	0
Violations>0.1 Å	9.8 ± 2.8
RMSD from idealized covalent geometry†	
Bonds (Å)	0.0031 ± 0.00017
Angles (°)	0.47 ± 0.0013
Impropers (°)	1.33 ± 4.97
Structural quality	
Ramachandran statistics*‡§	
Most favoured regions (%)	84.0 91.2
Allowed regions (%)	14.2/7.0
Generously allowed regions (%)	1.9/1.8
Disallowed regions (%)	0.0/0.0
CING ROG scores (R/O/G)* [1] (%)	20/22/58
Verify3D *Z*-score [2]	−2.57
Prosa II *Z*-score [3]	−0.74
Procheck *Z*-score (Φ/Ψ)‡ [4]	−1.14
Procheck *Z*-score (Φ/Ψ)‡ [4]	−1.71
MolProbity *Z*-score [5]	−1.57
Number of close contacts	2
Co-ordinates precision (RMSD)*§‖	
All backbone atoms (Å)	3.2/1.2/0.6
All heavy atoms (Å)	3.5/1.6/1.4

*Residues 5–59.
†Values reported by ARIA 2.3 [6].
‡Values reported by Procheck [4].
§Ordered residues (5–21, 23–32, 35–39 and 45–58) as calculated by PSVS 1.4 [3].
‖Residues in secondary structure (6–12, 16–19, 24–28, 35–39 and 50–58) as determined by DSSP [7].

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The chemical shifts and structure reported for HicA toxin from *Burkholderia pseudomallei* will appear in the Biological Magnetic Resonance Data Bank (BMRB) under accession number 19464 and in the PDB under code 4C26 respectively.

Figure S1 List of 75 HicA homologous sequences from differerent bacterial strains

These sequences were used for a subsequent ClustalW alignment and the most conserved residues are shown. A high-resolution version of Figure S1 is available to download (at http://www.biochemj.org/bj/459/bj4590333add.htm).

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