The Crystal Structure of YaeQ from Xanthomonas axonopodis pv citri.

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Xanthomonas axonopodis pv. citri (Xac) YaeQ (XAC2396) is a member of a family of bacterial proteins conserved in several gram negative pathogens. Here we describe the crystallization and structure determination of YaeQ. Recombinant YaeQ containing selenomethionine was crystallized in space group P2₁ and crystals diffracted up to 1.9 Å resolution at a synchrotron source. The unit cell parameters are a = 39.75, b = 91.88, c = 48.03 Å and β = 108.37°. Two YaeQ molecules are present in the asymmetric unit. Initial experimental phases were calculated by the multiple wavelength anomalous dispersion technique and an interpretable electron density map was obtained. The YaeQ structure reveals a novel protein fold characterized by a single helix sandwiched between two curved beta sheets. One beta strand stitches the two sheets together on one side to form an almost complete barrel with a lateral opening in which one face of the internal helix is exposed. Three adjacent parallel strands plus two external helices form a beta-alpha-beta-alpha-beta motif (Rossman fold). Though residues in the loops of the Rossman fold are not well-conserved in the YaeQ family, the C-termini of the beta strands in this motif point towards a number of well-conserved residues that are clustered on two loops located on the top of the YaeQ barrel and on the exposed face of the central helix. Analysis of the YaeQ structure has provided leads through which may be gained information regarding its function. The results of preliminary functional experiments will be presented.

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