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Publication Date

2005-03-20

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Poster presentation

Crystal Structure of a Hypothetical Mycoplasma Specific Protein, MP958 (GI: 1673958)

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The 193 amino acid residue long protein MP958 has sequence homologs only in other mycoplasma and ureaplasma species. Its function is unknown and could not be inferred by any of the sequence based methods such as phylogentic profile, Rosetta stone, gene neighbor, or gene cluster. We determined the crystal structure of the His-tagged protein to 2.8 Å to possibly extract information about the molecular function of the protein from its three-dimensional structure and any bound ligands, if some are present. Only the His-tagged version of the protein crystallized in space group C2 with four molecules in the asymmetric unit. Although the crystals grew to a very large size, they were useless due to severe twinning. Addition of various detergents improved crystal growths so that some untwinned data sets could be collected. The structure was eventually solved by SAD method from Se-Met derivatives of the protein. However, every step of the structure determination proved to be relatively difficult and required careful choosing and optimization of the methods available. Automated structure determination methods failed in this case. We are presenting here the methods used for structure determination, the description of the structure, and implications for the function of this molecule.