MS10-P10 Crystal structure of YwpF from *Staphylococcus aureus* reveals its architecture comprised of a β-barrel core domain resembling type VI secretion system proteins and a two-helix pair

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The *ywpF* gene (*SAV2097*) of the *Staphylococcus aureus* strain Mu50 encodes the YwpF protein, which may play a role in antibiotic resistance. Here, we report the first crystal structure of the YwpF superfamily from *S. aureus* at 2.5 Å resolution. The YwpF structure consists of two regions: an N-terminal core β-barrel domain that shows structural similarity to type VI secretion system (T6SS) proteins (e.g. Hcp1, Hcp3, and EvpC) and a C-terminal two-helix pair. Although the monomer structure of *S. aureus* YwpF resembles those of T6SS proteins, the dimer/tetramer model of *S. aureus* YwpF is distinct from the functionally important hexameric ring of T6SS proteins. We therefore suggest that the *S. aureus* YwpF may have a different function compared to T6SS proteins.

Keywords: Staphylococcus aureus, YwpF, SAV2097, type VI secretion system (T6SS) proteins

MS10-P11 PDB2INS - an interface to SHELXL refinements of macromolecules

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PDB2INS is an Open Source Python program that reads a PDB file and prepares an .ins file for macromolecular refinement with SHELXL. The necessary restraints for the refinement are taken from the CCP4 refmac monomer library, provided by the GRADE or PRODRG servers or extracted from a reference structure. The latter approach is particularly useful for refinement against neutron data where the reference structure has been refined already against higher resolution X-ray data. It may also be useful for mutants or protein complexes when a higher resolution structure is available for a wild-type or component protein. PDB2INS takes advantage of recent developments in SHELXL, e.g. for restrained anisotropic refinement or refinement against neutron data [1-3].

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