

W0452

Structure of Toprim Domain-containing Protein from *Bacillus stearothermophilus*. P. Rezacova¹, D. Borek¹, S. Moy², A. Joachimiak², Z. Otwinowski¹, ¹Dept. of Biochemistry, UT Southwestern Medical Center, Dallas, TX, ²Biosciences Div. and Structural Biology Center, Argonne National Laboratory, Argonne, IL.

The crystal structure of Midwest Center for Structural Genomics target APC35832, a 14.7-kDa protein from *Bacillus stearothermophilus*, has been determined at 1.6 Å by SAD from mercury soaked crystals.

APC35832 structure has a conserved Toprim fold with a 4-stranded β-sheet surrounded by 4 α-helices. Toprim domain is a part of the catalytic core in number of enzymes catalyzing formation or cleavage of phosphodiester bond. The closest structural homolog of APC35832 is domain in T7 primase, in which the conserved acetic residues coordinate Mg²⁺ ion and conserved glutamate was found to be critical for formation of phosphodiester bond.

In order to determine if the metal-binding function is preserved in APC35832, the protein was co-crystallized with MgCl₂ and the structure was determined at 1.6 Å. One Mg²⁺ ion is coordinated by side chains of conserved residues D58, D60 and E88.

The metal binding and the presence of conserved glutamate E14 suggest that Toprim domain of APC35832 can participate in a catalytic activity. Nevertheless, protein APC35832 lacks the additional domains necessary for catalytic activity of proteins belonging to Toprim superfamily. Protein consisting of Toprim domain alone thus might represent modules for construction of novel class of multimeric nucleotidyl transferases or nucleases. Potential interaction partners and biological function of the APC35832 protein are yet to be identified.

