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MCSG Case Study- A Difficult Structure Determination for *E. Coli* Yfce, a Predicted Phosphatase Demonstrating Mn Dependent Phosphodiesterase Activity. Darcie J. Miller^{1,2}, Ludmilla Shuvalova¹, Elena Evdokimova³, Alexei Savchenko³, Alexander F. Yakunin³, Wayne F. Anderson^{1,2}, ¹Dept. of Molecular Pharmacology & Biological Chemistry, ²Northwestern Drug Discovery Program, ^{1,2}Northwestern Univ. School of Medicine, Chicago, IL 60611, USA, ³C. H. Best Institute, Univ. of Toronto, Toronto, ON M5G 1L6, Canada.

As part of the Midwest Center for Structural Genomics, we have determined the X-ray crystal structure of a novel Mn dependent phosphatase from *E. coli*. The structure was not easily obtained, due to problems in finding isomorphous derivatives (diffraction quality Se-methionine substituted crystals were unavailable). Additionally, pseudosymmetry made these crystals appear to be of higher symmetry. After cross-comparison of several datasets, we were able to distinguish these crystals as P3₁, not P3₁21. The substructure was subsequently determined using SIRAS by comparing data from a CH₃HgCl₂ soaked crystal (“native”) with that from a K₂PtCl₄ doped crystal. An instructional description of the structure-determination is provided. The β-barrel topology and active site will also be discussed, and the biochemical assessment of Mn dependent phosphatase activity provided.