

W0467

Determination of ytrI Architecture. D. Borek¹, J. Osipiuk², R. Wu², S.F. Moy², A. Joachimiak² & Z. Otwinowski¹, ¹UT Southwestern, Dallas, TX, ²SBC-ANL, Argonne, IL.

ytrI is a structural protein specific for endospore-forming bacteria from *Bacillus* genus. It is implicated in maintaining spore integrity at the late stages of sporulation process. We solved the structure of ytrI soluble domain. The crystals we obtained diffracted anisotropically in the range 2.8-3.0 Å. Data analysis indicated six molecules in ASU with the solvent content ~70%. Heavy atom positions were found, but were poorly ordered due to only a single Se-site located on the protein surface. Initial NCS averaging was not successful as the protein forms only quasi-symmetric high order oligomeric assemblies. Due to unique pseudo-symmetry, the consequences of phase errors were not uniformly distributed, with two molecules having a particularly poor electron density. The solution of the structure integrated phasing and model building with an unusual procedure involving steps that increased bias, followed by returning to earlier phases to remove it.

The crystal structure consists of parallel fibers that are likely to be physiologically relevant. Interactions between flexible coil-coiled segments and alpha-beta core of the fiber are observed. The structure provides insight into the so far poorly understood group of the membrane-anchored, structural proteins.