Crystallization of the novel flavodoxine-like protein, WrbA, - on the way to three-dimensional structure

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Tryptophan (W)-repressor binding protein A, WrbA, identified as an *E. coli* stationary-phase protein was named for its reported effect on the interaction between tryptophan repressor and DNA [1]. Later work [2] showed that this effect was non-specific, leaving the physiological role of WrbA unknown. According to sequence analysis and homology modeling [3] WrbA was identified as the founding member of a new family of flavodoxin-like proteins, which displays low but structurally significant sequence similarity with the flavodoxins. The members of WrbA family are predicted to share the open, twisted α/β flavodoxin fold, but with a short conserved insertion unique for the new family. This structure motif could account for experimental observations that some family members are dimeric in solution, including also finding that WrbA creates a dimer-tetramer equilibrium at micromolar concentrations [2]. Unlike typical flavodoxins [4], these proteins bind FMN relatively weakly but still specifically. The computer analysis [3] indicated some structural differences in the flavin-binding pocket, which may explain the lower affinity of WrbA for FMN. Due to these peculiarities the structural analysis may aid in understanding the physiological roles of WrbA family members. These factors motivated our research for diffraction-quality crystals.Purified WrbA apoprotein and holoprotein were used for crystallization trials. Standard and advanced crystallization techniques were applied to crystallize mentioned proteins. WrbA apoprotein crystals grown in capillaries were measured directly at synchrotron DESY (beamline X13) in Hamburg (Germany). Crystals diffracted to a resolution of 2.2Å. Attempts with variable growing conditions are performed to improve quality of apo- and holoprotein crystals.

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