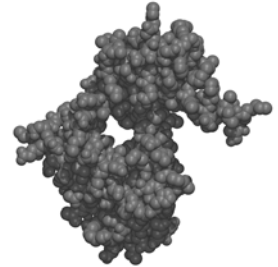


W0237

Crystal Structure of YfiR, a Putative Transcriptional Regulator from *Bacillus subtilis*. S.S. Rajan, X. Yang, L. Shuvalova, F. Collart¹, W.F. Anderson, Molecular Pharmacology & Biological Chemistry, Feinberg School of Medicine, Northwestern Univ., Chicago, IL, ¹Biosciences Div., Argonne National Laboratory, Argonne, IL.

YfiR is a putative transcriptional regulator from *Bacillus subtilis* similar in sequence to the tetracycline repressor (TetR) family. We have determined the crystal structure of YfiR to a resolution of 1.95 Å. YfiR is a two-domain all-helical protein with the N-terminal domain showing the characteristic helix-turn-helix (HTH) motif of DNA-binding proteins. YfiR exists as a dimer in crystals and in solution and is structurally similar to QacR, also a member of the TetR family. QacR can bind a wide range of structurally diverse xenobiotics and consequently allow the expression of the efflux pump QacA. The YfiR structure revealed the presence of an as yet unidentified ligand bound to the protein at the same relative position as in QacR structures. The ligand binding cavity in YfiR is a long winding tunnel that completely penetrates the subunit but is blocked at one end by the second subunit of the dimer. Efforts are underway to identify the ligand and DNA specificities of YfiR.



Diffraction data were collected at sector ID5B of DND-CAT beamline at APS. This work is supported by an NIH grant to the Midwest Center for Structural Genomics.