Crystal Structure of *Pfu* 838710: the First Model of a Pfam CYTH Domain

Hua Yang¹, Jessie Chang¹, Ashit Shah, Joe Ng², Wolfram Tempel¹, Florian Schubot¹, Zhi-Jie Liu¹, John Rose¹, Bi-Cheng Wang¹, Southeast Collaboratory for Structural Genomics, ¹Department of Biochemistry and Molecular Biology, University of Georgia, Athens, GA 30602, USA. ²Laboratory for Structural Biology, University of Alabama in Huntsville, Huntsville, AL 35899, U.S.A. E-mail: huayang@uga.edu

Pfu-838710 is a 21.4kDa protein from *Pyrococcus furiosus*, a hyperthermophile, belongs to a Pfam family [1] which includes the catalytic domains of CyaB-like adenylyl cyclase and thiamine triphosphatase (CYTH). The structure reported here represents the first structure for this Pfam.

Pfu-838710 crystallized in space group P3₁21 with cell dimensions a = 97.02Å and c = 127.59Å. A quick soak of a crystal in a K₂PtCl₄ solution produced a platinum derivative as determined by Patterson analysis. The initial 2.6Å phases and electron density map were generated from single wavelength anomalous scattering data (λ = 1.5418) using the SCA2Structure pipeline [2]. The model was built using XFIT and refined against a 2.3Å resolution data set collected at SER-CAT (www.ser-cat.org), Sector 22 APS. The protein contains an 8-stranded anti-parallel β barrel that forms a closed tunnel. The structure has been refined to R = 22.3%, R-free = 25.8% (PDB ID 1XKC).

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[1] Iyer L.M., Aravind L., *BMC Genomics* 2002, **3**, 33-33. [2] Liu, et al., *Acta Cryst. Section D*, 2005, *in press*.

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