

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

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Pfu-838710 is a 21.4kDa protein from *Pyrococcus furiosus*, a hyperthermophilic archaeon. Multiple sequence alignment [1] shows that *Pfu*-838710 belongs to a novel domain protein superfamily (Pfam) that includes the catalytic domains of CyaB-like adenylyl cyclase and thiamine triphosphatease (CYTH). The structure presented here represents the first structure reported for this Pfam.

The native protein crystallized in space group $P3_121$ with cell dimensions $a = b = 97.02\text{\AA}$ and $c = 127.59\text{\AA}$. A quick soak of a native crystal in a solution containing K_2PtCl_4 produced a platinum heavy atom derivative as determined from the analysis of the anomalous difference Patterson. The initial phases and electron density map were obtained using 2.6\AA single wavelength anomalous scattering data ($\delta = 1.5418\text{\AA}$) with SECSG SCA2Structure pipeline [2]. The model was built using XFIT and refined against a higher 2.3\AA resolution data set collected at SER-CAT (www.ser-cat.org), 22-ID, APS.

A *Pfu*-838710 dimer occupies the crystallographic asymmetric unit. Each monomer of the dimer contains an 8-stranded anti-parallel β barrel that forms a topologically closed tunnel. The structure has been refined to $R = 22.3\%$, $R\text{-free} = 25.8\%$ at 2.3\AA (PDB ID: 1XKC).

Work supported in part from funds from the National Institutes of Health (GM062407), the Georgia Research Alliance, and The University of Georgia Research Foundation.

[1] Iyer LM, Aravind L; BMC Genomics 2002; 3:33-33.

[2] Liu Z.J., Lin D.W. et al., Acta Cryst. D (61) 2005: 520-527.

Keywords: CYTH domain, *Pyrococcus furiosus*, Pfam, Sca2Structure