

## W0613

**Crystal Structure of Thiamine Monophosphate Kinase (thiL).** Subramaniam Eswaramoorthy, Subramanyam Swaminathan, Biology Dept., Brookhaven National Laboratory, Upton, NY 11973.

Thiamine monophosphate kinase is an enzyme that phosphorylates thiamine monophosphate. The enzyme thiL from *Aquifex aeolicus* was selected as a target by NYSGRG ([www.nysgrc.org](http://www.nysgrc.org)) and its crystal structure has been determined by the multiwavelength anomalous dispersion method (MAD). This representative structure of thiL family exists as a dimer. Each monomer has two domains, an  $\alpha\beta$ -domain comprising an anti-parallel  $\beta$ -sheet and  $\alpha$ -helices, and a small domain with an  $\alpha$  and  $\beta$  layers. The  $\alpha$  and  $\beta$  layers of two protomers come together and form an  $\alpha\beta\beta\alpha$  sandwich. A deep cavity is formed between the  $\alpha\beta$ -domain and the  $\alpha\beta\beta\alpha$  sandwich. A pyrophosphate molecule with a partial occupancy of one phosphate is located in a minor cleft further from this groove. The side chains of Glu58 has dual conformation with one of them competing with the partially occupied phosphate. As can be seen in the HSSP database more than 200 proteins with sequence identity >30% may be modeled using this structure. Fold of this protein resembles aminoimidazole ribonucleotide synthase (PurM). Details of the structure and active site will be discussed.

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