Crystal structures of Thiamine monophosphate kinase from *Acinetobacter baumannii* in complex with substrates and products

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Acinetobacter baumanii is a member of the ESKAPE pathogens (*Enterococcus faecium*, *Staphylococcus aureus*, *Klebsiella pneumonia*, *Acinetobacter baumanii*, *Pseudomonas aeruginosa*, and *Enterobacter* species), all of which have a high rate of antibiotic resistance, are opportunistic, and are responsible for a large number of hospital borne infections. Therefore, *A. baumanii* is one of the target organisms for SSGCID. Thiamine monophosphate kinase (ThiL) catalyzes the last step of the thiamine pyrophosphate synthesis, the ATP-dependent phosphorylation of Thiamine monophosphate (TMP) to Thiamine pyrophosphate (TPP). Humans lack ThiL, which might make ThiL an attractive drug target.

We solved the structure of *A. baumanii* ThiL in complex with its substrates TMP / AMPPNP, and in complex with its products TPP / ADP. High resolution of the data and anomalous diffraction allows for a detailed description of the binding mode of substrates and products, and the metal environment. The structures highlight the path of the reaction, and a distinct variability of metal content.