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Crystal structure of GMP synthetase from *Thermus thermophilus* HB8

高度好熱菌 *Thermus thermophilus* HB8 由来 GMP synthetase の結晶構造

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GMP synthetase (GuaA) catalyzes a reaction in which xanthosine 5'-monophosphate (XMP) is converted into GMP in the purine nucleotide biosynthetic pathway. According to the structure of *Escherichia coli* counterpart, GuaA consists of two catalytic domains, ATP pyrophosphatase domain and glutamine amidotransferase domain. In the purine nucleotide biosynthetic pathway, glutamine amidotransferase activity is also found in amidophosphoribosyltransferase (PurF) and FGAR amidotransferase I (PurQ). Thus, it must be important to compare the structures of these three enzymes.

We obtained crystals of GuaA in both of native and Se-Met modified forms with sizes of 0.5 x 0.3 x 0.2 mm^3 and 0.4 x 0.3 x 0.2 mm^3, respectively. Diffraction data for the crystals were collected in SPring-8 with a resolution of 2.1 Å, R factor of 9 % and a completeness of 96 % for native and 2.1 Å, 6 % and 65 % for Se-Met. MAD data were collected with the wavelengths of 0.9795 Å (peak), 0.9797 Å (edge) and 0.9840 Å (remote). Collected data were processed by using HKL2000 and crystallographic parameters were obtained as space group *C2*, a = 141.5 Å, b = 114.7 Å, c = 159.7 Å for native and *C2*, 140.3Å, 114.6 Å, 158.1 Å for Se-Met. The phase was determined by the MAD method using SOLVE/RESOLVE and it was found that two dimers are placed in an asymmetric unit (Fig. 1). The Cα model was obtained by program O, and model building is in progress. The overall folding is generally same with that of *E. coli* GuaA[1)]. Becasuse *T. thermophilus* GuaA did not bind ATP in the obtained crystal, electron density is missing in the ATP binding site, whereas electron density for both of ATP and the ATP binding site was clearly observed for the case of *E. coli* GuaA. In both structures, electron density was missing in the glutamine binding site. We are now trying to prepare co-crystals with substrate analogues such as AMPPNP by soaking or crystallization of the complex.

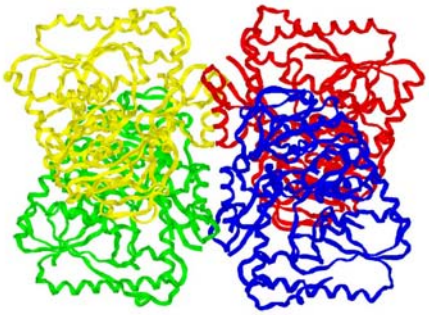

Fig. 1. Crystal structure of *T. thermophilus* GuaA.

Reference

[1] Tesmer J.J., Klem T.J., Deras M.L., Davisson V.J. and Smith J.L. *Nat Struct Biol.* Vol. 3, No. 1, pp. 74-86 (1996)