The crystal structure of peptide deformylase from *Thermus thermophilus* HB8.

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Peptide deformylase (PDF) catalyzes the hydrolytic removal of the N-terminal formyl group from nascent ribosome-synthesized polypeptide in eubacteria and organelle of certain eukaryotes. The gene encoding PDF (def) was shown to be essential in *Escherichia coli*, *Staphyrococcus aureus, and Streptococcus pneumoniae* and is present in all sequenced bacterial genomes. This has qualified PDF as an attractive target for the development of new antibacterial drugs. Subsequent analysis of diverse peptide deformylase sequences suggested that the enzyme family could be divided into two classes. The sequence homology to *E. coli* enzyme is 36 %. *T. thermophilus* is a gram-negative bacterium and is survived at 75 ºC. To gain further insight into the molecular mechanisms that nature uses to adapt to environmental temperature, we have tried to determine the crystal structure of *T. thermophilus* PDF (*Tth*PDF) and compare the ternary structure and biochemical characters with that of *E.coli*.(*Eco*PDF).

The crystals grown to the maximal dimension of 1.0 x 0.2 x 0.05 mm in a week were obtained with a reservoir solution consisting of 0.1 M Tris-HCl (pH 8.0), 20 % (w/v) PEG 4k and 0.2 M sodium acetate. Native X-ray diffraction data set were collected from cryocooled (100K) crystal at BL 41XU at SPring 8, Harima, Japan. The crystals diffracted X-rays up to 1.81 Å. The crystals belonged to the tetragonal space group $P4_3$ with unit-cell parameters of $a = b = 62.6$ Å and $c = 105.3$ Å and contained two molecules in an asymmetric unit, giving a crystal volume per protein mass (V_M) of 2.3 $Å^3$ Da^{-1} and solvent content of 46.7%.

The structure of *Tth*PDF has been solved by the molecular replacement method using the atomic coordinates of PDF from *Thermotoga maritima* (PDB code 1LME, Kreusch *et al*., 2003) as a search model (CCP4, 1994), which shares ca. 40% amino acid sequence identity to *Tth*PDF. Compared to the structure of *Eco*PDF, global structural difference occurred in the C-terminal region. The C-terminal helix of *Tth*PDF was kinked, whereas that of *Eco*PDF was straight. This would be one of the reasons why *Tth*PDF were thermostable.

The structural details will be discussed.