

## Crystal Structure of *Sulfolobus tokodaii* Aspartyl-tRNA Synthetase

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In the translation system, aspartyl-tRNA synthetase (AspRS) catalyzes aspartylation of the cognate tRNA through the two steps of reactions. At first, it strictly recognizes aspartic acid to produce aspartyl-AMP from ATP in the presence of  $Mg^{2+}$ . Then it is bound to the corresponding tRNA<sup>Asp</sup>, and transfers the aspartic acid to the 3' terminus of the tRNA. Two types of AspRS are known; discriminating and non-discriminating. The former is bound only tRNA<sup>Asp</sup>, while the latter is bound both tRNA<sup>Asp</sup> and tRNA<sup>Asn</sup>. Thermoacidophilic archaea *Sulfolobus tokodaii* (*St*) belongs to the non-discriminating type, missing AsnRS gene. The crystal structure of AspRS from *St* has been determined at 2.3 Å resolution. *St*-AspRS is a dimeric enzyme consisting of two identical subunits. This is the first AspRS structure from crenarchaea. Each subunit is composed of the catalytic, the anticodon-binding and the hinge domains. Structural comparison with those of the three published AspRS of different sources shows that the 3rd residue (C36) of the tRNA<sup>Asp</sup> anticodon is specifically recognized by the main chain amide group of discriminating AspRS, suggesting that C36 is the essential identity of tRNA<sup>Asp</sup>. However, in the case of non-discriminating AspRS, the contacting residue is replaced with proline, which has no amide group. Furthermore the Pro residue in question is put away from the 3rd residue of the anticodon so that the corresponding 3rd residue (U36) of tRNA<sup>Asn</sup> is also acceptable in this site. This situation is conserved in every non-discriminating AspRS.

**Keywords:** aspartyl-tRNA synthetase, *sulfolobus tokodaii*, x-ray crystal structure analysis