Crystal structure of aspartate α -decarboxylase from H. pylori

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L-Aspartate -decarboxylase (ADC), encoded by the panD gene, catalyses the conversion of L-aspartate into β -alanine. In the microorganisms, β -alanine is required for the synthesis of pantothenate (vitamin B₅), which is the precursor of 4'-phosphopantetheine and coenzyme A. We have determined the crystal structure of Helicobacter pyloriADC, a tetrameric enzyme, in two forms: the apo structure at 2.0 Åresolution and the isoasparagine complex structure at 1.55 Åresolution. All subunits of the tetramer are self-processed at Gly24Ser25 linkage, producing the chain (residues 124) and the larger achain (residues 25117). Each subunit smaller contains nine β -strands and three α -helices; it is folded into the double-psi -barrel structure. In the apo structure, the new amino terminus of the a chain, Ser25, is converted into a pyruvoyl group. In the isoasparagine complex structure, the substrate analog is covalently attached to the pyruvoyl group. This structure represents the enzyme-substrate Schiff base intermediate that was proposed to form prior to decarboxylation step in the catalytic cycle of ADC. Thus our study provides the direct structural evidence for the reaction mechanism of ADC.