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Crystal Structure of the Ternary Complex of Allantoate-Amidohydrolase with its Substrate and A Ligand: A Crucial Enzyme of Purine Catabolism from E. coli K12. Rakhi Agarwal, Subramanyam Swaminathan, Biology Dept., Brookhaven National Laboratory, Upton, NY, 11973 USA

Allantoate-amidohydrolase, one of the enzymes involved in purine degradation pathway, is responsible for the breakdown of allantoate to CO₂, NH₃ and ureidoglycine and is conserved among species. We determined the crystal structure of allantoate-amidohydrolase from E. coli K12 by Se-MAD at 2.25Å resolution. The protein is a homodimeric subunit, consisting of one large catalytic domain with a dizinc center and a small domain mainly involved in dimerization. Each domain has an interesting mixed α/β topology similar to the family of dizinc-dependant exopeptidases suggesting a common origin. The substrate allantoate binds to the deep cleft of the active site and the ligand binds close to the active site. Allantoate-amidohydrolase with the bound substrate and ligand provides insight into its mechanism of carbamoyl exopeptidase nature of action. The ligand sulfate anion presumably acts as an allosteric effector.

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