ESRF

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Report:

Insights into Enzyme Evolution Revealed by the Structure of Methylaspartate Ammonia Lyase

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Abstract

Methylaspartate ammonia lyase (MAL) catalyzes the magnesium-dependent reversible ,αβ-elimination of ammonia from L-*threo*-(2S,3S)-3-methylaspartic acid to mesaconic acid. The 1.3 Å MAD crystal structure of the dimeric *Citrobacter amalonaticus* MAL shows that each subunit comprises two domains, one of which adopts the classical TIM barrel fold, with the active site at the C-terminal end of the barrel. Despite very low sequence similarity, the structure of MAL is closely related to those of representative members of the enolase superfamily, indicating that the mechanism of MAL involves the initial abstraction of a proton α to the 3-carboxyl of (2S,3S)-3-methylasparic acid to yield an enolic intermediate. This analysis resolves the conflict that had linked MAL to the histidine and phenylalanine ammonia lyase family of enzymes.