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Crystal Structure of Molybdopterin-Guanine Biosynthesis Protein B (Mob B). Lakshminarasimhan Damodharan, Subramaniam Eswaramoorthy, Desigan Kumaran, Subramanyam Swaminathan, Biology Dept., Brookhaven National Laboratory, Upton, New York, NY 11973 USA.

Mob B from *Archaeoglobus fulgidus* DSM 4304 is involved in the biosynthesis of molybdopetirin guanine dinucleotide. We report the crystal structure of Mob B determined at 2.1Å resolution by the single wavelength anomalous dispersion method (SAD) using seleno-methionine protein. The protein crystallizes in the monoclinic space group P2₁ with the asymmetric unit containing a homodimer. The molecule has an α/β - fold with a major and a minor domain. The minor domain is involved in domain swapping between the protomers resulting in 16-stranded extended β -sheet. The protein contains two nucleotide binding motifs (Walker A) on the surface which might participate in GDP binding. During refinement, we identified a strong residual density that was modeled as praseodymium decahydrate which was used as an additive in crystallization. Praseodymium decahydrate solvent molecule is involved in molecular association.

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