Unique crystal structures of an SmtB/ArsR transcriptional factor from *Methanosarcina acetivorans*

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Archaea are a diverse group of organisms that exist in a wide array of environments. The first archaeal organisms to be identified were extremophiles – organisms that are able to survive in environments unsupportive of most life forms. *Methanosarcina acetivorans* is an archaeal organism that grows in sulfate-rich marine sediment. Screening of prokaryotic and archaeal genomes revealed the existence of a metal-responsive transcription factor involved in metal detoxification. *M. acetivorans* MA4344 was determined to be a potential metal-sensing repressor that belongs to the ArsR/SmtB family of metalloregulatory proteins. Based on sequence homology with other proteins within the ArsR/SmtB family, it was predicted that MA4344 has two putative metal binding sites. Here we report the X-ray crystal structure of a metal-deficient variant H99A form of MA4344. Data was collected at the SBC 19ID and 19BM beam lines at Argonne National Labs. The three-dimensional model reveals a homodimeric structure with a classic winged helix-turn-helix motif. The model demonstrates the potential for type I metal binding in a structural manner and confirms the presence of the type II metal binding site upon crystallization of the wild type protein with nickel. Here we discuss the purification, crystallization, structure determination, and refinement of the various MA4344 structures and demonstrate a clear structural shift upon metal binding.

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