Folding-analogs of ATPase RavA of Lokiarchaeota

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ATPase *RavA* is important membrane enzyme in prokaryotes. Genetic relationship of microorganisms can be associated with polymorphism of this enzyme. The aim of current scientific work was the modulation of the three-dimensional structure and search of folding-analogs of ATPase *RavA* of *Lokiarchaeota*. Models were built based on the target-template alignment using ProMod3. Coordinates which are conserved between the target and the template are copied from the template to the model. Insertions and deletions are remodeled using a fragment library.

The geometry of the resulting model is regularized by a force field. In case loop modelling with ProMod3 fails, an alternative model is built with PROMOD-II [1]. As result, three-dimensional structure of CaCA was calculated by folding-analogs (fig. 1). Three of them are statistically correct: Magnesium chelatase, DNA replication licensing factor MCM7 and Minichromosome maintenance protein MCM.

Fig. 1. Structure of ATPase *RavA* of *Lokiarchaeota*

1. Guex N., Peitsch M. C. SWISS-MODEL and the Swiss-PdbViewer: an environment for comparative protein modeling // Electrophoresis.-1997.-18, N 15.-P. 2714-2723.

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