Ab-initio Structure Determination of SMU.440 Protein from *Streptococcus mutans*

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SMU.440 is a 138 residue hypothetical protein from *Streptococcus mutans*, a primary pathogen for human dental caries. It's a function unknown protein with few sequence homologues. In this work, SMU.440 protein was expressed, purified and crystallized. Two sets of diffraction data were collected, including a native dataset to 2.4 Å resolution with satisfying statistics (Rsym= 3.8%), and Hg-derivative dataset to 2.4 Å resolution but with a high mosaicity of 1.9 and low completeness. The crystals belong to spacegroup $P2_12_12$ and there are 2 molecules per asymmetric unit (AU). The structure was determined by SIRAS method. Self rotation function showed a 2-fold NCS in the AU, but only one heavy atom site could be found per molecule, RESOLVE could only trace a partial (about 40%) structure and gave a poor density map. An initial NCS matrix was found using the lsq_etc. function of the O program. The partial structure combined with NCS information was input to Arp/Warp and Resolve for iterative model building and manually adjustment. Finally, a 130 residue model for structure refinement was obtained.

Keywords: SMU.440, ab-initio structure determination, iterative model building