In silico evaluation of crystallisation potential for conserved hypothetical proteins from the antarctic bacterium, Pedobacter cryoconitis BG5

ABSTRACT

The genome of Pedobacter cryoconitis BG5 highlighted the presence of conserved hypothetical proteins (HPs) with unique adaptive characteristics. Analysing and annotating the functions of these proteins was indeed essential for determining their suitability for X-ray crystallographic structure determination. The HPs were examined for the presence of transmembrane helices and signal peptides, and their structural and functional characteristics were analyzed using various bioinformatics tools and databases. The analysis revealed twelve conserved HPs with significant thermal stress response functions that met crystallisation criteria. Functional annotation showed that most of the proteins contain domains related to an enzyme or catalytic activity. Furthermore, the physicochemical properties of the shortlisted protein suggest a high probability of crystallisation based on the previously solved crystal structures of proteins with similar features. This early identification of protein eligibility for crystal screening has the potential to significantly reduce the time and cost involved in the structural determination of the unknown proteins in P. cryoconitis BG5.