Homology modeling of putative thioredoxin from Helicobacetr pylori

Abstract

The tertiary structure of putative thioredoxin (trx) of Helicobacter pylori was generated based on structural homology of the X-ray crystallographic structure of thioredoxin from Escherichia coli. Inspection of theoretically predicted structure indicates that the thioredoxin of H. pylori is similar to that of E. coli. Analysis of the structure revealed that thioredoxins have a common fold, characterized by a core of twisted β -pleated sheet flanked either side by helices. The amino terminal end of the molecule is occupied by β -a- β motif and carboxy terminal end by β - β -a motif. This molecule is characterized by five strands and four helices. Among the four helices, a2 is the longest helix which was disrupted near proline. Proline72 is identified as cis-proline. This structure retained overall trx-fold with the conservation of global shape and the secondary structures. This work determines the structure of thioredoxin and is found to be unique for further insight into molecular characterization.