

Abstract

Folding free energy of a protein is a delicate balance between stabilizing and destabilizing non-covalent interactions. In this work, we decompose folding free energy into physically meaningful contributions, in which we aim to find general trends. Empirical potential is used to calculate interaction energy between all protein fragments, which are classified based on their dominant term in multipolar expansion. Calculations are done using 1200 non-redundant structures from PDB database. Based on the general trends found in interactions between these fragments, we attempt to better understand relationships between interaction energies calculated using computational chemistry methods and their corresponding free energy contributions on stabilization.