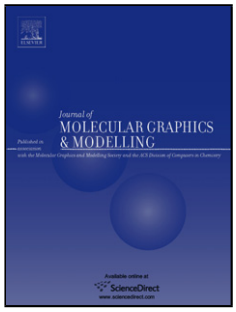

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Shielding effect in protein folding

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Abstract

One of the most important interactions responsible for protein folding and stability are hydrogen bonds between peptide groups. There is a constant competition between the water molecules and peptide groups in a hydrogen bond formation. Also side-chains take part in this process by reducing hydration of peptide group (shielding effect) that promotes the protein folding. In this paper, a new approach to take into account a shielding effect is presented. A modification of the energy function is derived and incorporated into the UNited RESidue (UNRES) force field. Canonical Molecular Dynamics and Replica Exchange Molecular Dynamics with UNRES force field is applied to study the influence of this effect on protein structure, folding kinetics and free energy landscapes. The results of test calculations suggest that even small contribution of this effect into energy function changes force field behavior as well as speeds up the folding process significantly.

keywords

proteins, UNRES force field, local interactions, physicochemical properties, potentials of mean force