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Reproducible In-Silico Folding of a Four Helix 60 Amino Acid Protein in a Transferable All-Atom Forcefield ALEXANDER SCHUG, Forschungszentrum Karlsruhe, Institut fr Nanotechnologie, WOLFGANG WENZEL — For predicting the protein tertiary structure one approach describes the native state of a protein as the global minimum of an appropiate free-energy forcefield. We have recently developed such a all-atom protein forcefield (PFF01). As major challenge remains the search for the global minimum for which we developed efficient methods. Using these we were able to predict the structure of helical proteins from different families ranging in size from 20 to 60 amino acids starting with random configurations. For the four helix 60 amino acid protein *Bacterial Ribosomal Protein L20* (pdb code: 1GYZ) we used a simple client-master model for distributed computing. Starting from a set of random structures three phases of different folding simulations refined this set to a final one with 50 configurations. During this process the amount of native-like structures increased strongly. Six out of the ten structures best in energy approached the native structure within 5 Å backbone rmsd. The conformation with the lowest energy had a backbone rmsd value of 4.6 Å therefore correctly predicting the tertiary structure of 1GYZ.
References
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