A minima hopping study of all-atom protein folding and structure prediction

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The minima hopping algorithm (MHOP) to find global minima on potential energy surfaces is used for protein structure prediction. The energy surface of the protein is represented with an all-atom OPLS force field and an implicit free energy solvation term. The system we studied here is the small 10-residue beta-hairpin mini-protein, chignolin. Starting from a completely extended structure, we found minima with <0.5 angstrom rms coordinate deviation from the geometry-optimized native experimental conformation. A few lowest-energy conformations were used for the calculation of NMR-restraint violations and chemical shifts, and the local minima found during each run leading to the global minimum were connected to trace out a search pathway of the folding process.

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