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Selection of optimal variants of Go-like models of proteins through studies of stretching JOANNA SULKOWSKA, Center of Theoretical Biological Physics, Department of Physics, UCSD, and Insititue of Physics Polish Academy of Science, Poland, MAREK CIEPLAK, Insititue of Physics Polish Academy of Science, Al. Lotnikow 32/48, Warsaw, Poland — The Go-like models of proteins are constructed based on the knowledge of the native conformation. However, there are many possible choices of a Hamiltonian for which the ground state coincides with the native state. Here, we propose to use experimental data on protein stretching to determine what choices are most adequate physically. This criterion is motivated by the fact that stretching processes usually start with the native structure, in the vicinity of which the Go-like models should work the best. Our selection procedure is applied to 62 different versions of the Go model and is based on 28 proteins. We consider different potentials, contact maps, local stiffness energies, and energy scales – uniform and non-uniform. In the latter case, the strength of the nonuniformity was governed either by specificity or by properties related to positioning of the side groups. Among them there is the simplest variant: uniform couplings and no$i, i+2$contacts. This choice also leads to good folding properties in most cases. We elucidate relationship between the local stiffness described by a potential which involves local chirality and the one which involves dihedral and bond angles. The latter stiffness improves folding but there is little difference between them when it comes to stretching.

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