Influence of Stereochemistry in a Local Approach for Calculating Protein Conformations

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Protein structure prediction is generally based on the use of local conformational information coupled with long-range distance restraints. Such restraints can be derived from the knowledge of a template structure or the analysis of protein sequence alignment in the framework of models arising from the physics of disordered systems. The accuracy of approaches based on sequence alignment, however, is limited in the case where the number of aligned sequences is small. Here, we derive protein conformations using only local conformations knowledge by means of the interval Branch-and-Prune algorithm. The computation efficiency is directly related to the knowledge of stereochemistry (bond angle and ω values) along the protein sequence and, in particular, to the variations of the torsion angle ω. The impact of stereochemistry variations is particularly strong in the case of protein topologies defined from numerous long-range restraints, as in the case of protein of β secondary structures. The systematic enumeration of the conformations improves the efficiency of the calculations. The analysis of DNA codons permits to connect the variations of torsion angle ω to the positions of rare DNA codons.