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Generation of protein-like structures via simple rules imposed on a cubic lattice¹ RAHMI OZISIK, DENIZ TURGUT, OSMAN B. OKAN, Rensselaer Polytechnic Institute, ARAVIND RAMMOHAN, Corning Inc., ANGEL E. GARCIA, Rensselaer Polytechnic Institute — In the current study, protein-like coarse-grained structures are generated by a simple set of rules on simple cubic lattice (SCL). The coarse-graining was based on individual amino acids. Detailed analysis of the average structure of 210 real proteins' radial distribution function (RDF) and number of neighbors as a function of cut-off distance suggest that SCL is an appropriate choice of lattice. Three simple rules were imposed to generate protein-like structures: finite size (presence of a molecular surface), random inclusion of voids, and a simple connectivity of remaining lattice sites. The set of on-lattice points (that mimic residues of a protein) satisfy many structural characteristics of real proteins. These on-lattice structures were subsequently relaxed either by random moves or by a combined Reverse Monte Carlo/Simulated Annealing (RMC/SA) algorithm that used the average RDF of proteins as its target function. The on-lattice and relaxed structures' characteristics were also analyzed via bond orientational order and graph theory. The results showed that although relaxation algorithms improved the structural characteristics of the generated structures, the improvement over the on-lattice structures are minimal. Based on various structural properties, our results indicate that the artificially generated structures closely resemble real proteins coarse-grained at the residue level.

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