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Predictive Computational Modeling of Chromatin Folding MIICHELE DI PIERRO, BIN ZHANG, PETER J. WOLYNES, JOSE N. ONUCHIC, Center for Theoretical Biological Physics, Rice University — In vivo, the human genome folds into well-determined and conserved three-dimensional structures. The mechanism driving the folding process remains unknown. We report a theoretical model (MiChroM) for chromatin derived by using the maximum entropy principle. The proposed model allows Molecular Dynamics simulations of the genome using as input the classification of loci into chromatin types and the presence of binding sites of loop forming protein CTCF. The model was trained to reproduce the Hi-C map of chromosome 10 of human lymphoblastoid cells. With no additional tuning the model was able to predict accurately the Hi-C maps of chromosomes 1-22 for the same cell line. Simulations show unknotted chromosomes, phase separation of chromatin types and a preference of chromatin of type A to sit at the periphery of the chromosomes.

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