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A lattice-based, coarse-grain tertiary structure model for RNA folding: predictive power and impact of excluded volume DANIEL JOST, RALF EVERAERS, Laboratoire de Physique and Centre Blaise Pascal of the Ecole Normale Superieure de Lyon, Lyon, France — We present a semi-quantitative lattice model of RNA folding which is able to reproduce complex folded structures like multi-loops and pseudoknots without relying on the frequently employed ad hoc generalization of the Jacobson-Stockmayer loop entropy. We derive the model parameters from the Turner description of simple secondary structural elements and pay particular attention to the unification of border and non- local loop parameters, resulting in a reduced, unified parameter set for simple loops of arbitrary type and size. For elementary structures, the predictive power of the model is comparable to standard secondary structure approaches. For complex structures, our approach offers a systematic treatment of generic effects of chain connectivity as well as of excluded volume interactions between and within all elements of the secondary structure.

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