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Coarse-grained modelling of RNA PETR SULC, The Rockefeller University, FLAVIO ROMANO, THOMAS OULDRIDGE, JONATHAN DOYE, ARD LOUIS, University of Oxford — We present a new, nucleotide-level model for RNA, oxRNA, based on the coarse-graining methodology recently developed for the oxDNA model of DNA. The model is designed to reproduce structural, mechanical and thermodynamic properties of RNA, and the coarse-graining level aims to retain the relevant physics for RNA hybridization and the structure of single- and double-stranded RNA. In order to explore its strengths and weaknesses, we test the model in a range of nanotechnological and biological settings. Applications explored include the folding thermodynamics of a pseudoknot, the formation of a kissing loop complex, the unzipping of a hairpin motif, and the thermodynamics and kinetics of RNA strand-displacement reaction. We argue that the model can be used for efficient simulations of the structure of systems with thousands of base pairs, and for the assembly of systems of up to hundreds of base pairs. The source code implementing the model is released for public use at dna.physics.ox.ac.uk.

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