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Moving Beyond Watson-Crick Models of Coarse Grained DNA KEVIN DORFMAN, MARGARET LINAK, University of Minnesota - Twin Cities, RICHARD TOURDOT, University of Pennsylvania — DNA structure possesses several levels of complexity, ranging from the sequence of bases (primary structure) to base pairing (secondary structure) to its three-dimensional shape (tertiary structure) and can produce a wide variety of conformations in addition to canonical double stranded DNA. By including non-Watson-Crick interactions in a coarse-grained model, we developed a system that not only can capture the traditional B-form double helix, but also can adopt a wide variety of other DNA conformations. In our experimentally parameterized, coarse-grained DNA model we are able to reproduce the microscopic features of double-stranded DNA without the need for explicit constraints and capture experimental melting curves for a number of short DNA hairpins. We demonstrate the utility of the model by simulating more complex tertiary structures such as the folding of the thrombin aptamer, which includes G-quartets, and strand invasion during triplex formation. Our results highlight the importance of non-canonical interactions in DNA coarse- grained models.

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