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Structural basis of pathway-dependent force profiles in DNA DANIEL ROE, ANNE CHAKA, Physics Laboratory, National Institute of Standards and Technology — Since DNA must bend and/or stretch to perform many of its functions, it is important to understand the mechanical properties of DNA. Single molecule experiments have been able to study the response of DNA to applied forces. One interesting result of such studies is that at high loading rates a greater force is required to stretch DNA when pulling from the 3' ends as opposed to the 5' ends. While these experiments provide valuable insights into the stability of DNA, it is often difficult to relate the results to specific structural changes. We have used molecular dynamics simulation methods to study the structure and dynamics of DNA under a tensile load. Simulations were performed on a variety of fully solvated DNA sequences up to 30 base-pairs in length, and were conducted under both non-equilibrium and equilibrium conditions. Different stretched DNA structures are observed depending on whether pulling occurs from the 5' ends or 3' ends. Detailed analysis of these structures provides a direct structural explanation of the observed difference between 3' and 5' pulling.

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