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Thermodynamic Model of Transcription Elongation VASISHT TADIGOTLA, Rutgers University, DAIBHID O'MAOILEIDIGH, Rutgers University, ANIRVAN SENGUPTA, Rutgers University, VITALY EPSHTEIN, New York University Medical Center, RICHARD EBRIGHT, Rutgers University, EVGENY NUDLER, New York University Medical Center, ANDREI RUCKENSTEIN, Rutgers University — We present a statistical mechanics approach to the prediction of backtracked pauses in prokaryotic transcription elongation derived from structural models of the transcription elongation complex (TEC). Our algorithm is based on the thermodynamic stability of TEC along the DNA template calculated from the sequence dependent free-energy of DNA-DNA, DNA-RNA and RNA-RNA base pairing associated with (a) the translocation and size fluctuations of the transcription bubble; (b) the changes in the DNA-RNA hybrid; and (c) the changes in the RNA folding free-energy. The calculations involve no adjustable parameters apart from a cutoff used to discriminate paused from non-paused complexes. When applied to 100 experimental pauses in transcription elongation by E. coli RNA polymerase on ten DNA templates the approach produces highly statistically significant results. Transcription elongation is an inherently kinetic process and a simplified kinetic model with the same predictive power is presented separately.

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