Abstract Submitted
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Interrogating Nucleosome Positioning Through Coarse-Grain Molecular Simulation[1] GORDON S. FREEMAN, DANIEL M. HINCKLEY, University of Wisconsin-Madison, VANESSA ORTIZ, Columbia University, JUAN J. DE PABLO, University of Wisconsin-Madison — Nucleosome positioning plays a crucial role in biology. As the fundamental unit in chromosome structure, the nucleosome core particle (NCP) binds to approximately 147 DNA base pairs. The location of bound NCPs in the genome, therefore, affects gene expression. The specific positioning of NCPs has been experimentally probed and competing viewpoints have been presented in the literature. Models for nucleosome positioning based on sequence-dependent flexibility (a genomic "code" for nucleosome positioning) have been demonstrated to explain available experimental data. However, so do statistical models with no built-in sequence preference; the driving force for NCP positioning therefore remains an open question. We use a coarse-grain model for the NCP in combination with advanced sampling techniques to probe the sequence preference of NCPs. We present a method for determining the relative affinity of two DNA sequences for the NCP and use this method to compare high- and low-affinity sequences. We discuss several coarse-grain protein models with varying level of detail to examine the impact of model resolution on the agreement of our results with experimental evidence. We also investigate the dynamics of the NCP-DNA complex and their dependence on system characteristics.

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