

The majority of eukaryotic DNA, about three quarter, is wrapped around histone proteins forming so-called nucleosomes. To study nucleosomal DNA we introduce a coarse-grained molecular dynamics model based on sequence-dependent harmonic rigid base pair step parameters of DNA and nucleosomal binding sites. Mixed parametrization based on all-atom molecular dynamics and crystallographic data of protein-DNA structures is used for the base pair step parameters. The binding site parameters are adjusted by experimental B-factor values of the nucleosome crystal structure. It is shown that the twist defect scenario together with the sequence-dependent elasticity of DNA can explain the slow time scales observed for nucleosome mobility along DNA. With this method we also show how the twist defect mechanism leads to a higher mobility of DNA in the presence of sin mutations near the dyad axis. Finally, by performing simulations on 5s rDNA, 601, and telomeric base pair sequences, it is demonstrated that the current model is a powerful tool to predict nucleosome positioning.