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Towards predictive molecular dynamics simulations of DNA: electrostatics and solution/crystal environments VOLODYMR BABIN, JASON BAUCOM, North Carolina State University, THOMAS DARDEN, National Institute of Environmental Health Sciences, CELESTE SAGUI, North Carolina State University — We have investigated to what extend molecular dynamics (MD) simulatons can reproduce DNA sequence-specific features, given different electrostatic descriptions and different cell environments. For this purpose, we have carried out multiple unrestrained MD simulations of the duplex d(CCAACGTTGG)2. With respect to the electrostatic descriptions, two different force fields were studied: a traditional description based on atomic point charges and a polarizable force field. With respect to the cell environment, the difference between crystal and solution environments is emphasized, as well as the structural importance of divalent ions. By imposing the correct experimental unit cell environment, an initial configuration with two ideal B-DNA duplexes in the unit cell is shown to converge to the crystallographic structure. To the best of our knowledge, this provides the first example of a multiple nanosecond MD trajectory that shows and ideal structure converging to an experimental one, with a significant decay of the RMSD.

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