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Development and Validation of the OL24 Force Field for DNA: Improved Modeling of Sugar Puckering and A/B Conformational Equilibria

The A/B conformational equilibrium of DNA is essential for many biological processes, including protein-DNA recognition and the formation of DNA/RNA hybrid duplexes. However, existing AMBER force fields such as OL15, OL21, and bsc1 significantly underestimate the stability of A-DNA, which may lead to unrealistic conformational behaviour or even destabilization of protein–DNA complexes in simulations. Here, we present a refined DNA force field that significantly improves the description of sugar puckering by increasing the stability of the north puckering present in A-DNA. The new OL24 parameters were validated through extensive molecular dynamics simulations of canonical DNA duplexes, DNA/RNA hybrids, and protein–DNA complexes. OL24 maintains an accurate representation of canonical B-DNA and improves the description of the A/B conformational equilibrium in B-DNA duplexes in water. In addition, it enables improved modeling of DNA/RNA hybrids and protein-DNA complexes. Overall, OL24 represents a significant advancement in the force field description of nucleic acids, enabling more reliable modeling of DNA structure and dynamics.

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