SUPPLEMENTARY DATA

Structure and dynamics of DNA loops on nucleosomes studied with atomistic, microsecond–scale molecular dynamics

Marco Pasi and Richard Lavery

MMSB, Univ. Lyon I/CNRS UMR 5086, Institut de Biologie et Chimie des Protéines, 7
passage du Vercors, 69367 Lyon, France

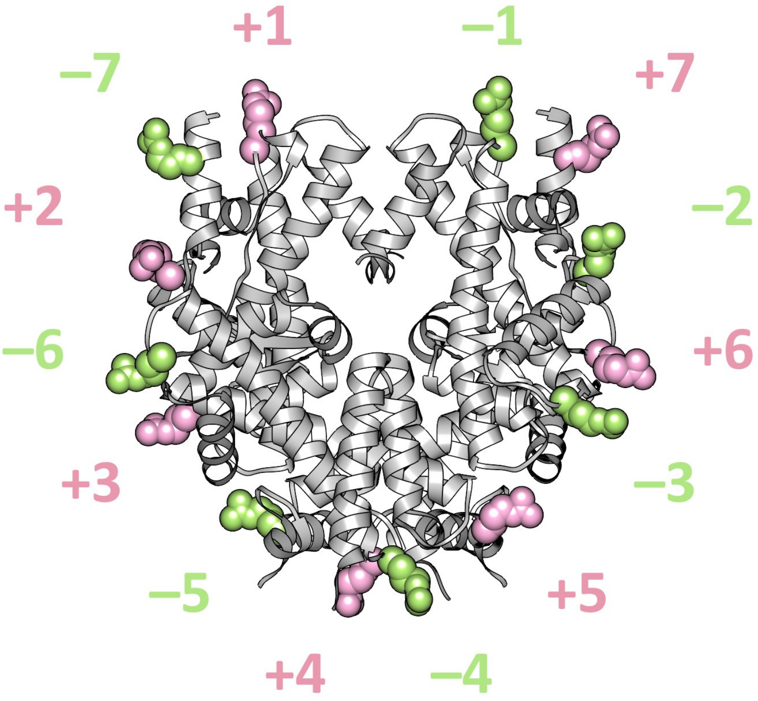

Figure S1. DNA-histone contacts. The histone octamer from crystal structure 1KX5 (1,2) is shown as gray ribbon, with the 14 arginines that contact the DNA minor groove once per helical turn shown as colored spheres, numbered -7 → -1 (green) and +1 → +7 (pink). Following the numbering of PDB entry 1KX5, arginines, from ±1 to ±7 are H4.R45, H3.R63, H3.R83, H2A.R42, H2A.R29, H2A.R77, H3.R49.

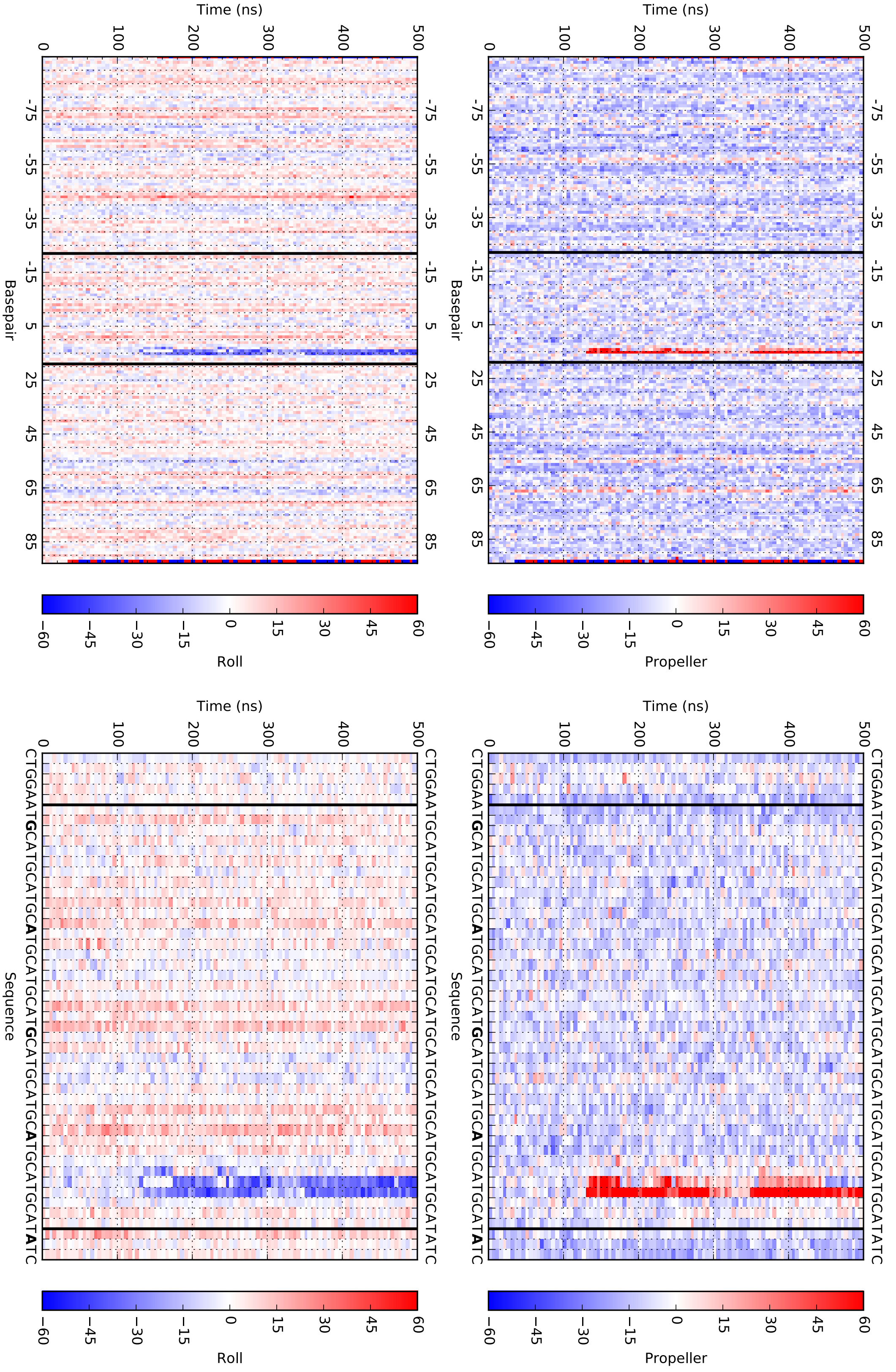

Figure S2. Time-evolution of roll and propeller for IN42. Time evolution of the propeller (top) and roll (bottom) helical parameters, highlighting the formation of a Type II kink. The two plots on the right focus on the region where the kink is formed.

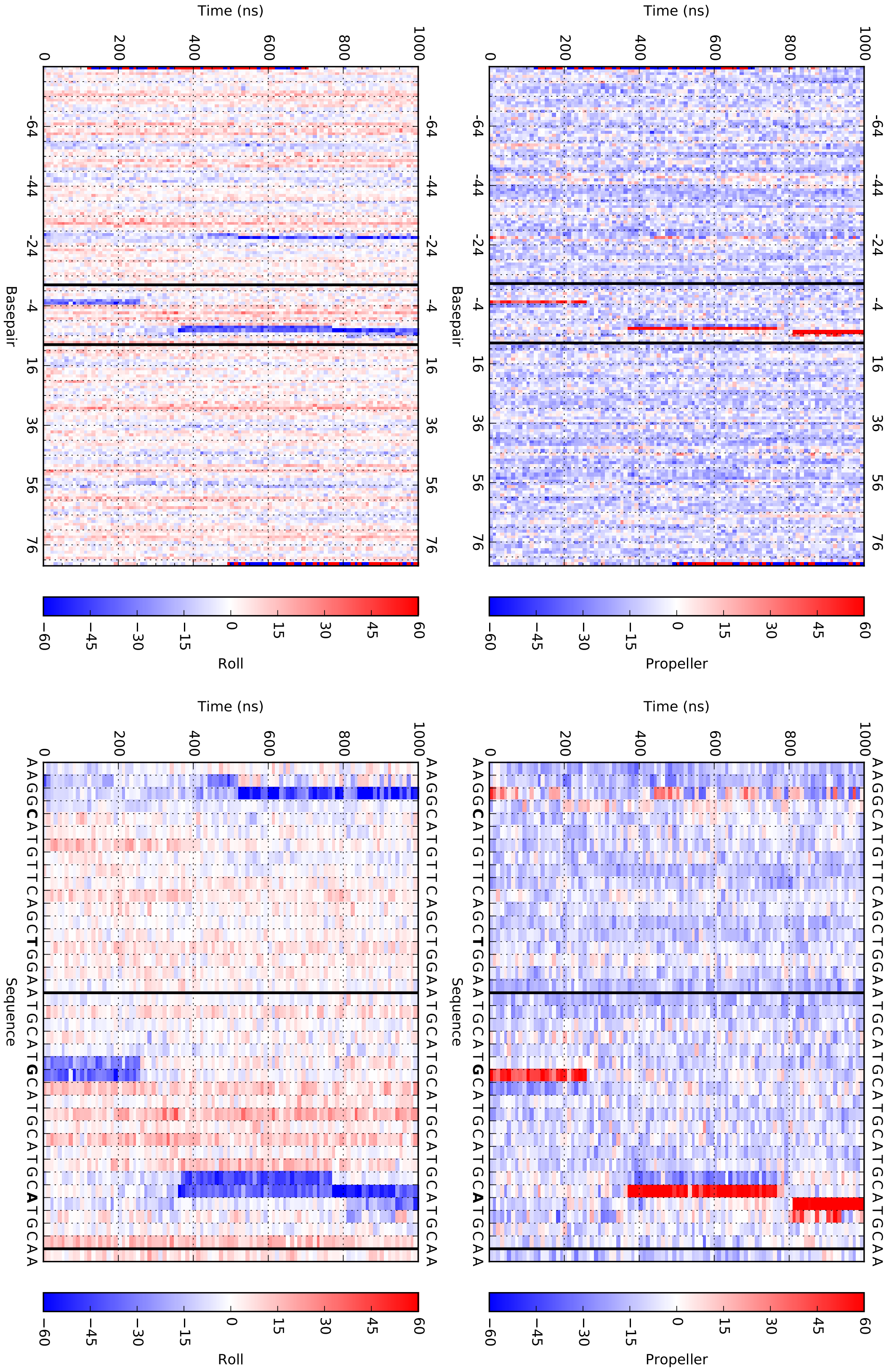

Figure S3. Time-evolution of roll and propeller for IN21. Time evolution of the propeller (top) and roll (bottom) helical parameters, highlighting the formation of Type II and Type III kinks. The two plots on the right focus on the insertion.

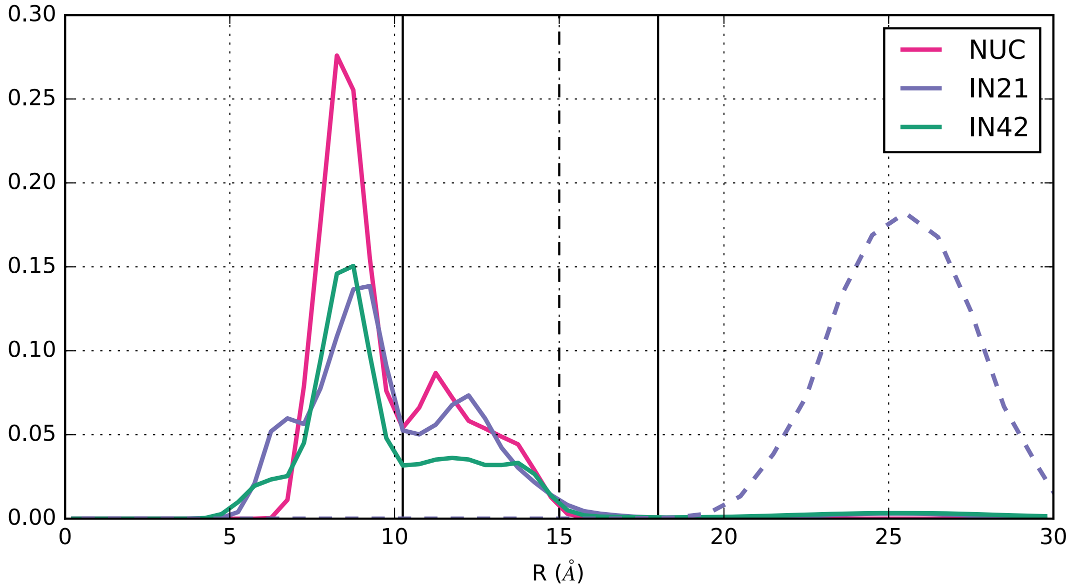

Figure S4. Arginine contacts. Histograms of the distance R between the DNA helical axis and the central carbon of the arginine head group for all 14 arginine contact points. The three line plots refer to the native nucleosome (NUC, magenta), the IN21 looped structure (purple) and the IN42 looped structure (green). The dashed purple line refers exclusively to arginine +1 of the IN21 looped structure, which is never bound to DNA during our simulation. Arginine side chains within the minor groove lie closer than 10.25 Å from the axis, while those in contact with the phosphate groups lie below 15 Å.

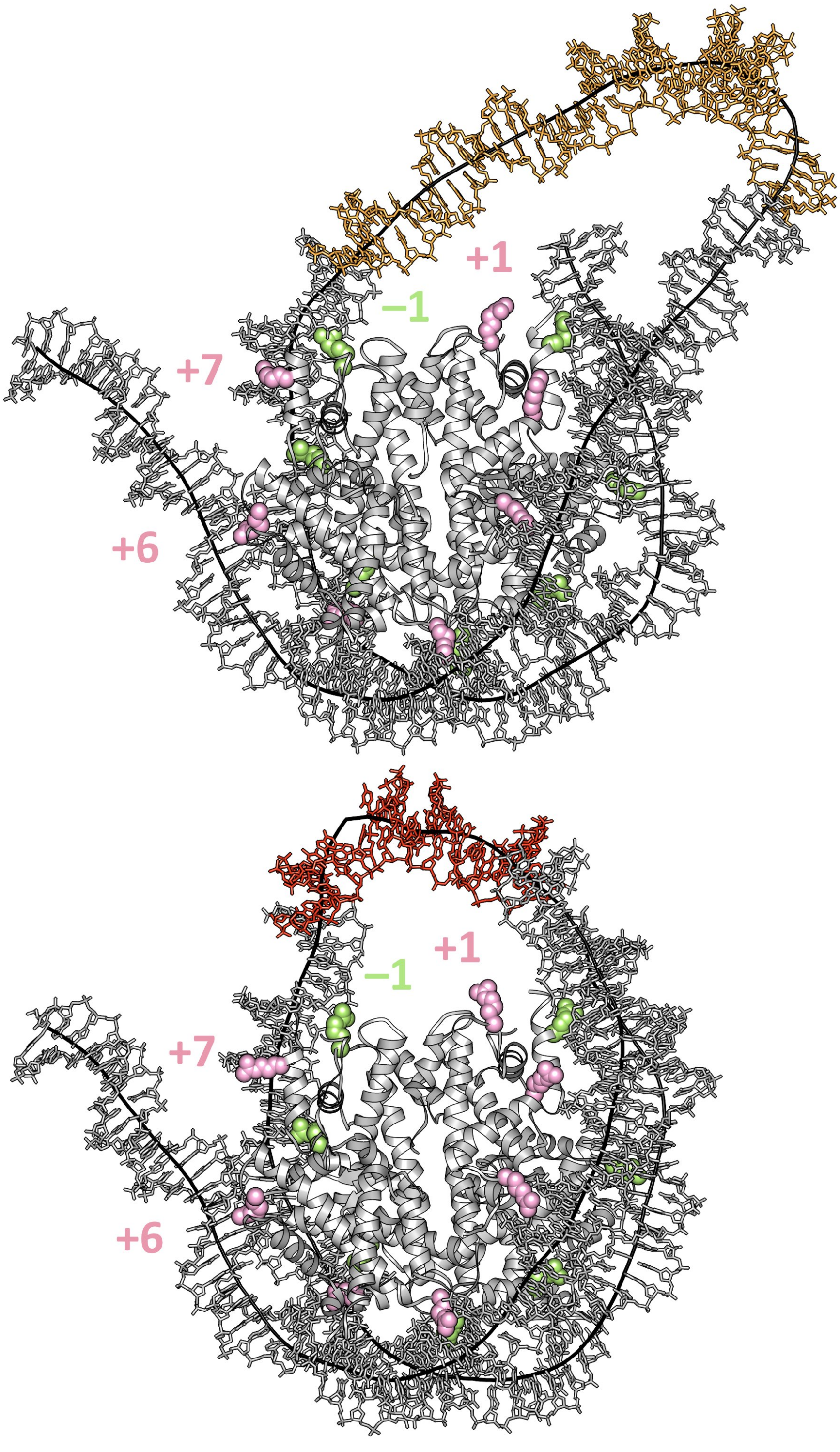

Figure S5. DNA-end dynamics. Snapshots along the trajectories of the IN42 (top, insert colored orange) and IN21 (bottom, insert colored red) simulations, showing large displacement of the positive end of DNA from the core. The distances between the positive end of the helical axis of DNA (shown as thick black lines) and the Cα carbon of arginine anchor +7 (shown as pink spheres and labeled) is of 51.0 Å (top) and 48.5 Å (bottom). Histones are shown in grey and the arginines contacting DNA are shown as green spheres (-1 → -7) and pink spheres (+1 → +7).

References

1. Davey, C.A., Sargent, D.F., Luger, K., Maeder, A.W. and Richmond, T.J. (2002) Solvent mediated interactions in the structure of the nucleosome core particle at 1.9 a resolution. *J Mol Biol,* **319**, 1097-1113.
2. Richmond, T.J. and Davey, C.A. (2003) The structure of DNA in the nucleosome core. *Nature,* **423**, 145-150.