Supplementary Table 1: Comparison between 20 ns [Ref. 19] and 100 ns nucleosome trajectories

		20 ns	100 ns
Intact nucleosome simulation			
Backbone RMSD	H3(1) H3(2)	~ 1.2 Å	1.31 ± 0.13 Å 1.32 ± 0.13 Å
	H4(1) H4(2)	~ 0.8 Å	1.32 ± 0.16 Å 1.15 ± 0.19 Å
	H2A(1) H2A(2)	~ 2.1 Å	1.41 ± 0.16 Å 1.50 ± 0.19 Å
	H2B(1) H2B(2)	~ 0.9 Å	1.56 ± 0.24 Å 1.37 ± 0.17 Å
Conservation of protein secondary structure		x	α-helics formation in H3 and H2B tail during simulation
DNA RMSD		~ 2.5 Å	3.2 ± 0.17 Å
DNA backbone conformation		B1 type	B1 type
Tail-truncated simulations			
Structural changes in the H2A2α3 domain		x	Structural changes in the sidechain hydrogen bonding Arg81 and Arg88 are observed in H3 and H2A tail-truncated simulations
Change of interaction between the H2A docking domain and contact residues		x	Interaction changes observed in H3 and H2A tail-truncated simulations.