Supplemental Information

Correlation among DNA Linker Length, Linker Histone Concentration, and Histone Tails in Chromatin

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A sensitive interplay between nucleosome repeat length, linker histone concentration, and histone tail interactions

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Supplementary Material

Figure S.1: Equilibrium configurations for 12-unit oligonucleosomes at 150 mM NaCl at different LH concentrations, $\rho_{LH}$ (rows), and NRLs (columns): (A) 173bp, (B) 182bp, (C) 191bp, (D) 200bp, (E) 209bp, (F) 218bp, and (G) 226bp. The green boxes highlight the critical LH concentration associated to the formation of well defined fibers at each NRL.
Figure S.2: Internucleosome interaction patterns for 12-unit oligonucleosomes at 150 mM NaCl at different NRLs: (A) 173bp, (B) 182bp, (C) 191bp, (D) 200bp, (E) 209bp, (F) 218bp, and (G) 226bp. For each NRL we analyze interaction patterns at different LH concentrations, $\rho_{LH}$. We also group all NRLs to compare the interactions for (H) $k=1$ and (I) $k=2$ against the LH concentration.
Figure S.3: Structural properties that capture the fiber transition for 12-unit oligonucleosomes at 150 mM NaCl at different LH concentrations, $\rho_{LH}$, and NRLs: (A) total energy, (B) fiber conformational effective energy ($E_{fib}(\rho_{LH}) = E_{tot}(\rho_{LH}) - n_c^2 \varepsilon_{LH} \rho_{LH}$), (C) effective volume per nucleosome ($v_{nc} = V/n_c$), and core-core frquency interaction between second nucleosome sequential neighbors ($k=2$).
Figure S.4: Structural properties for 12-unit oligonucleosomes at 150 mM NaCl at different NRLs: (A) sedimentation coefficient, (B) packing ratio, (C) dimer distance, (D) triplet distance, (E) triplet angle, (F) fiber length, (G) fiber width, and (H) length-width ratio.
Figure S.5: Core histone tail frequency interactions for 12-oligonucleosomes at 150 mM NaCl using the refined LH model at different concentrations (\(\rho_{LH}\)) and multiple NRLs: 173bp, 191bp, 209bp, and 226bp. At the top of the figure we show the main elements of a nucleosome core, including all histone tails: H2A1 (yellow), H2A2 (orange), H2B (purple), H3 (blue), and H4 (green). We show the interaction with (A) parental nucleosome core, (B) parental linker DNAs, (C) non-parental nucleosome cores, and (D) non-parental linker DNAs.