Supporting Information for 'Mesoscale Modeling Reveals Hierarchical Looping of Chromatin Fibers Near Gene Regulatory Elements'

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Supplemental Figures
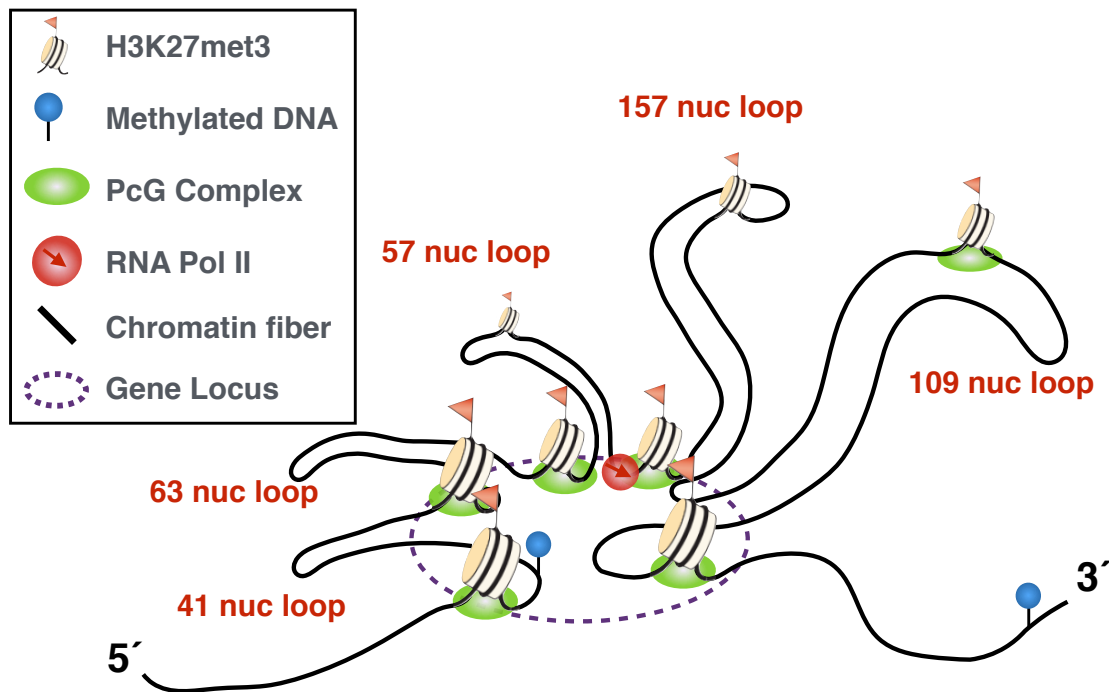
GATA-4 Gene Locus

Figure S1: Cartoon image of the GATA-4 gene locus connections adapted from Tiwari et. al.[1] The chromatin fiber is shown as a solid black line with observed H3 tail methylations (H3K27Me3), polycomb group proteins, DNA methylation, and RNA polymerase II indicated by orange flags, green ovals, blue balls, and a red ball/arrow, respectively. The arrow points in the direction of transcription, which runs from 5′ to 3′. Experimental 3C data shows five distinct loops of ~ 41, 63, 57, 157, and 109 nucleosomes respectively.

Initial Loops (Starting structures)

25nuc .4 Kb   50nuc 9.5Kb   75nuc 14.3Kb   100nuc 19.1Kb
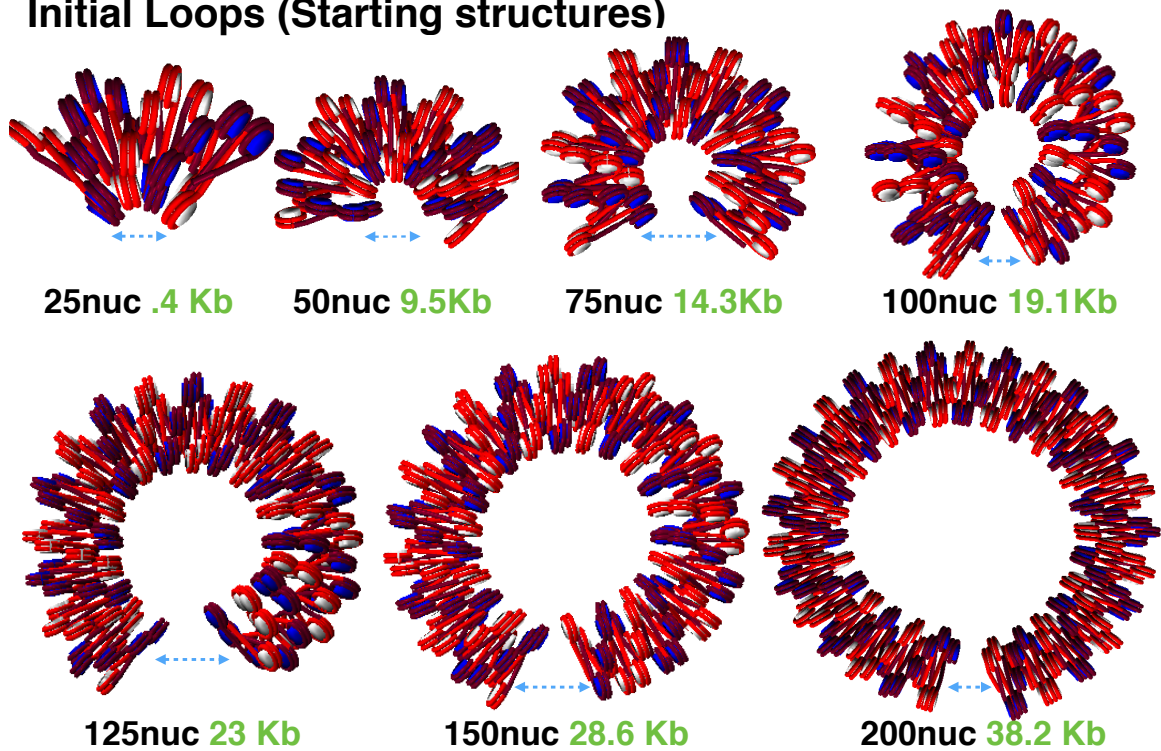
125nuc 23 Kb   150nuc 28.6 Kb   200nuc 38.2 Kb

Figure S2: Starting conformations for individually restrained loops. One harmonic distance restraint was applied per fiber, between the center of mass of terminal nucleosomal cores. Restraints are shown as blue dashed lines.
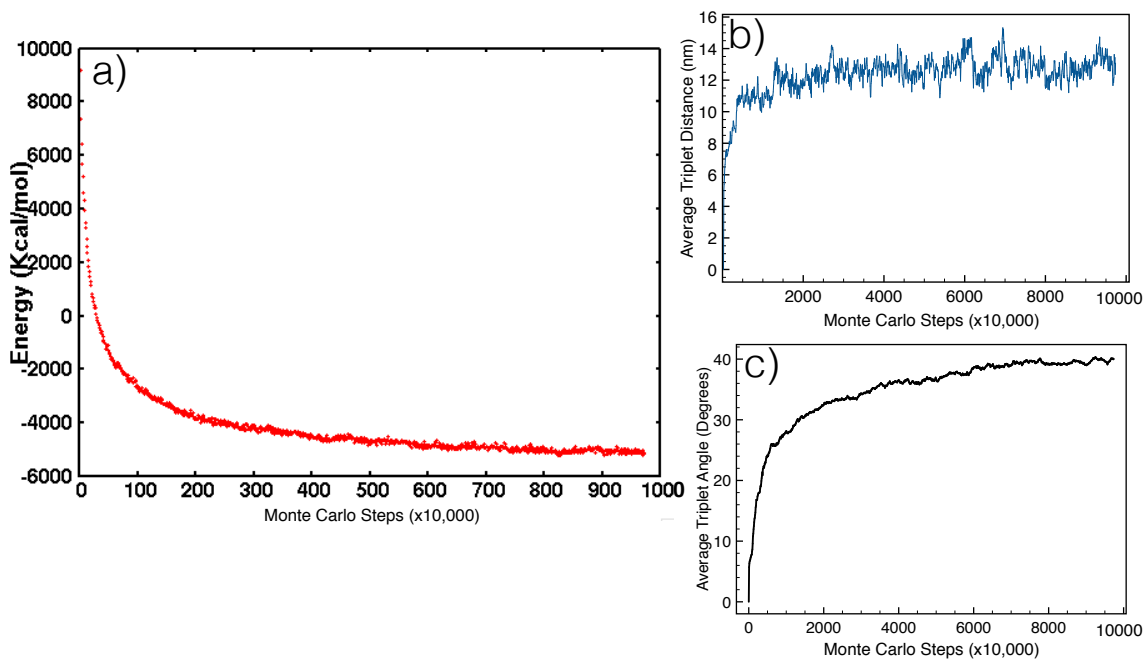
Figure S3: a) Sample energy evolution, b) average triplet distance, and c) average triplet angle for $\frac{1}{2}$LH restrained fibers of 125 nucleosomes across 100 million MC steps. All systems simulated were similarly monitored to show convergence in both energetic and geometric terms such as those shown above.
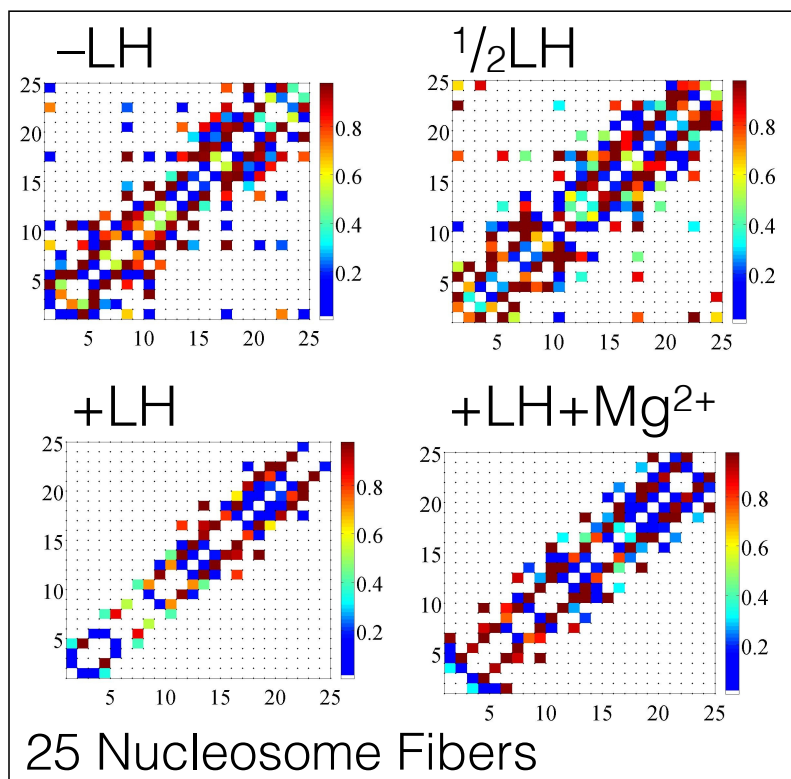
Figure S4: Interaction matrices of restrained loop fibers with 25 nucleosomes with $-LH$, $\frac{1}{2}LH$, $+LH$, and $+LH+Mg^{2+}$ (see caption to Fig 2a in the main text).
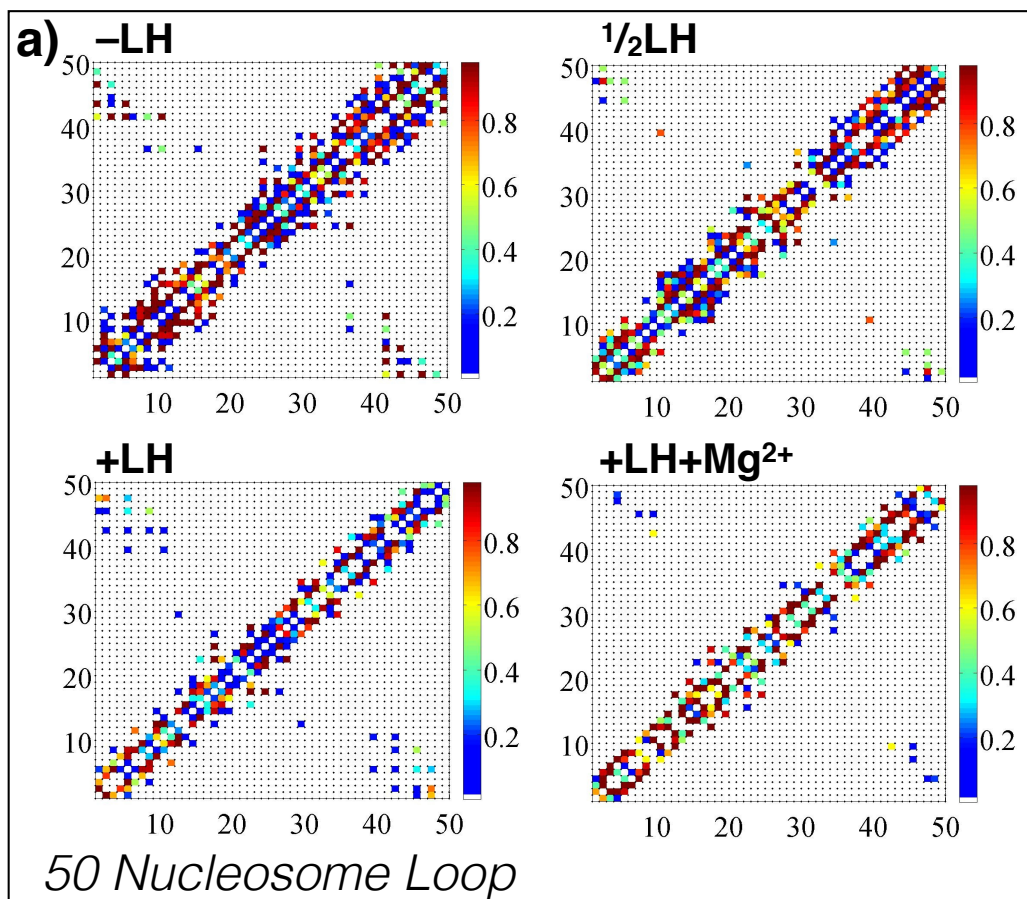
Figure S5: Interaction matrices of restrained loop fibers with 50 nucleosomes with $-$LH, $\frac{1}{2}$LH, $+$LH, and $+$LH$+$Mg^{2+} (see caption to Fig 2a in the main text).
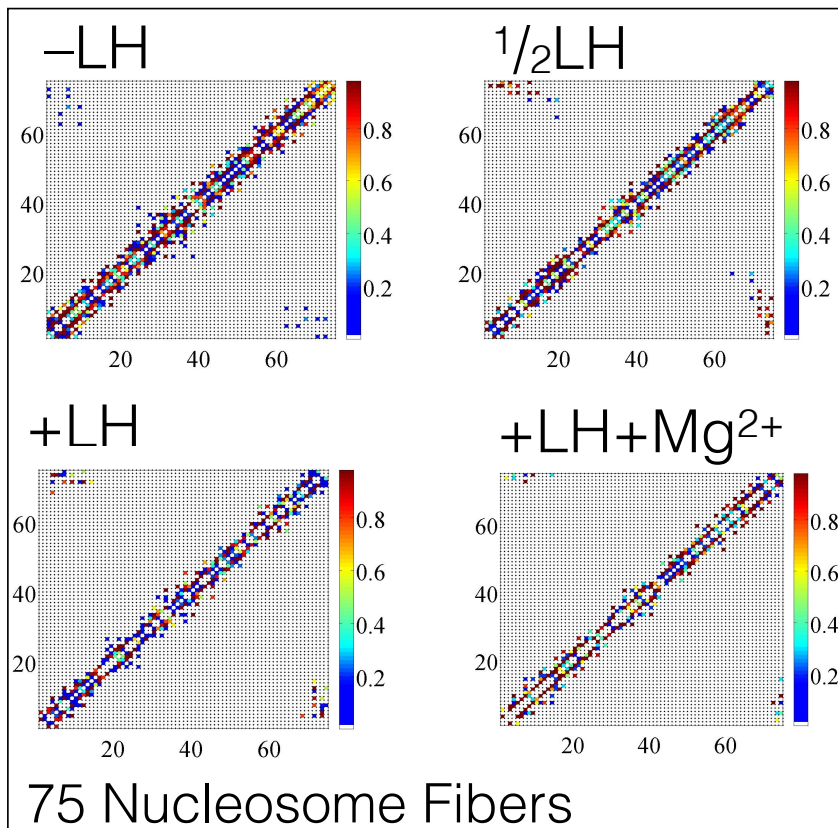
Figure S6: Interaction matrices of restrained loop fibers with 75 nucleosomes with $-$LH, $\frac{1}{2}$LH, $+$LH, and $+$LH$+$Mg^{2+} (see caption to Fig 2a in the main text).
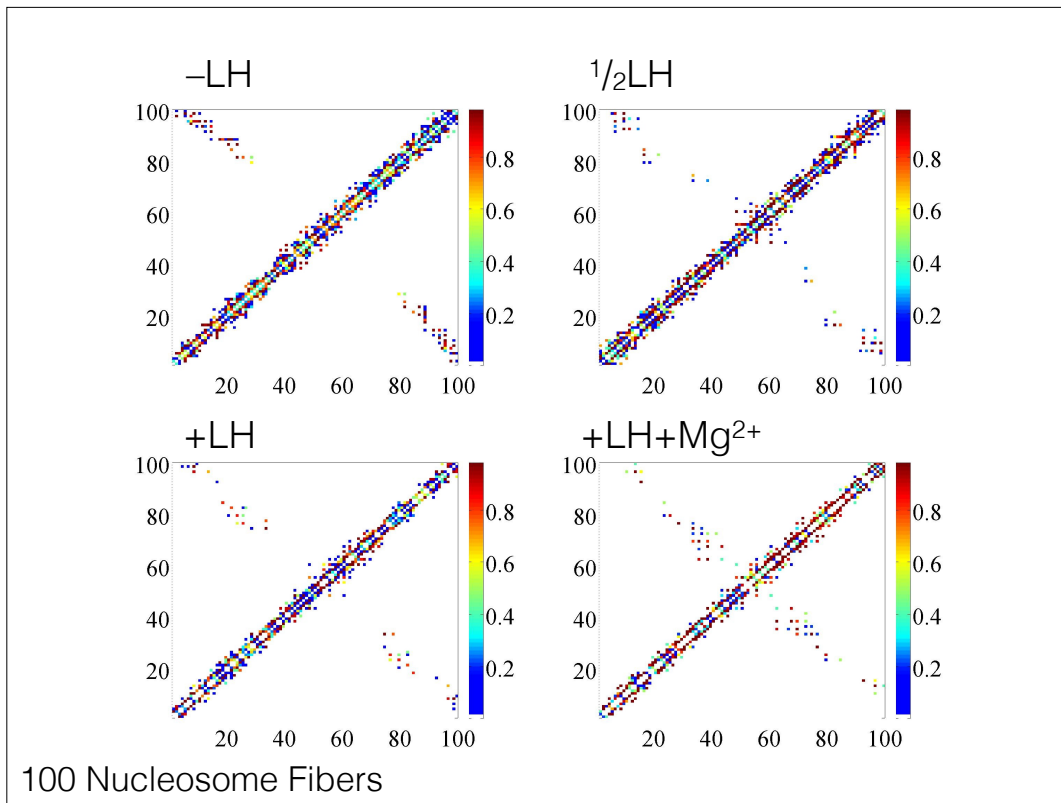
Figure S7: Interaction matrices of restrained loop fibers with 100 nucleosomes with $-$LH, $\frac{1}{2}$LH, $+$LH, and $+$LH$+$Mg^{2+} (see caption to Fig 2a in the main text).
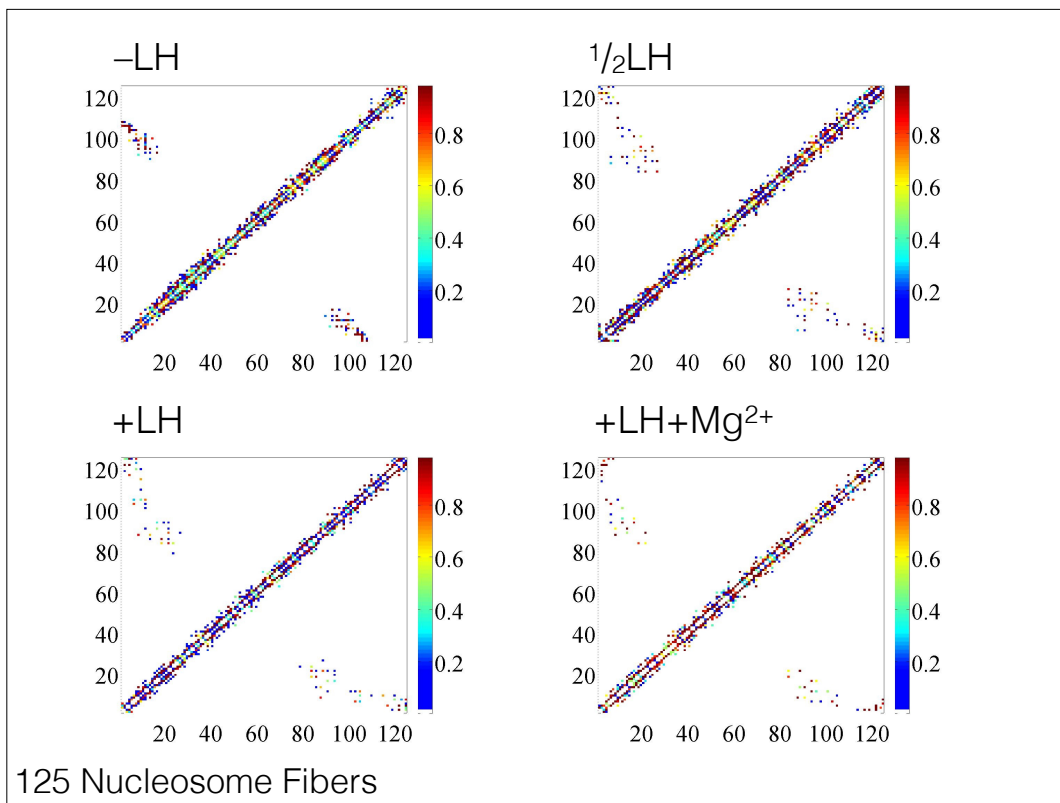
Figure S8: Interaction matrices of restrained loop fibers with 125 nucleosomes with $-$LH, $\frac{1}{2}$LH, $+$LH, and $+$LH$+$Mg^{2+} (see caption to Fig 2a in the main text).

Figure S9: Interaction matrices of restrained loop fibers with 150 nucleosomes with $-$LH, $\frac{1}{2}$LH, $+$LH, and $+$LH$+$Mg^{2+} (see caption to Fig 2a in the main text).
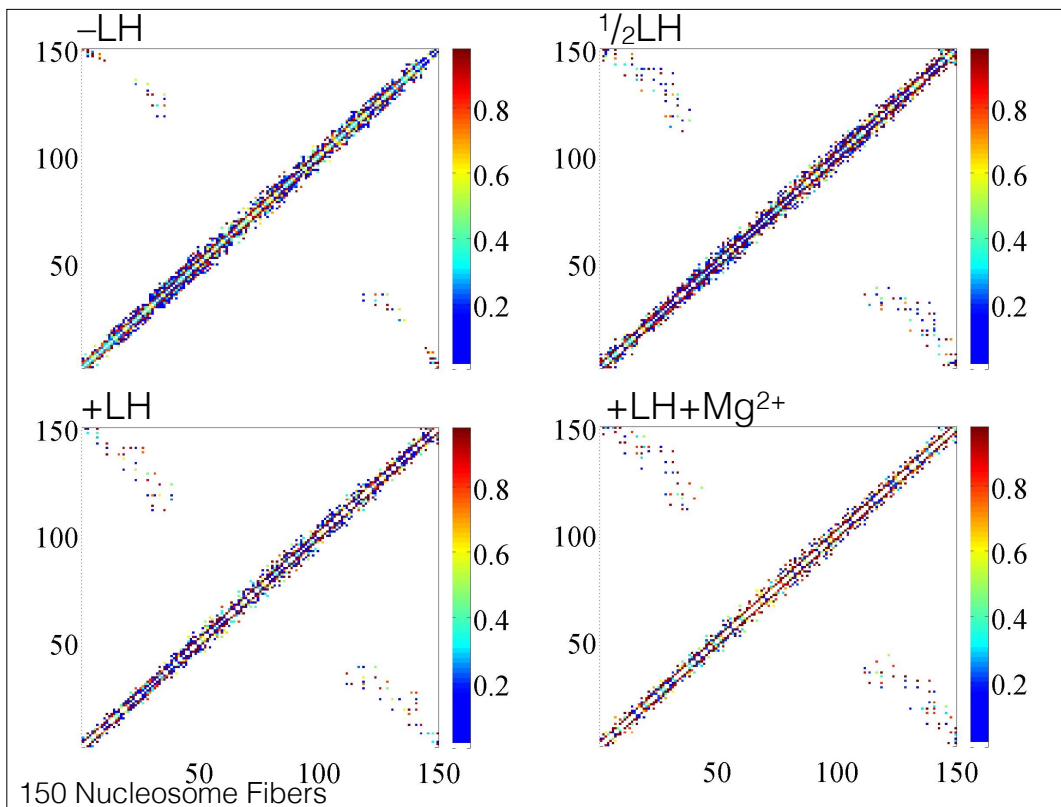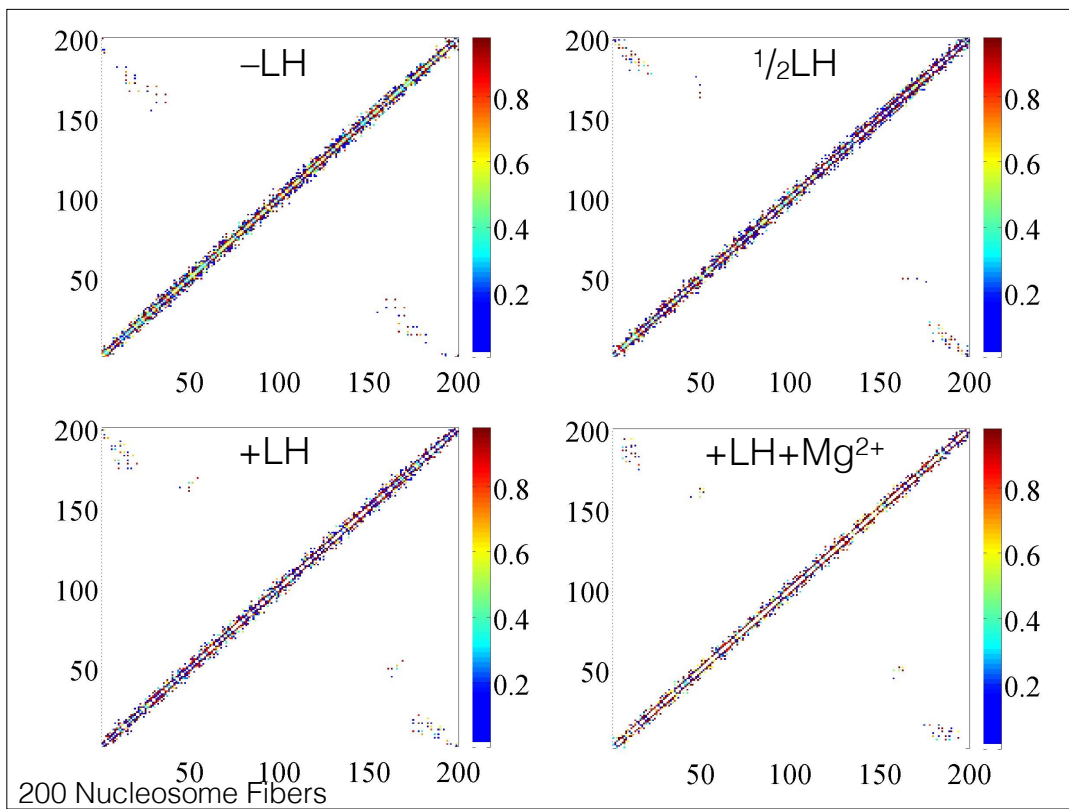
Figure S10: Interaction matrices of restrained loop fibers with 200 nucleosomes with $-$LH, $\frac{1}{2}$LH, $+$LH, and $+$LH$+$Mg^{2+} (see caption to Fig 2a in the main text).

Parameter	Value
DNA Persistence Length ($-Mg^{2+}$)	50 nm
DNA Persistence Length ($+Mg^{2+}$)	30 nm
DNA Stretching rigidity h	6.4 kcal/mol/nm^2
DNA Bending Rigidity g	5.8 kcal/mol
DNA Twisting Rigidity s	14.3 kcal/mol
DNA Equilibrium Twist Value ϕ_0	$.033 \pm .209$ rad ($0 \pm 12\,^\circ$)
Electrostatic Long Range Cutoff	7 nm
Lennard-Jones Long Range Cutoff	4 nm
Temperature	293 K
Salt Concentration (NaCl)	150 mM

References

(1) Tiwari, V. K.; McGarvey, K. M.; Licchesi, J. D.; Ohm, J. E.; Herman, J. G.; Schübeler, D.; Baylin, S. B. PcG proteins, DNA methylation, and gene repression by chromatin looping. *PLoS Biol.* **2008**, *6*, 2911–2927.