SUPPLEMENTAL DATA

Supplemental Table 1. Set of DMD constraints and interaction radii used to model the nucleosomal DNA. S^i, P^i, A^i, C^i, G^i and T^i represent the i^{th} nucleotide's sugar, phosphate, adenine-base, cytosine-base, guanine-base and thymine-base beads, respectively. r_0, r_1, r_2, r_3 are the corresponding interaction radii used in the model, modeled (refer: Fig. 2). K^j and R^j denote the side chain beads of j^{th} lysine and arginine amino acids, respectively.

(a) *Distance constraints:*

Interacting Pair	r_0 (Å)	r_1 (Å)
S^i-P^i	4.050	4.394
S^i-P^{i+1}	3.794	3.954
A^i-S^i	4.901	5.101
C^i-S^i	3.801	3.956
G^i-S^i	4.868	5.066
T^i-S^i	3.795	3.949

(b) *Angular constraints:*

Interacting Pair	r_0 (Å)	r_1 (Å)
A^i-P^i	7.130	8.214
C^i-P^i	5.887	6.703
G^i-P^i	7.137	8.289
T^i-P^i	5.865	6.703
P^i-P^{i+1}	6.450	6.990
S^i-S^{i+1}	5.284	5.696
A^i-P^{i+1}	7.479	7.979
C^i-P^{i+1}	6.884	7.452
G^i-P^{i+1}	7.484	7.990
T^i-P^{i+1}	6.801	7.276

(c) *Dihedral constraints:*

Interacting Pair	r_0 (Å)	r_1 (Å)
P^i-S^{i+1}	9.041	9.709
A^i-S^{i+1}	5.648	6.530
C^i-S^{i+1}	6.294	7.468
G^i-S^{i+1}	5.710	6.806
T^i-S^{i+1}	5.993	7.049
S^i-P^{i+2}	8.881	9.367
S^i-A^{i+1}	5.907	7.155
S^i-C^{i+1}	5.055	5.715
S^i-G^{i+1}	5.876	6.936
S^i-T^{i+1}	5.403	6.213

(d) *Adenine-Thymine base pairing:*

Interacting Pair	r_0 (Å)	r_1 (Å)	r_2 (Å)
A^i-T^j	5.375	5.813	6.251

(e) *Cytosine-Guanine base pairing:*

Interacting Pair	r_0 (Å)	r_1 (Å)	r_2 (Å)
C^i-G^j	5.464	5.758	6.052

(f) *Lysine-Phosphate attraction:*

Interacting Pair	r_0 (Å)	r_1 (Å)	r_2 (Å)	r_3 (Å)
P^i-K^j	3.306	4.0	6.0	8.0

(g) *Arginine-Phosphate attraction:*

Interacting Pair	r_0 (Å)	r_1 (Å)	r_2 (Å)	r_3 (Å)
P^i-R^j	3.306	4.0	6.0	8.0

(h) *Base stacking*

Interacting Pair	r_0 (Å)	r_1 (Å)
A^i-A^{i+1}	3.425	4.697
A^i-C^{i+1}	3.582	4.686
A^i-G^{i+1}	3.376	5.816
A^i-T^{i+1}	3.481	4.441
C^i-A^{i+1}	4.111	6.791
C^i-C^{i+1}	3.85	6.602
C^i-G^{i+1}	3.901	6.701
C^i-T^{i+1}	3.927	6.623
G^i-A^{i+1}	3.582	4.798
G^i-C^{i+1}	3.824	6.912
G^i-G^{i+1}	3.408	5.128
G^i-T^{i+1}	3.627	4.395
T^i-A^{i+1}	4.527	6.407
T^i-C^{i+1}	3.735	4.999
T^i-G^{i+1}	4.207	6.871
T^i-T^{i+1}	3.791	5.263

(i) *Base-Sugar repulsion:*

Interacting Pair	r_0 (Å)

A^i-S^j	8.296
C^i-S^j	10.325
G^i-S^j	8.348
T^i-S^j	10.259

Supplemental Figure Legends

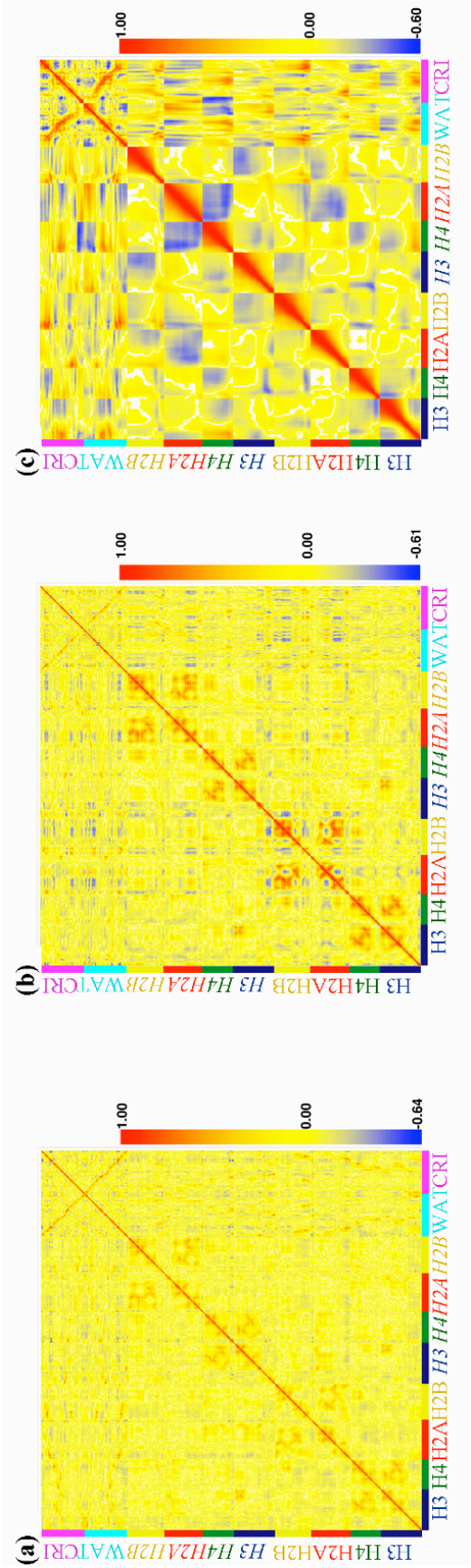
Supplemental Fig. S1 Temperature dependence of normalized correlation matrices of the nucleosome core particle for temperature range ((a) $T = 0.1\varepsilon/k_B$; (b) $T = 0.8\varepsilon/k_B$; (c) $T = 1.2\varepsilon/k_B$). These normalized correlation matrices depict regions of the nucleosome undergoing correlated, uncorrelated and anti-correlated motions in the fixed temperature DMD simulation of the nucleosome core particle. Observed correlation in motion is color coded as anti-correlated (blue), uncorrelated (yellow) and correlated (red).

Supplemental Fig. S2 Per-residue contact map of frequencies of intra/inter-histone contacts. Detailed per-residue contact map of frequencies of intra- and inter- histone contacts is plotted for (*A*) $T = 0.1$, corresponding to low temperature regime; and (*B*) $T = 0.8$, corresponding to near-transition temperature regime of constant-temperature DMD simulations of the nucleosome core particle. Contact frequency data is averaged over five independent simulation runs starting with different initial velocity distributions.

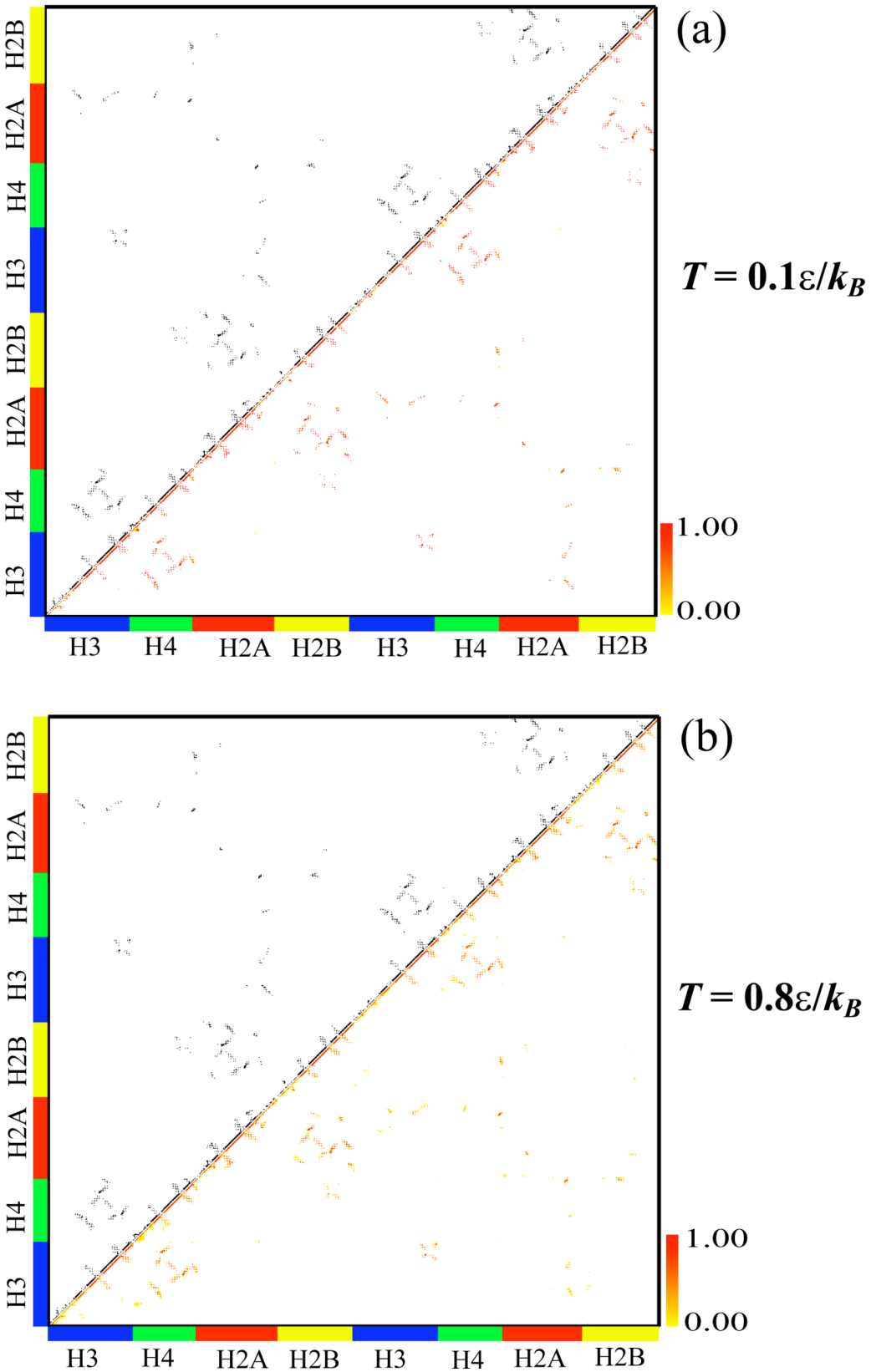
Supplemental Fig. S3 Trajectory of the nucleosome core particle, i.e. the potential energy of the nucleosome core particle system as observed in constant temperature DMD simulations is shown as a function of time for temperatures shown in the adjoining legend. Temperature is measured in units of E/k_B and energy in DMD units (*cf.* Materials and Methods). Equilibration of simulations occurs in the initial 5×10^4 t.u.

Supplemental Fig. S4 Thermodynamics of the histone octamer assembly. The dependence on temperature of the energy, E is shown. The error bars represent a standard deviation of energy fluctuations. (B), Variation of the constant volume heat capacity, C_v of the histone octamer assembly with temperature. The error bars are the standard deviation of C_v fluctuations. The unfolding of histone octamer occurs at temperature $T = 0.8$.

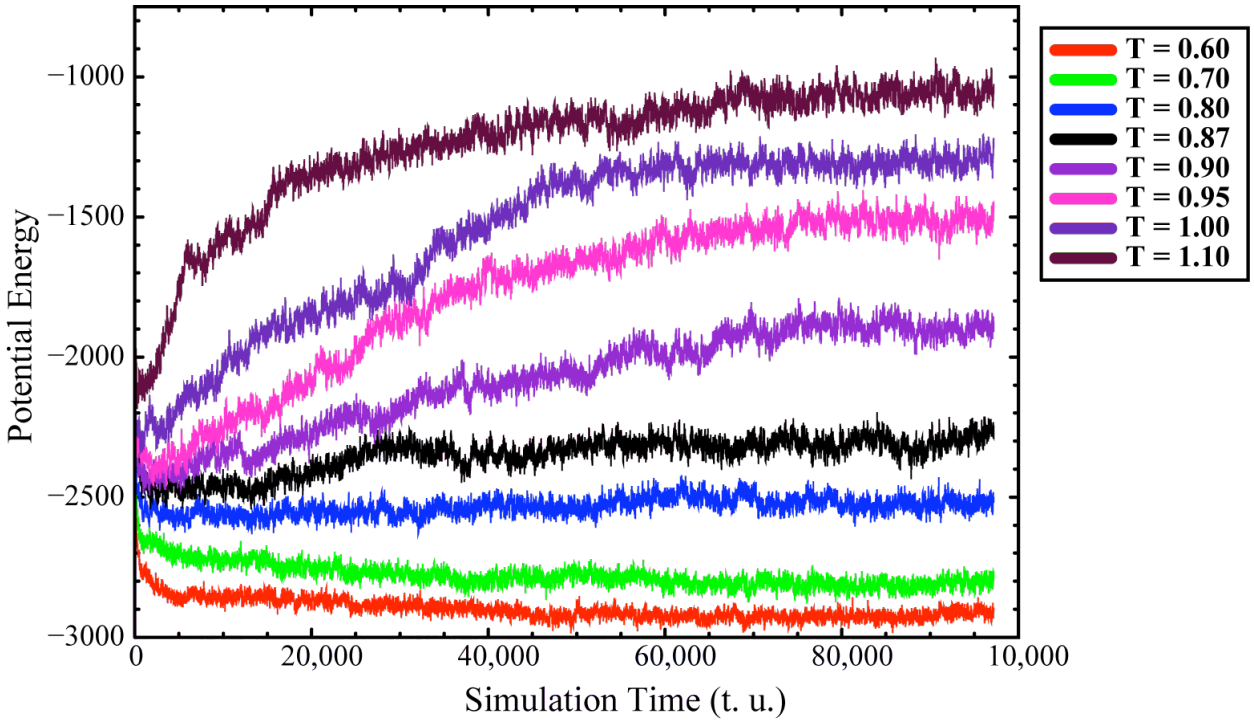
Supplemental Figure S1



Supplemental Figure S2



Supplemental Fig. S3



Supplemental Fig. S4