SUPPLEMENTARY MATERIALS

Nucleosome geometry and internucleosomal interactions control the chromatin fiber conformation

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SUPPLEMENTARY TABLES

TABLE S1: Parameters used in the MC simulations

Parameter	Value
Stretching module DNA	$1.10 \cdot 10^{-18}$ J nm
Bending module DNA	$2.06 \cdot 10^{-19}$ J nm
Torsion module DNA	$2.67 \cdot 10^{-19}$ J nm
Electrostatic radius DNA	1.2 nm
Stretching module chromatosome	$1.10 \cdot 10^{-18}$ J nm
Torsion module chromatosome	$1.30 \cdot 10^{-18}$ J nm
Temperature	293 K
Ionic strength	100 mM NaCl
S-function parameters (cylinder)	S000 = 1.6957
	Scc2 = -0.7641
	S220 = -0.1480
	S222 = -0.2582
	S224 = 0.5112
	E000 = 2.7206
	Ecc2 = 6.0995
	E220 = 3.3826
	E222 = 7.1036
	E224 = 3.2870
	$\sigma_0 = 5.5\,\mathrm{nm}$

SUPPLEMENTARY FIGURES

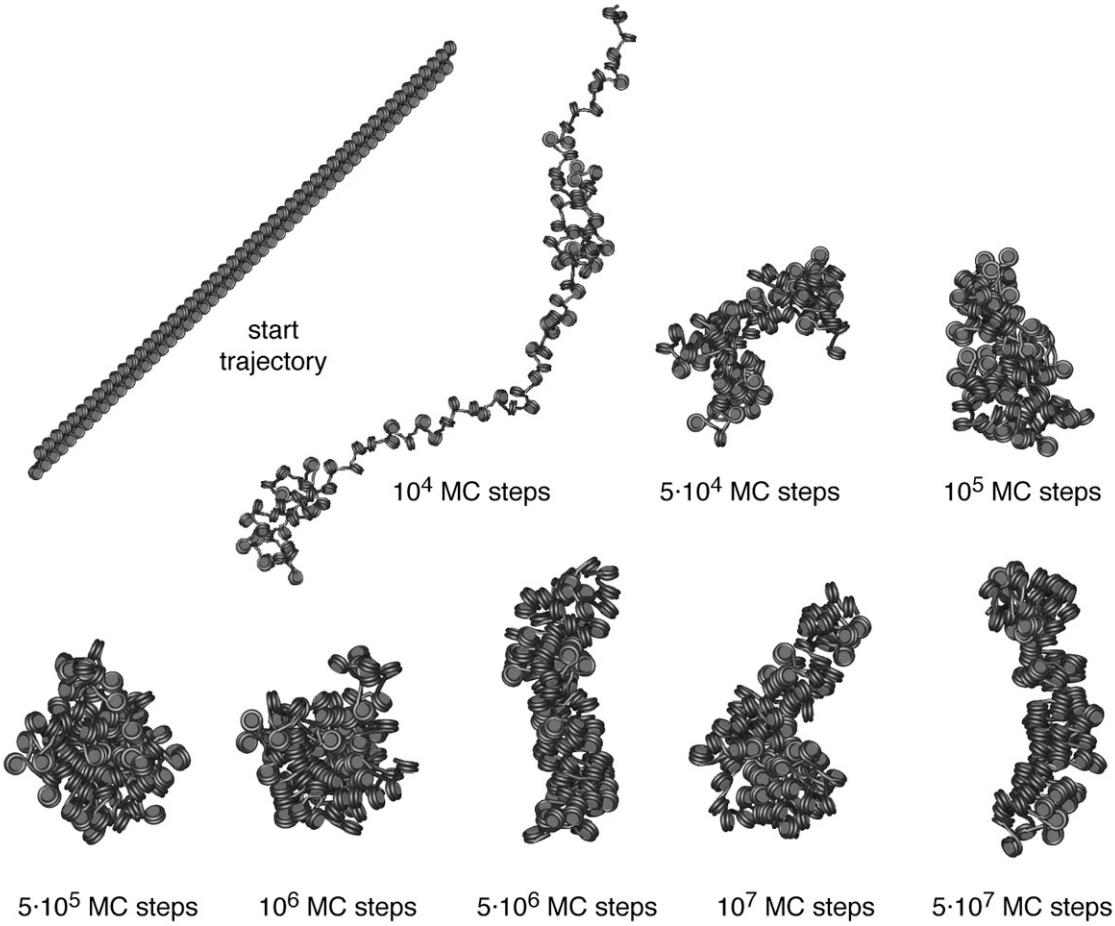

FIGURE S1. Examples of Monte Carlo simulations with alternative start configuration. To test the influence of the start geometry, the MC simulations were started also from a stretched linear conformation for geometries listed in Tables 1 to 3. The example shown here has the same local chromatosome geometry as the fiber in Fig. S3B. After about $5 \cdot 10^6$ MC steps this simulation reached thermal equilibrium at the same energies as the simulation started from a mechanically relaxed structure (Fig. S3B).

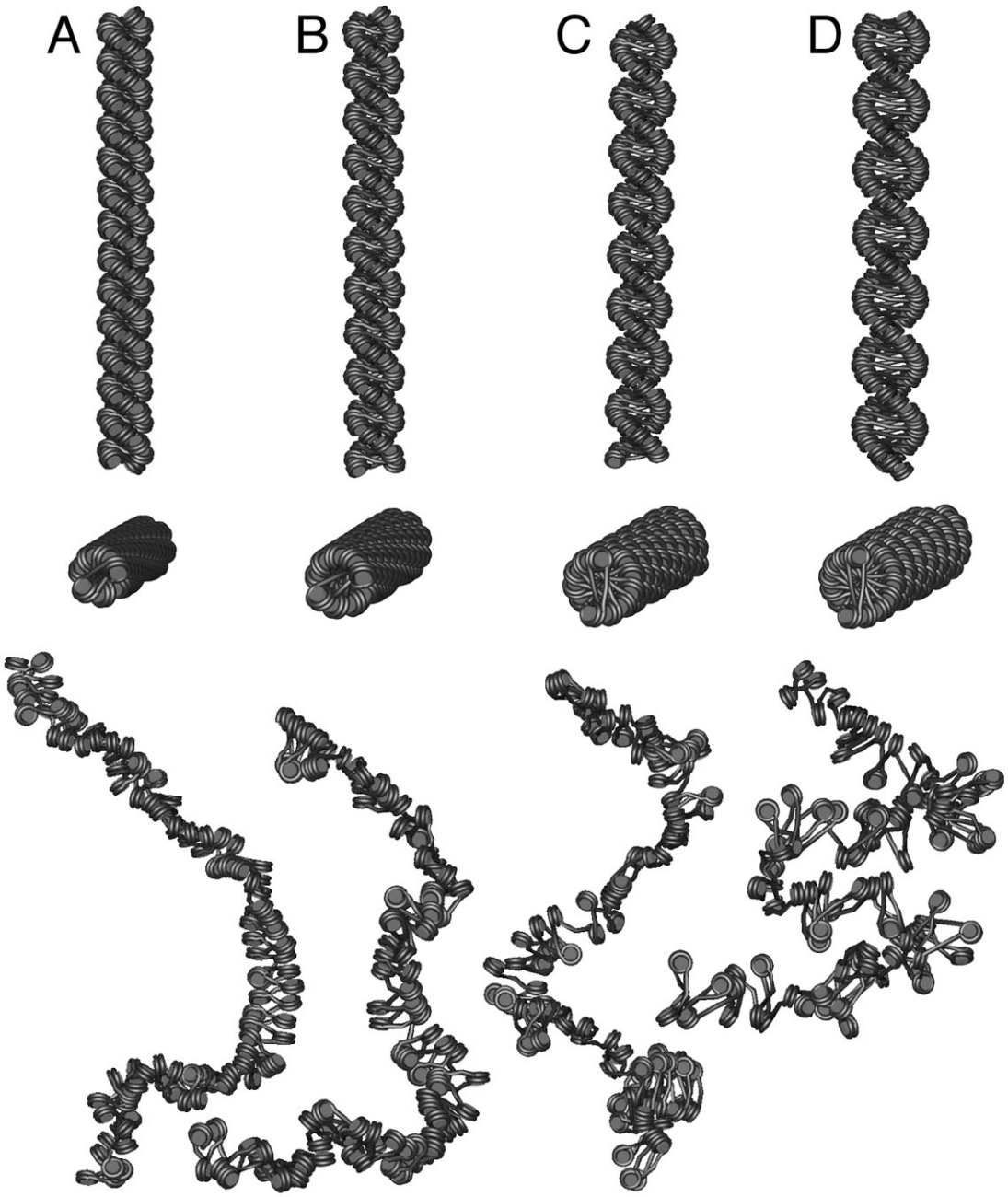

FIGURE S2. Monte Carlo simulations of two-start helix crossed-linker fiber conformation (CL). Simulations of a chain of 100 nucleosomes with NRLs of 169 bp (A), 179 bp (B), 189 bp (C), and 199 bp (D). Side and top views of the start structures are displayed in the first and second row. The bottom row depicts representative configurations at equilibrium, indicating a reduction of mass densities with increasing NRLs to 3.1, 2.8, 2.5, and 2.2 nucleosomes per 11 nm fiber length (Table 1).

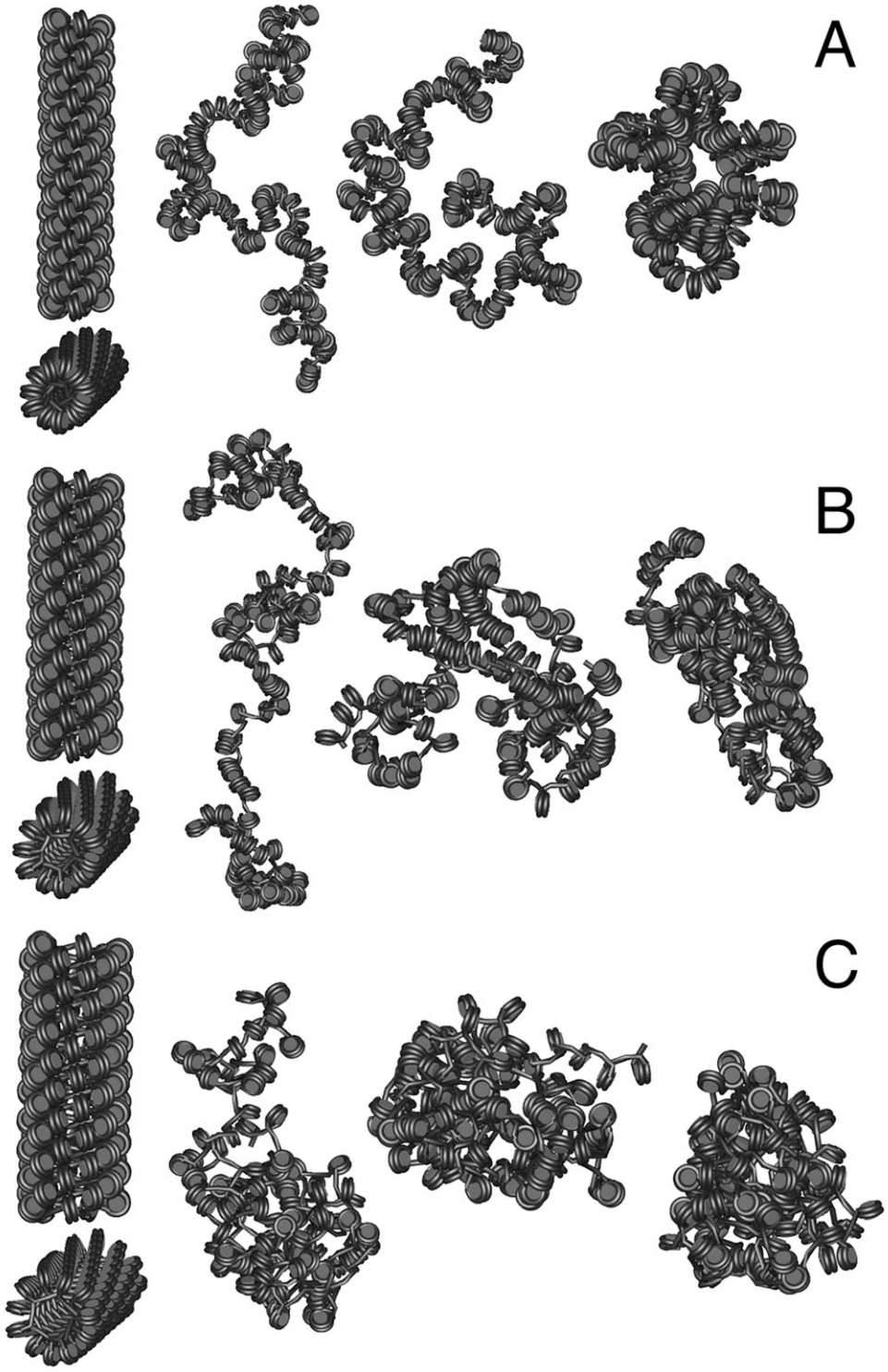

FIGURE S3. Monte Carlo simulations of interdigitated one-start helix fibers with low nucleosome tilt (ID20). Simulations of a chain of 100 nucleosomes with NRLs of 187 bp (A), 197 bp (B), and 207 bp. (C) are shown. Initial configurations are displayed in the first column. The second to last columns show representative configurations at thermal equilibrium. The initial interdigitated fiber conformation is lost during the MC simulations for all NRLs (Table 2).

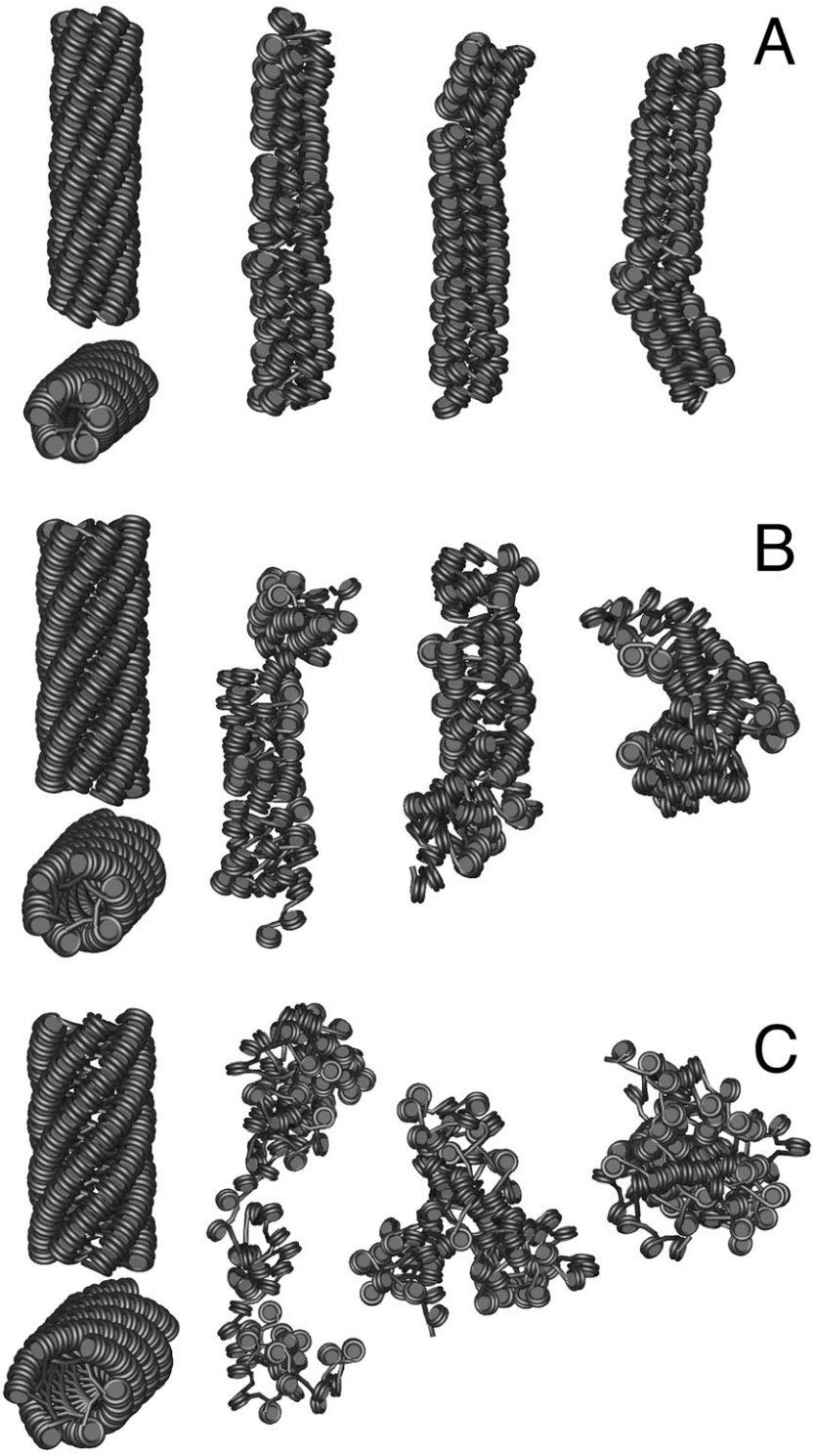

FIGURE S4. Monte Carlo simulations of interdigitated one-start helix fibers with high nucleosome tilt angle (ID40+). Simulations of a chain of 100 nucleosomes with 5.8 chromatosomes per turn and NRLs of 189 bp (A), 199 bp (B), and 207 bp (C) are shown. Initial configurations are displayed in the first column. The mass densities of the starting structures vary between 9 and 11 nucleosomes per 11 nm fiber. In the following three columns the variations in shape and average mass density at thermal equilibrium are depicted. The mass density increased from left to right (Table 3).

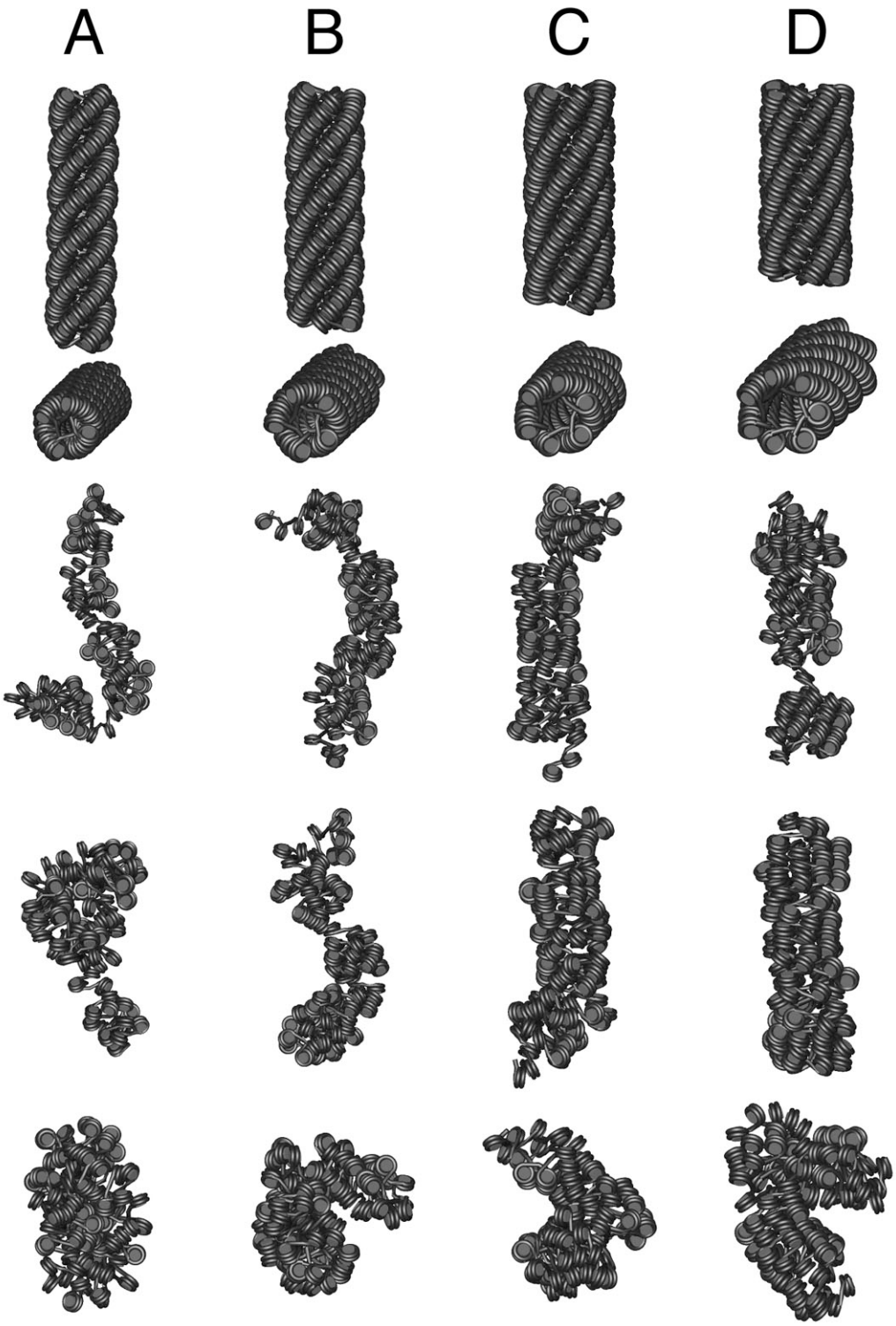

FIGURE S5. Monte Carlo simulations of ID40+ conformations with different numbers of nucleosomes per turn. ID40+ fibers with a NRL of 197 bp and 3.8 (A), 4.7 (B), 5.8 (C), or 6.8 (D) chromatosomes per turn were simulated. The local nucleosome tilt angle was adapted between 45-60° to obtain an optimal stacking of the nucleosomes in the different structures. A higher number of nucleosomes per turn increased the diameter of the fiber and also its stability as inferred from the MC simulations (Table 3).

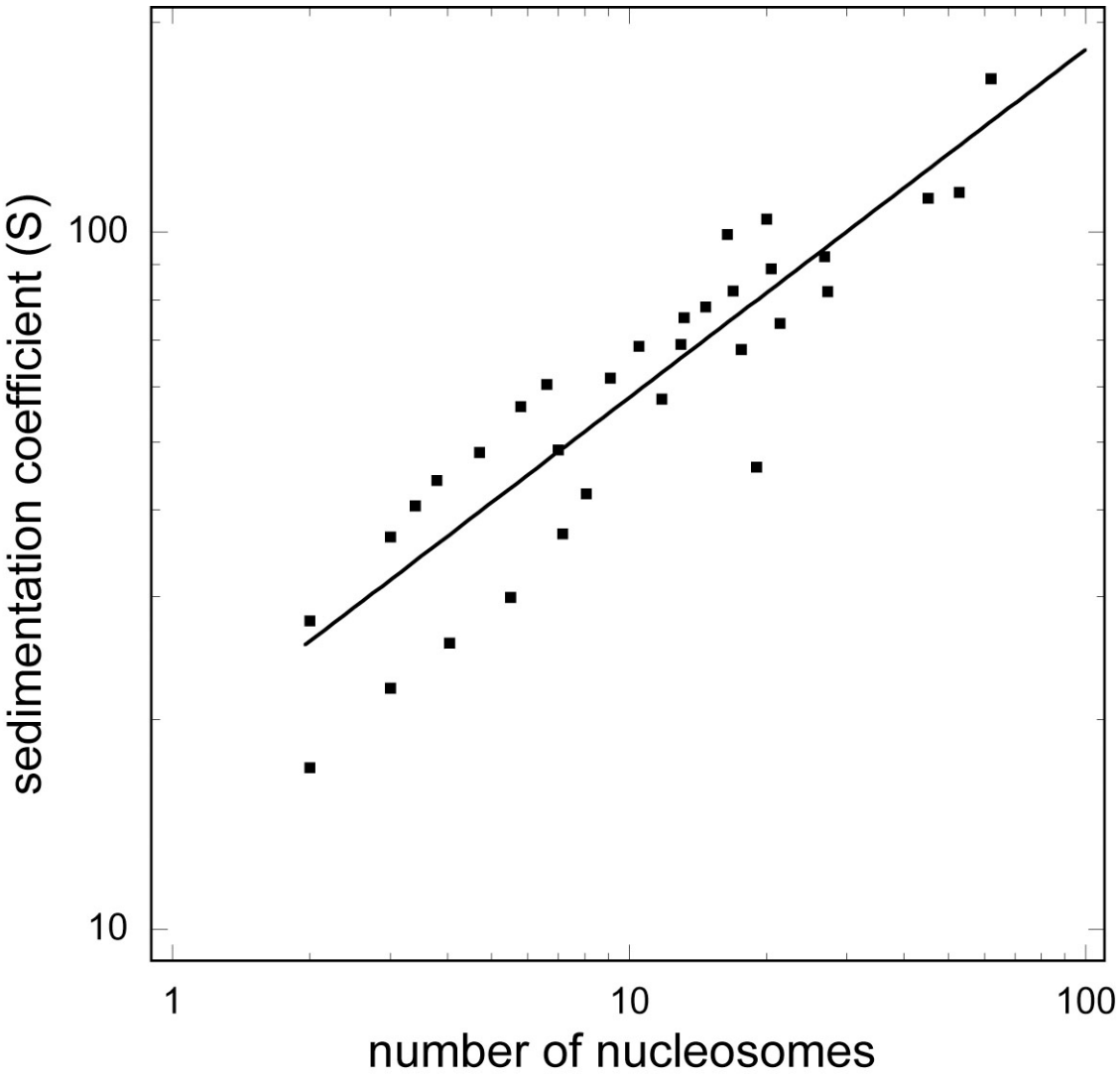

FIGURE S6. Dependence of experimentally determined sedimentation coefficients on the number of nucleosomes. Sedimentation coefficient data for native nucleosome chains with 2 to 60 nucleosomes at 0.1 M salt reported for rat liver nuclei (49,50), chicken erythrocytes (51), nuclei from bovine thymus (52) and HeLa cells (15) are plotted versus the number of nucleosomes (references are given in the main text). The line represents an empirical fit function $s(n) = 21.1 \cdot n^{0.466} - 3.2$, from which a sedimentation coefficient of ~180 S for chromatin fibers of 100 nucleosomes at a NRL of 200 bp is estimated.