



Research article

Topological diversity of chromatin fibers: Interplay between nucleosome repeat length, DNA linking number and the level of transcription

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Supplementary

For $L = 20$ bp, our structure has the inclination angle $\rho = -45^\circ$ and rise = 27 Å. The “direct” model by Schalch et al. [7] is based on the X-ray tetranucleosome structure; it has inclination about $-50^\circ/-40^\circ$ and low rise = 17 Å. Note, however, that this model has “steric overlaps” [7]; the authors suggest that these overlaps can be relieved by increasing the separation of tetranucleosomes. On the other hand, using the EM images for $L = 20$ bp [9,16], one can estimate the rise to be ~ 25 Å, which is close to 27 Å in our energetically optimal fiber (**A**).

For $L = 30$ bp, Song et al. [8] built the high-resolution model based on the Cryo-EM data, with the inclination angle $\rho \approx -60^\circ$ and rise = 24 Å (**E**). Our optimal structure is very close to this model: $\rho = -60^\circ$ and rise = 25 Å (**B**).

For $L = 40$ bp, the Cryo-EM-based model has $\rho \approx -60^\circ$ and rise = 22.5 Å, compared to $\rho = -70^\circ$ and rise = 20 Å in our optimal structure (**C**). Note that in both the theoretical (**B**, **C**) and the Cryo-EM-based models (**E**, **F**) the linker increase from $L = 30$ to 40 bp is accompanied by a decrease in superhelical rise and increase in the diameter of fibers.

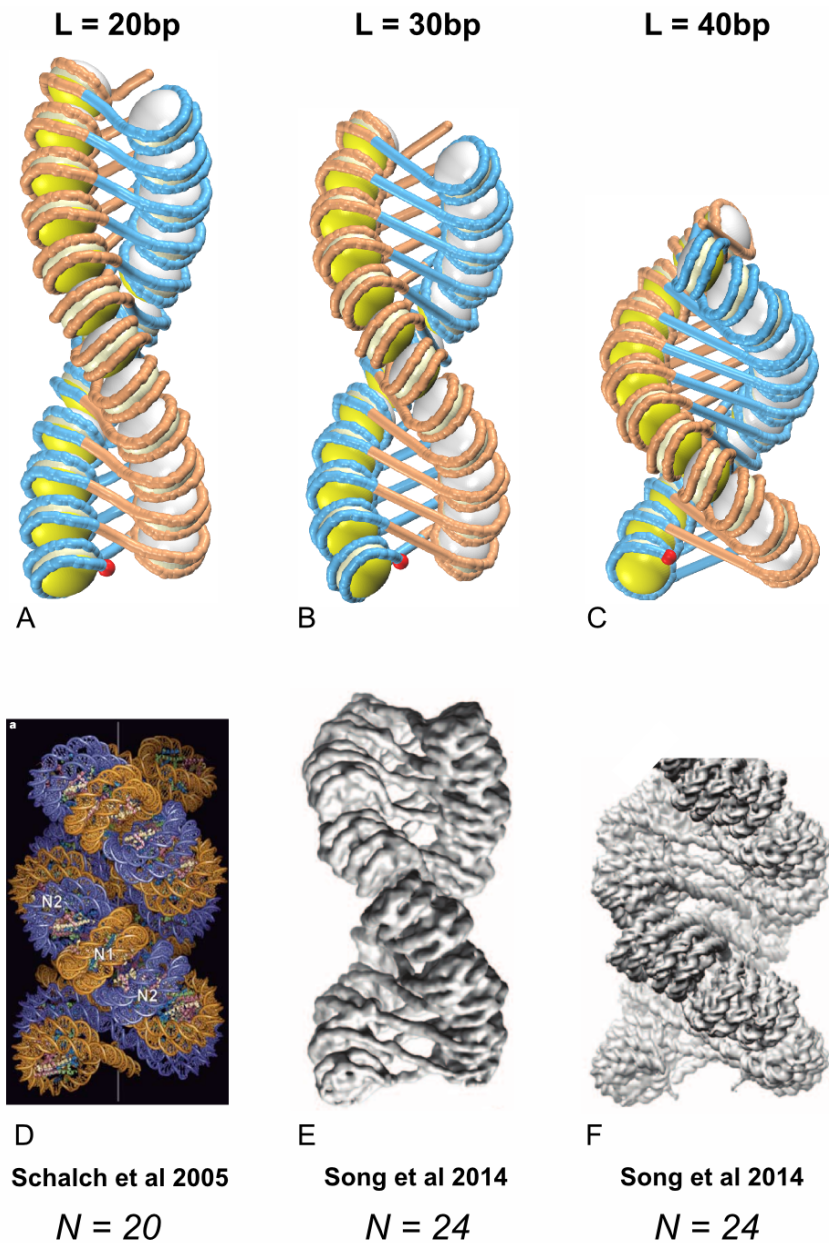


Figure S1. Comparison of the energetically optimal fibers with the experiment-based models. The computed structures for $L=20, 30, 40$ bp (A, B, C) are the same as shown in Figure 3. In each case, the number of nucleosomes, N , is 24. (D–F) The published experiment-based models are shown for comparison, with the N values given below.



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