

Fig. S1. Time evolution of RMSD values from the starting structure for the DSL (black lines) and SSL (red lines) nanocages. In figure are reported the values calculated over all the atoms (A), the structural DNA double helices (B) and the linkers (C), respectively.

Fig. S2. Time evolution of the gyration radius for the DSL (black line) and SSL (red line) nanocages.

Fig. S3. Per nucleotide RMSF projection along the second (A) and third (B) eigenvector for each of the two strands of the 12 structural DNA double helices (i.e. non linker helices) for the DSL (black and red lines) and SSL (green and blue lines) nanocages.

Fig. S4. Graphical representation of the Cartesian reference system used to compute the rotation angle of each DNA double helix (A). Time evolution of the rotation angles evaluated for some helices (DH1, DH2, DH5, DH7, DH11, DH12), for the SSL cage (B) and the DSL cage (C).

Fig. S5. Tube representation of the motion projections along the second (DSL A, SSL B) and third (DSL C, SSL D) eigenvectors for the two nanocage structures. The width of the ribbon, generated by the flanking tubes, indicates the amplitude of the motion, the direction going from the red to the blue color. This picture was produced using the VMD program.⁴⁰

Fig. S1

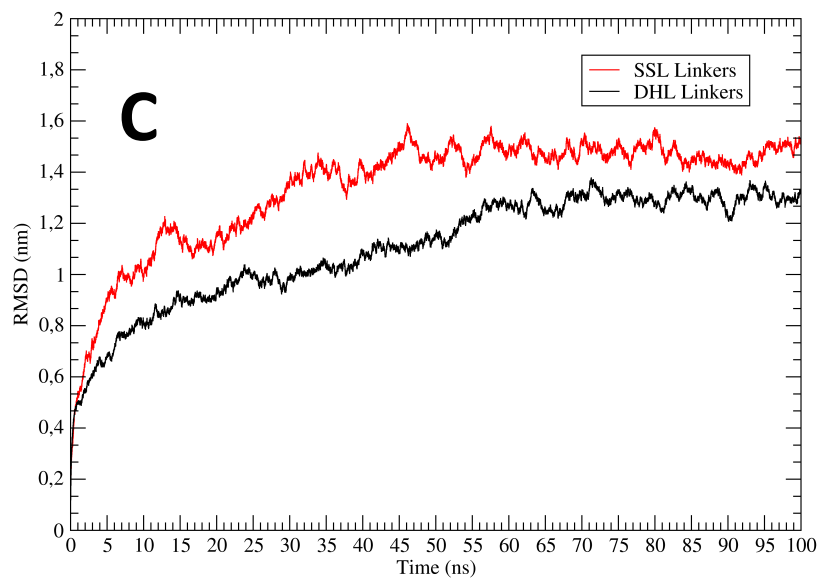
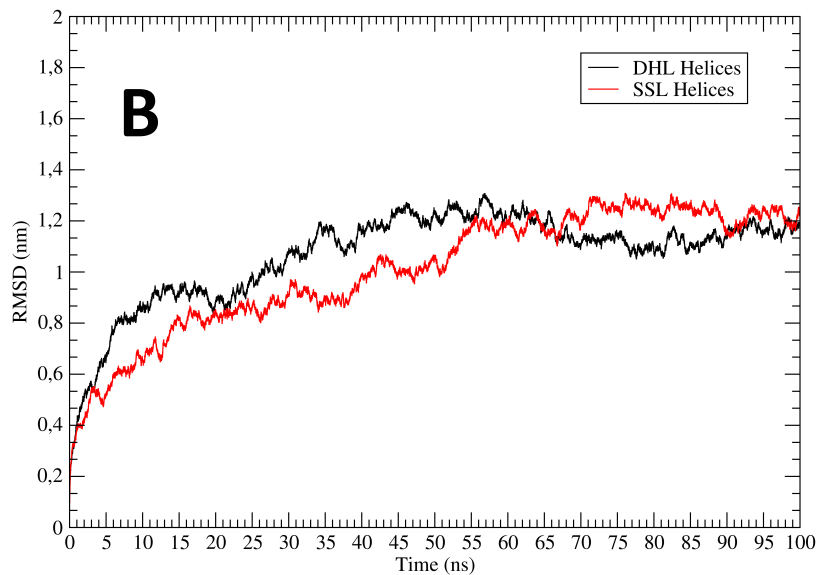
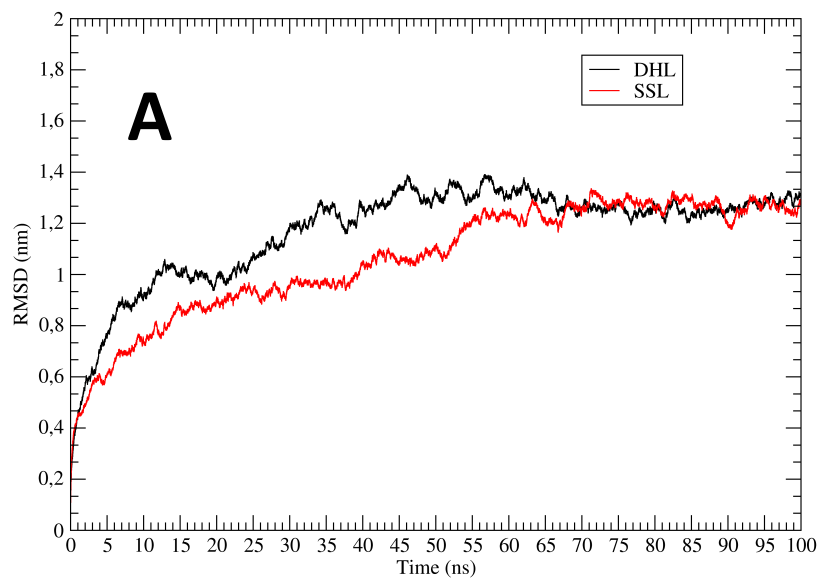


Fig. S2

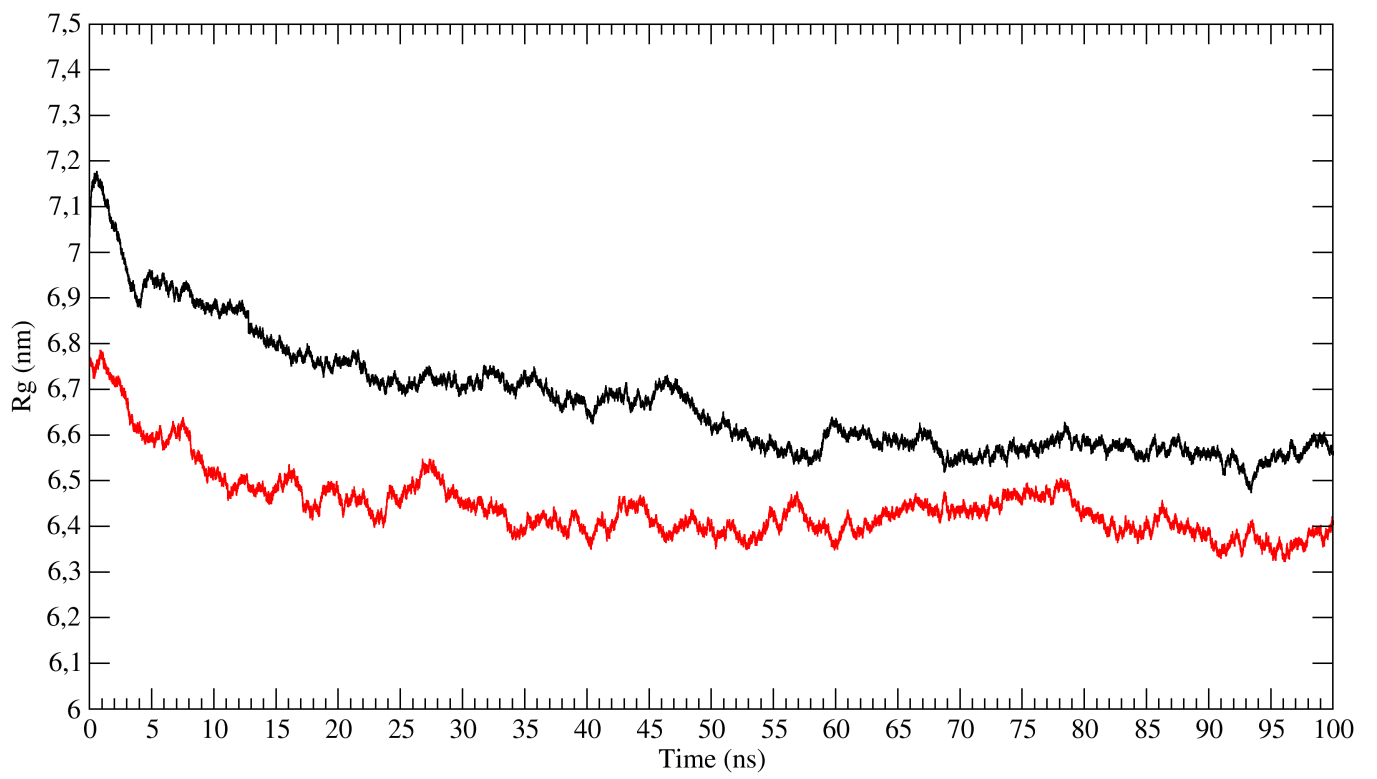
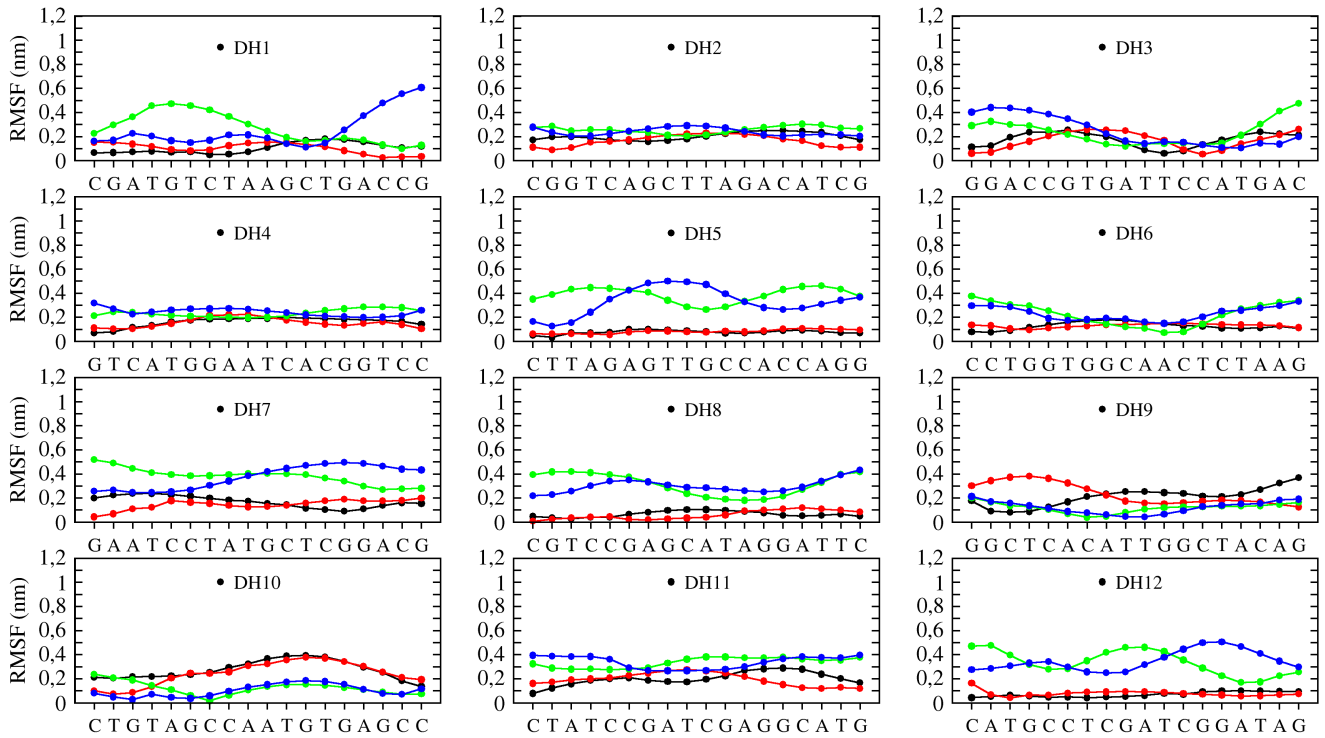


Fig. S3

A



B

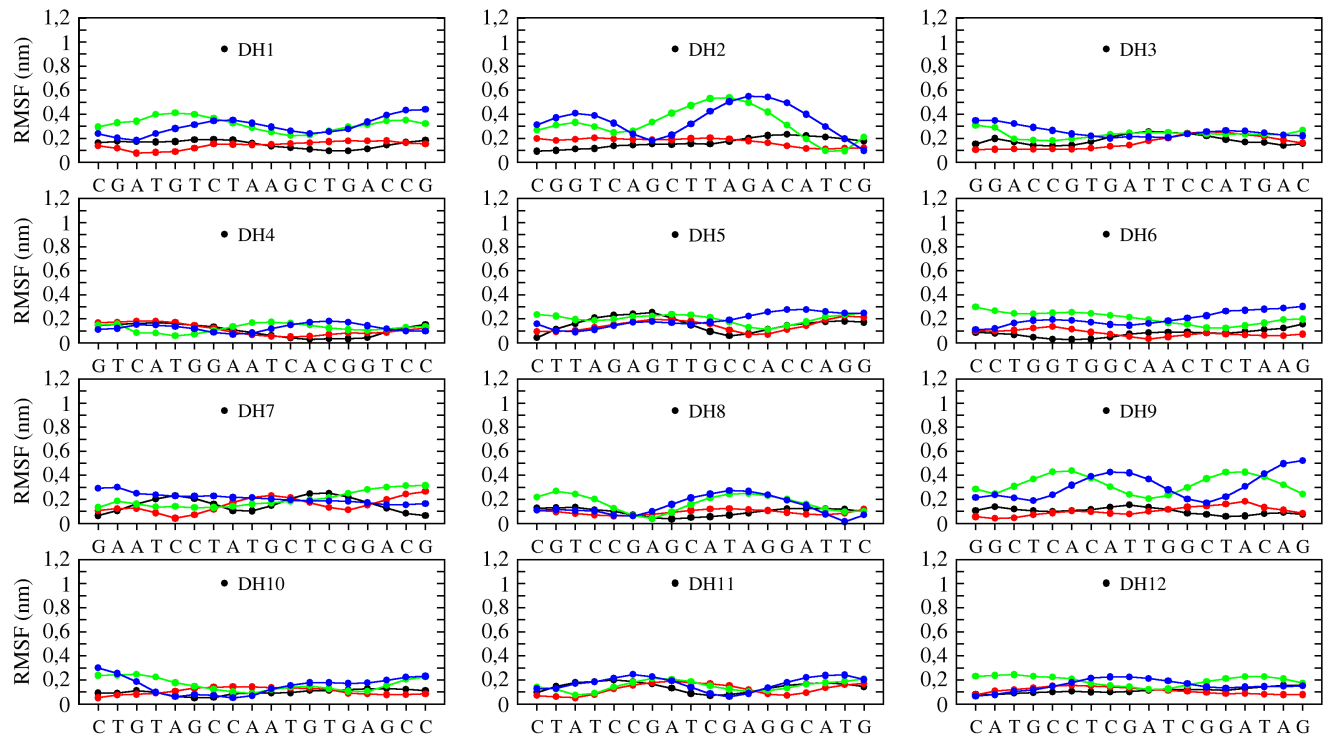


Fig. S4

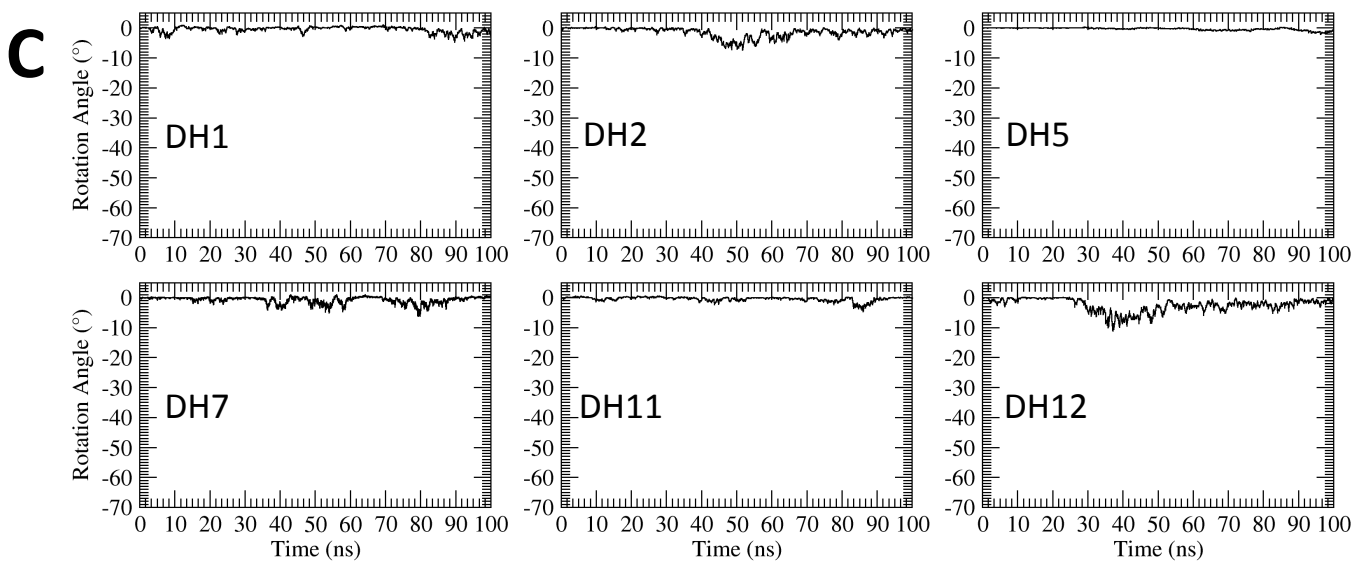
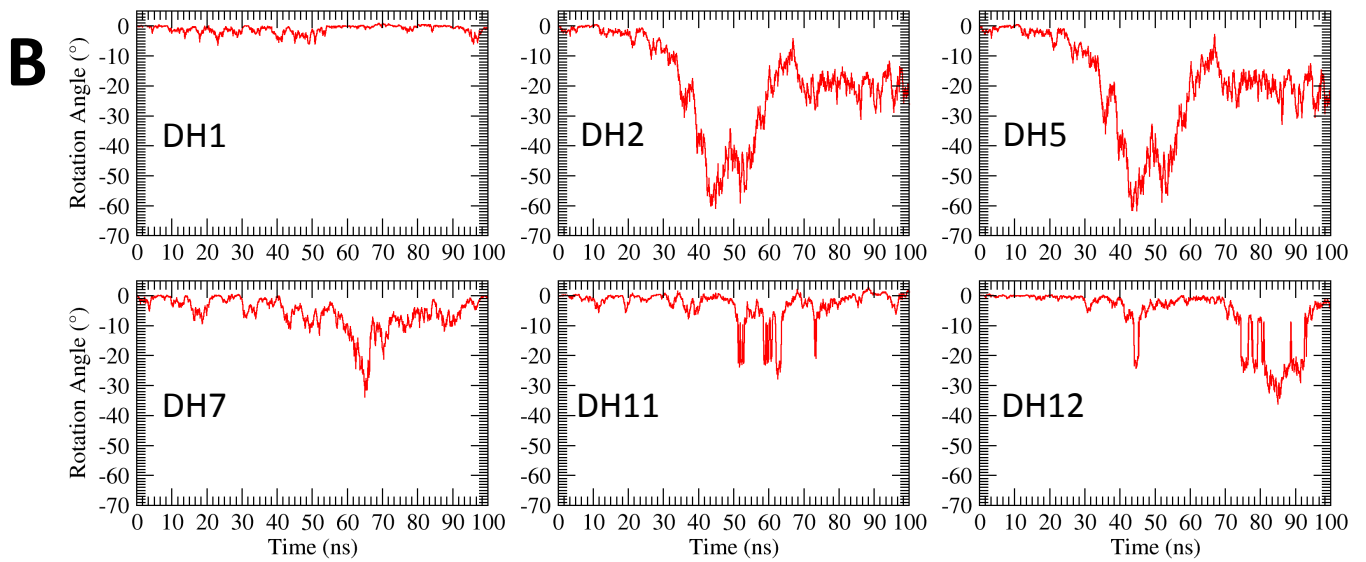
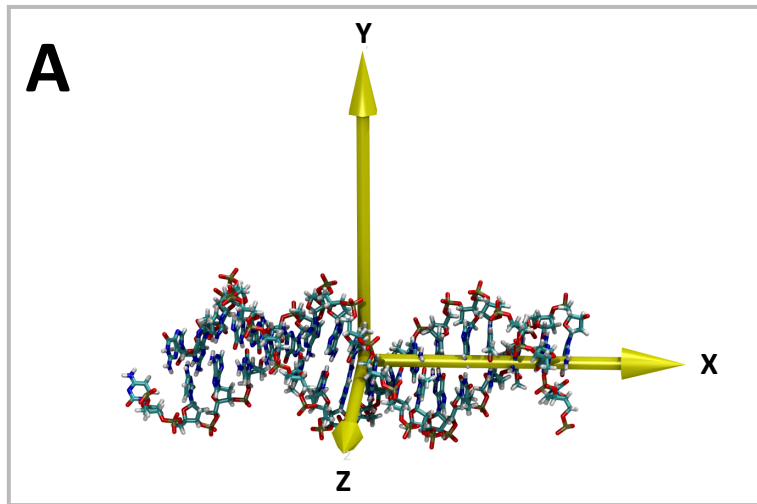


Fig. S5

