

Twist-Induced Defects of the P-SSP7 Genome Revealed by Modeling Cryo-EM Density

Qian Wang¹, Christopher G. Myers² and B. Montgomery Pettitt^{1,2*}

1 Department of Biochemistry and Molecular Biology, Sealy Center for Structural Biology and Molecular Biophysics, University of Texas Medical Branch, Galveston, TX 77555-0304

2 Structural and Computational Biology and Molecular Biophysics Program, Baylor College of Medicine, Houston, TX, 77030

DNA sequences (from 3' to 5'). The base pairs corresponding to the hole in the density map are colored in red.

Sequence A:

GCGAATTGTGTCCGCACAGACATATTACGCGCCGACGGACGCAATTAAGTAGCGCA
TACGCGGGTATACGGGTGCAGTGT

Sequence B:

CAAGAGCGACCTAATGTATAGATCGCGCCCCGTTTAGGCTGGGGGGATGCCCCAA
AAACGCAGGACACATGTAGCATAT

Figure S1. Density map produced from simulations of a twisted DNA (Sequence B) without cryo-EM fitting. $\sigma = -0.33$. $T = 310\text{K}$.



Figure S2. Density map produced from simulations of a twisted DNA (sequence A) without cryo-EM fitting and without position constraint. $\sigma = -0.33$. $T = 310\text{K}$.

