

SUPPLEMENTARY MATERIAL

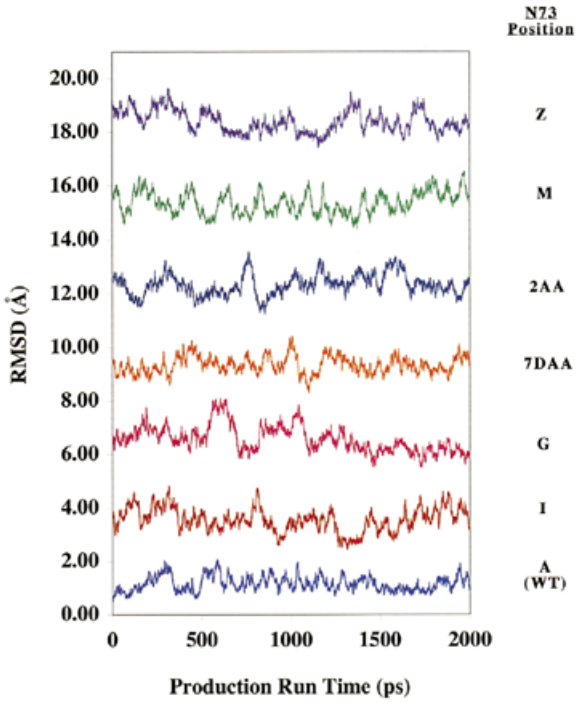


Figure S1. RMSDs (Å) from initial structures taken over the production run portion of each trajectory. Values have an arbitrary 0 and are calculated excluding the single-stranded region of the microhelix.

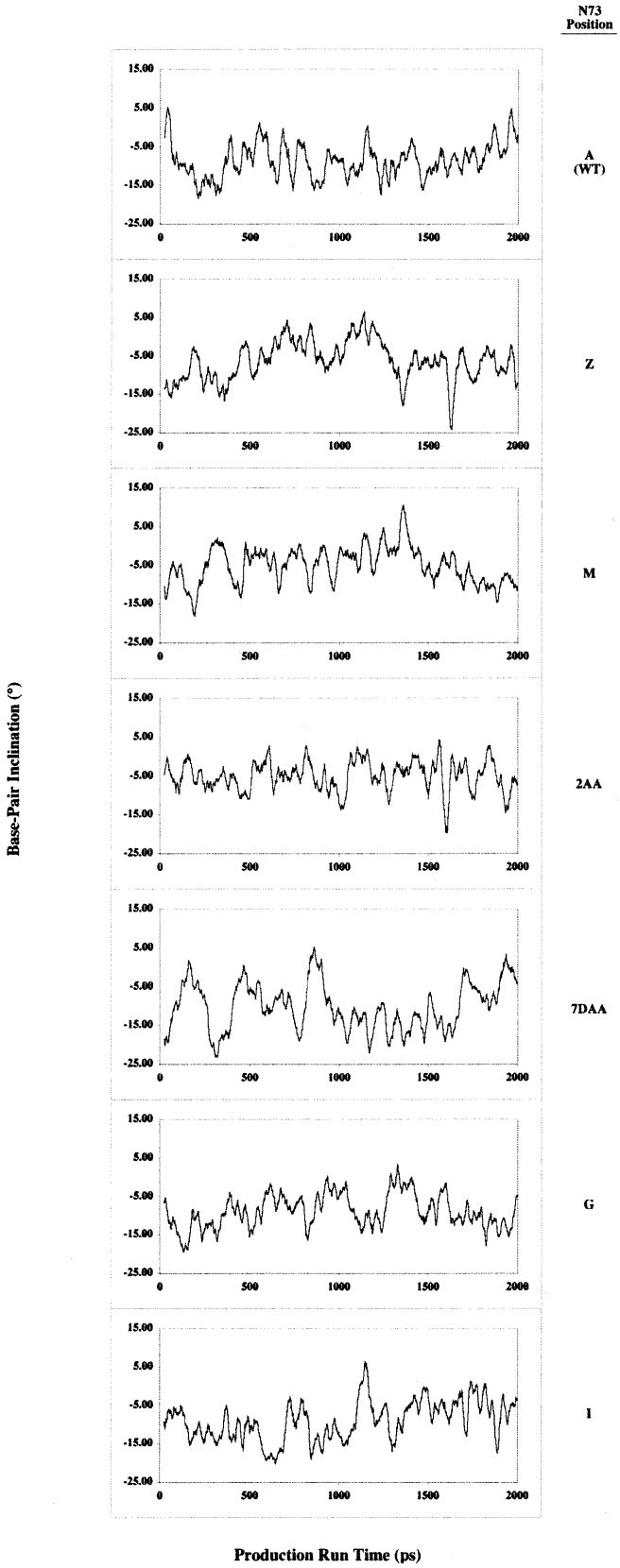


Figure S2. Average base pair inclinations (°) taken over the production run portion of each trajectory.

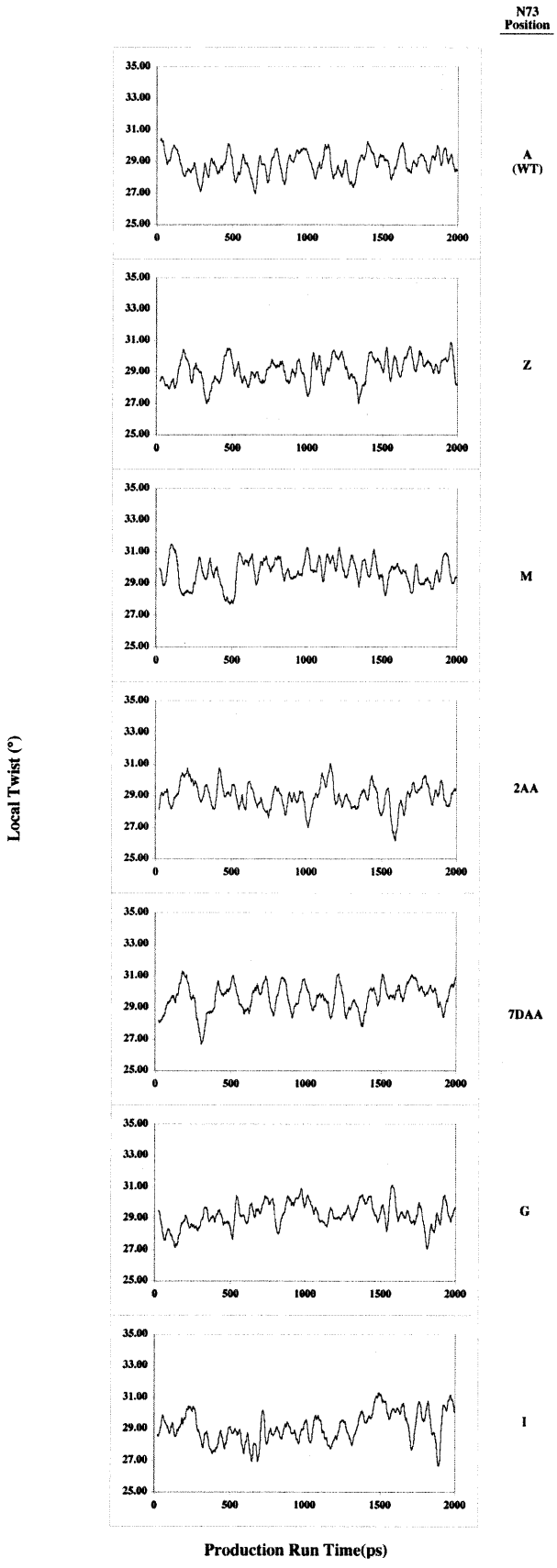


Figure S3. Average local helical twist (°) taken over the production run portion of each trajectory.

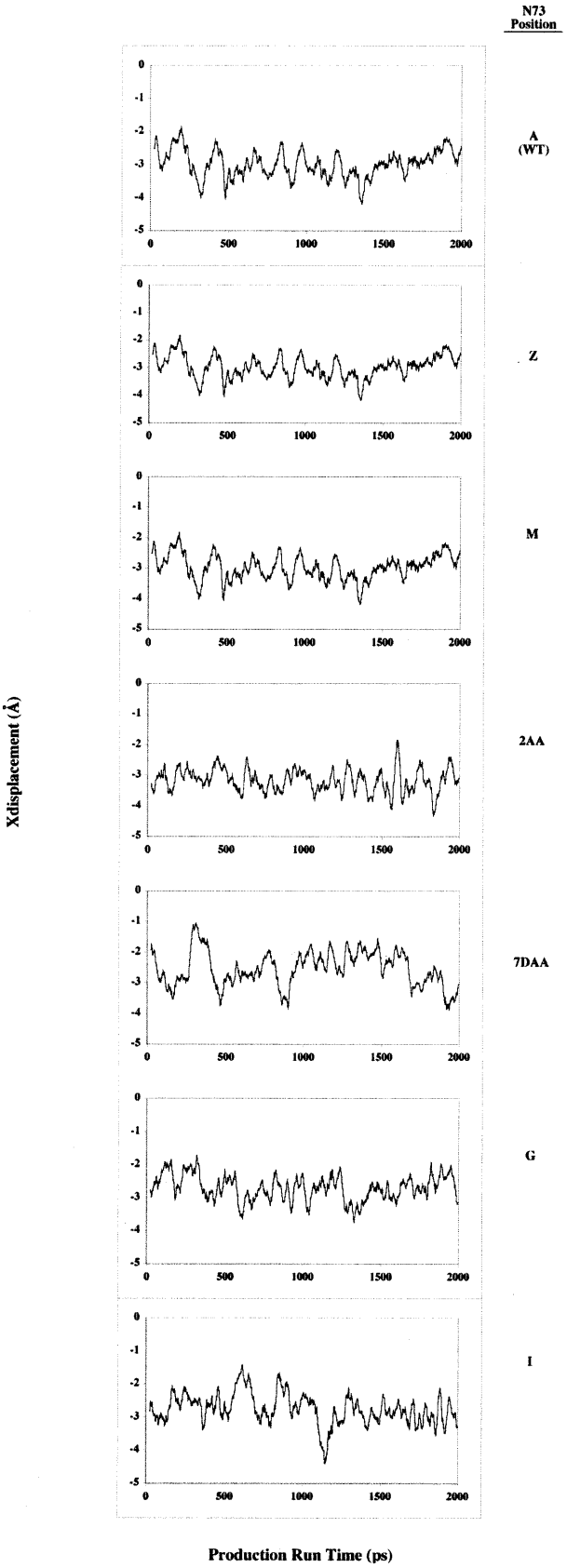


Figure S4. Average x displacement (Å) taken over the production run portion of each trajectory.

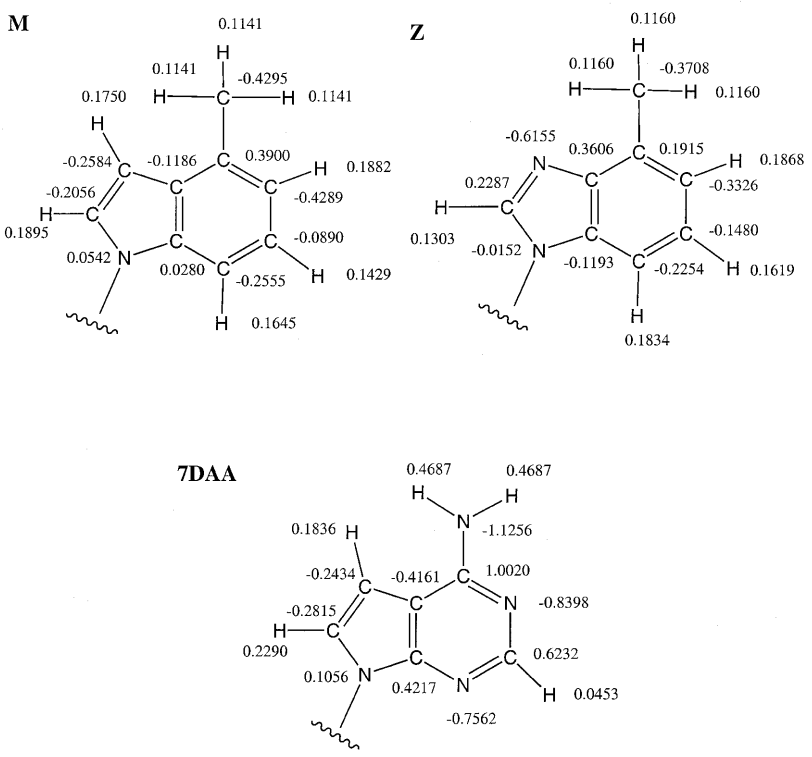
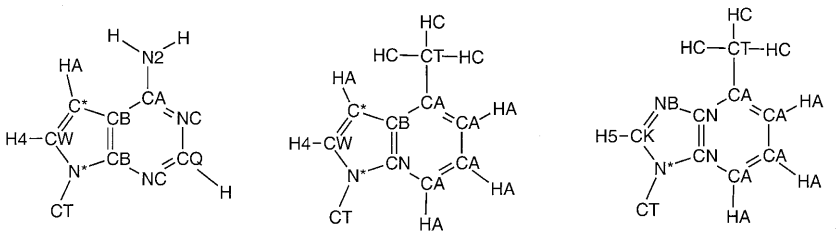


Figure S5. Partial atomic charges employed for non-standard bases 7DAA, M and Z.



7-deazaadenine (7DAA) **4-methylindole (M)** **4-methylbenzimidazole (Z)**

Figure S6. Atom types [as defined in Cornell,W.D., Cieplak,P., Bayly,C.I., Gould,I.R., Merz,K.M., Ferguson,D.M., Spellmeyer,D.C., Fox,T., Caldwell,J.W. and Kollman,P.A. (1995) *J. Am. Chem. Soc.*, **117**, 5179–5197] employed for non-standard bases 7DAA, M and Z.