SUPPORTING INFORMATION

Impact of Bistrand Abasic Sites and Proximate Orientation on DNA Global Structure and Duplex Energetics

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TABLE S1. Summary of van't Hoff Thermodynamic Parameters derived via Shape Analysis of Temperature-dependent Profiles acquired for the Tridecameric Duplexes.

Acronym	ΔH^{o}_{shape} (kcal·mol^{-1})	$T\Delta S^{o}_{shape}$ (kcal·mol^{-1})	ΔG^{o}_{shape} (kcal·mol^{-1})
CCC/GGG	**113.7**	**91.1**	**22.5**
FCC/GGG	**69.9**	**56.7**	**13.2**
CFC/GGG	**86.7**	**72.2**	**14.5**
CCF/GGG	**70.8**	**57.6**	**13.2**
CCC/GFG	**79.0**	**65.1**	**13.9**
FCC/GFG	**85.8**	**71.2**	**14.5**
CFC/GFG	**81.9**	**68.2**	**13.6**
CCF/GFG	**77.0**	**64.1**	**12.9**

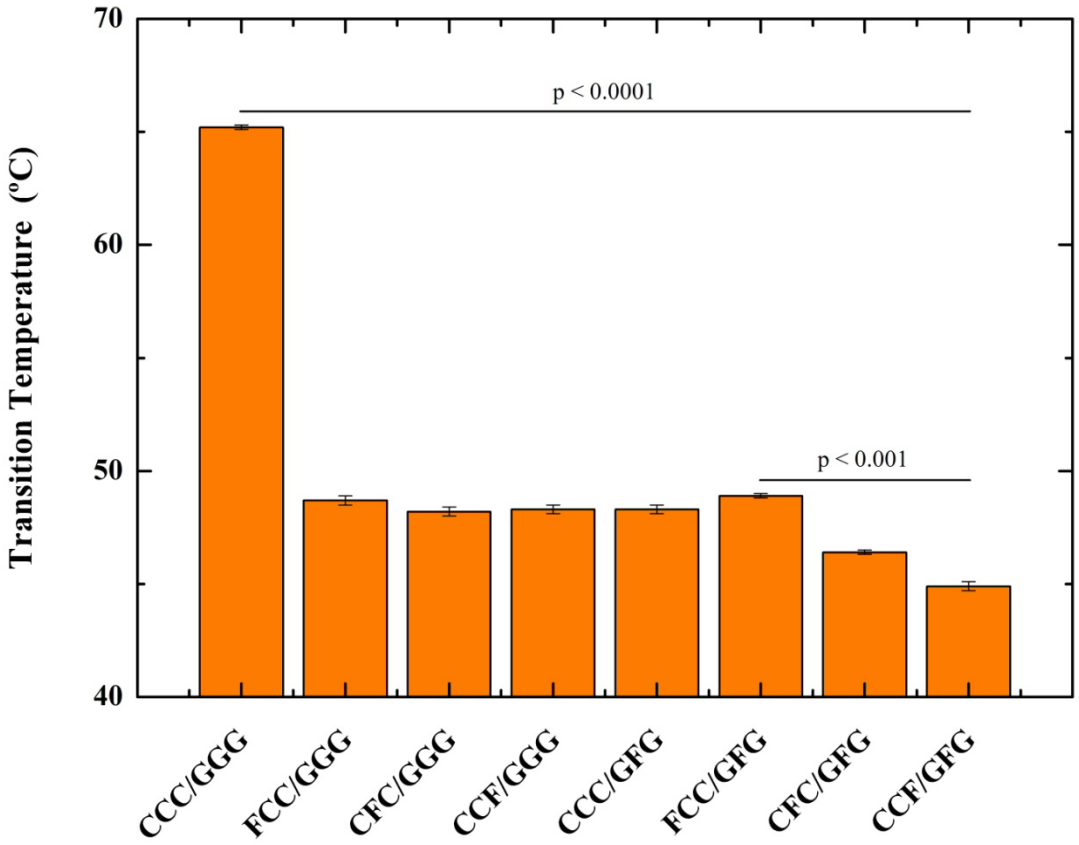
Thermodynamic data correspond to a DNA duplex of 45.4 μM total strand concentration (C_T). Standard errors for ΔG^{o}, ΔH^{o}, and $T\Delta S^{o}$ are within 2.0, 4.5, and 5.0 kcal·mol^{-1}, respectively.

TABLE S2. Heat-Capacity Corrected Thermodynamic Dissociation Parameters.

Acronym	$\Delta H°_{25\ °C}$ (kcal·mol^{-1})	$T\Delta S°_{25\ °C}$ (kcal·mol^{-1})	$\Delta G°_{25\ °C}$ (kcal·mol^{-1})
CCC/GGG	**79.32**	**63.3**	**16.0**
FCC/GGG	**80.56**	**69.2**	**11.4**
CFC/GGG	**74.16**	**63.4**	**10.8**
CCF/GGG	**76.07**	**65.1**	**10.9**
CCC/GFG	**72.51**	**61.8**	**10.7**
FCC/GFG	**60.65**	**50.7**	**10.0**
CFC/GFG	**74.20**	**63.9**	**10.3**
CCF/GFG	**58.55**	**49.6**	**8.9**

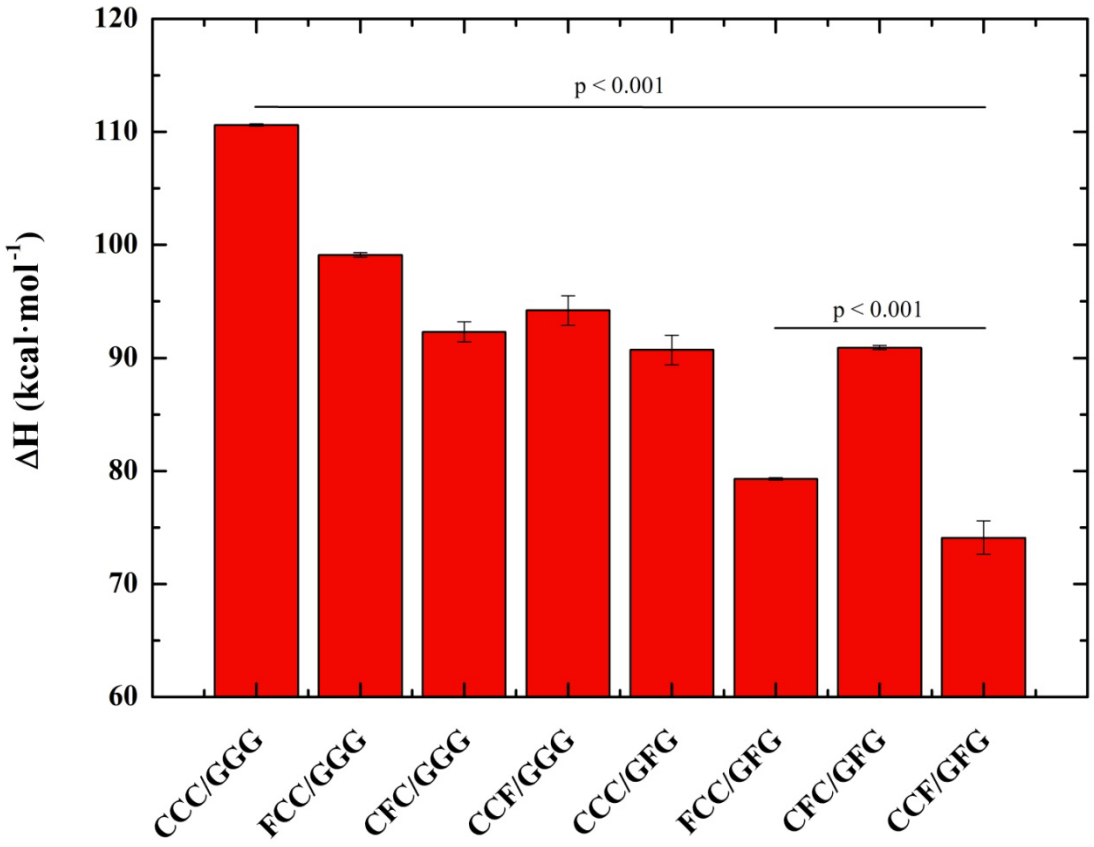
Values extrapolated to 25 ºC using a ΔC_p of 780 cal·mol^{-1}·deg $^{-1}$ (i.e., 60 cal·mol^{-1}·deg $^{-1}$·bp^{-1}) applying the following relations: $\Delta H\ (T) = \Delta H\ (T_m) - \Delta C_p\ (T_m - T)$; $\Delta S\ (T) = \Delta H/T_m + \Delta C_p\ ln(T/T_m) + R\ ln\ (C_T/4)$; $\Delta G\ (T) = \Delta H(T_m)\ (1 - T/T_m) + \Delta C_p\ [T - T_m - T\ ln\ (T/T_m)] - RT\ ln\ (C_T/4)$, *whereby T = 25 ºC.*

FIGURE S1. Thermal Stability of Canonical, Single, and Bistrand AP-Site Duplexes.



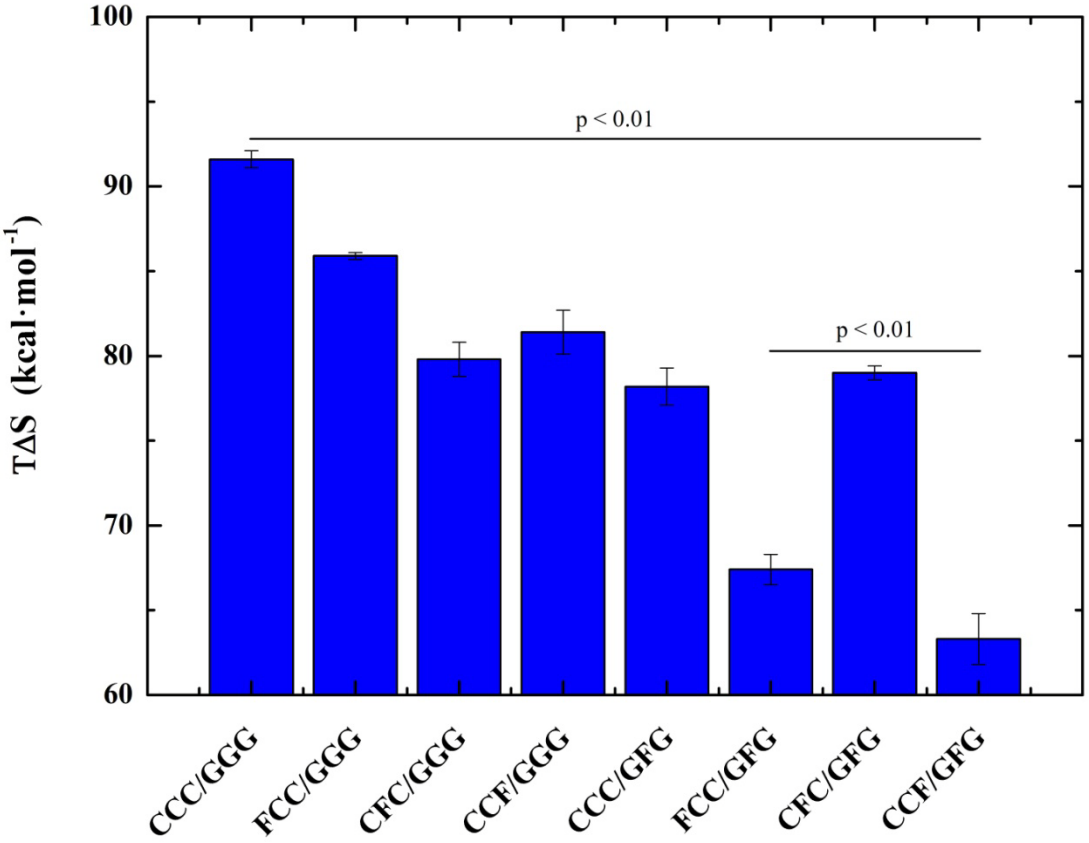
The single and bistrand abasic site duplexes exhibit statistically significant differences in thermal stability ($p < 0.0001$) relative to the undamaged parent tridecamer. The differential thermal stability of CFC/GFG and CCF/GFG are statistically significant ($p < 0.001$) when compared to the corresponding single AP-site reference duplexes CFC/GGG and CCF/GGG The bistrand CFC/GFG and CCF/GFG duplexes are thermally destabilized with CCF/GFG > CFC/GFG ($p < 0.001$). Thermal destabilization of FCC/GFG does *not* differ significantly ($p > 0.5$) relative to the single AP-site CCC/GFG and FCC/GGG duplexes.

FIGURE S2. Dissociation Enthalpies of Canonical, Single, and Bistrand AP-Site Duplexes.



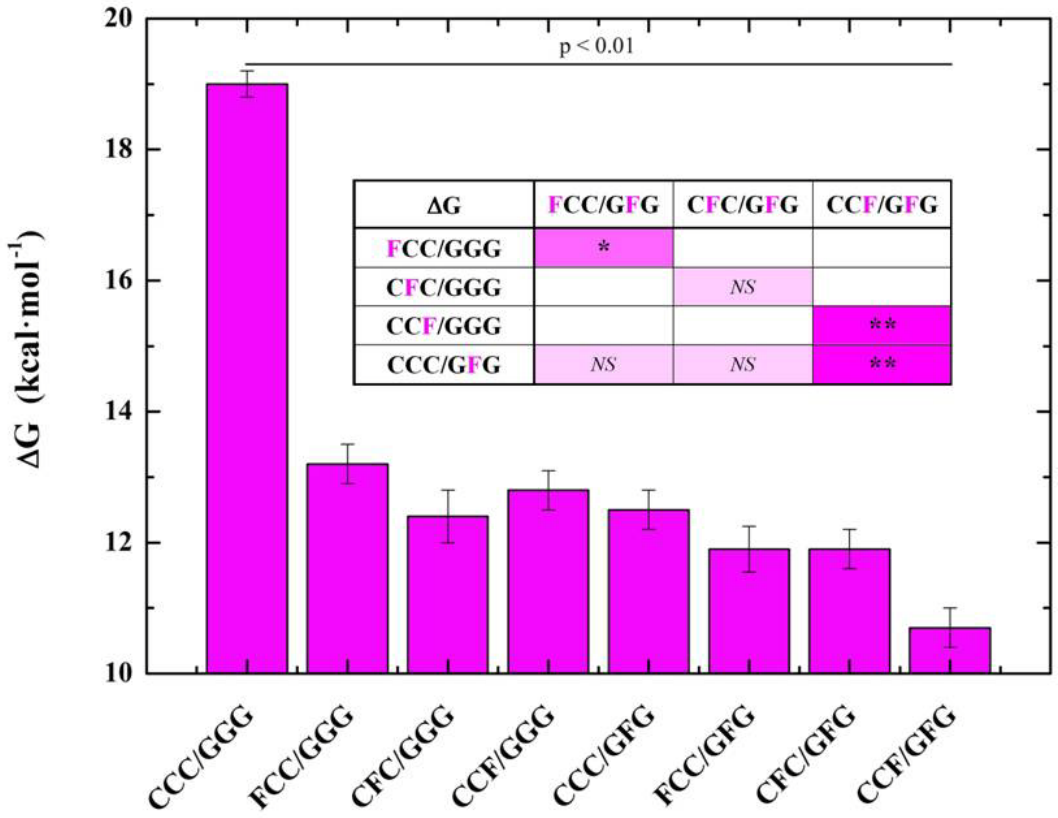
The single and bistrand abasic site duplexes exhibit statistically significant differences in enthalpic stability ($p < 0.001$) relative to the undamaged parent tridecamer. The differential enthalpic stability of FCC/GFG and CCF/GFG are statistically significant ($p < 0.001$) when compared to the corresponding single AP-site reference duplexes FCC/GGG and CCF/GGG. Enthalpic destabilization of the bistrand FCC/GFG and CCF/GFG duplexes are comparable ($p > 0.5$). The dissociation enthalpy of CFC/GFG does *not* differ significantly ($p > 0.5$) relative to the single AP-site CCC/GFG and CFC/GGG duplexes.

FIGURE S3. Dissociation Entropies of Canonical, Single, and Bistrand AP-Site Duplexes.



The single and bistrand abasic site duplexes exhibit statistically significant differences in entropic stability ($p < 0.01$) relative to the undamaged parent tridecamer. The differential entropic stability of FCC/GFG and CCF/GFG are statistically significant ($p < 0.001$) when compared to the corresponding single AP-site reference duplexes FCC/GGG and CCF/GGG. Entropic stabilization of the bistrand FCC/GFG and CCF/GFG duplexes are comparable ($p > 0.5$). The dissociation entropy of CFC/GFG is *not* significantly different ($p > 0.5$) relative to the single AP-site CCC/GFG and CFC/GGG duplexes.

FIGURE S4. Dissociation Free Energies of Canonical, Single, and Bistrand AP-Site Duplexes.



The single and bistrand abasic duplexes exhibit statistically significant differences in thermodynamic stability ($p < 0.01$) relative to the undamaged parent tridecamer. INSET: Statistical significance of dissociation free energy (ΔG) differences employing ANOVA and Tukey tests. Meaningful comparisons are designated as ** and * signifying that the corresponding means differ at a level of $p < 0.05$ and $p < 0.1$, respectively. An *NS* designation indicates that the values differ somewhat albeit not significantly.