Electronic Supplementary Information for

"Temperature-induced twisting and swelling of double-stranded DNA"

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This PDF file includes the parameters under various temperatures:

Figure S1

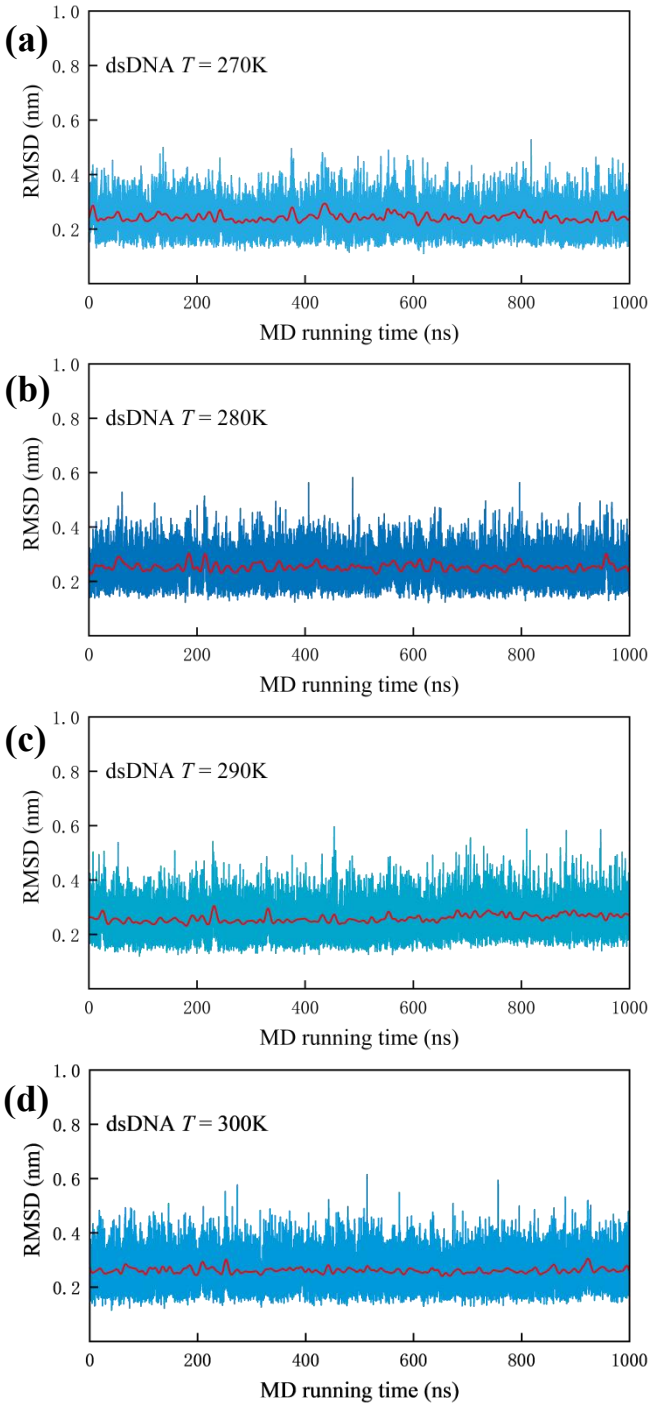
(a)
dsDNA T = 270K
(b)
dsDNA T = 280K
(c)
dsDNA T = 290K
(d)
dsDNA T = 300K
RMSD (nm)
1.0
0.8
0.6
0.4
0.2
0
200
400
600
800
1000
MD running time (ns)

Figure S1

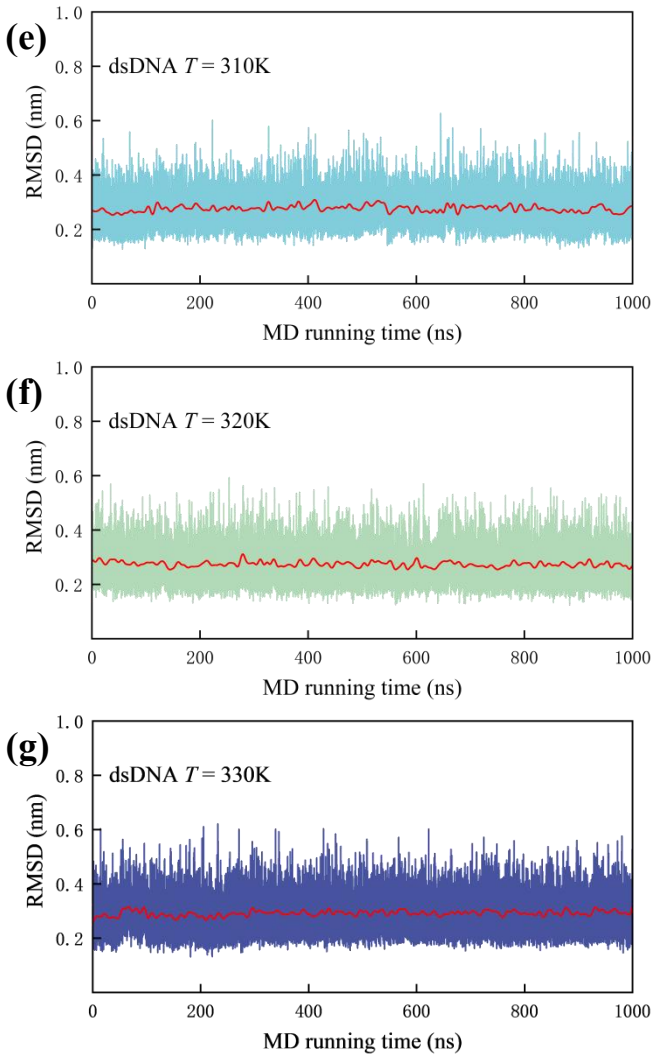

Fig. S1

The root mean square deviation (RMSD) curve of 14 base fragments in dsDNA center at various temperatures, where the red line represents the average of the relevant parameters every 5 ns .The The temperature T varies from 270 K to 330 K, with a step of 10 K.

Figure S2

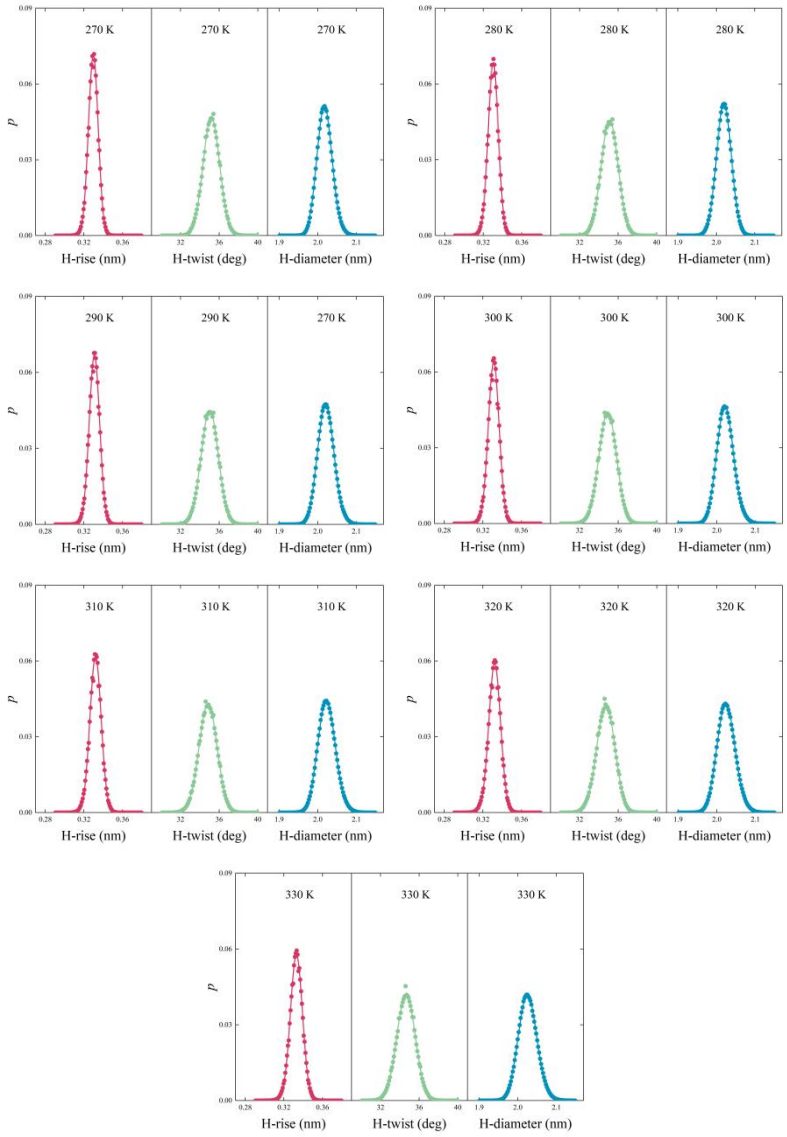

Fig. S2

The Gaussian distributions for H-rise, H-twist and H-diameter under various temperatures *T*, where the temperature varies from 270 K to 330 K, with a step of 10 K.

Figure S3

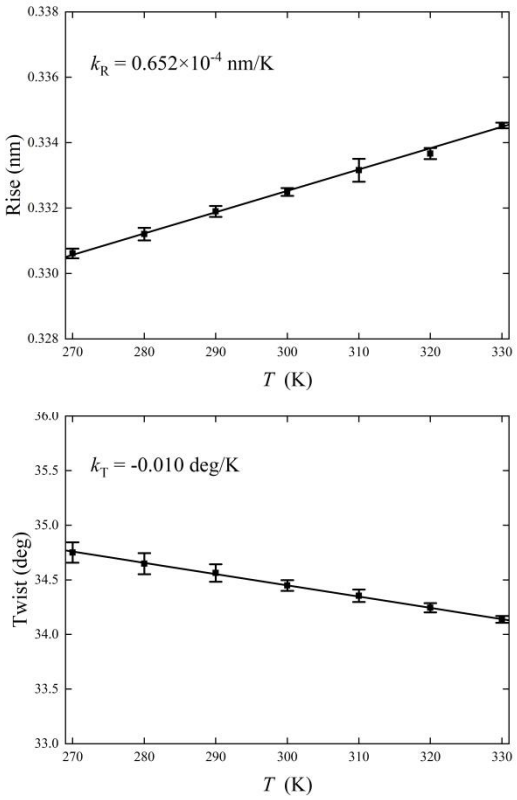

Fig. S3

The temperature dependent Rise and Twist.The temperature *T* varies from 270 K to 330 K , with a step of 10 K. The data points are mean values and standard deviations for the five measurement samples, while the solid lines are fitting results.

Figure S4

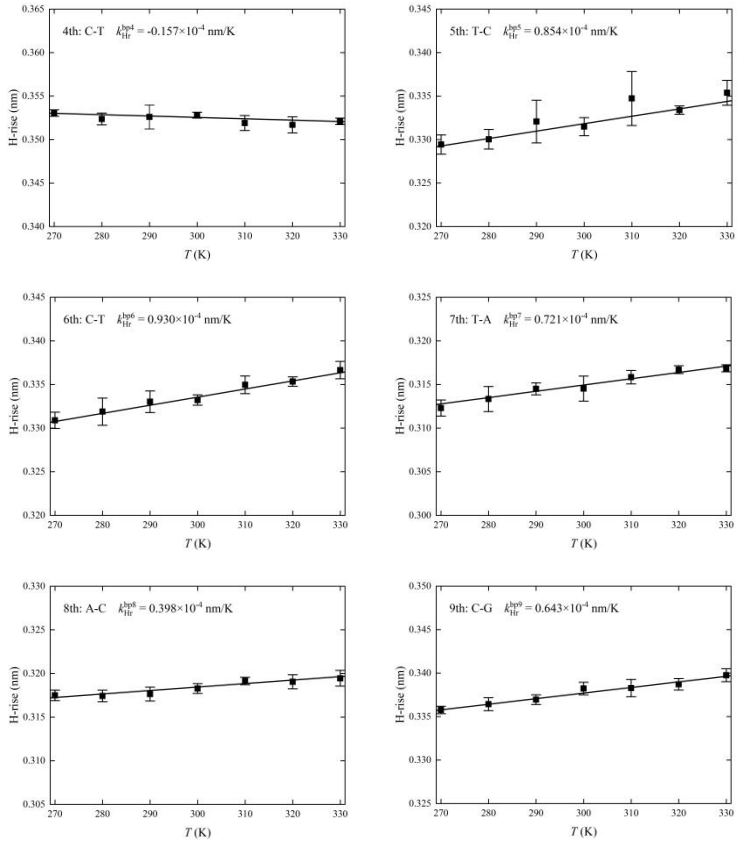
4th: C-T k_{Hr}^{bp4} = -0.157×10^{-4} nm/K
5th: T-C k_{Hr}^{bp5} = 0.854×10^{-4} nm/K
6th: C-T k_{Hr}^{bp6} = 0.930×10^{-4} nm/K
7th: T-A k_{Hr}^{bp7} = 0.721×10^{-4} nm/K
8th: A-C k_{Hr}^{bp8} = 0.398×10^{-4} nm/K
9th: C-G k_{Hr}^{bp9} = 0.643×10^{-4} nm/K
H-rise (nm)
T (K)

Figure S4

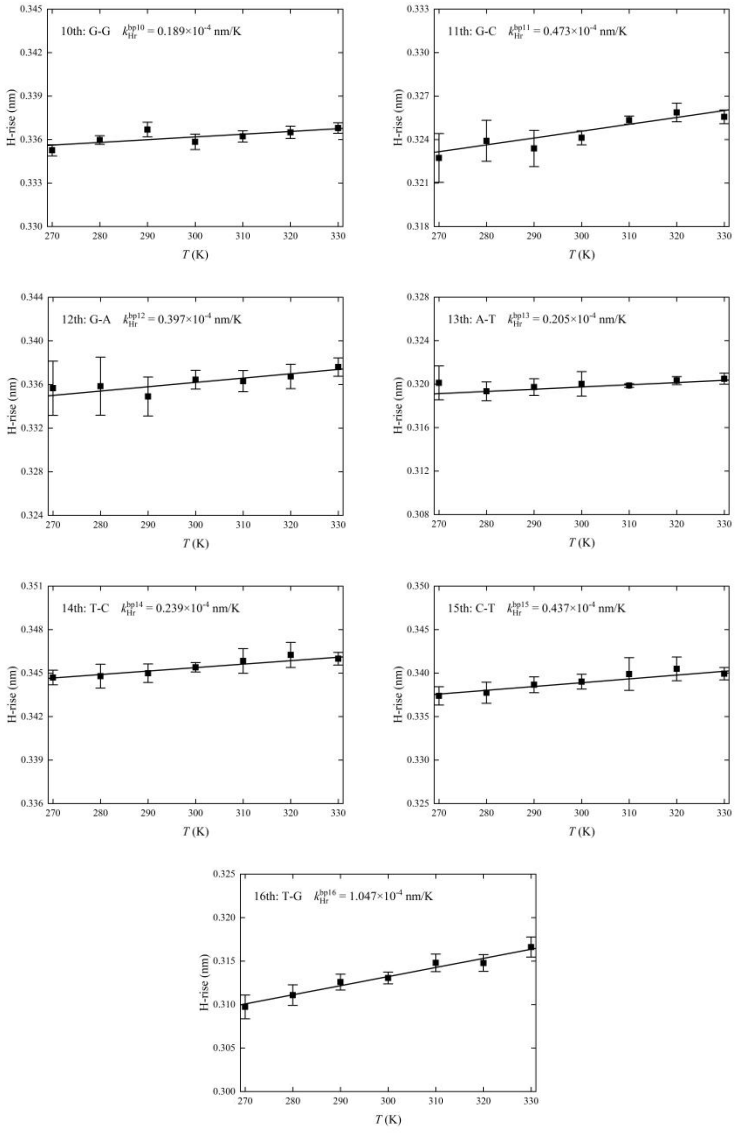
10th: G-G $k_{Hr}^{bp10} = 0.189\times10^{-4}$ nm/K
11th: G-C $k_{Hr}^{bp11} = 0.473\times10^{-4}$ nm/K
12th: G-A $k_{Hr}^{bp12} = 0.397\times10^{-4}$ nm/K
13th: A-T $k_{Hr}^{bp13} = 0.205\times10^{-4}$ nm/K
14th: T-C $k_{Hr}^{bp14} = 0.239\times10^{-4}$ nm/K
15th: C-T $k_{Hr}^{bp15} = 0.437\times10^{-4}$ nm/K
16th: T-G $k_{Hr}^{bp16} = 1.047\times10^{-4}$ nm/K
H-rise (nm)
T (K)

Figure S4

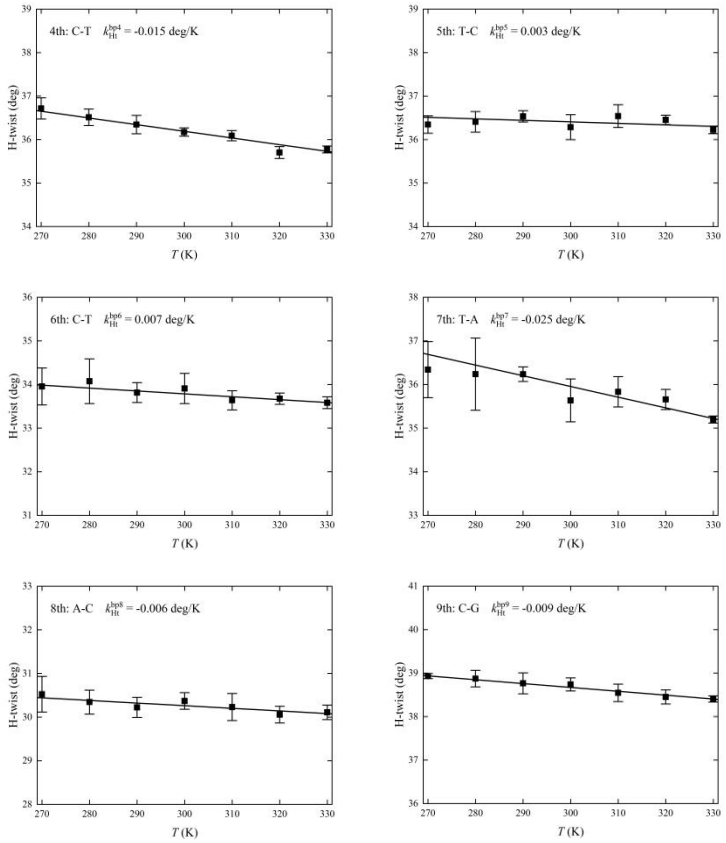
4th: C-T k_{Ht}^{bp4} = -0.015 deg/K
5th: T-C k_{Ht}^{bp5} = 0.003 deg/K
6th: C-T k_{Ht}^{bp6} = 0.007 deg/K
7th: T-A k_{Ht}^{bp7} = -0.025 deg/K
8th: A-C k_{Ht}^{bp8} = -0.006 deg/K
9th: C-G k_{Ht}^{bp9} = -0.009 deg/K
H-twist (deg)
T (K)

Figure S4

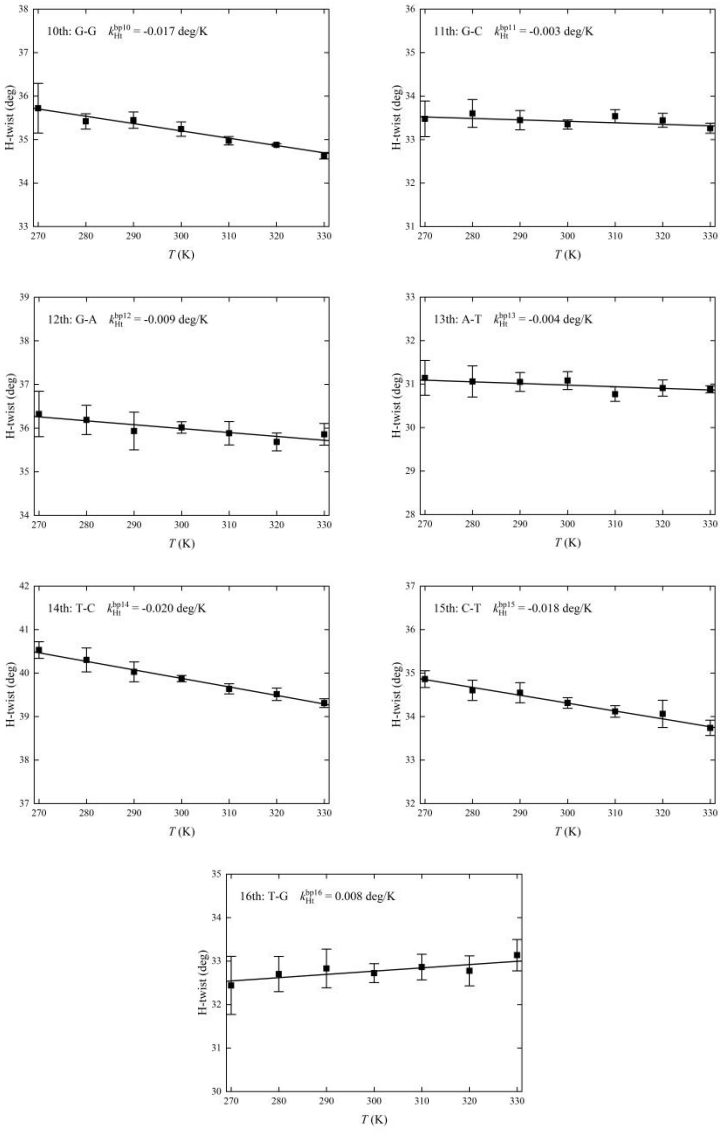
10th: G-G k_{Ht}^{bp10} = -0.017 deg/K
11th: G-C k_{Ht}^{bp11} = -0.003 deg/K
12th: G-A k_{Ht}^{bp12} = -0.009 deg/K
13th: A-T k_{Ht}^{bp13} = -0.004 deg/K
14th: T-C k_{Ht}^{bp14} = -0.020 deg/K
15th: C-T k_{Ht}^{bp15} = -0.018 deg/K
16th: T-G k_{Ht}^{bp16} = 0.008 deg/K
H-twist (deg)
T (K)

Figure S4

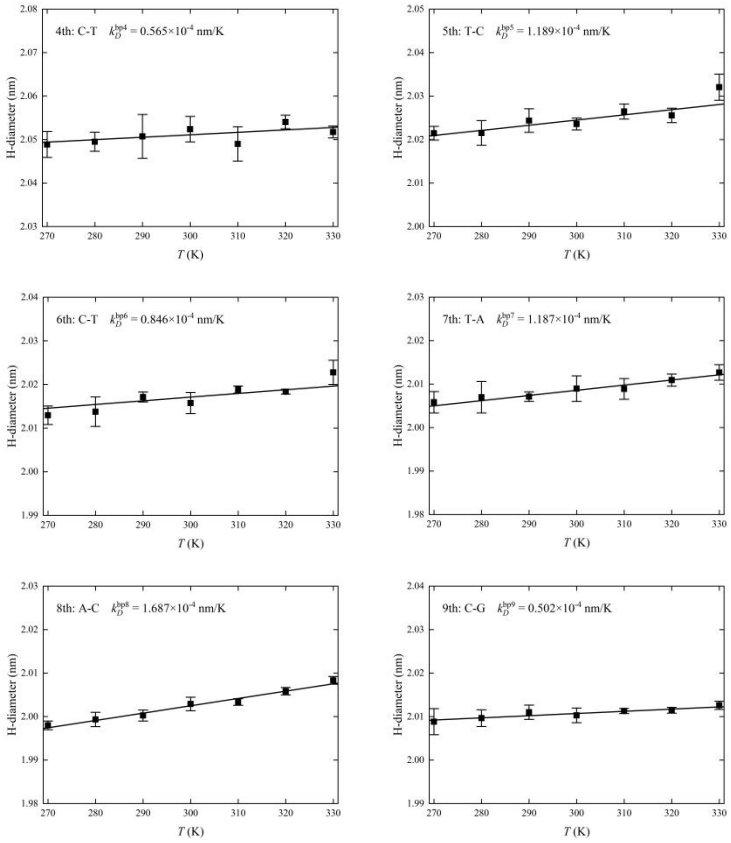
4th: C-T k_D^{bp4} = 0.565×10^{-4} nm/K
5th: T-C k_D^{bp5} = 1.189×10^{-4} nm/K
6th: C-T k_D^{bp6} = 0.846×10^{-4} nm/K
7th: T-A k_D^{bp7} = 1.187×10^{-4} nm/K
8th: A-C k_D^{bp8} = 1.687×10^{-4} nm/K
9th: C-G k_D^{bp9} = 0.502×10^{-4} nm/K
H-diameter (nm)
T (K)

Figure S4

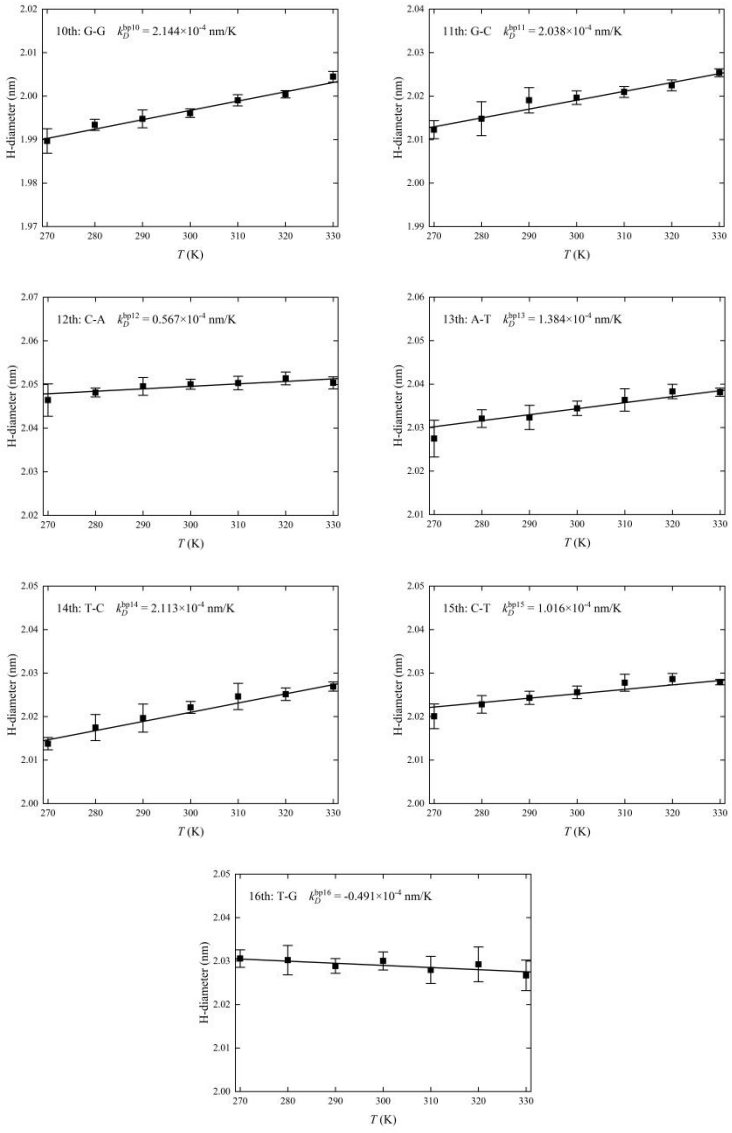

Fig. S4

The temperature dependent H-rise, H-twist and H-diameter for individual bp at various temperatures *T*. The temperature *T* varies from 270 K to 330 K , with a step of 10 K. The data points are mean values and standard deviations for the five measurement samples, while the solid lines are fitting results.

Figure S5

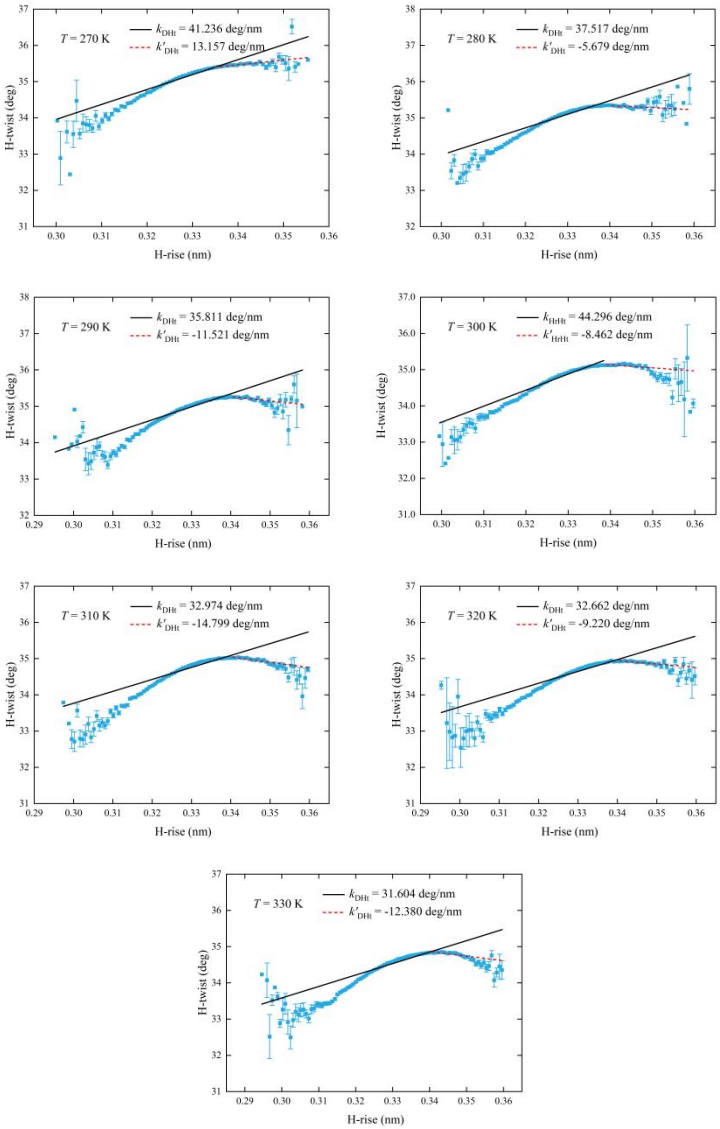
T = 270 K
k_DHt = 41.236 deg/nm
k'_DHt = 13.157 deg/nm
T = 280 K
k_DHt = 37.517 deg/nm
k'_DHt = -5.679 deg/nm
T = 290 K
k_DHt = 35.811 deg/nm
k'_DHt = -11.521 deg/nm
T = 300 K
k_HrHt = 44.296 deg/nm
k'_HrHt = -8.462 deg/nm
T = 310 K
k_DHt = 32.974 deg/nm
k'_DHt = -14.799 deg/nm
T = 320 K
k_DHt = 32.662 deg/nm
k'_DHt = -9.220 deg/nm
T = 330 K
k_DHt = 31.604 deg/nm
k'_DHt = -12.380 deg/nm
H-twist (deg)
H-rise (nm)

Figure S5

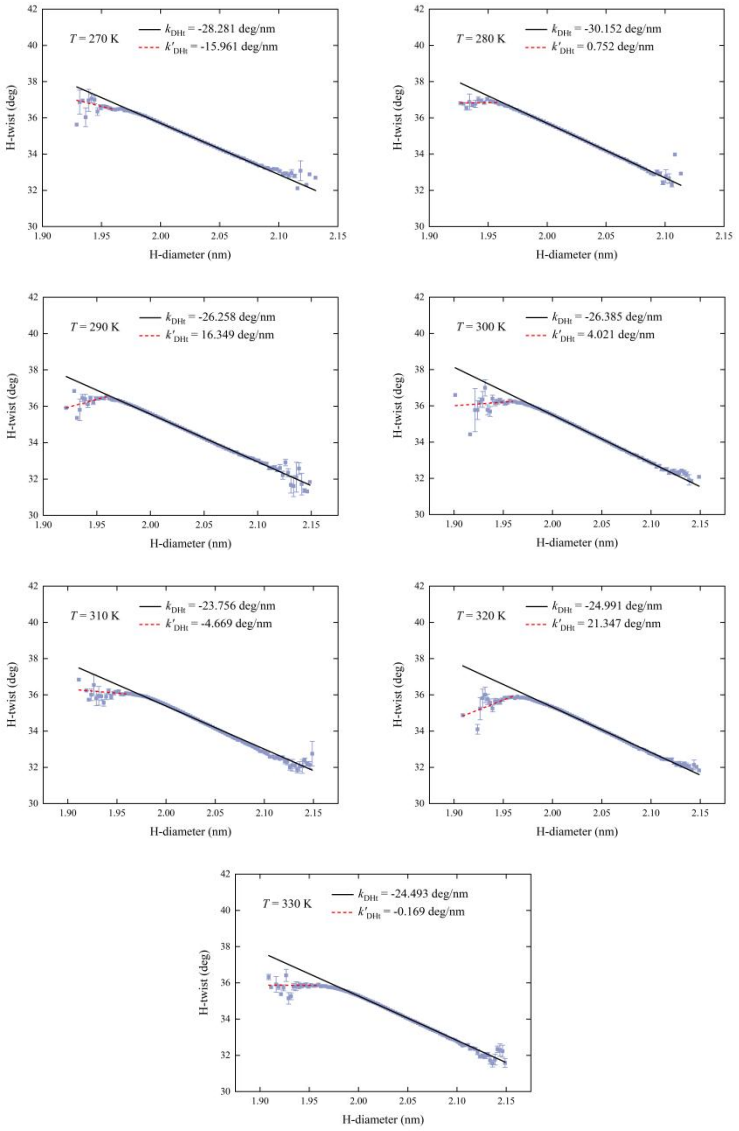
T = 270 K
k_{DHt} = -28.281 deg/nm
k'_{DHt} = -15.961 deg/nm
T = 280 K
k_{DHt} = -30.152 deg/nm
k'_{DHt} = 0.752 deg/nm
T = 290 K
k_{DHt} = -26.258 deg/nm
k'_{DHt} = 16.349 deg/nm
T = 300 K
k_{DHt} = -26.385 deg/nm
k'_{DHt} = 4.021 deg/nm
T = 310 K
k_{DHt} = -23.756 deg/nm
k'_{DHt} = -4.669 deg/nm
T = 320 K
k_{DHt} = -24.991 deg/nm
k'_{DHt} = 21.347 deg/nm
T = 330 K
k_{DHt} = -24.493 deg/nm
k'_{DHt} = -0.169 deg/nm
H-twist (deg)
H-diameter (nm)

Figure S5

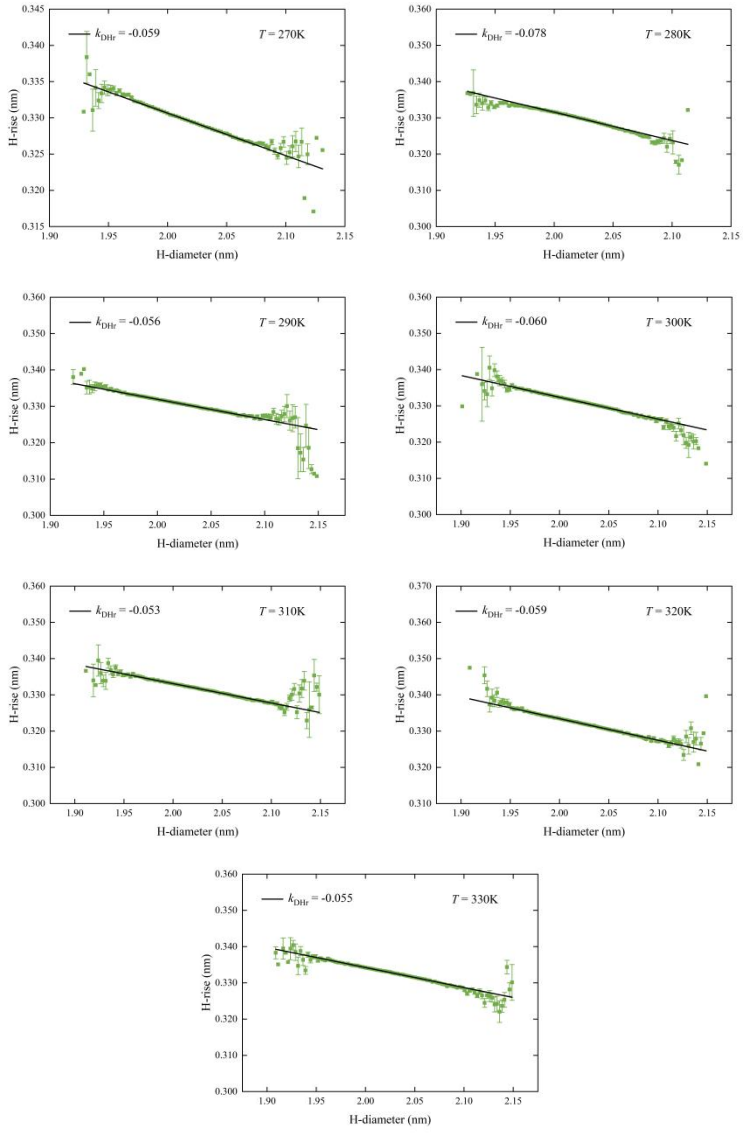

Fig. S5

The coupling between H-twist and H-rise, H-twist and H-diameter, H-rise and H-diameter at various temperatures *T*. The temperature *T* varies from 270 K to 330 K , with a step of 10 K. The data points are mean values and standard deviations, while the solid lines are fitting results.

Figure S6

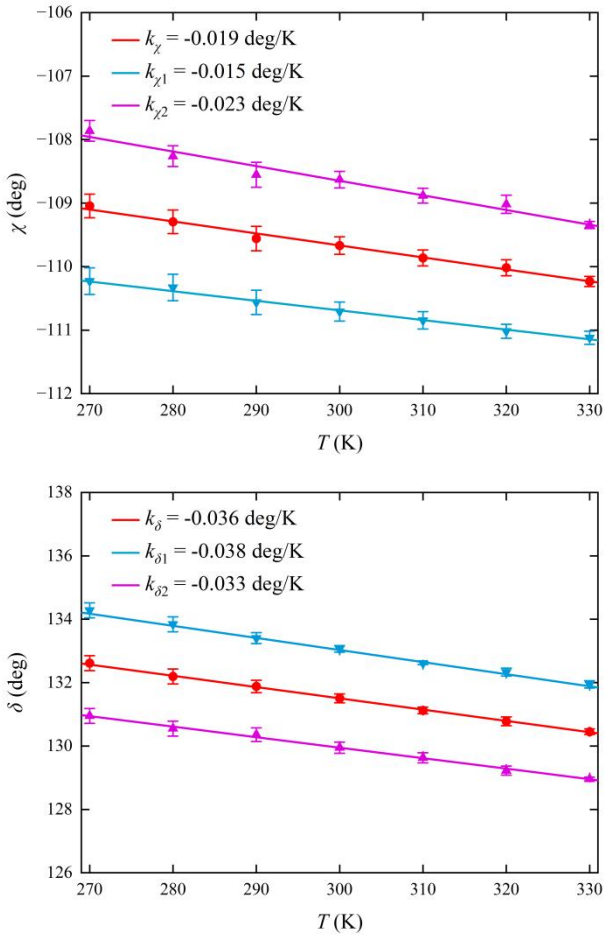

Fig. S6

The two dihedral angles χ and δ at various temperatures *T*. The temperature *T* varies from 270 K to 330 K , with a step of 10 K. The data points are mean values and standard deviations for the five measurement samples, while the solid lines are fitting results.

Figure S7

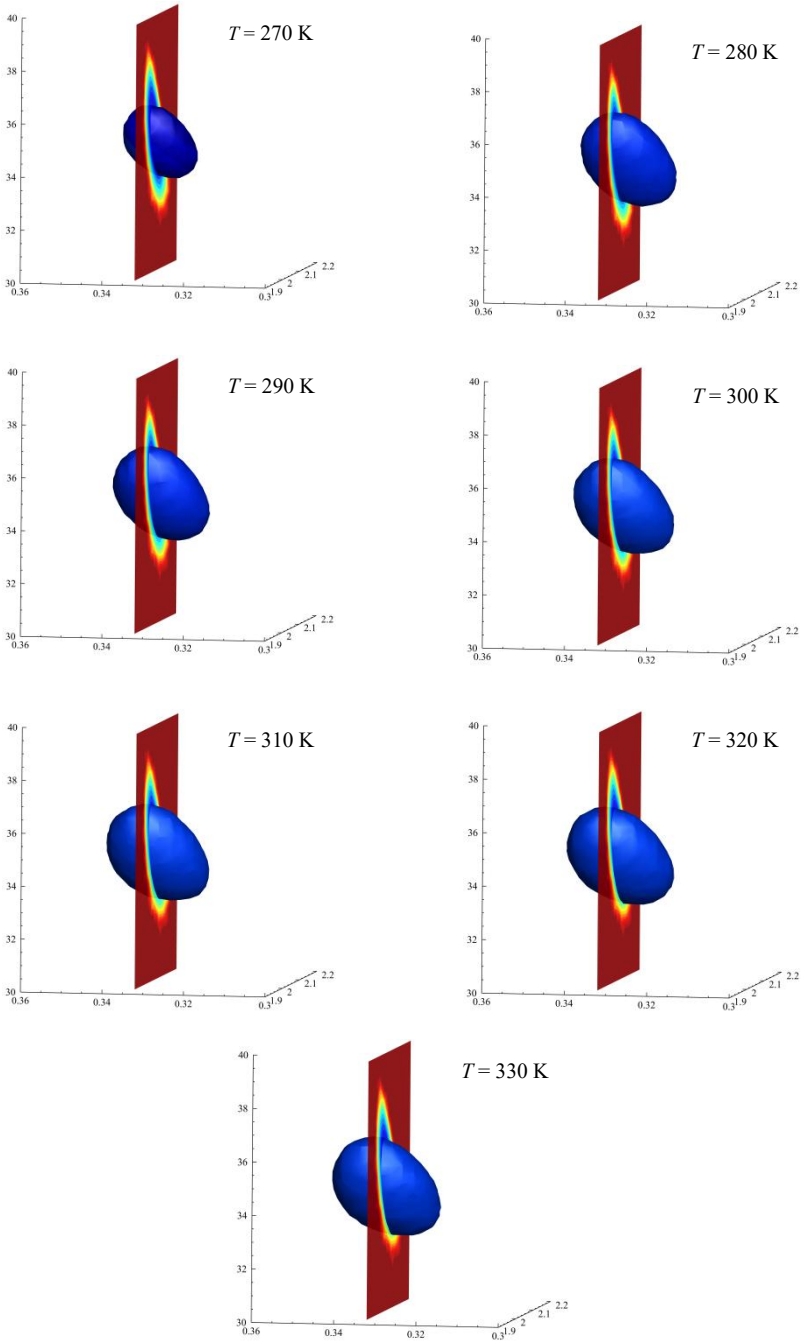

Fig. S7

The three-dimensional PMF with respect to H-rise, H-diameter, and H-twist at various temperature *T*. The temperature *T* varies from 270 K to 330 K , with a step of 10 K.

Figure S8

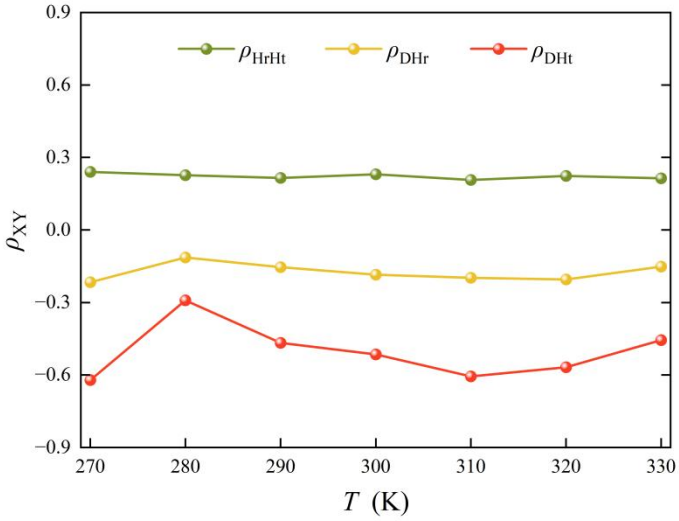

Fig. S8

The Pearson correlation coefficients ρ_{XY} among the H-rise Hr, H-twist Ht, and H-diameter D at various temperature T.The temperature T varies from 270 K to 330 K , with a step of 10 K.

Figure S9

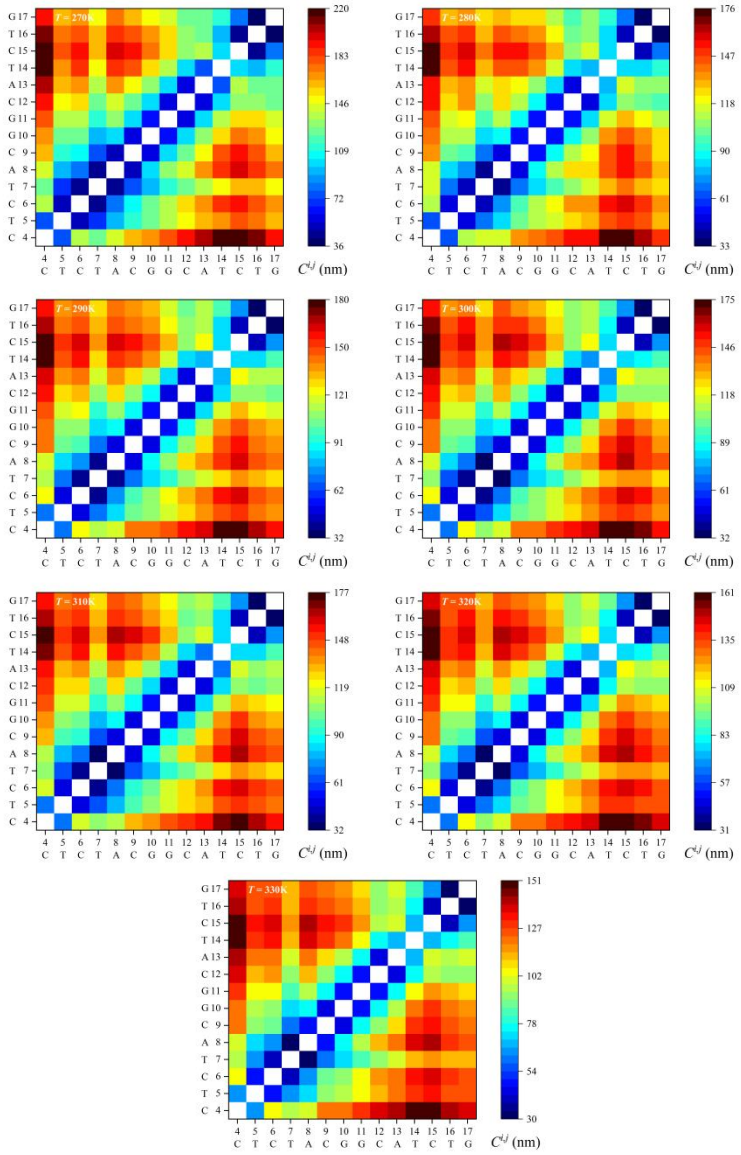

Fig. S9

The two-dimensional distributions of twist stiffness C^{ij} about the bp step at various temperature T. The temperature T varies from 270 K to 330 K , with a step of 10 K.

Figure S10

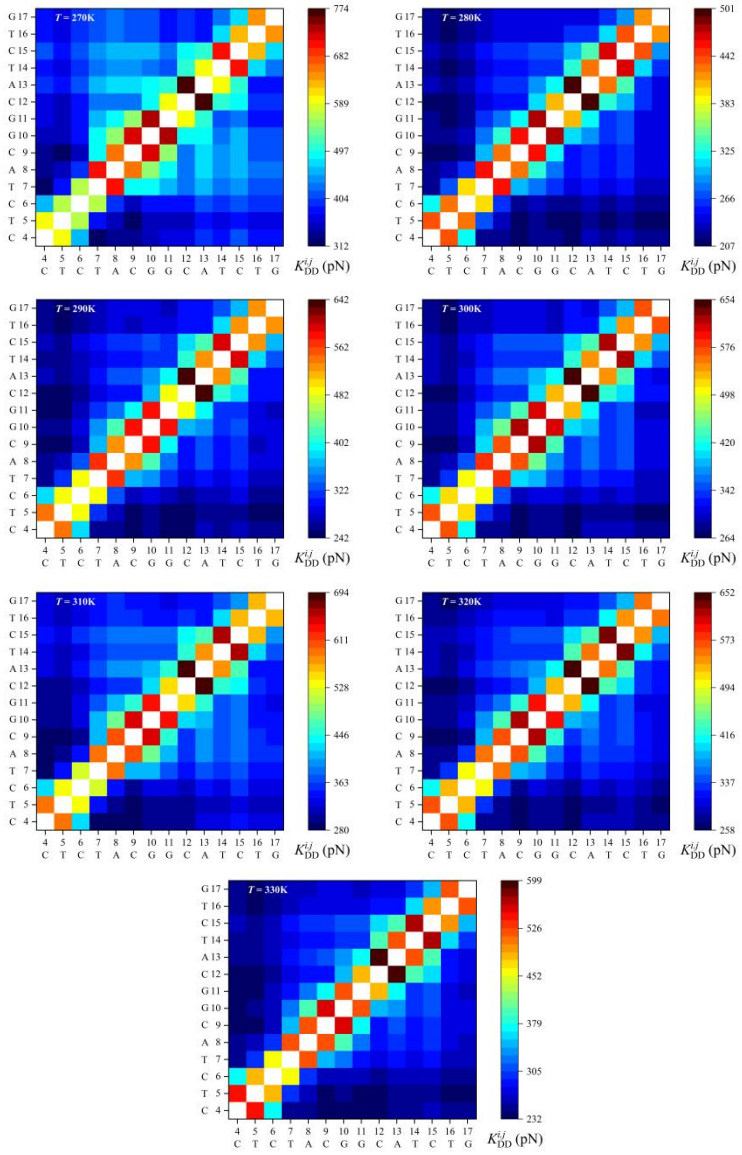

Fig. S10

The two-dimensional distributions of H-diameter stiffness K_{DD}^{ij} about the bp step at various temperature T. The temperature T varies from 270 K to 330 K , with a step of 10 K.

Figure S11

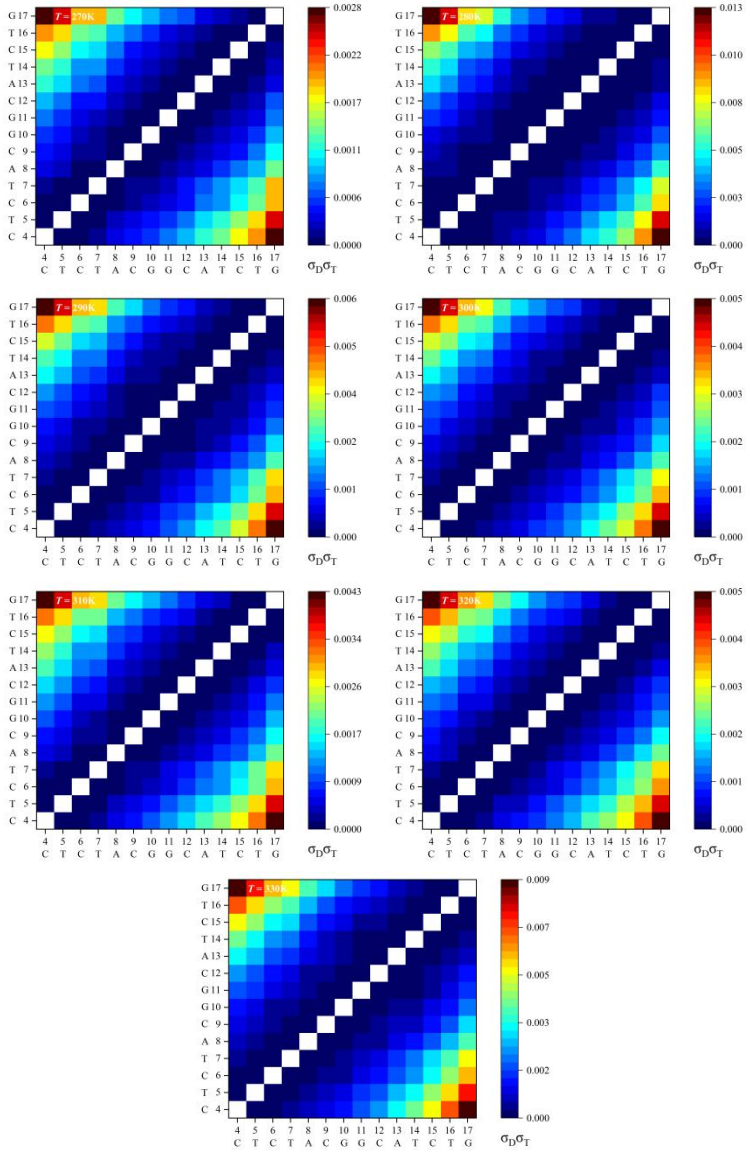

Fig. S11

The two-dimensional distributions of $\sigma_{\mathrm{T}}^{ij}\sigma_{\mathrm{T}}^{ij}$ about the bp step at various temperature T. The temperature T varies from 270 K to 330 K , with a step of 10 K.

Figure S12

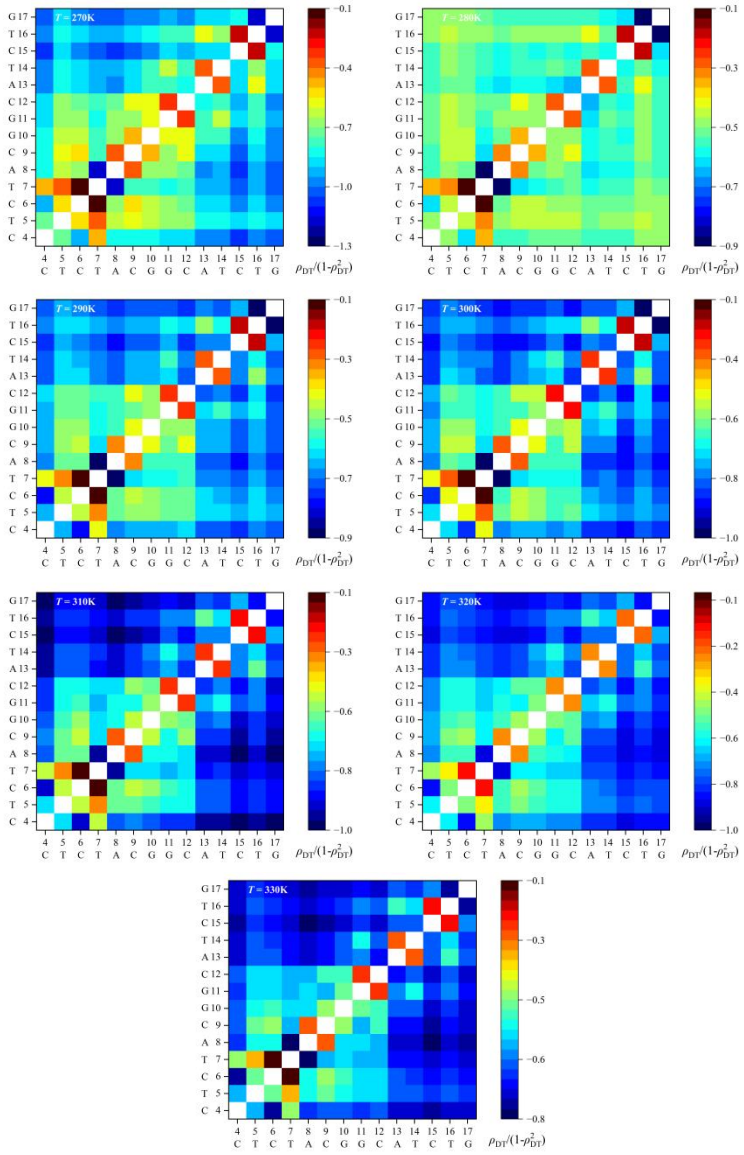

Fig. S12

The two-dimensional distributions of $\rho_{\mathrm{DT}}^{ij}/\left(1-\rho_{\mathrm{DT}}^{ij}\rho_{\mathrm{DT}}^{ij}\right)$ about the bp step at various temperature T.The temperature T varies from 270 K to 330 K , with a step of 10 K.

Figure S13

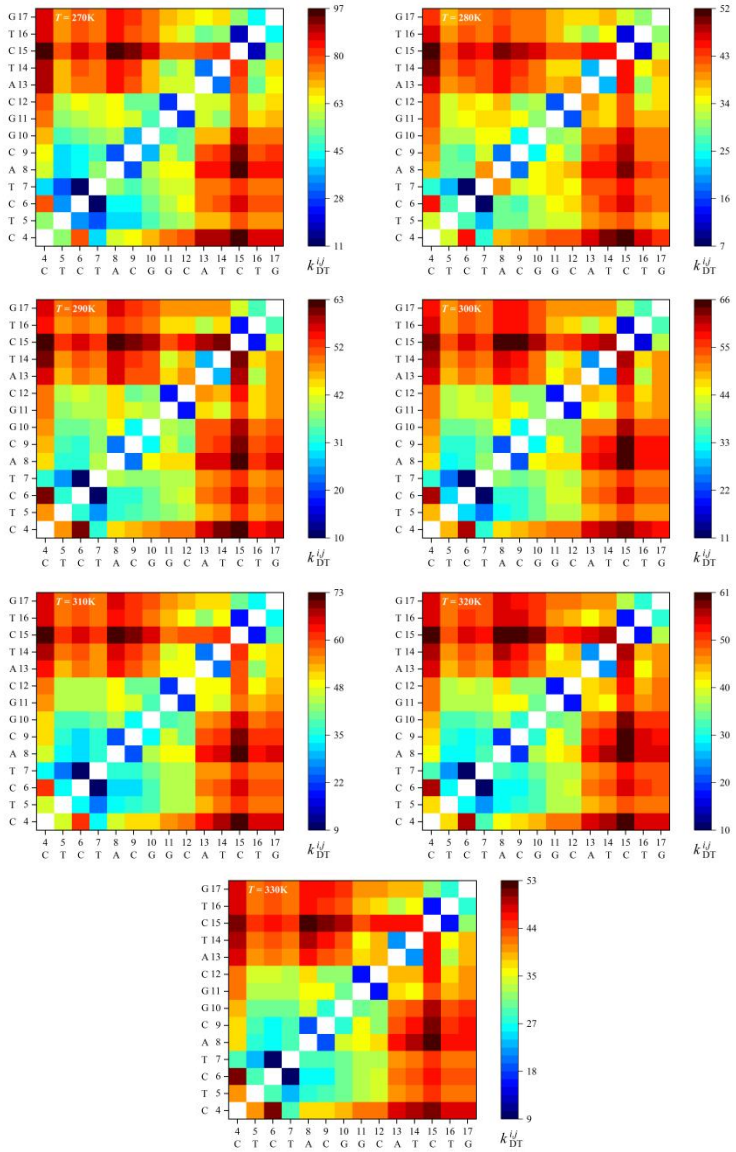

Fig. S13

The two-dimensional distributions of H-twist and H-diameter coupling k_{DT}^{ij} about the bp step at various temperature *T*.The temperature *T* varies from 270 K to 330 K , with a step of 10 K.