

SUPPORTING INFORMATION

Homologous BHLH transcription factors induce distinct deformations of torsionally-stressed DNA: a potential transcription regulation mechanism

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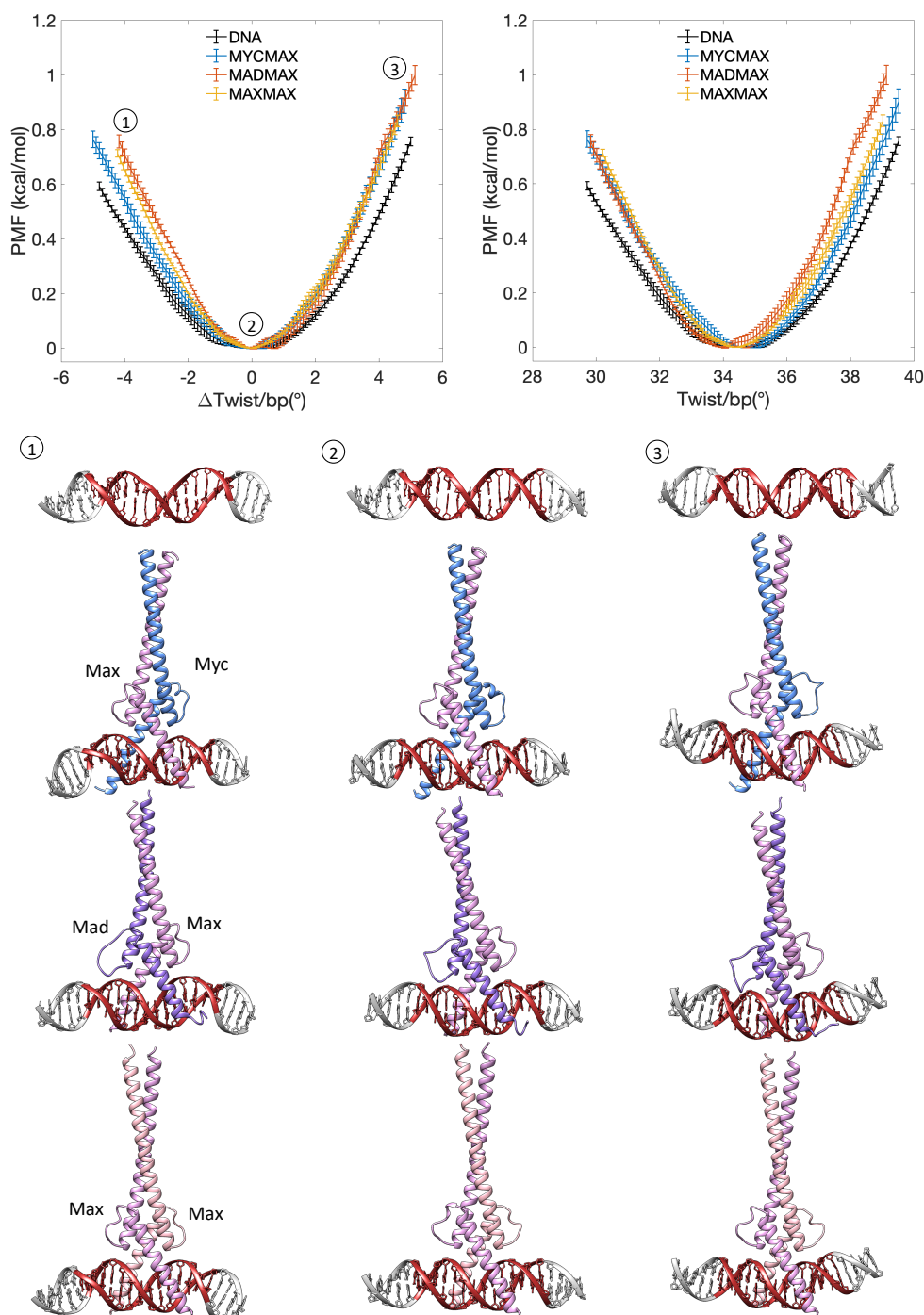


Figure S1: PMF profiles of DNA twisting transitions for unbound DNA and MycMax- (blue), MadMax- (orange) and MaxMax- (yellow) bound DNA. Standard deviations of the 500 ns windows are highlighted as error bars. DNA deformations for unbound DNA, MycMax-, MadMax- and MaxMax-bound DNA are shown for (1) underwound regime ($-4.5^\circ/\text{bp}$), (2) torsionally relaxed regime and (3) overwound regime ($+4.5^\circ/\text{bp}$). The restrained DNA region (GTAGCACGTGCTAC) is highlighted with red colour.

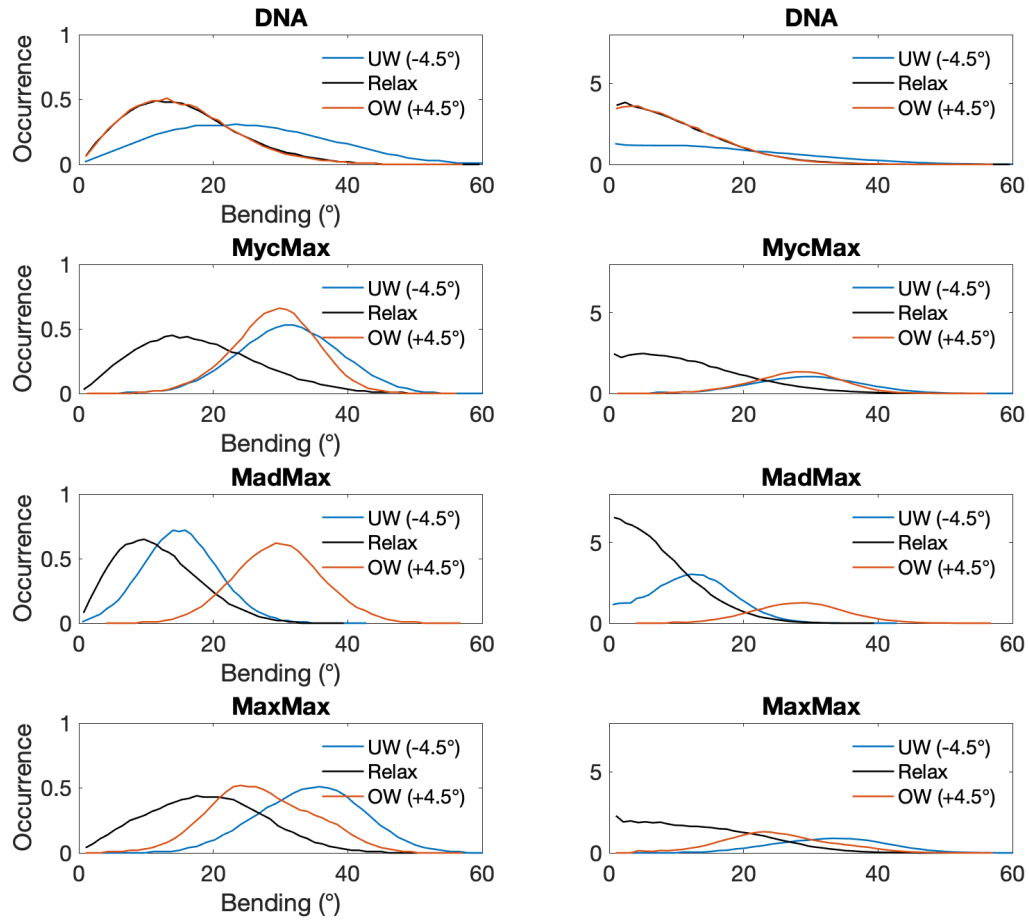


Figure S2: Bending distributions of the restrained region (GTAGCACGTGCTAC) for unbound DNA, MycMax-, MadMax- and MaxMax-bound DNA. For the right-hand panels, the histograms have been divided by $\sin(\theta)$, where θ corresponds to the bending angle at the middle of each histogram bin, to compensate for the increasing area of the spherical ring segment sampled as the bending angle increases.

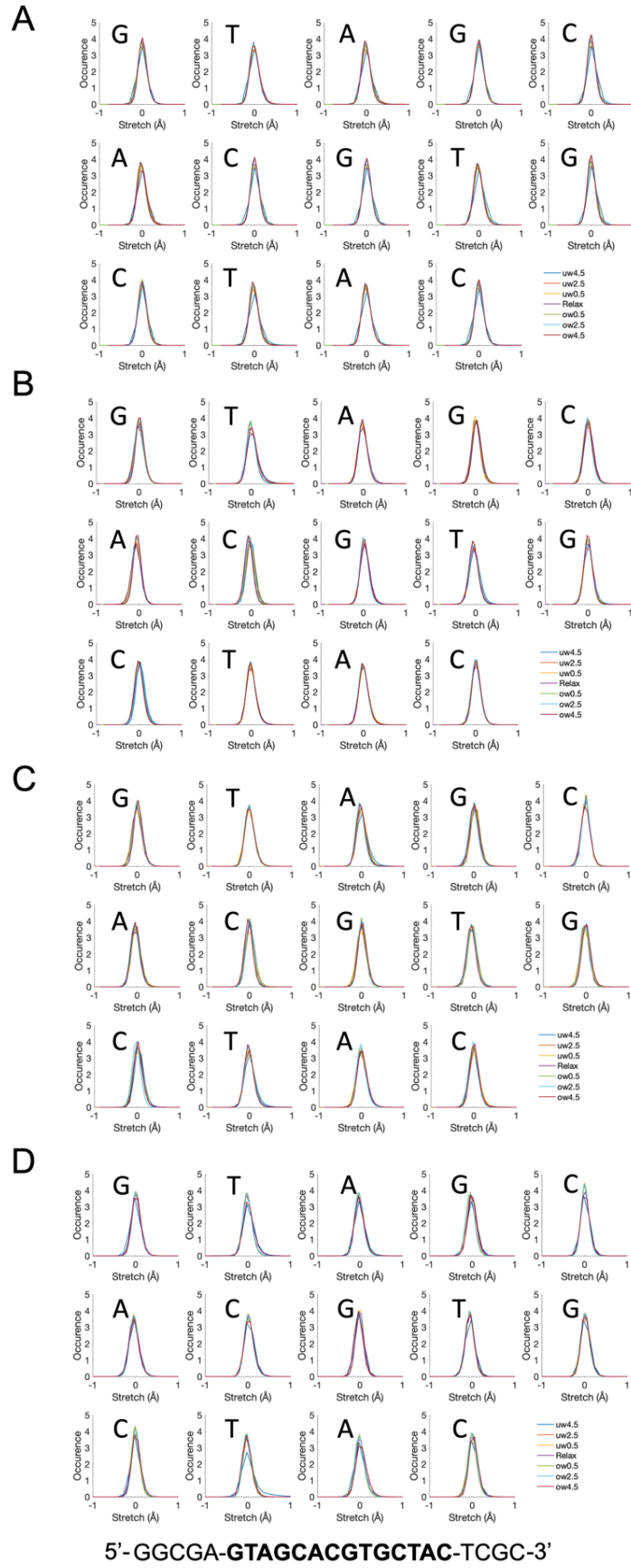


Figure S3: Stretch distributions for b.p. of the restrained region for different torsional regimes. **A.** DNA, **B.** MycMax-DNA, **C.** MadMax-DNA, **D.** MaxMax-DNA.

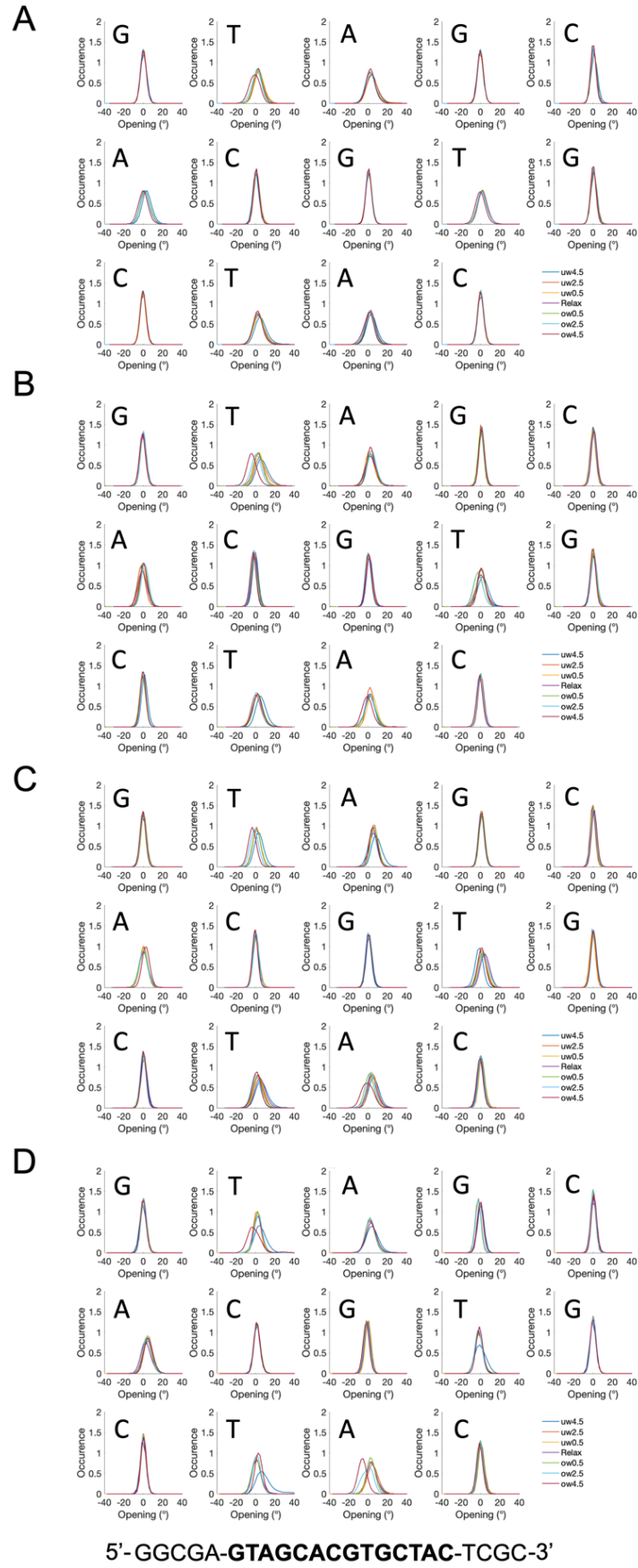


Figure S4: Opening distributions for b.p. of the restrained region for different torsional regimes. **A.** DNA, **B.** MycMax-DNA, **C.** MadMax-DNA, **D.** MaxMax-DNA.

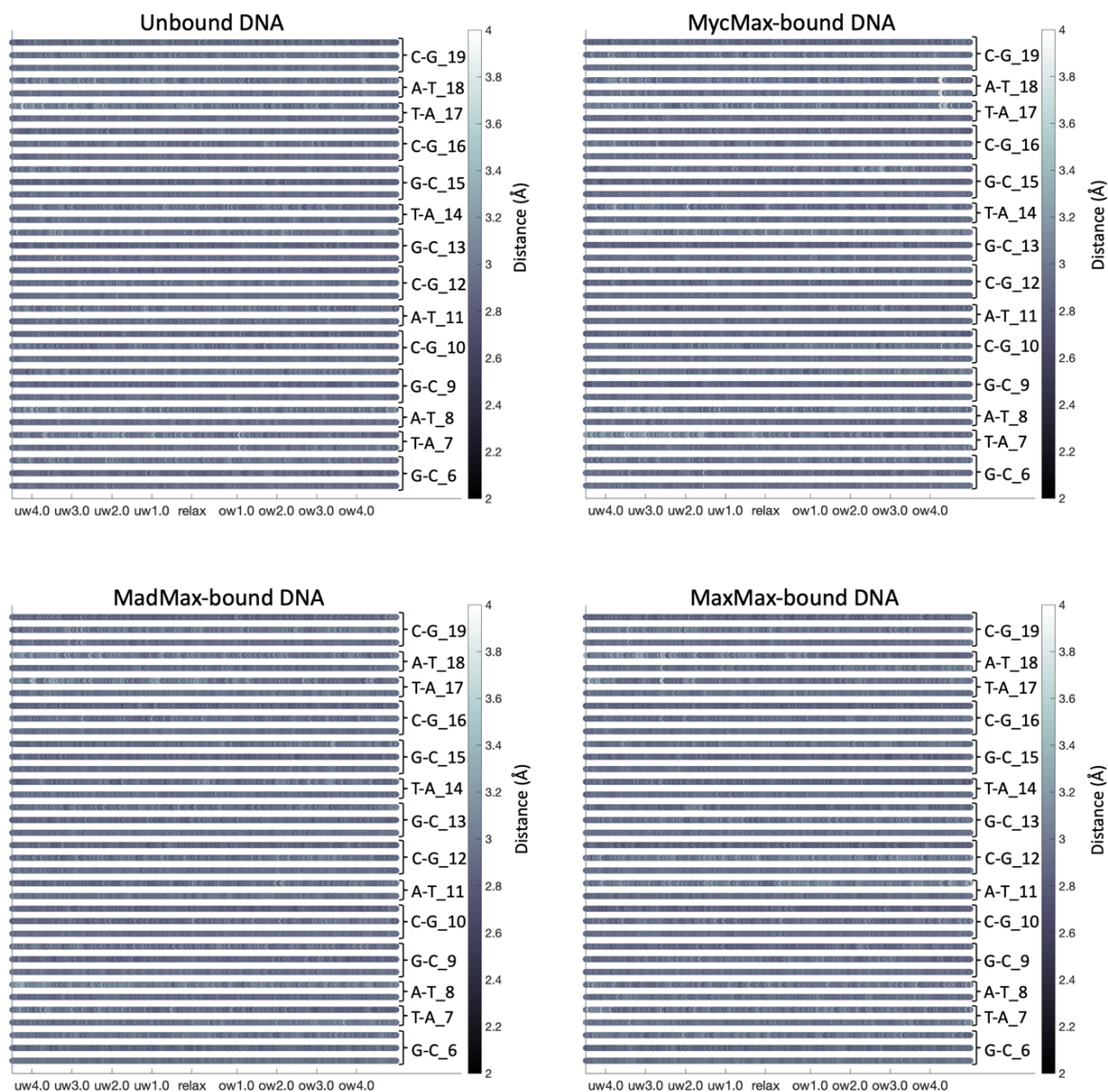


Figure S5: Evolution of hydrogen bond distances between heavy atoms of the b.ps within the restraint region (GTAGCACGTGCTAC) along the different torsional regimes for unbound DNA and MycMax-, MadMax and MaxMax-bound DNA. Distances are denoted with a colorbar.

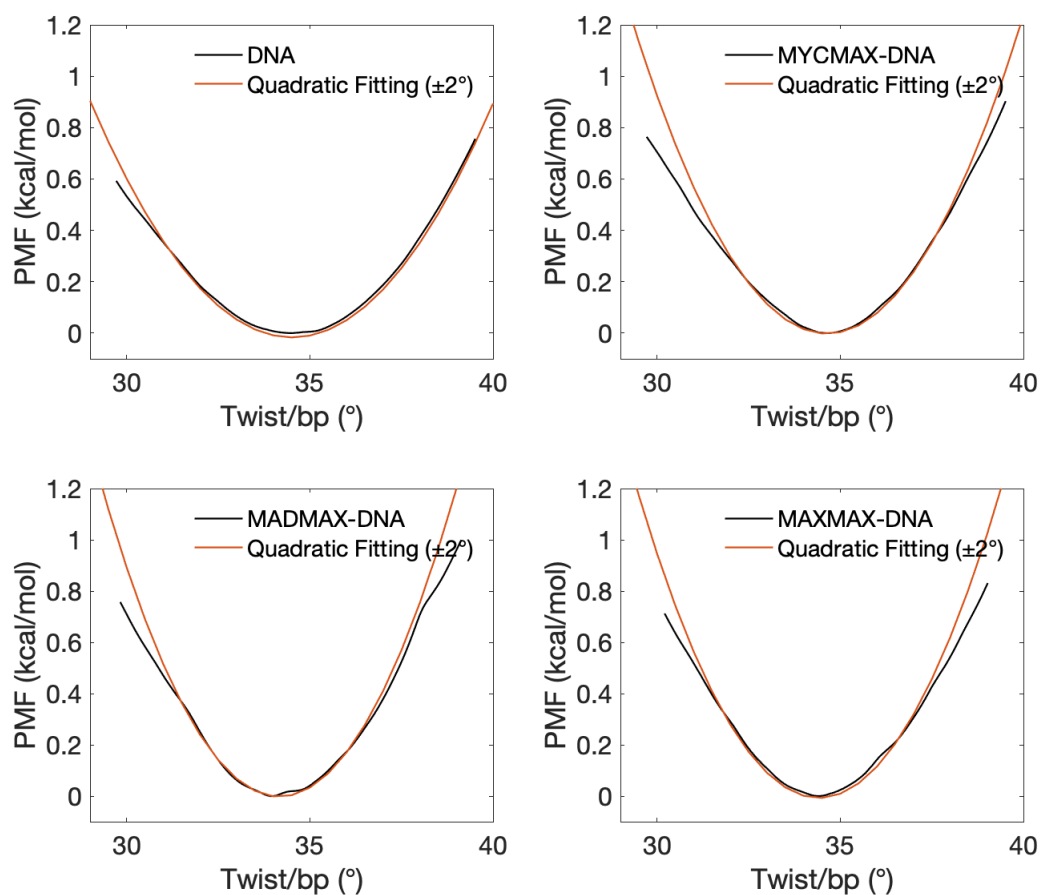


Figure S6: Quadratic regression ($\pm 2^\circ$) of PMF profiles of unbound DNA and MycMax-, MadMax- and MaxMax bound DNA is shown in orange lines.

Table S1: Calculated average relaxed twists, torsional constants ‘K’, torsional moduli ‘C’, and torsional persistence lengths ‘P’ for unbound DNA BHLH bound DNA.

	DNA	MycMax-DNA	MadMax-DNA	MaxMax-DNA
Relaxed twist (°)	34.5	34.7	34.0	34.4
K (kcal/mol*deg ²)	0.059	0.081	0.089	0.087
C (nm)	111	153	168	163

Supplementary figures S7-S12 are also available as separate supplementary figures if a reader would like to investigate them closer.

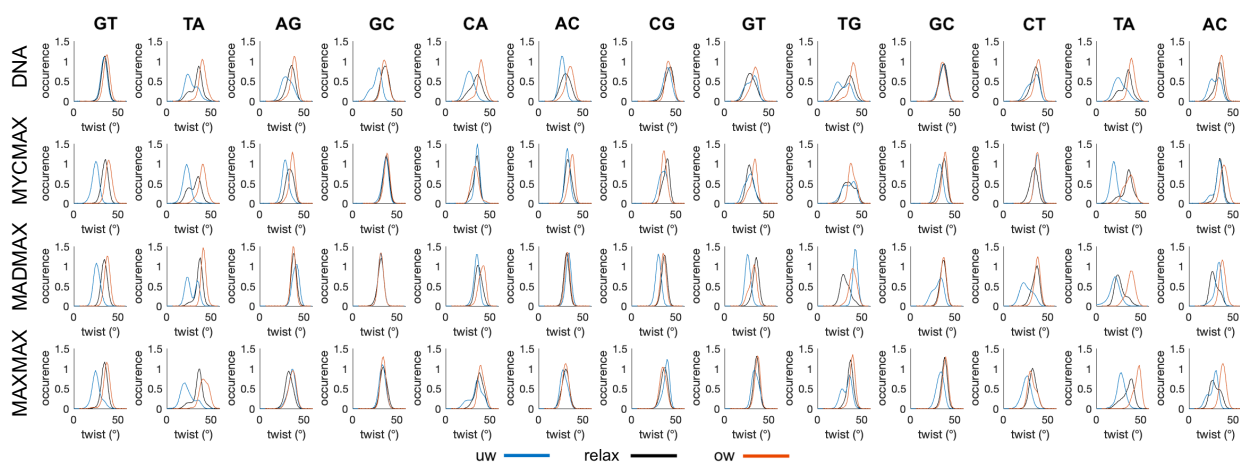


Figure S7: Twist distributions of the restrained DNA region (GTAGCACGTGCTAC) for underwound (-4.5), relaxed and overwound (+4.5) state.

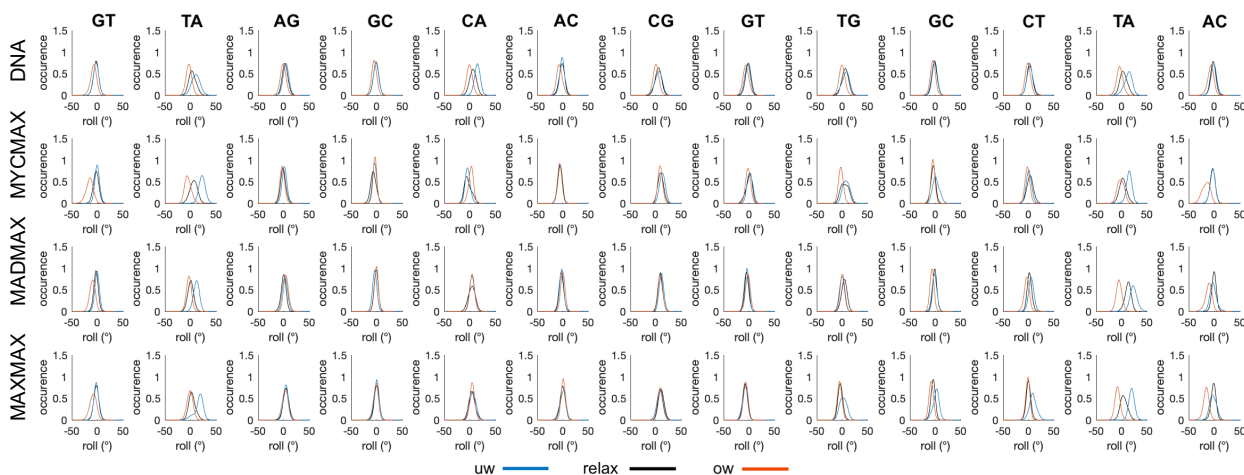


Figure S8: Roll distributions of the restrained DNA region (GTAGCACGTGCTAC) for underwound (-4.5), relaxed and overwound (+4.5) state.

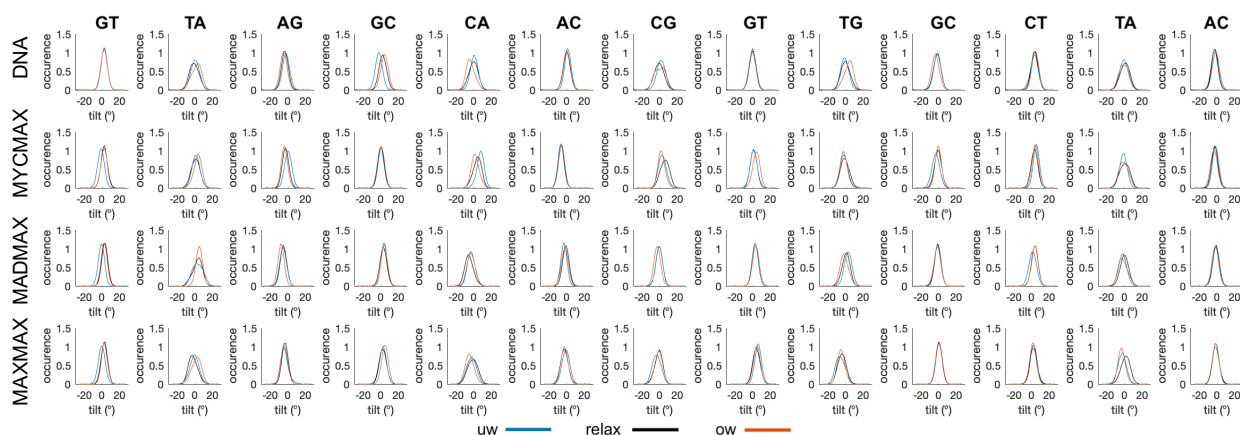


Figure S9: Tilt distributions of the restrained DNA region (GTAGCACGTGCTAC) for underwound (-4.5), relaxed and overwound (+4.5) state.

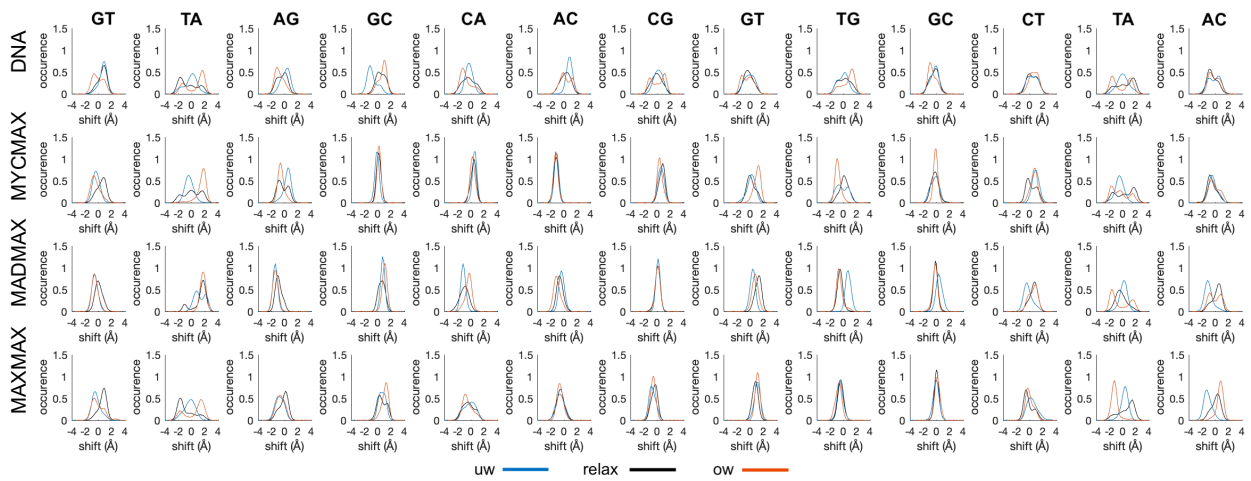


Figure S10: Shift distributions of the restrained DNA region (GTAGCACGTGCTAC) for underwound (-4.5), relaxed and overwound (+4.5) state.

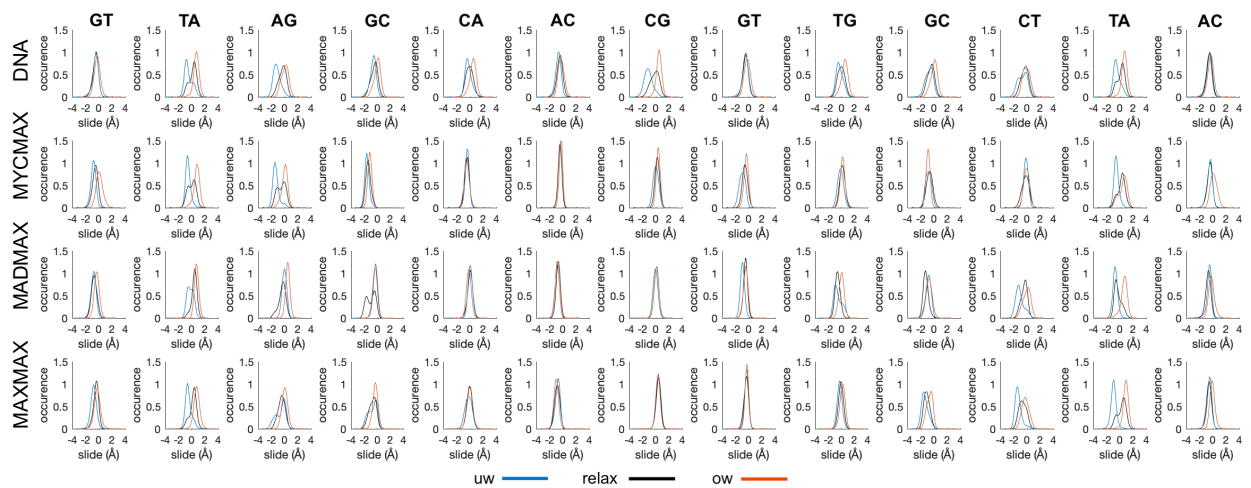


Figure S11: Slide distributions of the restrained DNA region (GTAGCACGTGCTAC) for underwound (-4.5), relaxed and overwound (+4.5) state.

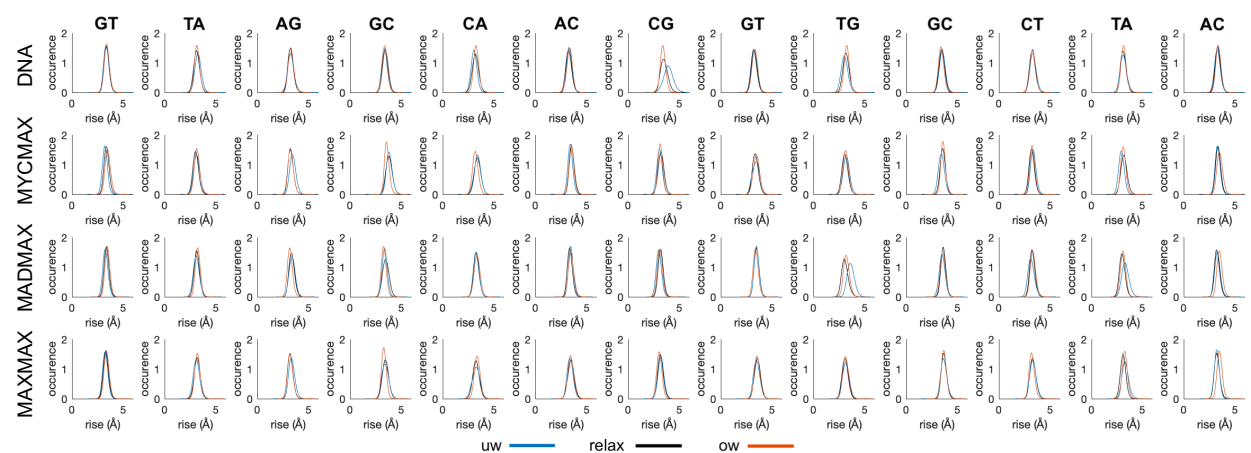


Figure S12: Rise distributions of the restrained DNA region (GTAGCACGTGCTAC) for underwound (-4.5), relaxed and overwound (+4.5) state.

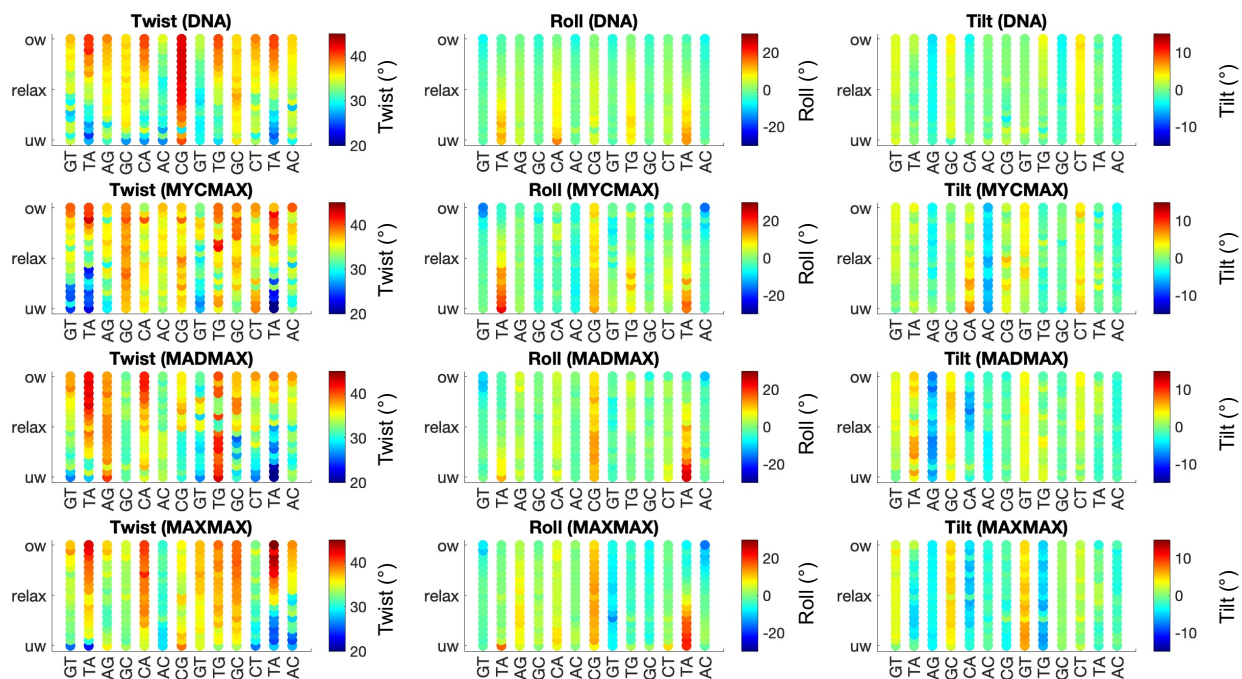


Figure S13: Change in average twist, roll and tilt of b.p. steps of the restrained DNA region (GTAGCACGTGCTAC) along the torsional regimes denoted with a colorbar.

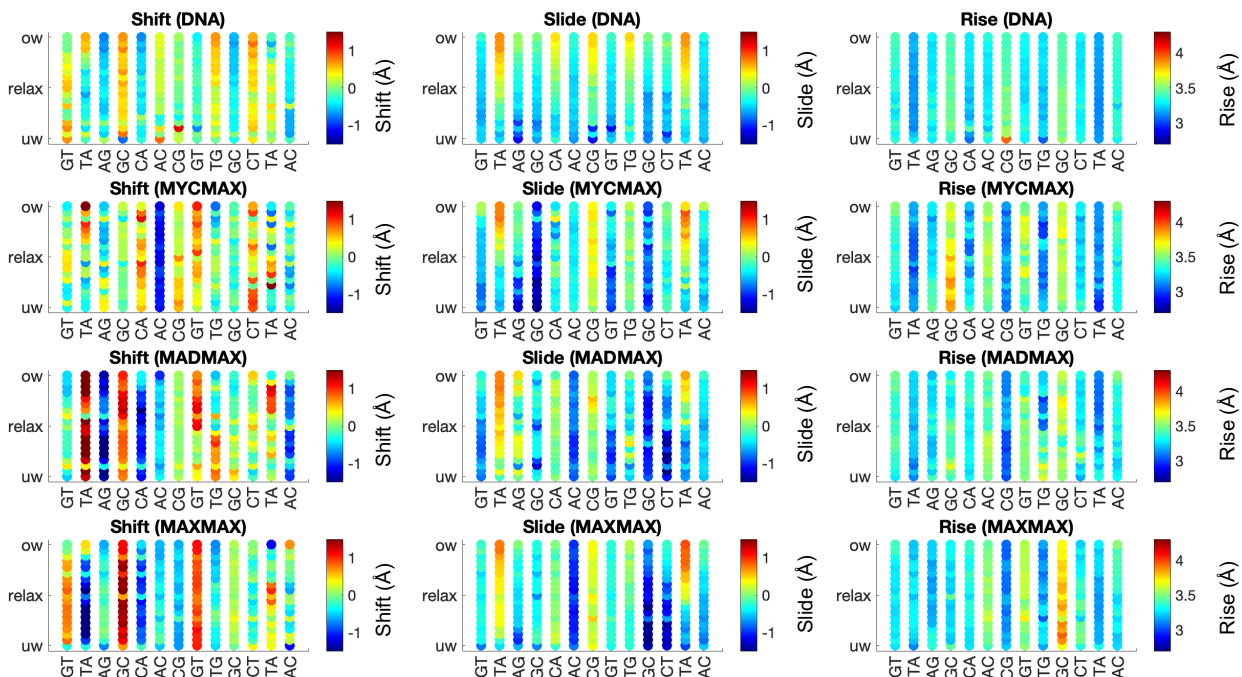


Figure S14: Change in average shift, slide and rise of b.p. steps of the restrained DNA region (GTAGCACGTGCTAC) along the torsional regimes denoted with a colorbar.

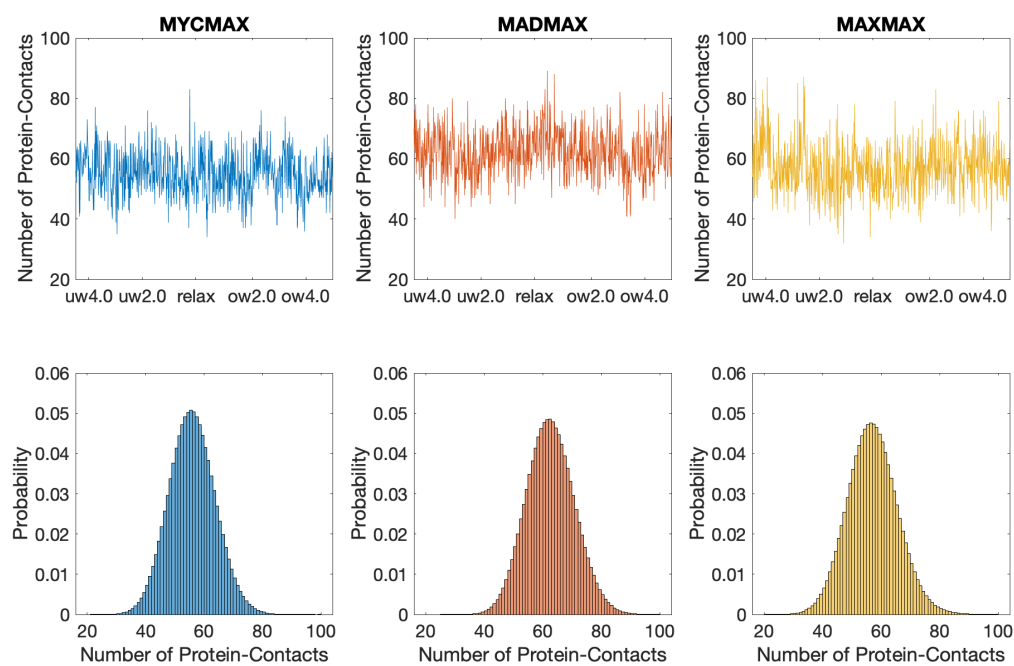
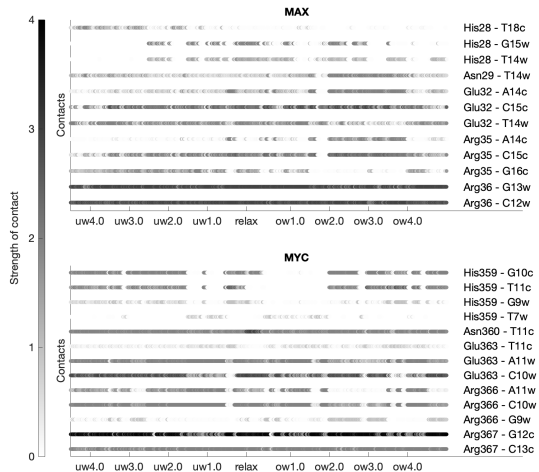
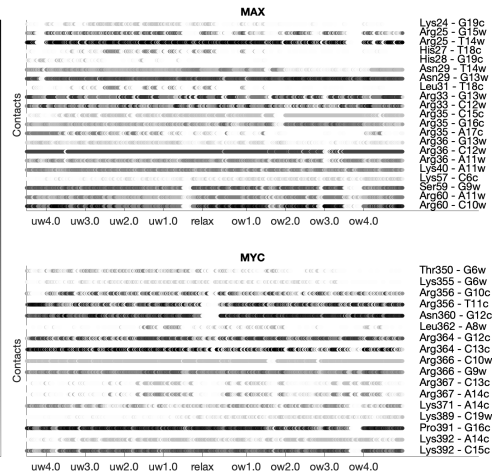


Figure S15: Upper panel: fluctuations of the total number of protein-DNA contacts along the torsional regimes. Bottom panel: distributions of the total number of protein-DNA contacts for the different BHLH-DNA complexes.

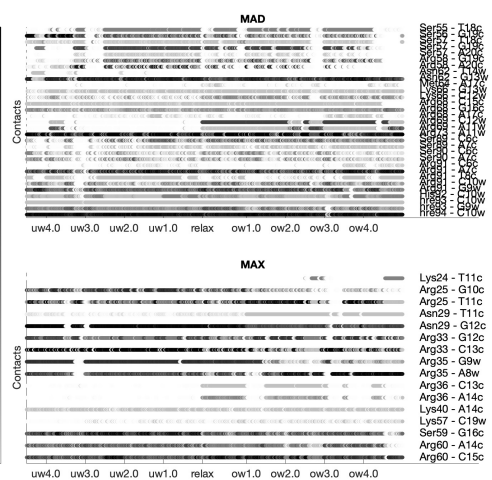
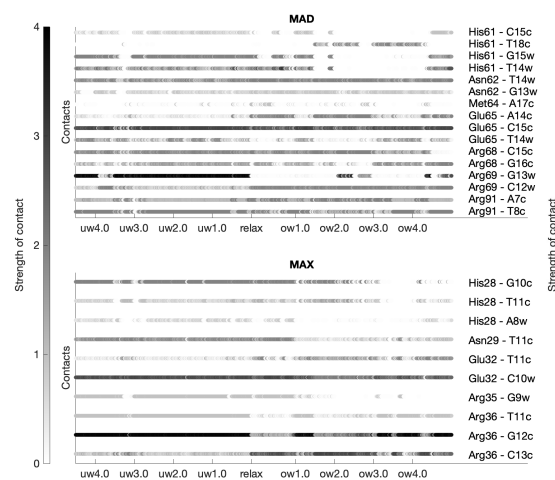
Specific Contacts



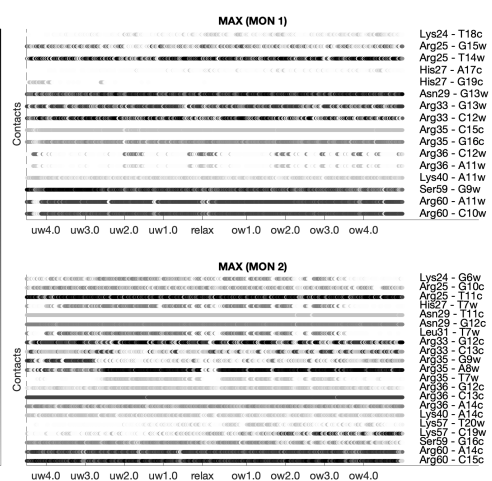
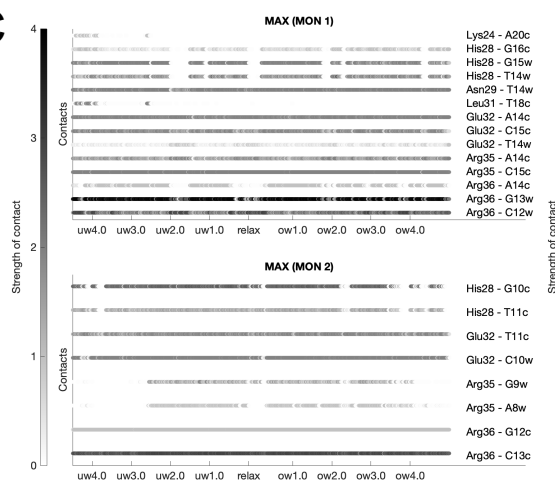
Non-specific Contacts



B

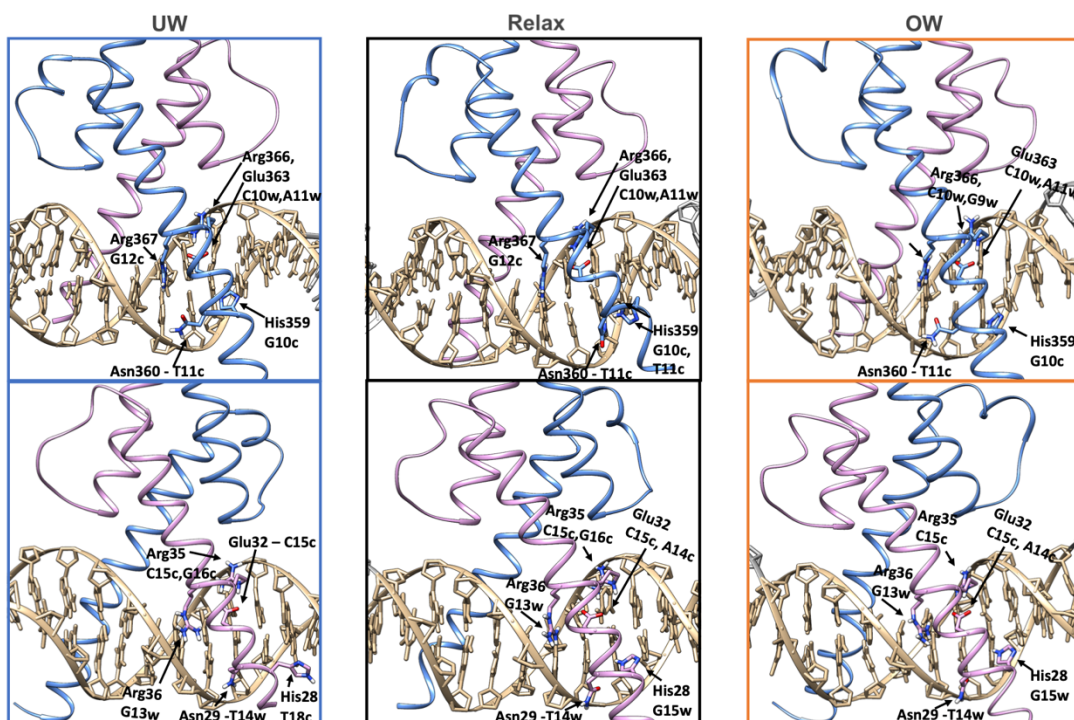
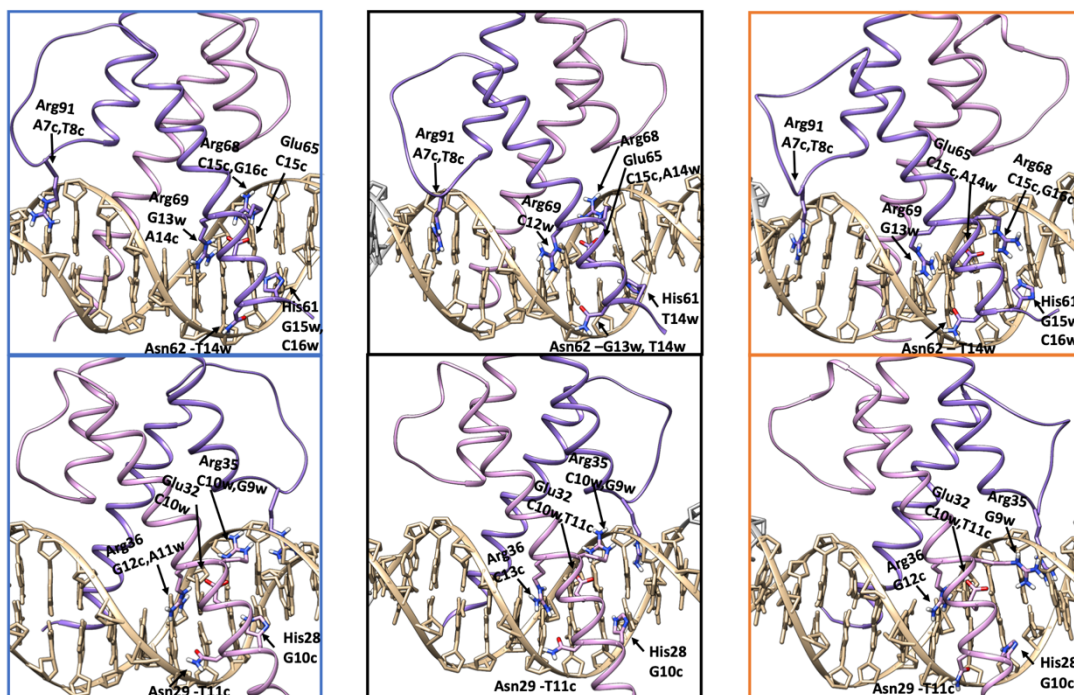


C



W-Strand 5'- G G C G A G T A G C A C G T G C T A C T C G C -3'
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
C-Strand 3'- C C G C T C A T C G T G C A C G A T G A G C G -5'

Figure S16: Dynamic interactions maps of specific and non-specific contacts along the different torsional regimes for **A.** MycMax, **B.** MadMax and **C.** MaxMax. The contacts between pairs of residues are characterized by strength and occurrence

A**B**

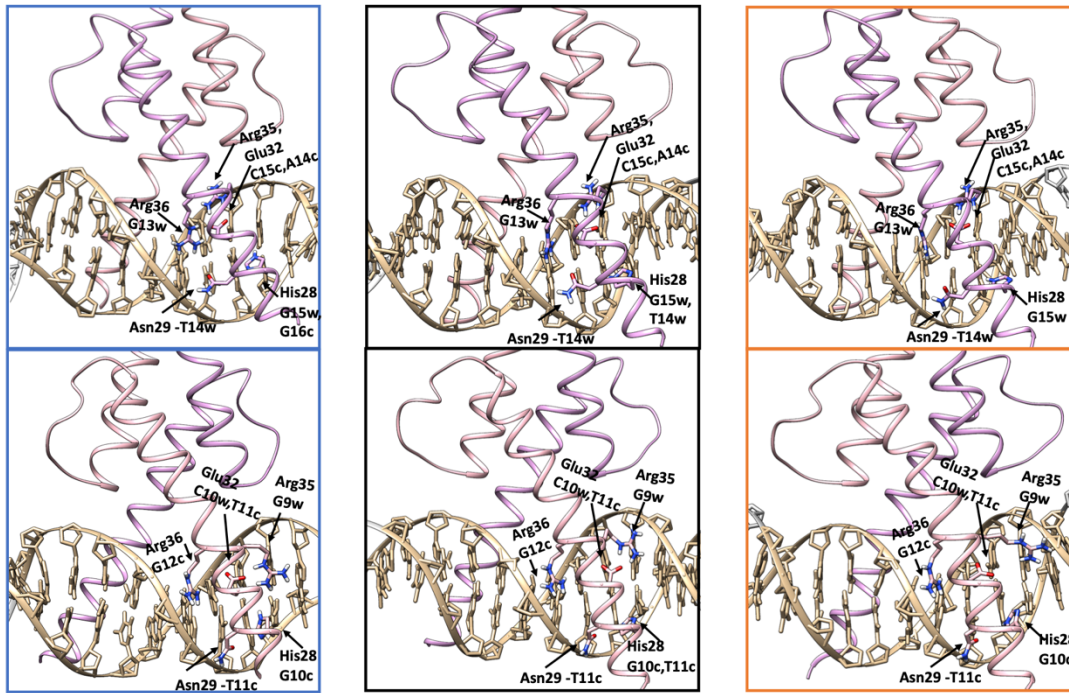
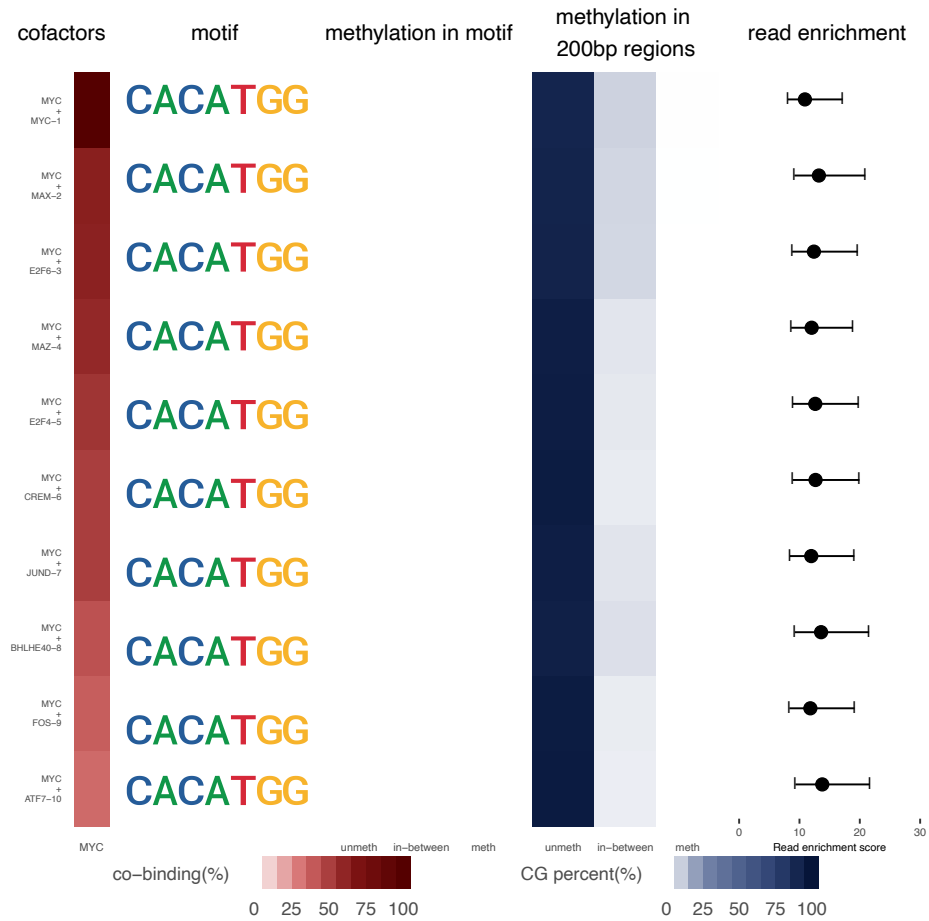
C

Figure S17: BHLH-DNA contacts exploited by the five-residues motif (HNxxExxRR) for underwinding regime ($-4.5^\circ/\text{bp}$), relaxed state and overwinding regime ($+4.5^\circ/\text{bp}$). Restrained DNA region (GTAGCACGTGCTAC) is denoted with tan colour. **A.** Upper panel: Myc-DNA contacts. Bottom panel: Max-DNA contacts. **B.** Upper panel: Mad-DNA contacts. Specific contacts exploited by Mad loop is also shown. Bottom panel: Max-DNA contacts. **C.** Upper panel: Max(monomer 1)-DNA contacts. Bottom panel: Max(monomer 2)-DNA contacts.

A



B

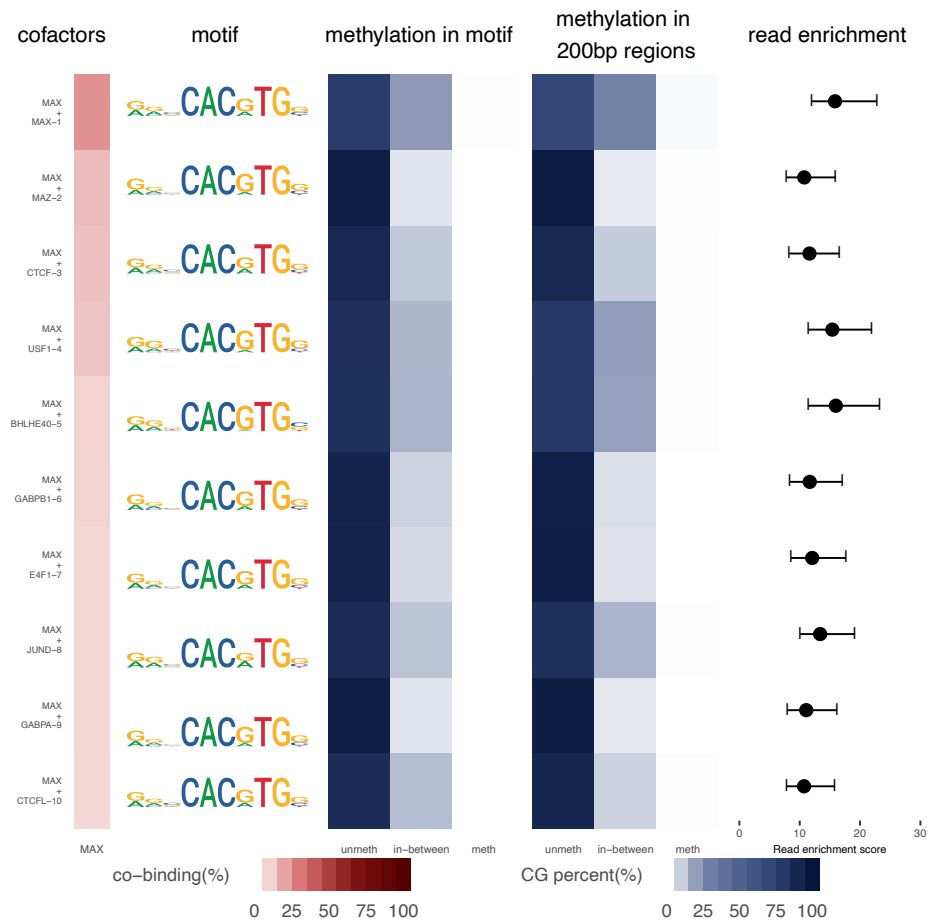


Figure S18: A. Myc and B. Max co-factors summary as reported by TFregulomeR. Information reported are, from left to right, the name of transcription factors detected as potential co-factors to either Myc or Max, with the corresponding co-binding percentage in shade of red; the sequence motif for the main protein of interest (Myc or Max); the methylation percentage of cytosine inside the binding motif and in a window of 200bp around the binding motif, represented in shade of blue; the reads enrichment from the ChIP-seq profile of the considered proteins.