Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Probing helical transitions in a DNA duplex

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Supporting Information

List of Figures

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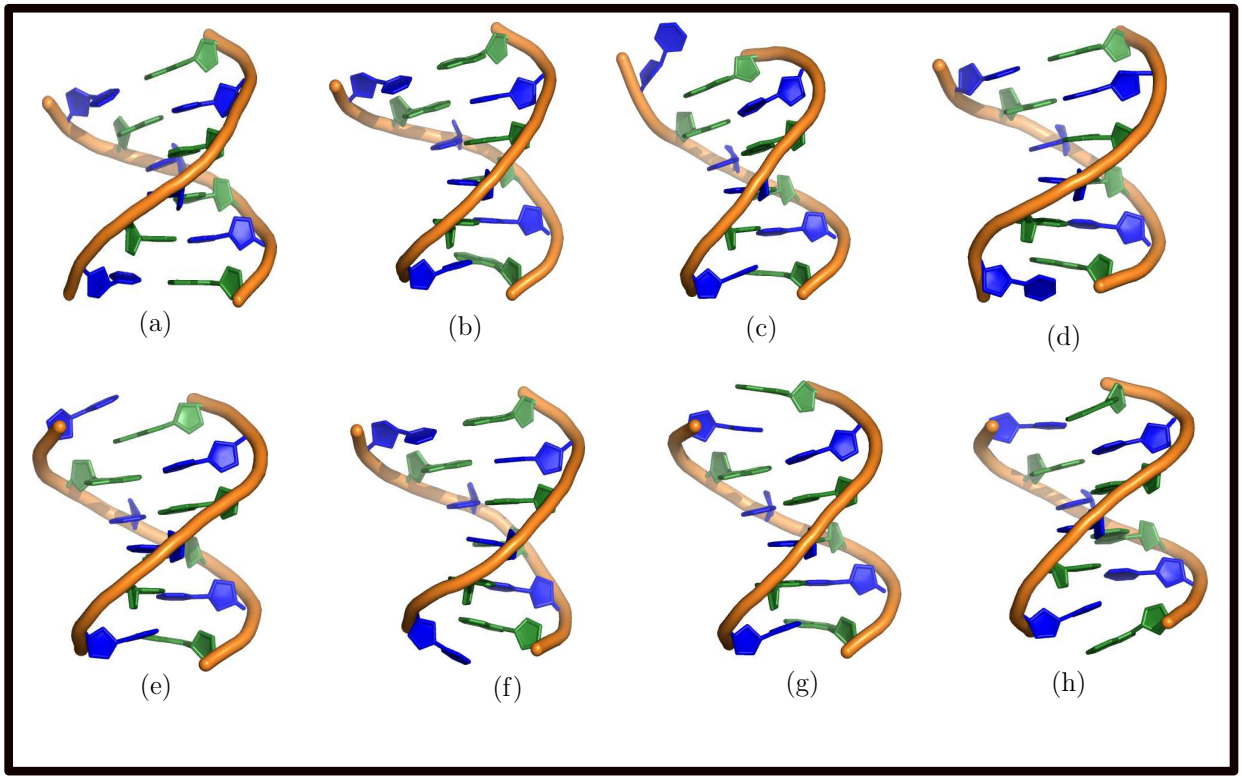

Figure 1. (a) Canonical B-DNA duplex with all base-pairs in the WC orientation. (b)-(h) are representative snapshots of the different duplexes constituting the lowest free energy group. (b) tWS base-pair between G6 and C7. (c) C1 frayed out of the helix. (d) C7 frayed out of the helix. (e) C1 stacked on top of G12. (f) C7 stacked on top of G6. (g) G12 stacked on top of C1. (h) G6 stacked on top of C7.

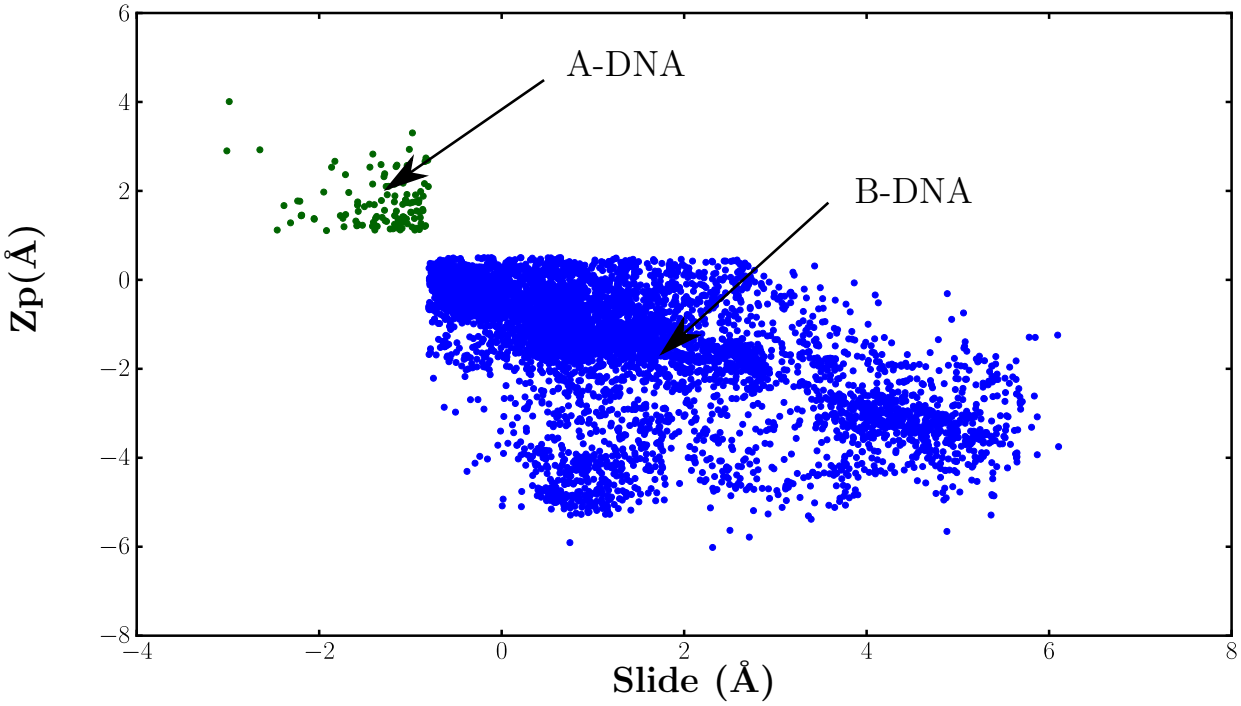

Figure 2. Plot of Slide vs Zp for distinguishing between the B-DNA and A-DNA structures.

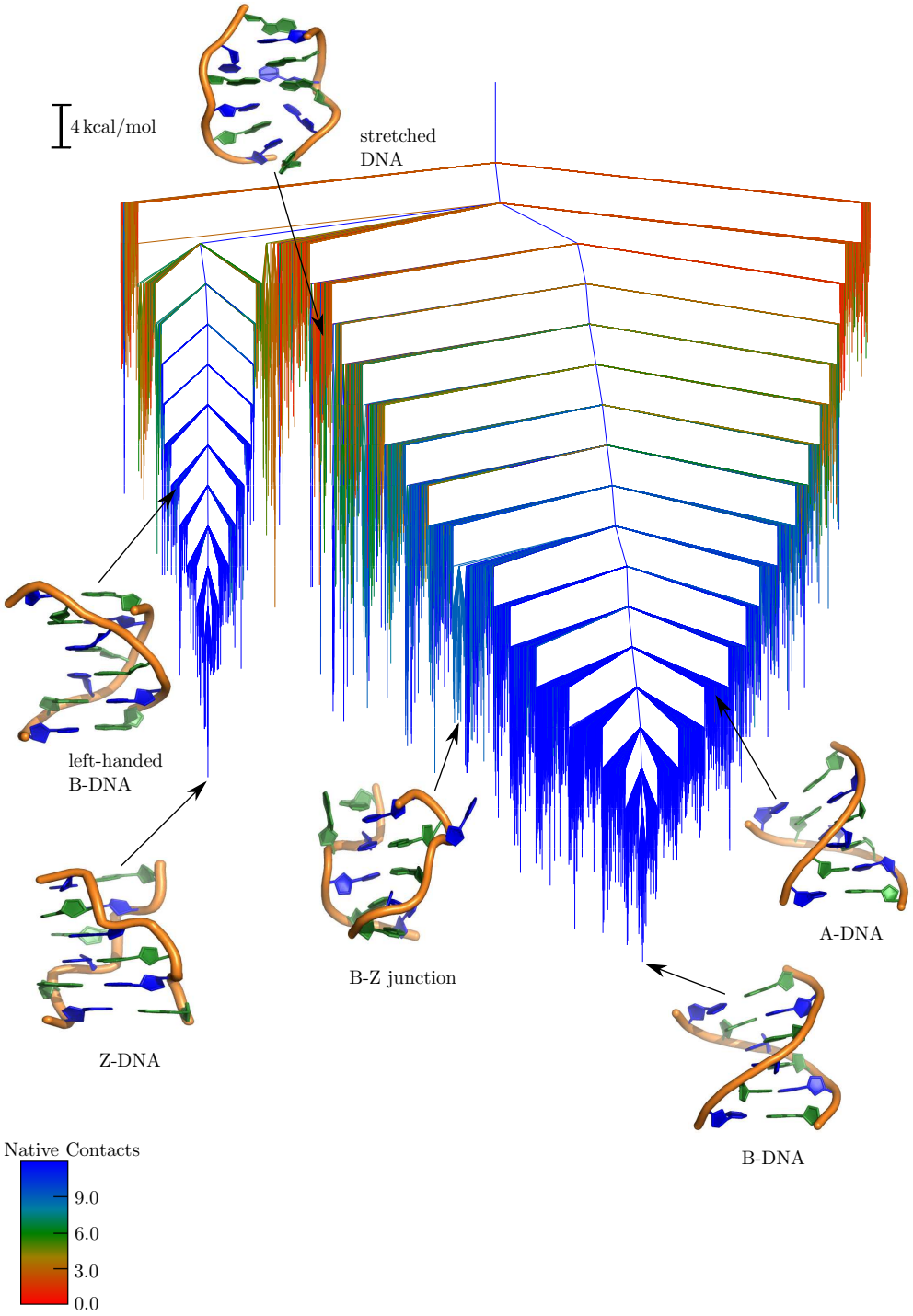

Figure 3. Free energy disconnectivity graph computed at 298 K using a regrouping threshold of 5 kcal/mol. The branches are coloured according to the number of Watson-Crick base pairs in the helix (from blue to red, with blue representing structures having all the native contacts, and red representing structures without any native contacts). Representative snapshots from the different ensembles are also shown.