Correlations and helical coherence in DNA structure: "straightening" the helix upon crystal packing

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The twist, rise, and other parameters that define the arrangement of adjacent DNA base pairs depend on the identity of the constituent bases. This dependence may provide a structural fingerprint of the underlying DNA sequence, which could be important for DNA sequence recognition by proteins, packaging and maintenance of genetic material, and other interactions involving DNA. The conformation of a specific DNA sequence, however, may not be fully realized knowing average values of these parameters alone as variations exist in the stacking geometry of the same adjoining base pairs within different sequence contexts. Hence, we have investigated the problem of sequence-dependent DNA conformation through a statistical analysis of X-ray and NMR structures of DNA oligomers, determining how these parameters are correlated along a sequence. We define a corresponding helical coherence length, which is a cumulative parameter quantifying sequence-dependent deviations from the ideal double helix geometry. We find, e.g., that the solution structure of synthetic oligomers is characterized by a 100 - 200 Angstrom coherence length, which is similar to the 150 Angstrom coherence length of natural, salmon-sperm DNA. Packing of oligomers in crystals dramatically alters their helical coherence, however. Here, the coherence length increases to 800 - 1200 Angstroms, consistent with theoretical predictions of its role in interactions between DNA at close separations.