

Abstract

DNA is the fundamental molecule in all domains of life, its role in heredity is well established. Although the famous double helical complementary form is indispensable for replication mechanism DNA can occupy wide range of conformations. In the past studies performed in the laboratory, DNA oligomers related to single stranded bacterial Repetitive Extragenic Palindromic (REP) showed spectral behavior suggesting complex equilibria including double helical, hairpin, and tetraplex conformations. The studies presented in this thesis extended the scope of analyzed sequences and employed circular dichroism spectroscopy and X-ray crystallography. We report spectral data and X-ray structures of three successfully crystalized oligonucleotides. All three structures acquire double helical architecture with two consecutive T-T mismatches in the center. To improve the convergence of the refinement process of the crystal structures we used novel dinucleotide conformational classes, NtC classes. The NtC class classification was also used to analyze geometries of selected non-canonical base pairs in all DNA crystal structures in the Protein Data Bank. We measured the fit between geometries of the dinucleotides involved in the non-canonical base pairing and the NtC classes and correlated this fit to the electron density of the analyzed dinucleotides. This new type of the quality measure revealed that dinucleotides involved in non-canonical base pairing show no significant geometrical difference from the Watson-Crick paired dinucleotides. We also suggest that a large fraction of so far unclassified dinucleotides can be re-refined into the known geometries.

Key words: single stranded DNA, structural database, X-ray crystallography, circular dichroism, NtC, base pairing, mismatch