

23. STRUCTURAL ANALYSIS AND CLASSIFICATION

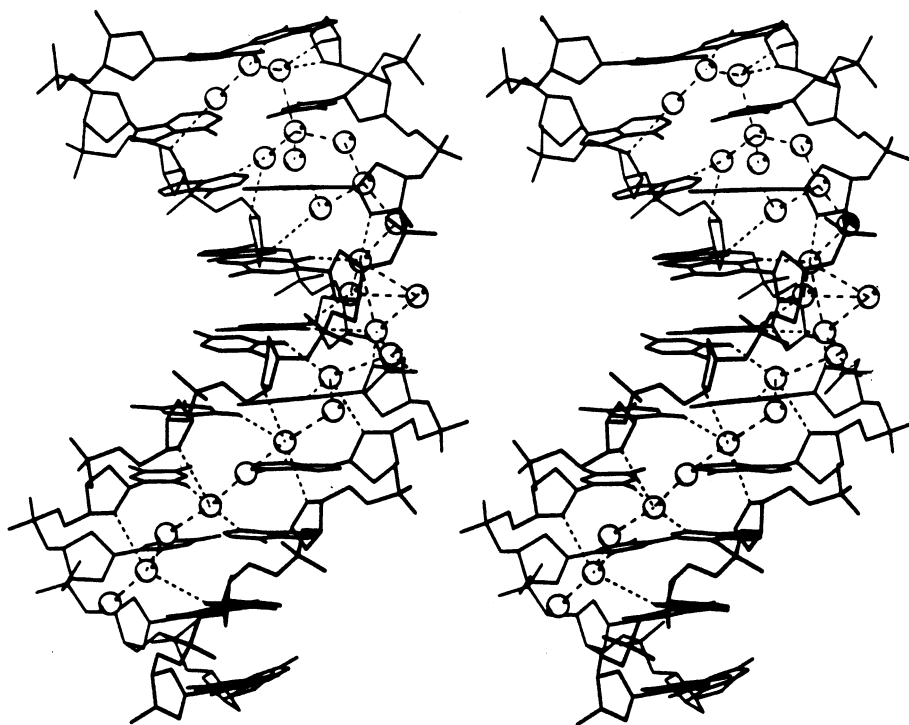


Fig. 23.3.4.1. Structure of C-A-A-A-G-A-A-A-G (B107). The lower half of the helix, with -A-A-A-A-G, exhibits the narrow minor groove commonly associated with the AT region of the helix and a single zigzag spine of hydration, as was first seen in C-G-C-G-A-A-T-T-C-G-C-G (B1-B6). The upper half, with C-A-A-A-G-, has the wider minor groove of general-sequence B-DNA and two separate rows of hydrating water molecules along the two walls of the wider groove.

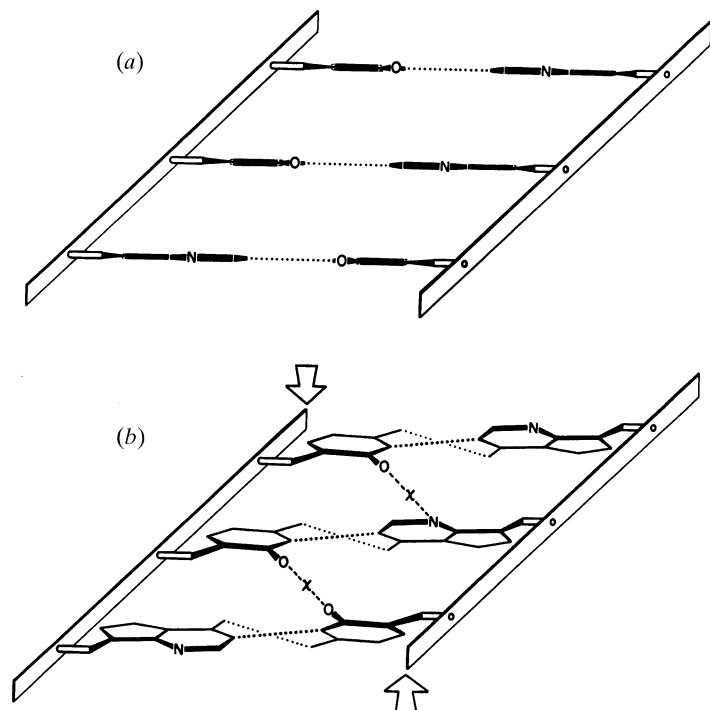


Fig. 23.3.4.2. Relationship between minor groove width and propeller twist. (a) View into the minor groove of B-DNA, with base pairs seen on edge and with the sugar-phosphate backbones shown schematically as inclined ladder uprights. (b) Consequences of propeller twisting the base pairs. Glycosyl bonds connected to sugar C1' atoms are all displaced upward in the right strand and downward in the left strand. This shifts the backbone chains as indicated by the arrows. Hence, the gap between the chains is decreased, and the minor groove is narrowed.

The Ansevin-Wang helix has been sedulously ignored since its publication in 1990, especially by crystallographers. The Science Citation Index lists an average of *one* citation of their paper per year since publication, most commonly by spectroscopists. Ho & Mooers (1996) are almost alone among crystallographers in coupling the B-to-Z interconversion dilemma to the possible existence of a different kind of left-handed structure in long polynucleotides. Of course the Z(WC)-DNA structure, as presented here, is only a model; it could be far from the true structure in many respects. But its interest lies in the fact that a left-handed alternating helix with 'standard' backbone directions *can* be built with reasonable bond geometries and with properties that fit the various physical measurements as well as Z-DNA. It calls into question not the correctness of the Z-DNA structure obtained from short oligomers with free helix ends, but the relevance of that structure to the production of left-handed regions in longer duplexes with constrained ends.

23.3.4. Sequence-structure relationships in B-DNA

Two channels of information exist in B-DNA by which base sequence is expressed to the outside world. One of these is the Watson-Crick base pairing of A with T and G with C that is used in the storage of genetic information and in replication and transcription. The other channel, used in control and regulation of the expression of this genetic information, involves the hydrogen-bonding patterns of base-pair edges along the floors of the grooves and any systematic deformations of local helix structure that result explicitly from the base sequence.

The simplest and most direct expression of this second channel is the passive reading of hydrogen-bonding patterns along the floor of the major and minor grooves. This readout mechanism was first