23.3.2.5. *Syn/anti glycosyl bond geometry*

The glycosyl bond angle, χ, about the bond connecting a sugar ring to a base is a special case of torsion angle, and is defined by O4′—C1′—N1—C2 for pyrimidines and O4′—C1′—N9—C4 for purines. In A- and B-DNA, the normal range of χ is 160 to 300°. This is known as the *anti* conformation (right-hand side of Fig. 23.3.2.13) and swings the sugar ring out away from the minor groove edge of the base pair. In Z-DNA, pyrimidines also exhibit the *anti* glycosyl bond conformation, but purines adopt the *syn* geometry shown on the left-hand side of Fig. 23.3.2.13. Now the sugar ring is rotated so that it intrudes into the minor groove, and χ lies in the range 50 to 90°.

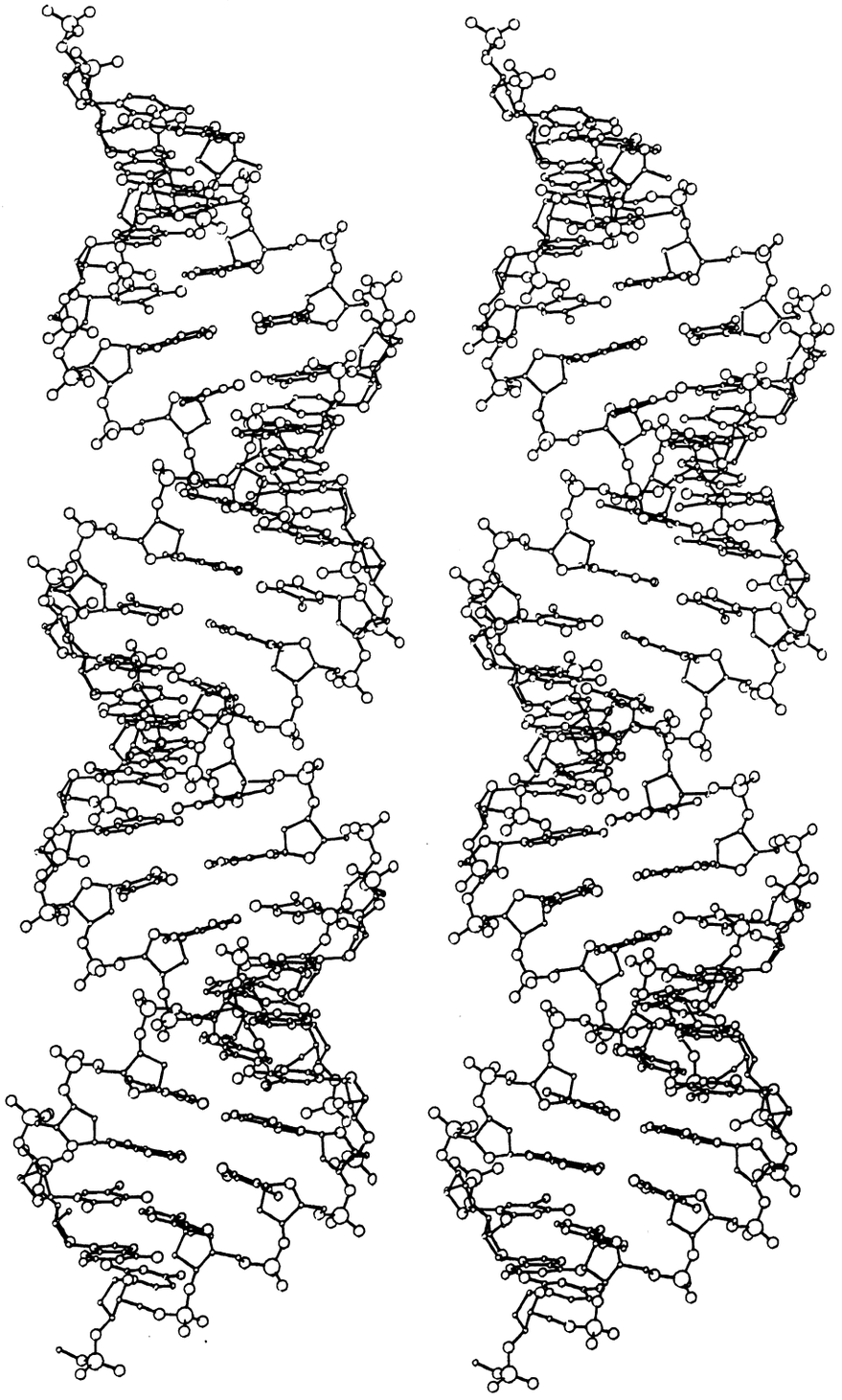

Fig. 23.3.3.1. The A-DNA stereo pair drawing from which Fig. 23.3.1.2 was derived, with repeating sequence -(G-T-A-T-A-C)$_n$-. The impression of the A helix as a ribbon wrapped around an imaginary core is even more strongly developed in this stereo. (From Dickerson, 1983.)

23.3.3. Comparison of A, B and Z helices

Figs. 23.3.3.1–23.3.3.3 show the original stereo pairs that were re-drawn by Irving Geis in preparing Figs. 23.3.1.2–23.3.1.4. These stereo pairs were constructed from X-ray structures of A-, B- and Z-DNA oligomers by deleting the outermost base pair from each end, eliminating the backbone as far as the first phosphate group, and then stacking these trimmed-down helices on top of one another, with phosphate groups overlapping, to create an infinite helix. They are improvements over the idealized infinite helices generated from fibre diffraction in that they display local variation in helix parameters that only single-crystal analyses can reveal. In the present context, they are good subjects for discussion of the differences between the three helix types.

23.3.3.1. *x displacement and groove depth*

A-DNA (Wahl & Sundaralingam, 1996, 1998), B-DNA (Berman, 1996; Dickerson, 1998*b*) and Z-DNA (Ho & Mooers, 1996; Basham *et al.*, 1998) have each been the subject of recent reviews, to which the reader is referred for details that cannot be covered here. The distinctive properties of the three helices are listed in Table 23.3.3.1. The most obvious distinction is handedness: A and B are right-handed helices, whereas Z is left-handed. Moreover, the position of each base pair relative to the helix axis is quite different. As noted in Fig. 23.3.2.13, the helix axis passes through base pairs in B-DNA, lies on the minor groove side of base pairs in Z-DNA, and on the major groove side in A-DNA. In terms of the helix parameters of Fig. 23.3.2.12, A-DNA has a typical *x* displacement of $d_x = +3$ to $+5$ Å, B-DNA has $d_x = -1$ to 0 Å, and Z-DNA has $d_x = -3$ to -4 Å. There is virtually no overlap between these three ranges; *x* displacement, d_x, in fact, is a better criterion for differentiating the three classes of helix than is sugar ring conformation.

A direct consequence of these *x* displacement values is great differences in depths of major and minor grooves. Both grooves are of equivalent depth in B-DNA because base pairs sit on the helix axis. In A-DNA, a base pair is pushed off-axis so

references