Table 23.3.3.1. *Comparison of structures of A, B and Z helices*

	A	B	Z
Handedness	Right	Right	Left
Helix axis relative to base pairs	Major groove side	Through centre of base pair	Minor groove side
Major groove	Very deep and narrow	Wide, same depth as minor	Very shallow and broad
Minor groove	Shallow and broad	Variable, same depth as major	Very deep and narrow
Glycosydic bonds	*anti*	*anti*	C: *anti* G: *syn*
Minor groove backbone chain sense *	Clockwise	Clockwise	Counterclockwise
Sugar conformation	C3′-*endo* (narrow range)	C1′-*exo*/C2′-*endo* (broad range)	C: C2′-*endo* G: C3′-*endo*
Base pairs per helix repeat	1	1	2
Base sequence limitations	None	None	Alternating $(C\text{-}G)_n$ or close variants
Rise per base pair (average)	2.9 Å	3.4 Å	C-G: 4.1 Å G-C: 3.5 Å
Base pair inclination	10–20°	*ca* 0°	*ca* 0°
Mean twist angle	30–33°	34–36°	C-G: −8° G-C: −52°
Helix repeats per turn	11–12	10–10.5	6 (2 base pairs)
Propeller twist	Often substantial, 0–25°	Often substantial, 0–25°	Usually small
Common biological occurrence	RNA	DNA	None?

* Relative 5′-to-3′ directions of the two backbone chains, when viewed into the minor groove.

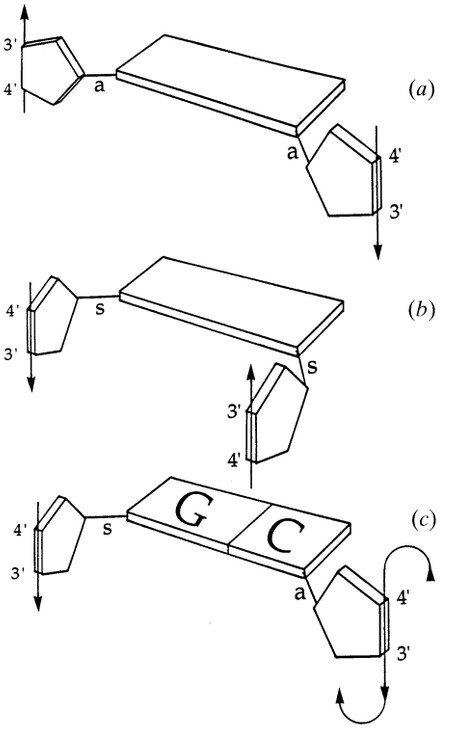

Fig. 23.3.3.4. Glycosyl conformation and chain sense. (*a*) Glycosyl conformations *anti/anti*, backbone chains antiparallel, with clockwise sense when viewed into the minor groove, as here. This is typical for A- and B-DNA. (*b*) Glycosyl conformation *syn/syn*, backbone chains antiparallel, with counterclockwise sense viewed into minor groove. This is not known for any nucleic acid duplex. (*c*) Glycosyl conformation *syn* at G and *anti* at C, with the C4′—C3′ edge of the sugar pointing downward in both strands, which would seem to imply a parallel-stranded helix. However, in Z-DNA, antiparallel strands are achieved by a local reversal of chain direction at each C, as shown here. This produces the zigzag backbone pathway that is characteristic of the Z helix, visible in Fig. 23.3.3.3.

Z-DNA is larger because it involves stacking of a sugar oxygen on each purine ring, not ring stacked on ring. For A-DNA, the rise along the helix axis can actually be less than the thickness of a base pair, because adjacent base pairs are stacked at an incline. The perpendicular distance from one base pair to the next in A-DNA is still 3.4 Å. Both A- and B-DNA exhibit considerable base pair propeller twist, especially at A·T pairs with only two hydrogen bonds rather than three. In contrast, Z-DNA, with predominately G·C pairs, shows only a small propeller twist.

The stacking of base pairs has immediate consequences for crystal growth. For Z-DNA, four base pairs are one-third of a helical turn, and six base pairs are a half turn. Hexamers are the most common crystal form in Table A23.3.1.3 by a large majority. In contrast, octamers and decamers are not simple fractions of a turn, and they stack in a disordered manner. One would predict that dodecamers of Z-DNA might crystallize well if the oligomers were not so long as to fall prey to cylindrical disorder.

By the same principles, B-DNA decamers stack easily and well to build pseudo-infinite helices through the crystal, with ordered cylindrical rods packed in six different space groups. The other common crystallization mode for B-DNA, the dodecamer, has a two-base-pair overlap of ends that both stablizes the crystals and yields a functional ten-base-pair repeat. (See Fig. 2 of Dickerson *et al.*, 1987.) Because the dodecamers are held by their outer two base pairs, the central eight pairs are unobstructed and accessible in the crystal, making dodecamers particularly good subjects for the study of minor-groove binding drugs.

A-RNA duplexes [Table A23.3.1.1, part (*k*)] also stack end-for-end in a manner simulating an infinite A helix, even though the end base pairs are inclined and are not perpendicular to the helix axis. This behaviour has been seen for octamers with roughly two-thirds of a helical turn, for nonamers, and for dodecamers with roughly a full turn.

In contrast, crystals of A-DNA behave quite differently. Regardless of chain length, A-DNA helices crystallize with the outer base pair of one helix packed against one wall of the broad, open and relatively hydrophobic minor groove of another helix.

references