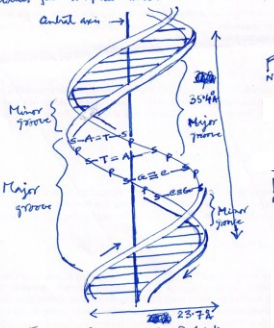
DNA:

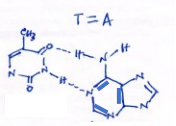
Erwin Chargaff observed that the constraint on the base composition in DNA is much less: $\chi_A = \chi_T$ and $\chi_G = \chi_C$ where χ represents mole fraction and only a single variable $\chi_{at}\left(= 1 - \chi_{A+T}\right)$ is needed to describe the composition of DNA.

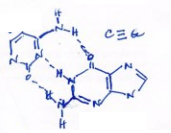
The X-ray diffraction data of DNA molecule and the observation of Chargaff led Watson and Crick to propose a model of double stranded DNA molecules.

1. Two polynucleotide chains running in opposite direction coil around a common axis to form a right-handed double helix
2. Purine and pyrimidine bases are on the inside of the helix, whereas phosphate and deoxyribose units are on the outside
3. Adenine (A) is paired with thymine (T), and guanine (G) with cytosine (C). An A-T base pair is held together by two hydrogen bonds and that of a G-C base pair by three such bonds.

The common form of DNA is right handed base residues form a spiral in a clockwise direction.

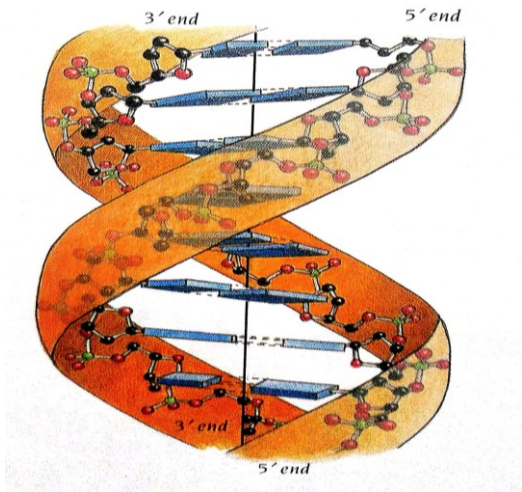


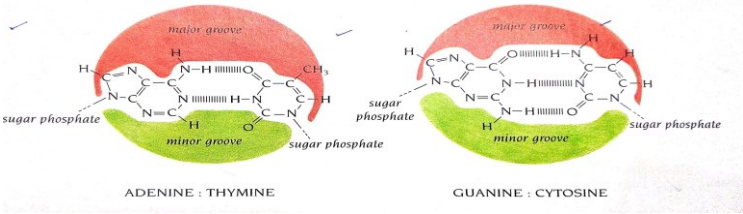




Diagrammatic representation of Watson and Crick model of the double helical structure of the B-form A-DNA width ≈ 20Å, ● one complete turn ≈ 35Å one turn of B-DNA includes ten base pairs (bp) ⇒ rise is 3.5Å per bp

P → Phosphate; S → sugar (deoxyribose)





ADENINE : THYMINE

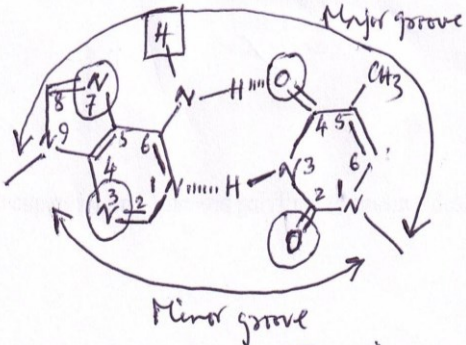
GUANINE : CYTOSINE

The most important feature of DNA double helix is the specificity of the pairing of bases. Adenine must pair with thymine and guanine with cytosine. The glycosidic bonds that are attached to a bonded pair of bases are very nearly 10·8 Å apart. A purine-pyrimidine base pair fits perfectly into this space. In contrast there is insufficient room for two purines and there is more than enough space for two pyrimidines, but they would be too far apart to form H-bonds. Adenine cannot pair with cytosine because there would be two hydrogens near one of the bonding positions and none at the other. Likewise, guanine cannot pair with thymine. The two strands of the double helix, each of which possess a polarity, are antiparallel, i.e, one strand runs in the 5′ to 3′ direction and the other in the 3′ to 5′ direction. This is analogous to two parallel streets, each running one way but carrying traffic in opposite direction.

Different forms of the double helix are possible. In B-DNA, the most abundant form of DNA in the cell, the double helix is right handed with a diameter of 2·37 nm and a pitch of 3·54 nm. The base pairs are approximately parallel to each other and perpendicular to the central axis. In A-DNA, the double helix is right handed but slightly wider, with a diameter of approximately 2·55 nm and a pitch of 2·53 nm. The base pairs are parallel to each other but not perpendicular to the central axis of the helix. Double-stranded RNA and hybrid RNA-DNA, the assembly of one strand of ribonucleic acid strand with a DNA strand, assume the A-form. The third form of DNA, called Z-DNA, is left handed helix with a diameter of 1·84 nm, a pitch of 4·56 nm and a slightly tilted arrangement of the base pairs relative to the central axis of the helix. The physiological role of Z-DNA is not certain.

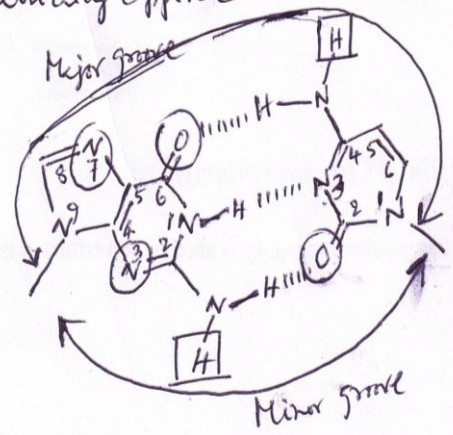
DNA helix has major and minor grooves:

B-DNA contains two kind of grooves, called major groove (12 Å wide) and the minor groove (6 Å wide). They arise because the glycosidic bonds of a base pair are not diametrically opposite to each other.



Adenine : Thymine

O ← H-bond acceptor, □ → H-bond donor



Guanine : Cytosine

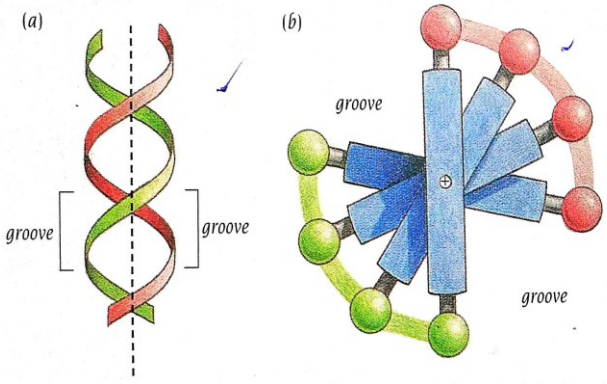
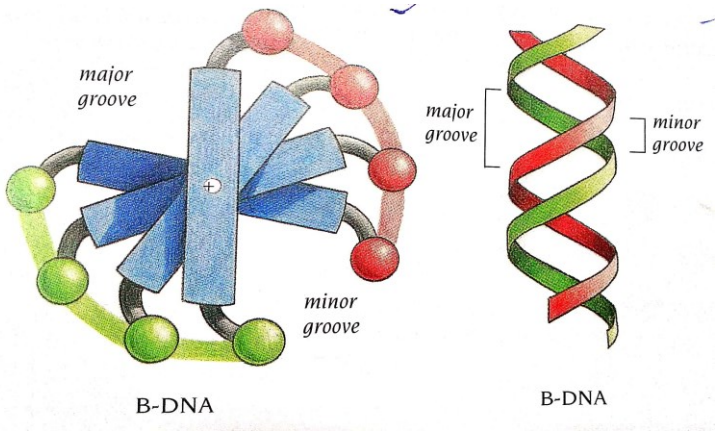


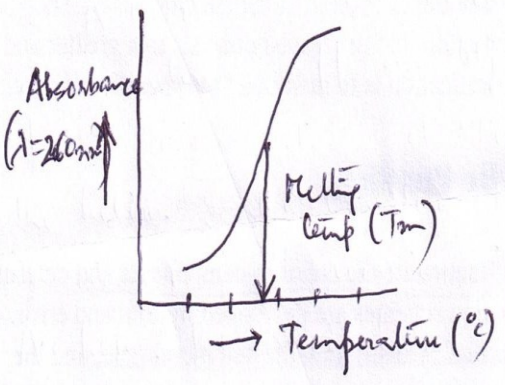
Figure 7.3 Schematic diagram illustrating that there are two similar grooves in a helical staircase. Four rungs are viewed from the top of the staircase in (b).

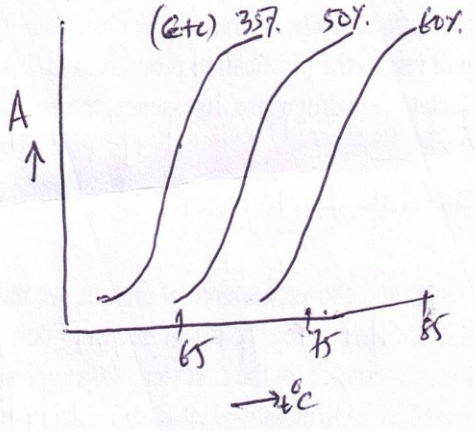


The minor groove contains the pyrimidine O-2 and the purine N-3 of the base pair, and the major groove is on the opposite side of the pair. Each groove is lined by potential hydrogen bond donor and acceptor atoms. The major groove is wider and deeper than minor one. In these grooves, protein can interact specifically with exposed atoms of the nucleotide, usually by H bonding, and thereby recognize and bind to specific nucleotide sequences without disrupting the base pairing of the double helical DNA molecule.

Denaturation (Melting) of DNA:

The double-stranded structure of DNA can be separated into two component strands (melted) in solution by increasing the temperature. The strands of a given molecule of DNA separate over a range of temperature. The melting temperature (T_m) is defined as the temperature at which half the helical structure is lost. The melting of DNA is readily monitored by measuring its absorbance at $\lambda = 260$ nm.





T_m is influenced by the base composition of the DNA. DNA rich in G-C pairs, which have three hydrogen bonds, melts at a higher temperature than that rich in A-T pairs, which have two hydrogen bonds.