A *nucleotide* consists of a nitrogenous base, a sugar (ribose sugar) and one or more phosphate groups. *Nucleosides* are formed by the condensation of nitrogenous bases with ribose sugars (i.e. pentose sugar). The nitrogenous base is a **purine or pyrimidine** derivative. The *purine bases are adenine (A) and guanine (G), and the pyrimidine bases are cytosine (C), uracil (U) and thymine (T)* (i.e. 5-methyl uracil).
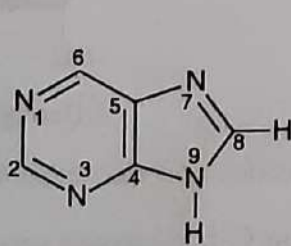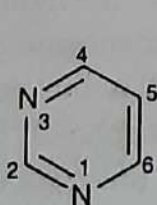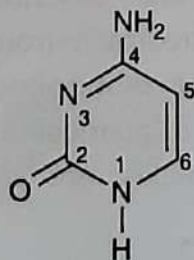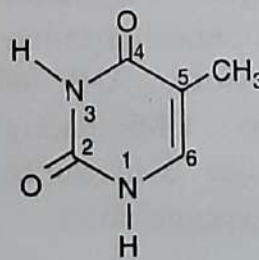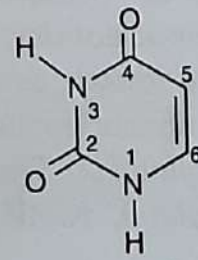

Purine
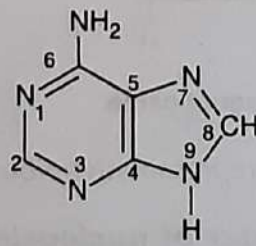
Adenine
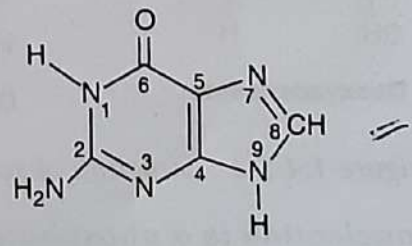
Guanine

Pyrimidine

Cytosine

Thymine

Uracil

A nucleoside consists of a purine or pyrimidine base linked to a **pentose sugar**. The pentose sugar is D-ribose or 2-deoxy-D-ribose. **The nucleosides are chemically N-glycosides of purine or pyrimidine bases.** The glycosidic linkage is formed between the C-1 atom of the pentose sugar and N-1 of the pyrimidine or N-9 of the purine base. In *ribonucleosides*, the pentose sugar is ribose. Some common ribonucleosides are : *adenosine, guanosine, uridine* and *cytidine*. In *deoxyribonucleosides*, the pentose sugar is 2-deoxy-ribose. The common *deoxyribonucleosides* are : *deoxyadenosine, deoxyguanosine, deoxythymidine* and *deoxycytidine*.
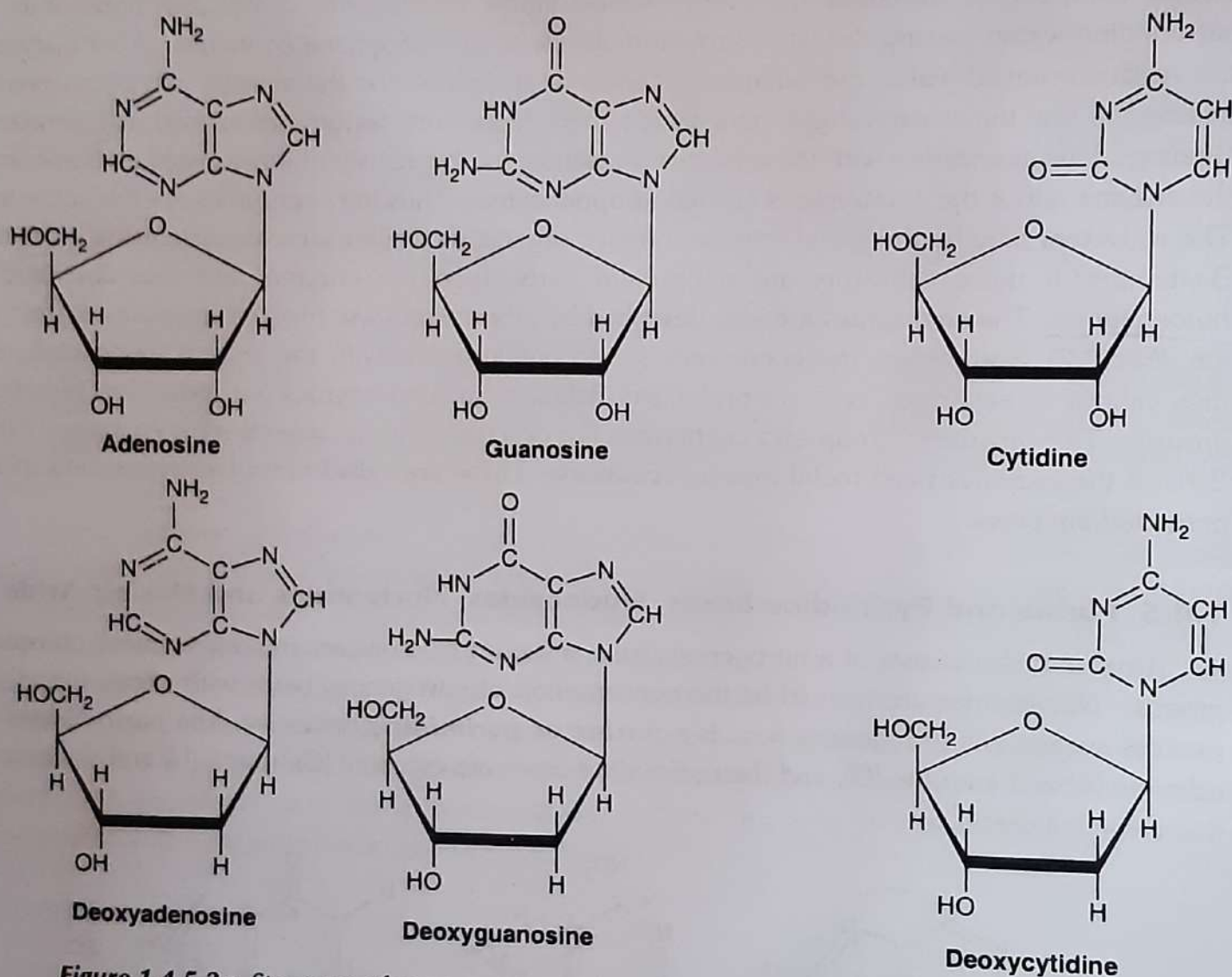

Figure 1.4.5.2 : *Structure of some representative ribonucleosides and deoxyribonucleosides.*

A nucleotide is a phosphate ester of nucleoside. The C-5 hydroxyl group of the pentose sugar is phosphorylated. **Thus, a nucleoside-5′-phosphate is a 5′-nucleotide.** Depending on the nature of pentose sugar, the nucleotides are described as 5′-ribonucleotides and 5′-deoxyribonucleotides. On phosphorylation of 5′-hydroxyl group of adenosine gives adenosine-5′-phosphate known as *adenylate*. AMP (adenosine monophosphate) is the adenylate. Other common 5′-ribonucleotides are : GMP (*guanylate, i.e.* guanosine-5′-phosphate), UMP (*uridylate*), CMP (*cytidylate*). The major 5′-deoxyribonucleotides are dAMP (*deoxyadenylate*), dGMP (*deoxyguanylate*), dCMP (*deoxycytidylate*).

The different adenine ribonucleotides, AMP (adenosine-5′-monophosphate), ADP (adenosine-5′-diphosphate) and ATP (adenosine-5′-triphosphate) are very much important in bioenergetics. AMP, ADP and ATP contain monophosphate (PO_4), diphosphate (P_2O_7) and triphosphate (P_3O_{10}) groups attached with the 5-carbon atom of ribose.
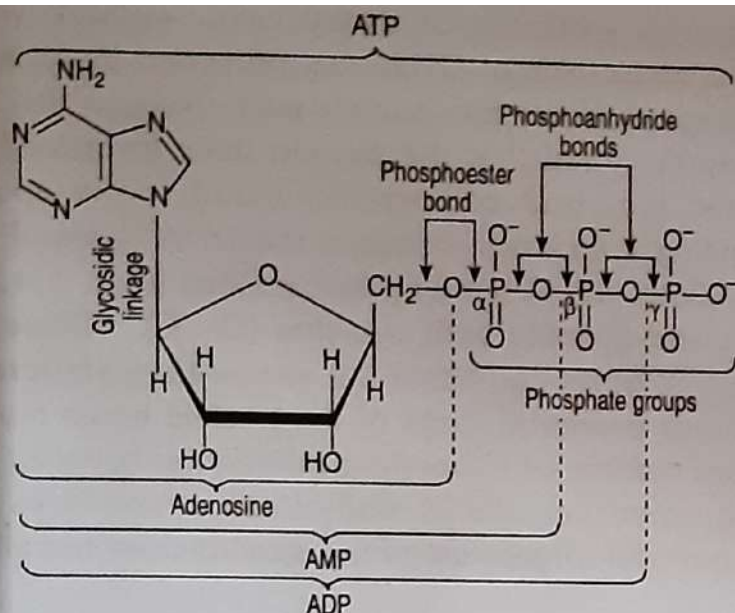
Figure 1.4.5.3 : *Structure of adenine ribonucleotides ATP, ADP and AMP. These ribonucleotides are actually rATP, rADP and rAMP.*

The nucleic acids are polynucleotides. The nucleic acids are DNA (deoxyribonucleic acid) and RNA (ribonucleic acid). DNA contains two purine bases (adenine and guanine), and two pyrimidine bases (cytosine and thymine). **RNA contains uracil instead of thymine.** In DNA, the purine and pyrimidine bases carry the genetic information, and the sugar and phosphate groups perform the structural roles. DNA is the molecule of heredity. **The primary structure of the nucleic acids consists of repeating sequence of simple nucleotide units.**

In the nucleic acids (DNA and RNA), C-1' of the pentose sugar is linked with the nitrogenous base; and the 3'-hydroxyl group of the pentose sugar of one nucleotide is joined with the 5'-hydroxyl group of the sugar unit of the adjacent nucleotide by a *phosphodiester bond*. In the nucleic acid chain one end bears a 5'-OH group and the other end bears a 3'-OH group. The base sequence is written in the 5'→3' direction. It may be pointed out that the amino acid sequence of a polypeptide chain is written in the direction, N-terminal end → C-terminal end direction.
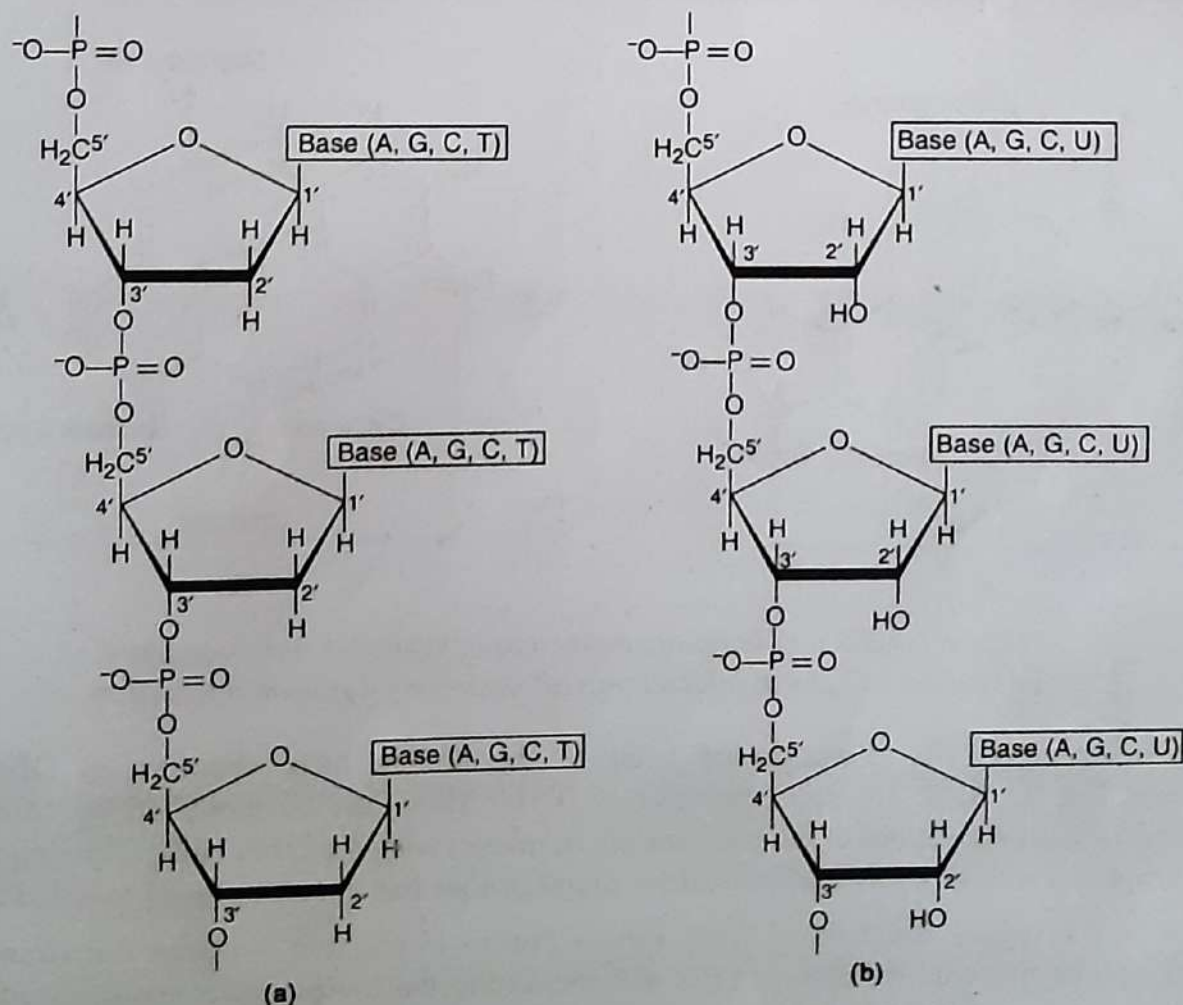

Figure 1.4.5.4 : *Structure of DNA (a) and RNA (b) chain*

The **primary structure** of DNA gives the sequence of deoxyribonucleotides in its strands (cf. Fig. 1.4.5.4). The **double helix structure** of DNA was proposed by Watson and Crick (1953). The double helix DNA structure bears two nucleic acid chains which are twisted together about the same axis. It may be noted that the protein helix (proposed by Pauling and Corey, 1951) is single stranded (i.e. one polypeptide chain). The double stranded helix of DNA is stabilised by H-bonding interaction between the DNA bases of the two chains. This Watson-Crick base pairing allows the H-bonding interactions (Figs. 1.4.5.5 and 1.4.5.6) : adenine with thymine (A⋯T), and guanine with cytosine (G⋯C). These H-bonding interactions between the complementary bases constitute the **secondary structure** of DNA (Fig. 1.4.5.6). Orientation of the *planar aromatic rings* of the nucleic bases causes the double helix to *twist* to allow the maximum number of H-bonding interaction between the strands. The strands are *antiparallel to each other* (i.e., the 5′ -end of one strand faces the 3′-end of the other end and vice versa). The *parallel alignment* of the strands does not allow the complementary bases pairing.

The *polar groups* (i.e., sugar moieties and *phosphodiester backbone*) are exposed to the surrounding aqueous medium to allow *hydrophilic interaction*. On the other hand, the relatively hydrophobic nucleic bases are located within the helix and thus these are shielded from water. **These nucleic bases produce both hydrophobic interaction and H-bonding interaction (i.e., Watson-Crick base pairing) to stabilise the DNA structure.** The negative charges of phosphate groups are to be stabilised by the metal ions like Mg^{2+}. The metal ions like Cu^{2+} which interact with the DNA bases will destroy the Watson-Crick base pairing interaction to destabilise the DNA structure. These aspects have been discussed in Sec. 2.3.1.
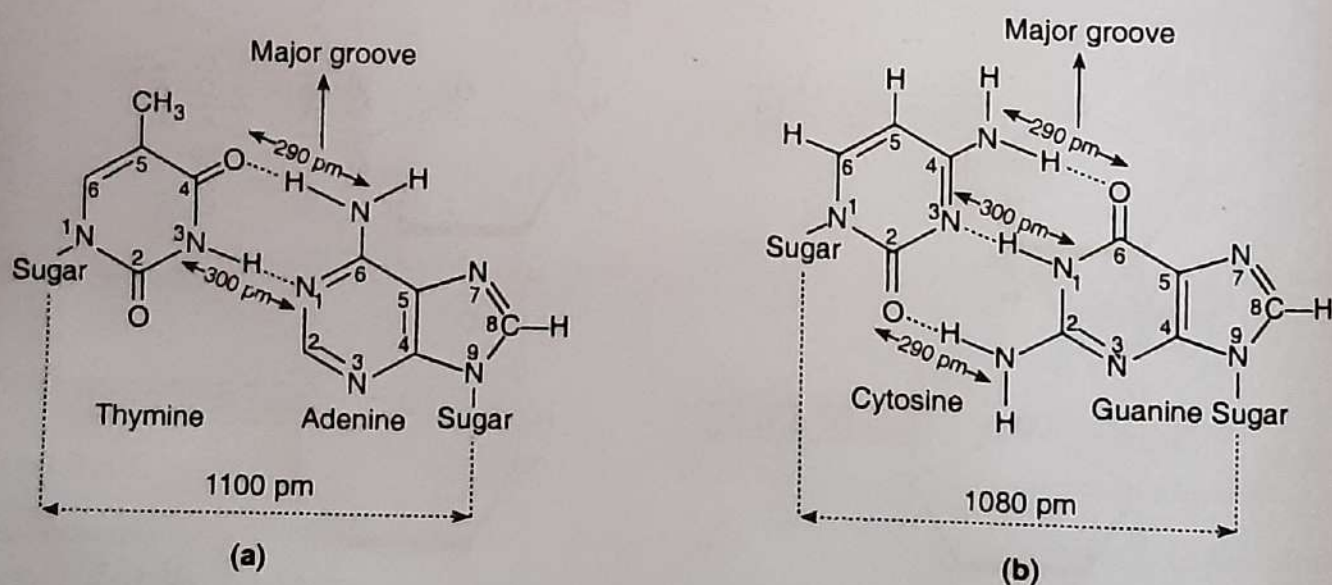

Figure 1.4.5.5 : H-bonding interaction in Watson-Crick base pairs.
(a) Adenine-Thymine interaction; (b) Guanine - Cytosine interaction.

Depending upon *the direction of twist* in the double helix structure of DNA, different conformers like **A, B, Z** are produced (Sec. 2.5.1). They can be identified by considering the interaction (e.g. intercalation) of different metal complexes with the DNA helix. Binding of transition metal complexes with DNA as nucleic acid structural probes has been discussed in detail in Sec. 2.5.

The double helical structure of DNA survies due to H-bonding between the strands. This H-bonding may be ruptured (by chinging the pH, increasing the temperature, metal coordination with DNA-bases, etc.) and then the two strands get separated. The loss of helical structure of DNA is

called **denaturation of DNA** (Fig. 1.4.5.6). It may be noted that in the separated strands, the **phosphodiester bonds** are not broken. *Thus in denaturation, only the H-bonding breaks down but the sugar-phosphate back-bone remains unchanged.*
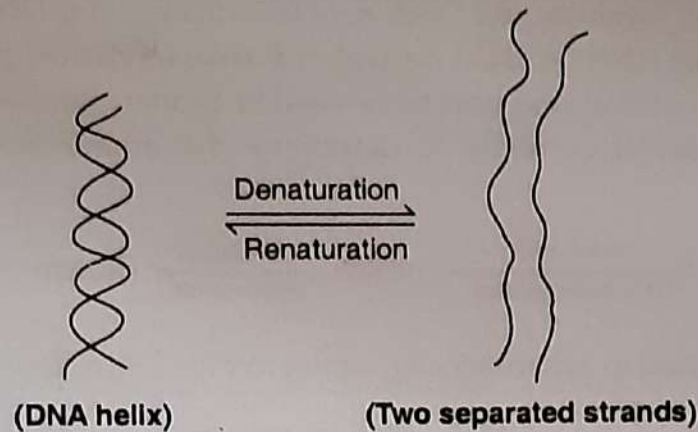

(DNA helix)　　　　　　(Two separated strands)

Figure 1.4.5.6 : *Schematic representation of denaturation and renaturation of DNA.*

In contrast to DNA, RNA helix is *single stranded*. RNA consists of the bases adenine, guanine, cytosine and uracil but no thymine. The RNA molecule is much smaller than the DNA molecule.
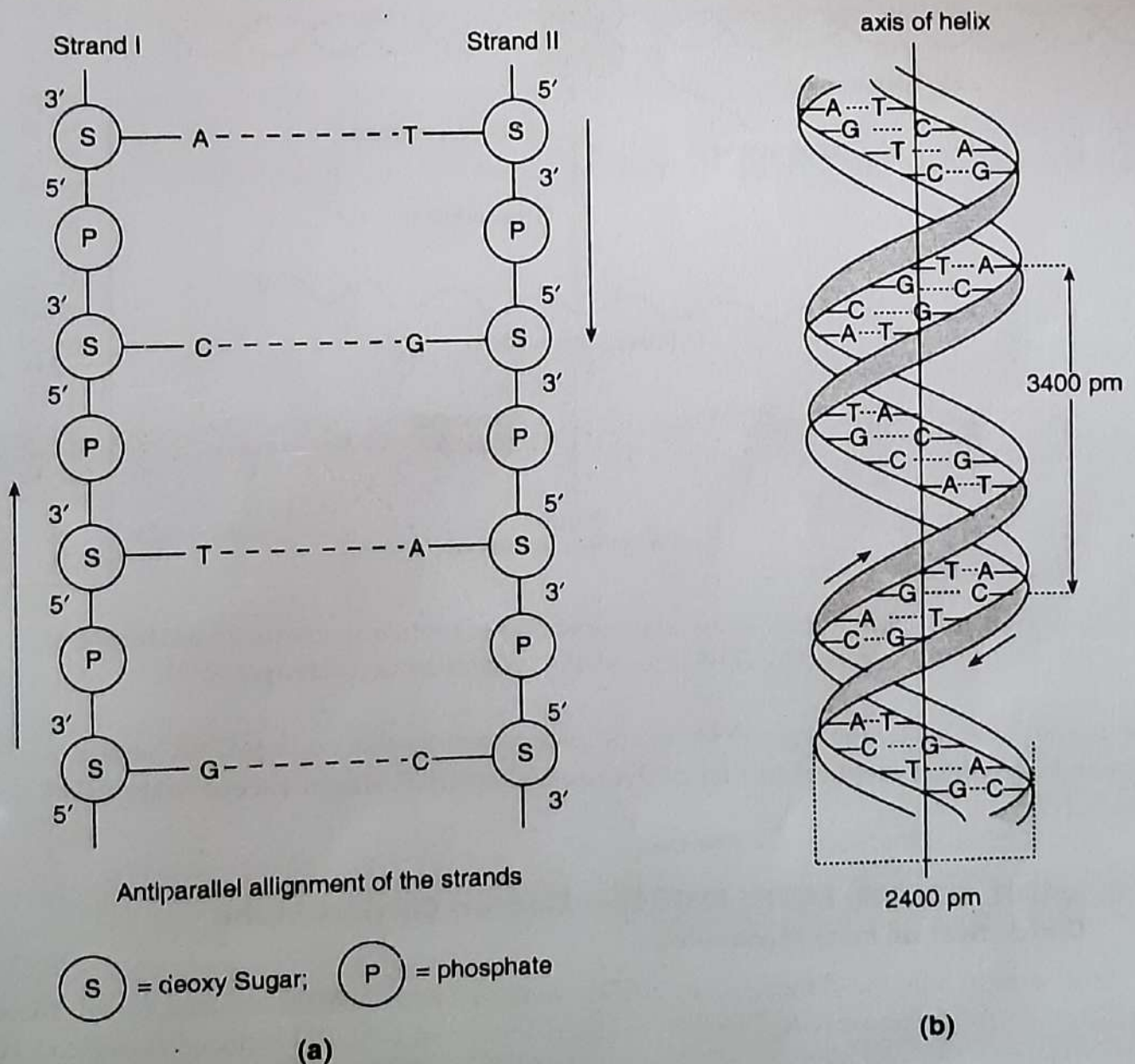

Antiparallel allignment of the strands

$\left(S\right)$ = deoxy Sugar;　$\left(P\right)$ = phosphate

(a)

(b)

Figure 1.4.5.7 : *Double helix structure of DNA.*