

Fragment of ribonucleic acid (RNA) with sequence adenosine (A), guanosine (G), uridine (U), cytidine (C) linked by 3',5'-phosphodiester bonds. Chain direction is from 5'- to 3'-end as shown by arrow. Atom numbering scheme is indicated in one framed nucleotide unit, 5'-GMP. All hydrogen atoms drawn in A and only functional hydrogens in other nucleotides. In short notation, this fragment would be pApGpUpCp or pAGUCp. In deoxyribonucleic acid (DNA), the hydroxyl attached to  $C_{2'}$  is replaced by hydrogen and uracil, by thymine.

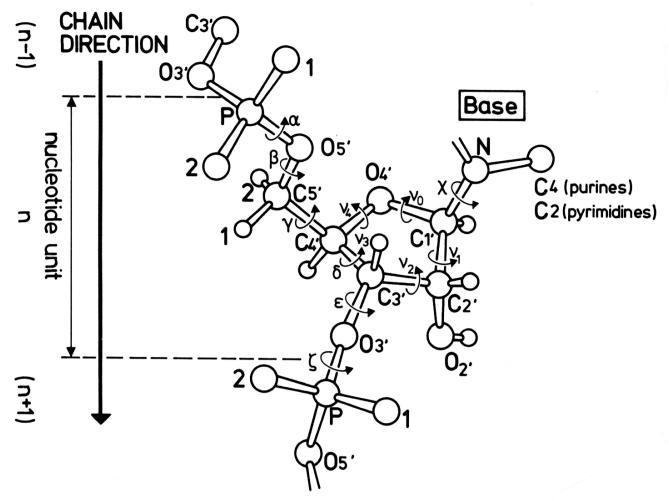


Figure 2-3. Atomic numbering scheme and definition of torsion angles for a polyribonucleotide chain. Counting of nucleotides is from top to bottom, i.e., in the direction  $O_{5'} \rightarrow O_{3'}$ . Hydrogens at  $C_{5'}$  and oxygens at P are differentiated by 1 and 2 according to the rule given in the text. In deoxyribose, the hydrogen replacing  $O_{2'}$  is labeled 1, the other one, 2. For a full description of torsion angles, see Table 2-2.

$$\begin{array}{c} H \\ N_{6} \\ N_{7} \\ \downarrow \\ N_{9} \\ \downarrow \\ N_{3} \\ \end{array}$$

Adenine Ade

Guanine Gua

Cytosine Cyd

Uracil Ura

Thymine Thy

Two minor purines

Nº-Methyladenine

2-Methylguanine

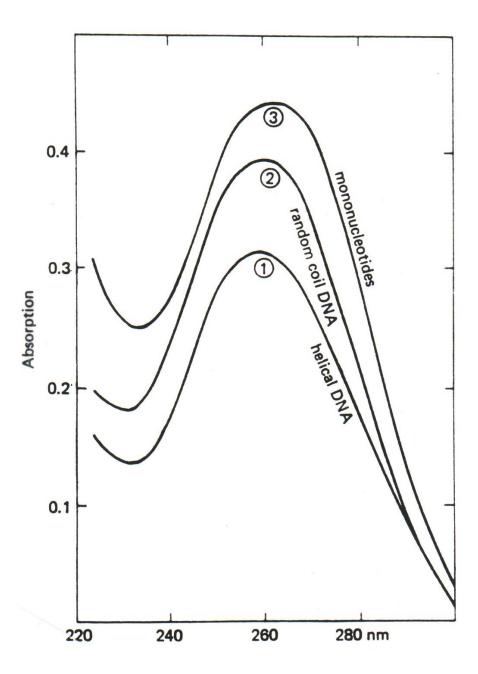
Two minor pyrimidines

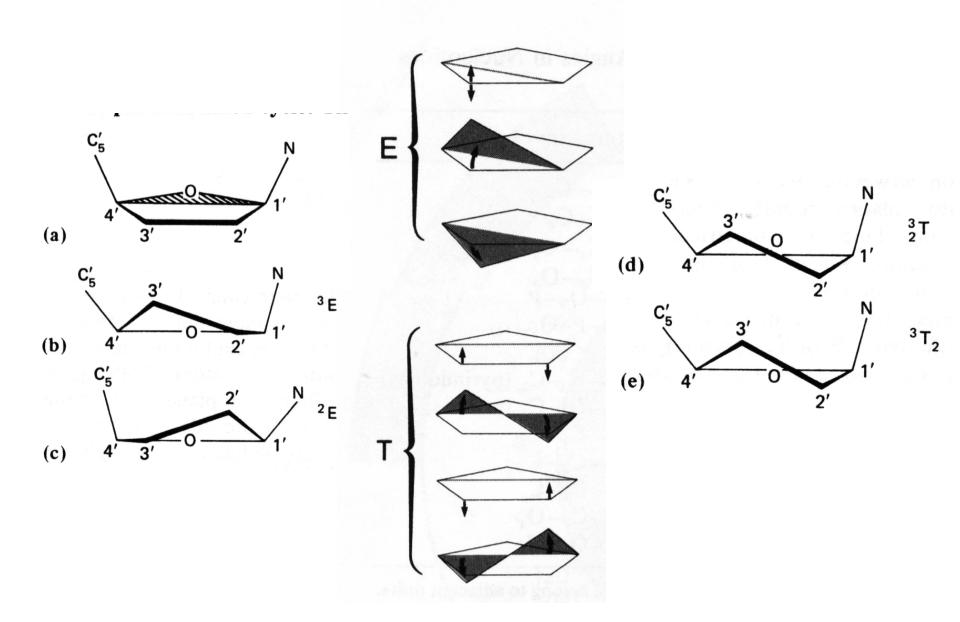
5-Methylcytosine

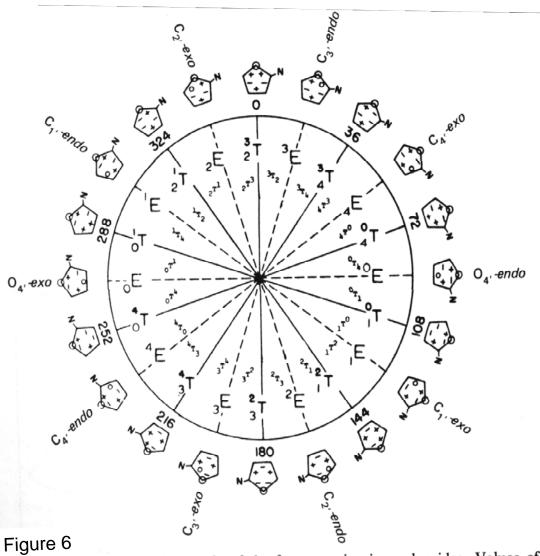
5-Hydroxymethylcytosine

Table 1 Other rare bases found in nucleic acids

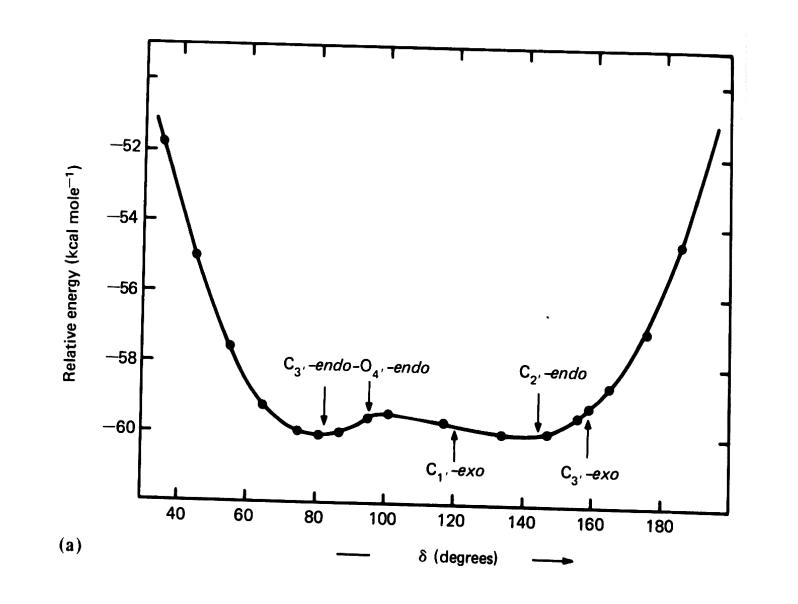
- 5,6-Dihydrouracil
- 1-Methyluracil
- 3-Methyluracil
- 5-Hydroxymethyluracil
- 2-Thiouracil
- N4-Acetylcytosine
- 3-Methylcytosine
- 5-Methylcytosine
- 5-Hydroxymethylcytosine
- 1-Methyladenine
- 2-Methyladenine
- 7-Methyladenine
- Nº-Methyladenine
- Nº Nº Dimethyladenine
- $N^{8}$ - $(\Delta^{2}$ -Isopentenyl)adenine
- 1-Methylguanine
- 7-Methylguanine
- N2-Methylguanine
- Nº Nº-Dimethylguanine







Pseudorotation cycle of the furanose ring in nucleosides. Values of phase angles given in multiples of 36°. Envelope E and twist T forms alternate every 18°. After rotation by 180° the mirror image of the starting position is found. On the periphery of the cycle, riboses with signs of endocyclic torsion angles are indicated. (+) Positive, (-) Negative, (0) angle at 0°. From (31).



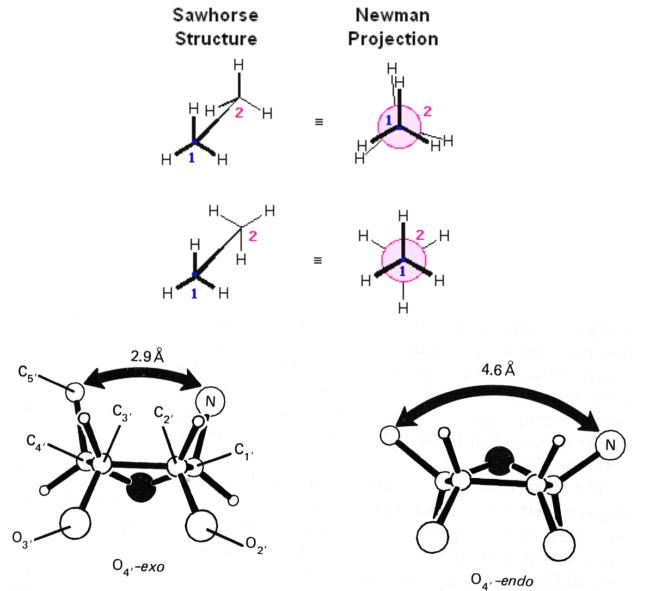
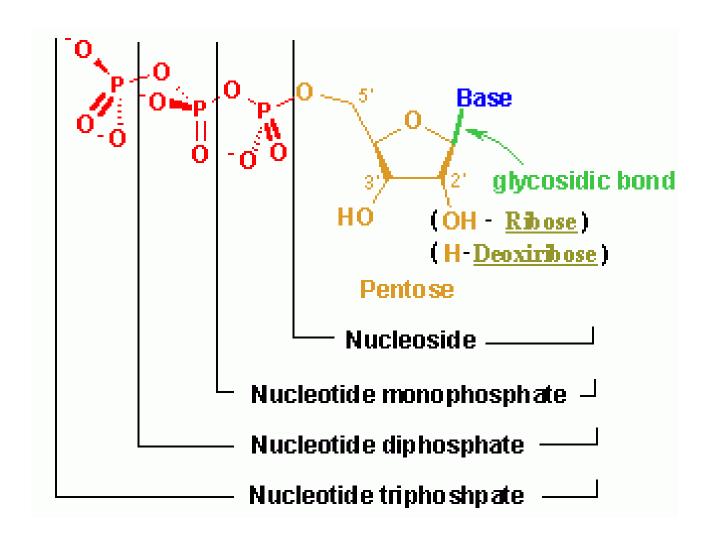


Figure 4-5. Equatorial and axial positioning of substituents N (base) and  $C_{5'}$  in sugar puckering modes  $O_{4'}$ -exo (left) and  $O_{4'}$ -endo (right). In  $O_{4'}$ -exo,  $C_{5'}$  and N interfere sterically and therefore the  $C_{2'}$ -endo  $\rightleftharpoons C_{3'}$ -endo interchange occurs via  $O_{4'}$ -endo as intermediate.



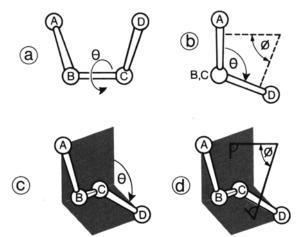


Figure 2-4. Definition of torsion and dihedral angles. (a) Torsion angle  $\theta$  (A-B-C -D) describing orientations of bonds A-B and C-D with respect to the central bond B-C. (b) View along B $\rightarrow$ C.  $\theta$  is the torsion angle between the projected bonds A-B and C-D; the complement  $\phi$  is called the dihedral angle. If A-B and C-D are cis-planar (coinciding in projection), angles  $\theta$  and  $\phi$  are 0°; they are counted positive if the far bond C-D rotates clockwise with respect to the near bond A-B. (c)  $\theta$  is defined as the angle between planes A-B-C and B-C-D. (d) The dihedral angle  $\phi$  represents the angle between normals to these planes.

