

Figure 2-4. Definition of *torsion* and *dihedral* angles. (a) *Torsion* angle θ (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→C. θ is the torsion angle between the projected bonds A–B and C–D; the complement ϕ is called the *dihedral* angle. If A–B and C–D are *cis*-planar (coinciding in projection), angles θ and ϕ are 0° ; they are counted positive if the far bond C–D rotates clockwise with respect to the near bond A–B. (c) θ is defined as the angle between planes A–B–C and B–C–D. (d) The *dihedral* angle ϕ represents the angle between normals to these planes.

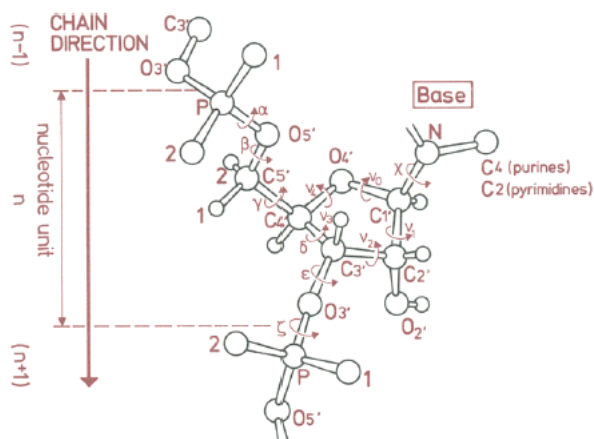


Figure 2-3. Atomic numbering scheme and definition of torsion angles for a polynucleotide chain. Counting of nucleotides is from top to bottom, i.e., in the direction $O_3 \rightarrow O_{3'}$. Hydrogens at $C_{2'}$ and oxygens at P are differentiated by 1 and 2 according to the rule given in the text. 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.

Table 2-2. Definition of Torsion Angles in Nucleotides [From (16).]^a

Torsion angle	Atoms involved
α	${}^{(n-1)}O_{3'}-P-O_{5'}-C_{5'}$
β	$P-O_{5'}-C_{5'}-C_{4'}$
γ	$O_{5'}-C_{5'}-C_{4'}-C_{3'}$
δ	$C_{5'}-C_{4'}-C_{3'}-O_{3'}$
ϵ	$C_{4'}-C_{3'}-O_{3'}-P$
ζ	$C_{3'}-O_{3'}-P-O_{5'}^{(n+1)}$
χ	$O_4-C_1-N_1-C_2$ (pyrimidines) $O_4-C_1-N_9-C_4$ (purines)
ν_0	$C_4'-O_4'-C_1'-C_2'$
ν_1	$O_4'-C_1'-C_2'-C_3'$
ν_2	$C_1'-C_2'-C_3'-C_4'$
ν_3	$C_2'-C_3'-C_4'-O_4'$
ν_4	$C_3'-C_4'-O_4'-C_1'$

^a Atoms designated $(n-1)$ and $(n+1)$ belong to adjacent units.