e) Consequences of Watson-Crick base pair geometry for double helix geometry

Features 1), 2) and 3) in the previous paragraph c) indicate that:

i) base pairs are nearly isomorphous, no matter whether we have A:T(U), T(U):A, G:C or C:G. They can therefore substitute each other without disturbing the geometry of the double helix

ii) the pseudo-dyad symmetry axis requires that the direction of the sugar-phosphate backbone attached to the C1′ of one base is opposite to that attached to the C1′ of the other base. This implies that the two strands of a double helix are antiparallel, and that they are related by (pseudo)-dyad symmetry axes located within each base pair and also (for geometrical reasons) between all base pairs

iii) because the glycosyl bonds are positioned on the same side of the base pair, the sugars are closer together on the (purine N3, pyrimidine O2) side than on the (purine O6/N6, pyrimidine N4/O4) side. This gives rise to a *minor groove* and a *major groove* which determine macroscopically the picture of a double helix (Fig. 14). The dimensions of the grooves can be given in Å units, as defined in chapter 2.2.

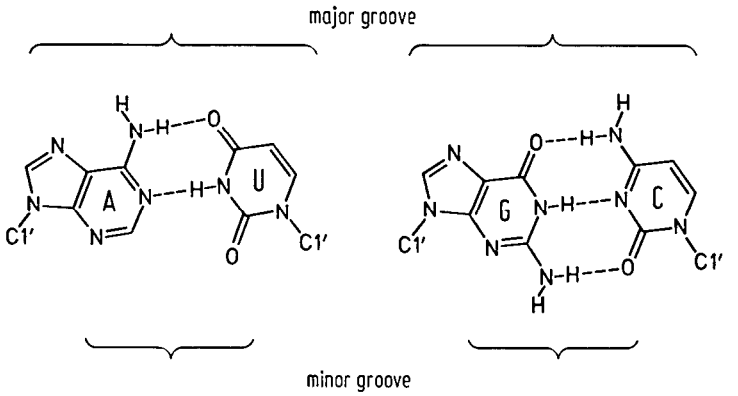


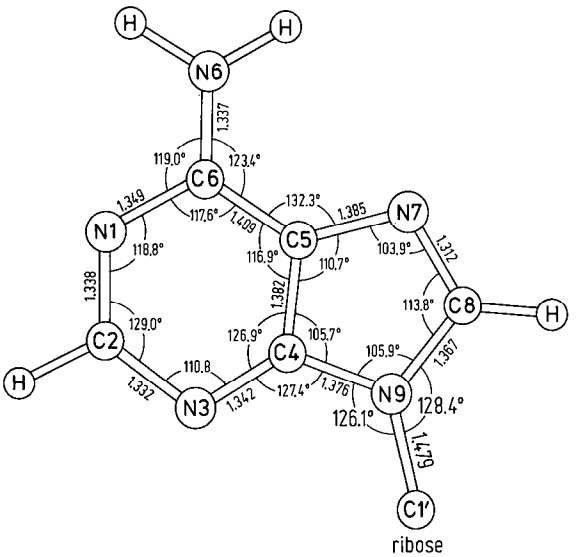
Fig. 14. Schematic description for A:U(T) and G:C base pairs occurring in RNA (DNA). Hydrogen bonds N-H---N and N-H---O indicated by dashed lines. Minor and major groove sides of base pairs are defined [84S1].

f) Base pair propeller, twist, roll, tilt, dislocation, slide

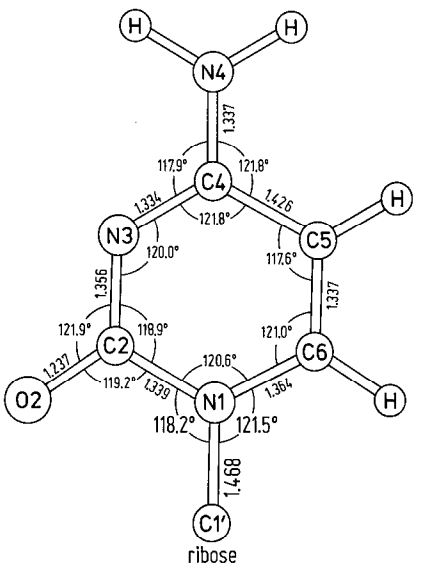
The geometry of a base pair and its position in a double helix and relative to the helix axis is characterized by several parameters. These are all defined in chapter 2.2 and therefore not described here.

1.4 Geometry of bases, sugars, and phosphate groups

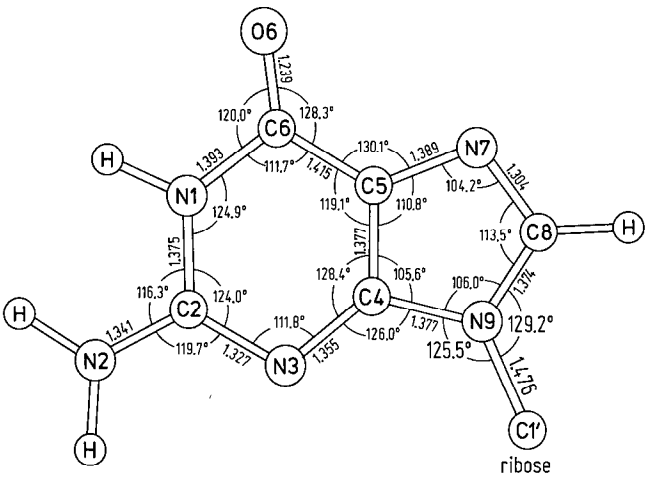
The binding geometry of a molecule is defined by bond angles and bond distances. These parameters were averaged for the base, sugar and phosphate moieties in the four common nucleosides. They are given in Fig. 15a···c, with details indicated in the respective legends. For the phosphate group, Fig. 15c, data are given for (i) deprotonated monophosphate group, (ii) protonated monophosphate group, (iii) phosphodiester group, (iv) protonated pyrophosphate ester group as it occurs in ADP etc. Figs. 15a···c were taken from [84S1].



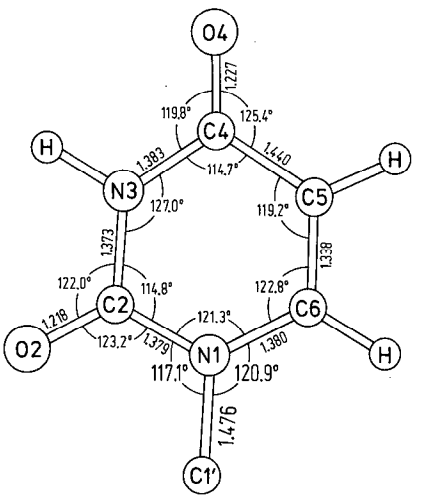
adenine



cytosine



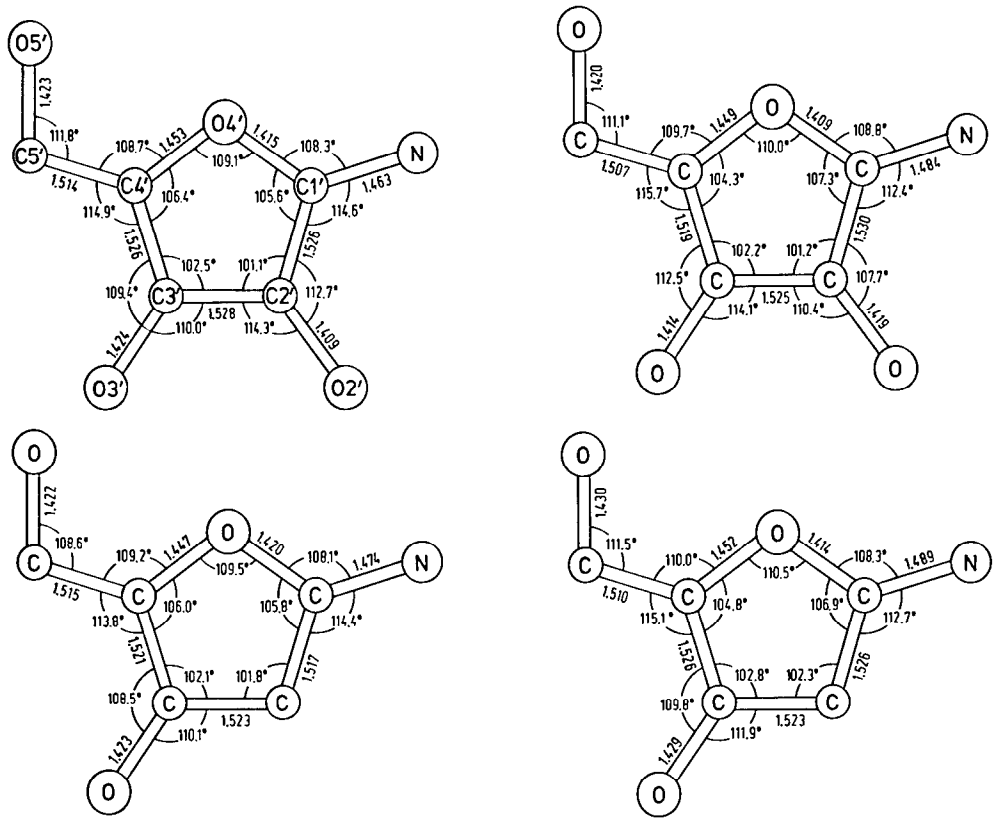
guanine



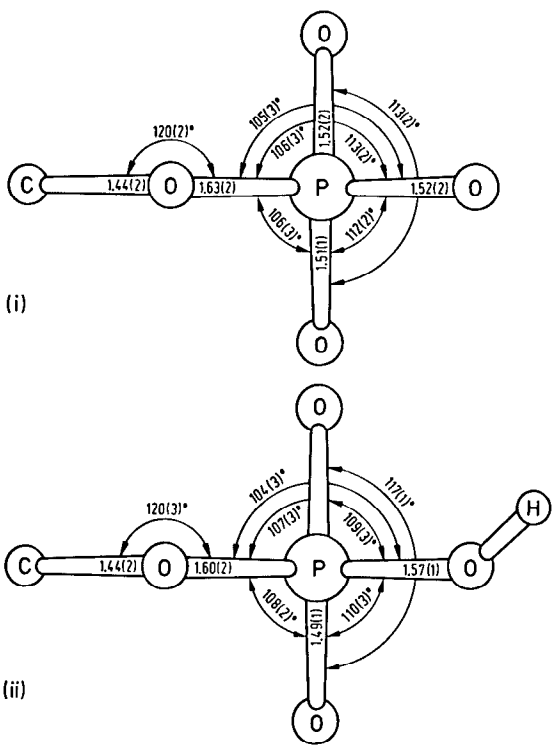
uracil

a

Fig. 15a···c. Average bond angles (in degrees) and distances (in Å) for the constituents of nucleotides. (a) Geometrical data for 1-substituted cytosine and uracil and for 9-substituted adenine and guanine. Data are from [82T1]; standard deviations are defined as $\sigma=[\Sigma(X_i-\bar{X})^2/(N-1)]^{1/2}$, where X_i and $\bar{X}$ denote individual and mean values, and N is the number of observations. For angles, σ's are in the range 0.3°···1°, and for distances, 0.005···0.016 Å. N is 32 for uracil, 14 for cytosine, 21 for adenine, and 7 for guanine. Data in capital numbers involve glycosyl C–N linkages taken from [70V1]. They are less accurate because they depend on orientation of base and on furanose pucker [84S1]. (b) Geometrical data for ribose and deoxyribose in nucleosides with C2′-*endo* and C3′-*endo* puckering. For other averaged data, see [72A1]. Data are averages obtained from well-refined crystal structures ($R<0.08$); standard deviations σ calculated according to formula given in legend to (a). For C2′-*endo* and C3′-*endo* riboses, $N=35$, $\sigma_{distances}=0.006\cdots0.014$ Å, $\sigma_{angles}=0.6\cdots2.3°$, for C2′-*endo* deoxyribose, $N=7$, $\sigma_{distances}=0.009\cdots0.018$ Å, $\sigma_{angles}=0.5°\cdots3.2°$, for C3′-*endo* deoxyribose, $N=8$, $\sigma_{distances}=0.007\cdots0.024$ Å, $\sigma_{angles}=0.5°\cdots2.1°$ [84S1]. (c) Geometrical data for phosphate mono- and diesters and pyrophosphate. Data for monoesters from [82T1]; those for diesters and pyrophosphate ester from [79A1]. Standard deviations σ obtained with formula given in legend to (a) are presented in parentheses. Numbers of observations, N, are 11 and 15 for monoester di- and monoanion (i) and (ii), respectively, 33 for diester (iii), and 4 for pyrophosphate ester (iv) [84S1].



b



c

Fig. 15b, c. For figure caption, see p. 19.

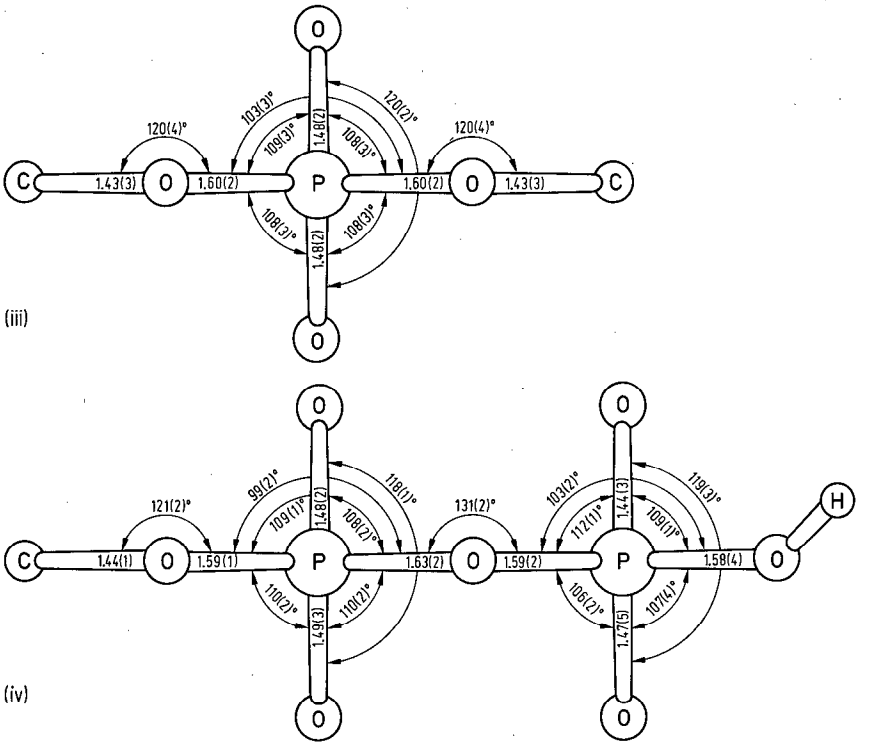


Fig. 15c, continued.

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