

APPENDIX 1: Structures of Base Pairs Involving at Least Two Hydrogen Bonds

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The structures of 29 possible base pairs that involve at least two hydrogen bonds are given in Figures 1–5 (for further descriptions, see Saenger, in *Principles of nucleic acid structure*, p. 120. Springer-Verlag [1984]). A base pair that is not a Watson-Crick pair or a G·U wobble pair is called a base-base mismatch, or an internal loop of two nucleotides. All the base pairs can be divided into two classes: normal and flipped. The normal class is defined by the arrangement of the Watson-Crick base pairs. The hydrogen bonding occurs for nucleotides with antiparallel strands and *anti* orientation of the bases relative to the ribose rings. The 11 base pairs that can be made with this same arrangement of nucleotides are called normal; they are shown in Figures 1 and 2. The remaining 18 base pairs require that one of the bases be flipped (inverted) by either reversing the direction of the strand or by switching the base from *anti* to *syn*. (Figs. 3–5). Normal base-base mismatches are found more often than flipped mismatches.

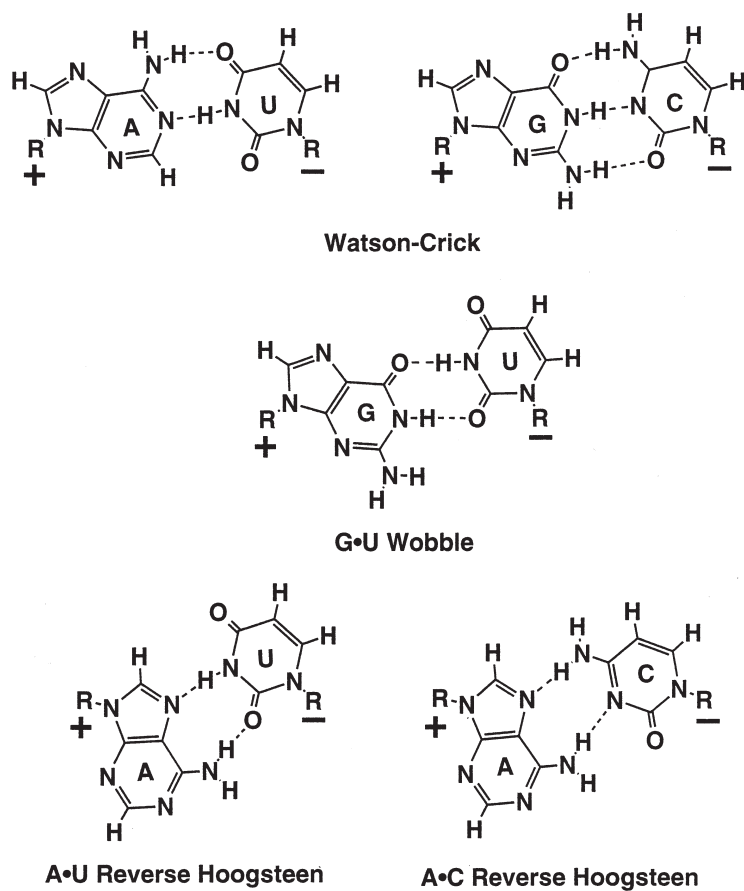


Figure 1 Five possible **normal** purine-pyrimidine base pairs. The Watson-Crick A·U, Watson-Crick G·C, and G·U wobble pairs fit into a double helix with very little distortion; A·U and A·C reverse Hoogsteen are mismatches. The plus and minus signs represent the direction of the strands (antiparallel) for *anti* nucleotides. The same orientation of each base can be obtained by reversing the direction of the strand and rotating the base around the glycosidic bond to *syn*.

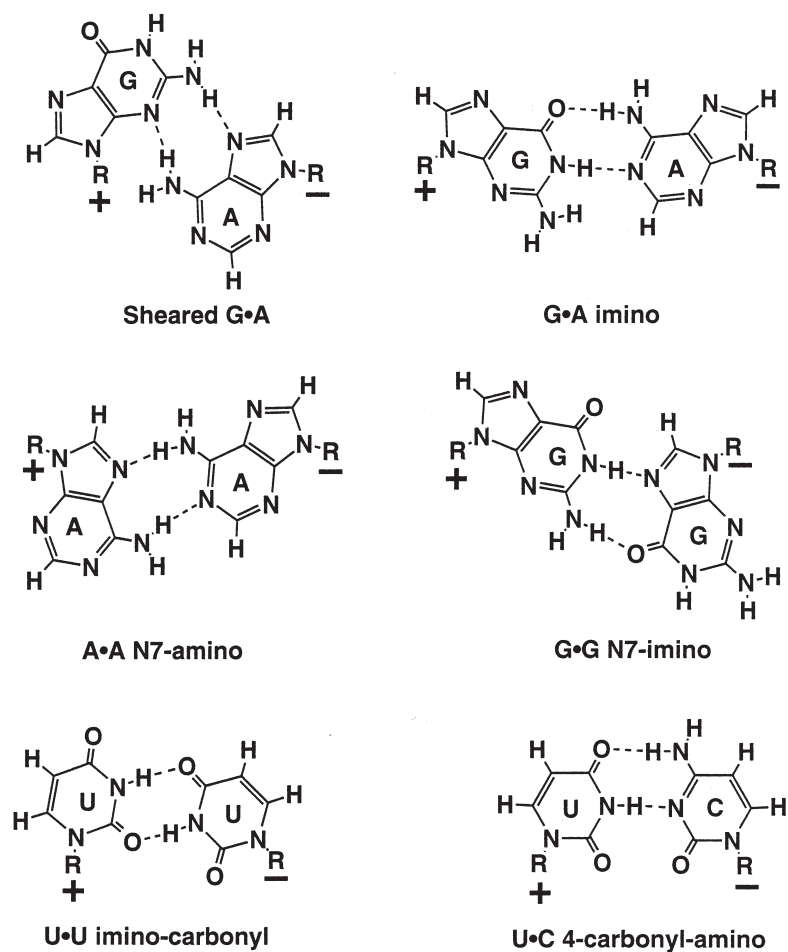


Figure 2 Six possible **normal** purine-purine and pyrimidine-pyrimidine base pairs. The plus and minus signs represent the direction of the strands for *anti* nucleotides. The significance of the pluses and minuses is clear from the fact that no rotation of the bases in the plane of the figure can superimpose, for example, a +A base on a -A base. To superimpose two bases, either one strand must be reversed or the base must be changed from *anti* to *syn*. Sheared and imino G•A mismatches are found often in RNA structures.

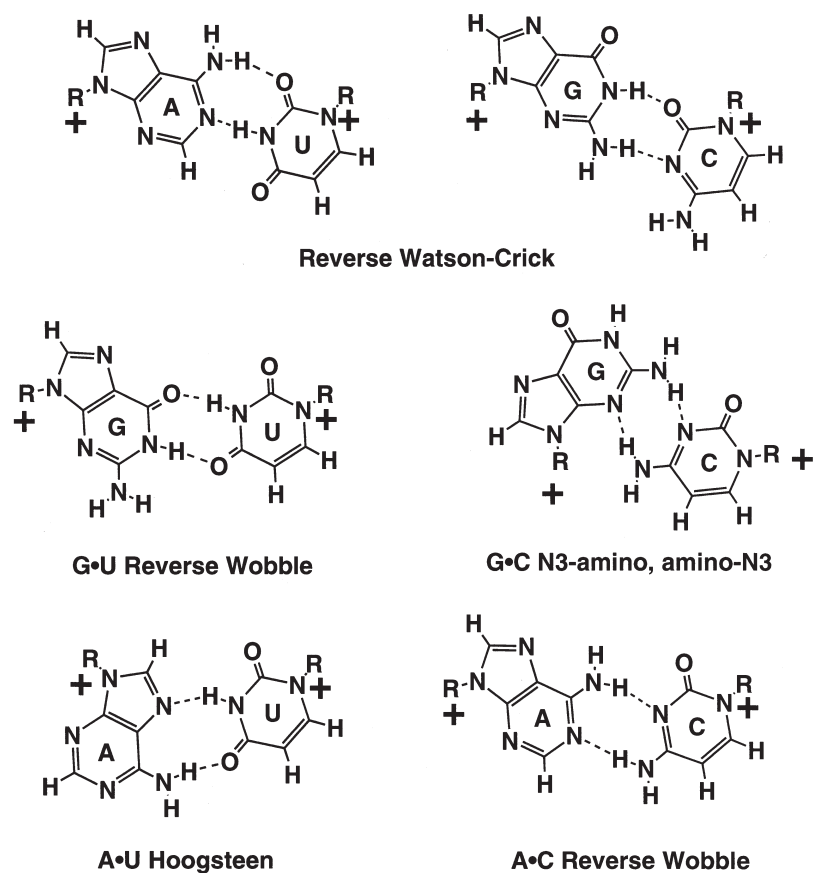


Figure 3 Six possible **flipped** purine-pyrimidine mismatches. Note that all the nucleotides are labeled +. Each base pair could as well have been rotated 180° around an axis in the plane of the figure and labeled -. These base pairs can be formed from parallel strands with *anti* bases, or from antiparallel strands with one base changed to *syn*. *Syn* bases are higher energy conformations than *anti* bases.

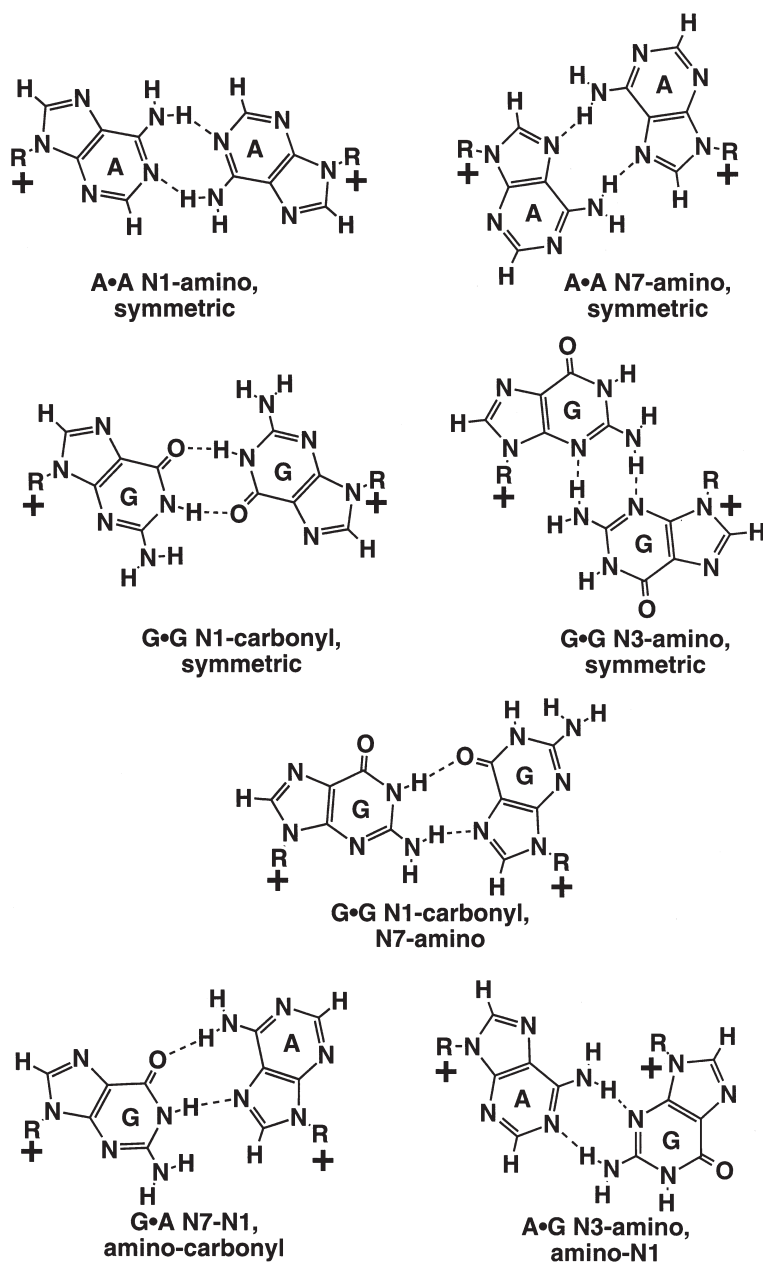


Figure 4 Seven possible **flipped** purine-purine mismatches. Note that all the nucleotides are labeled +. Each base pair could as well have been rotated 180° around an axis in the plane of the figure and labeled -. These base pairs can be formed from parallel strands with *anti* bases, or from antiparallel strands with one of the purine bases changed to *syn*. *Syn* purines are higher energy than *anti* purines, but they have been found in several RNA molecules.

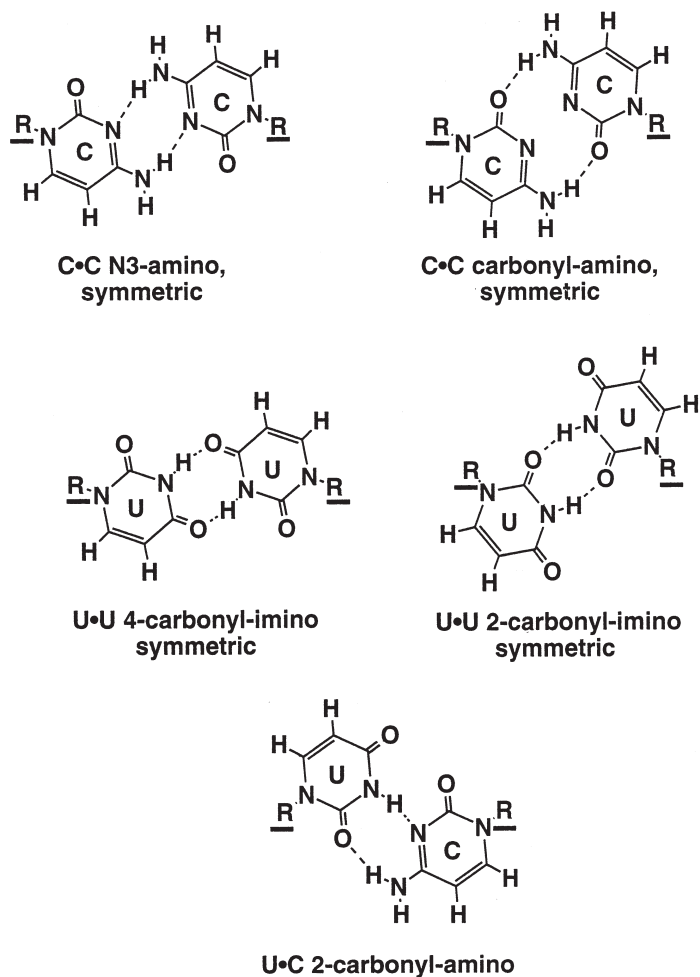


Figure 5 Five possible **flipped** pyrimidine-pyrimidine mismatches. Note that all the nucleotides are labeled -. Each base pair could as well have been rotated 180° around an axis in the plane of the figure and labeled +. These base pairs can be formed from parallel strands with *anti* bases, or from antiparallel strands with one of the pyrimidine bases changed to *syn*. *Syn* pyrimidines are high-energy conformations that have been very rarely identified, but they do occur.