Sugar

5' end

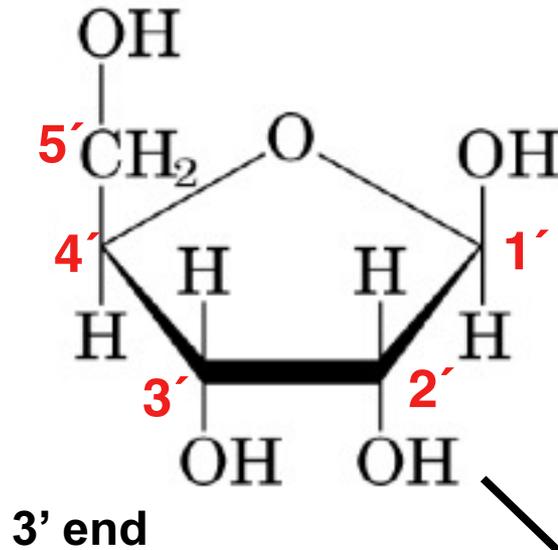**Ribose: (RNA)**

3' end

or

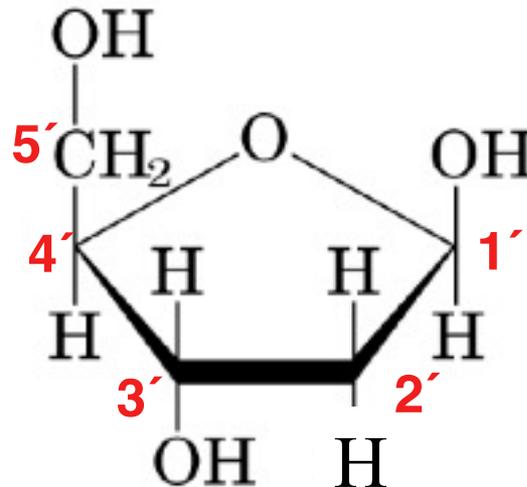**Deoxyribose: (DNA)**

Numbering is the same in DNA and RNA

Numbering of carbons: C1′, C2′...
(′ used to prevent confusion with the numbering of atoms in bases).

The base is connected at the 1' position.

The presence of the **2′OH** confers special chemical reactivity and structural properties to RNA compared to DNA

The sugar is not actually flat!
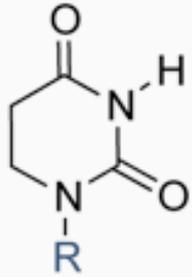
PyMol: G_C3'endo.pse
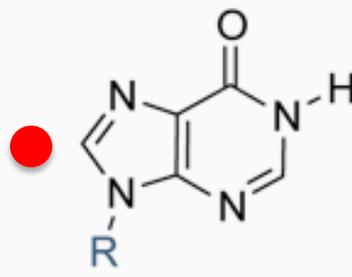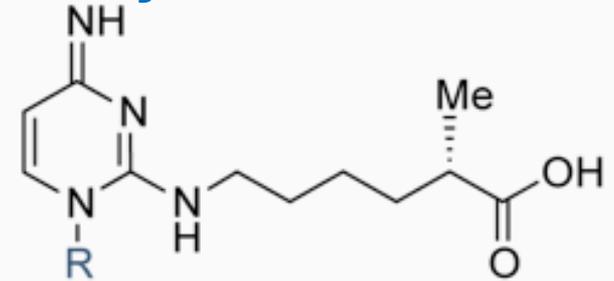
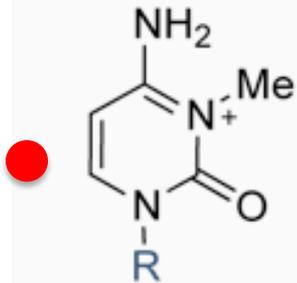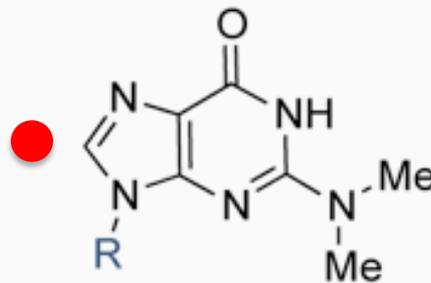# RNA (and to some extent DNA) can contain chemically modified bases which can impact the ability to form H-bonds
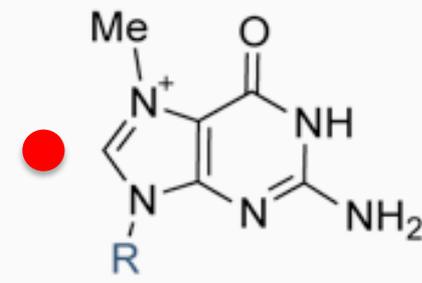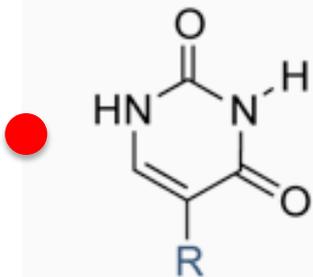

dihydrouridine

inosine

lysidine

3-methylcytidine

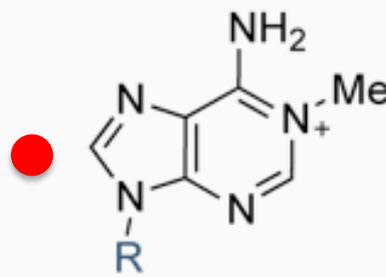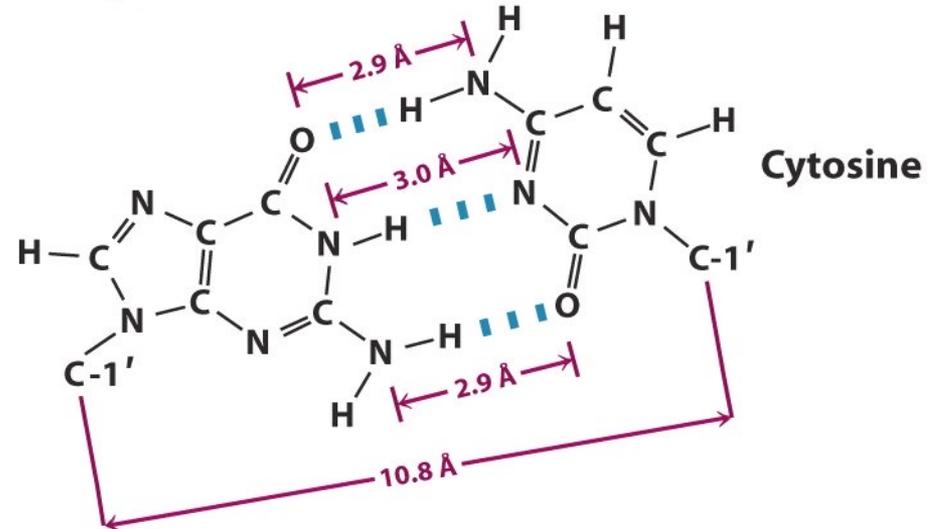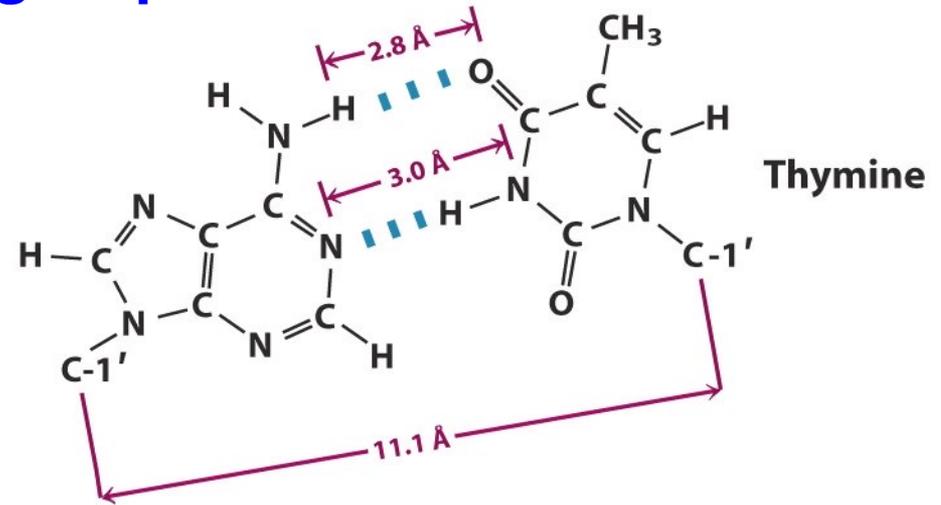N(2)-dimethylguanosine

7-methylguanosine

pseudouridine

1-methyladenosine

Modifications generated by modifying enzymes on the polymers

● **= structures need to be known**

R = ribose

Watson-Crick base pairs: complementary sets of donors and acceptor groups on bases
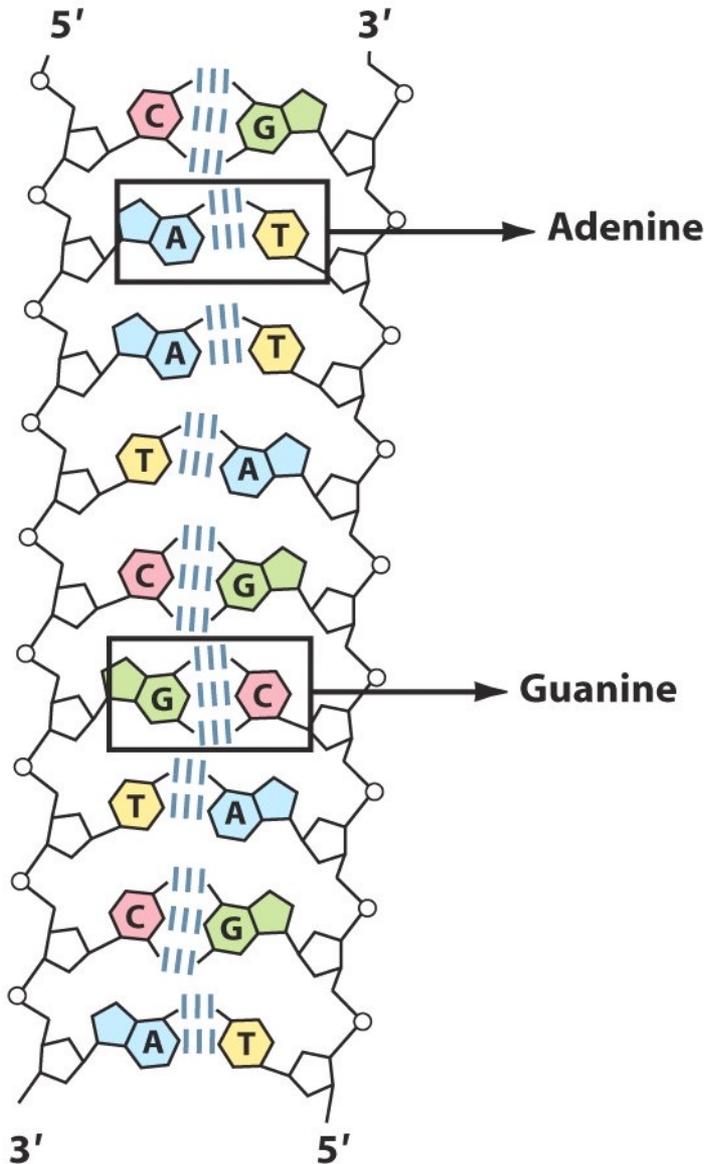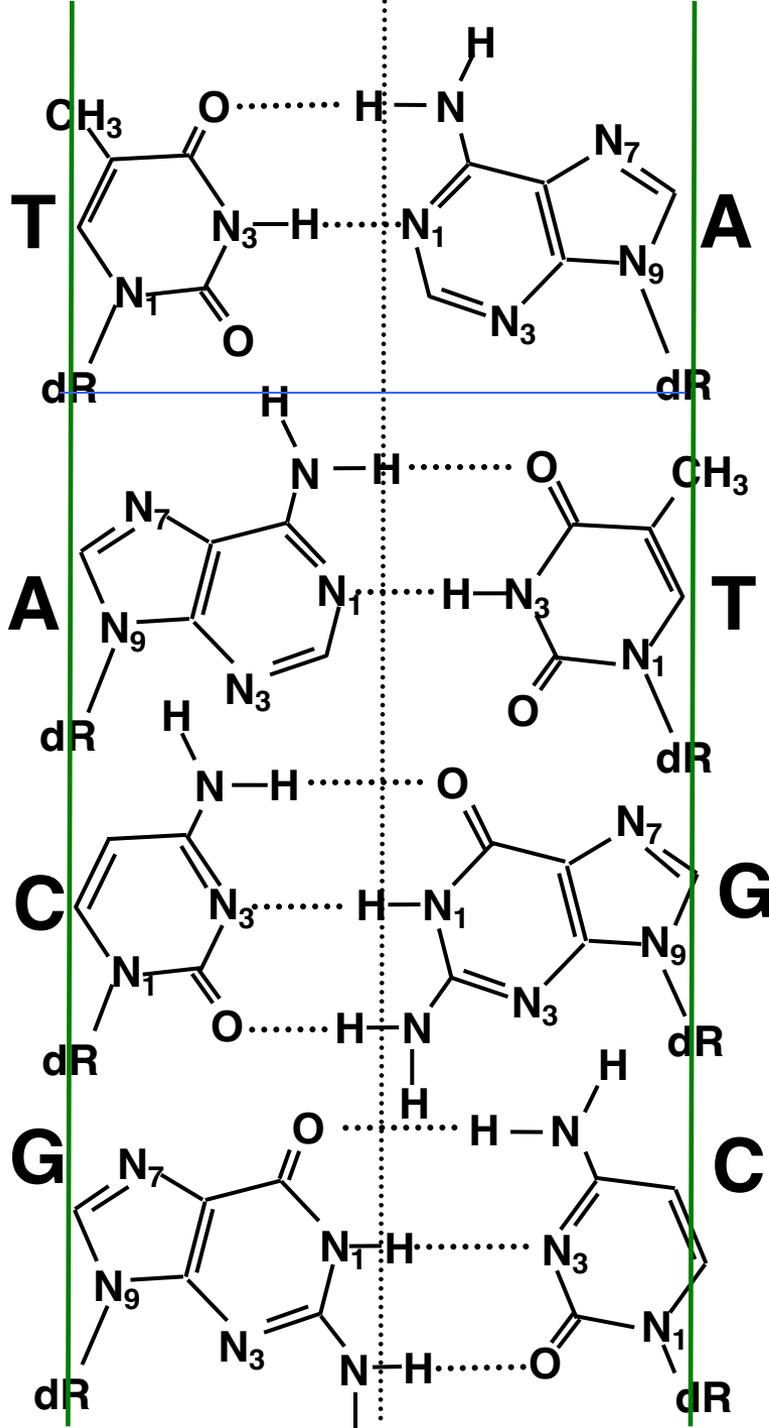
Isostericity of Watson-Crick Base Pairs (and non isostericity of non WC base pairs)

Example of a G-T non WC base pair
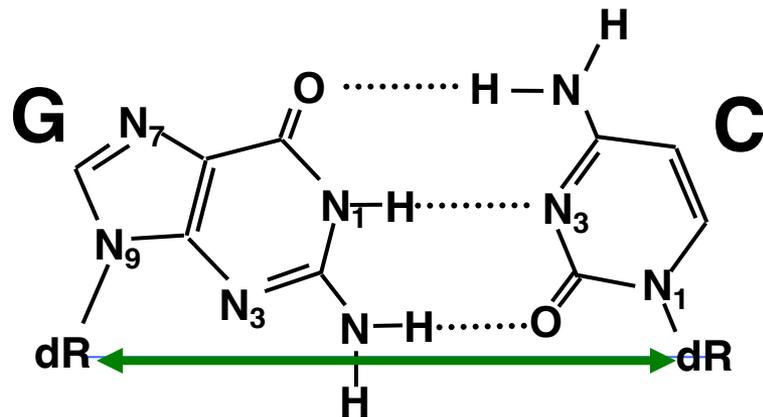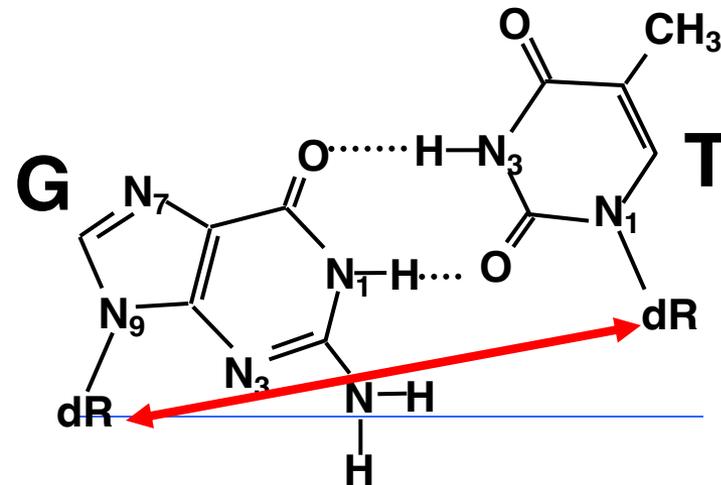
RNA secondary structure dot bracket notation

- Unpaired nucleotides are represented as dots
- Base pairs are represented as parentheses (Watson-Crick pairs)

GGCACUAGAUAACUAGGUGCC

((((((((. . . .))) .)))))

Predicting RNA secondary structure

Nearest neighbor parameters

Table 4: RNA Thermodynamic Parameters for INN-HB Nearest-Neighbor Model, 1 M NaCl, pH 7[a]

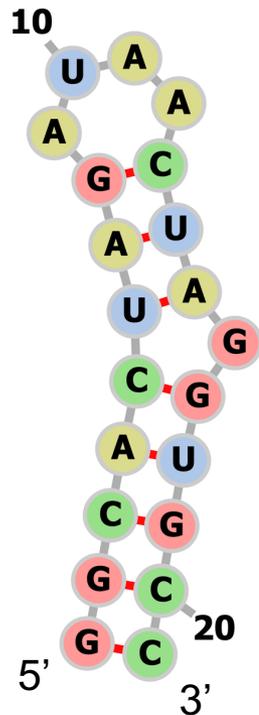| parameters	$\Delta G°_{37}$ (kcal/mol)
5'AA3' 3'UU5'	−0.93
5'AU3' 3'UA5'	−1.10
5'UA3' 3'AU5'	−1.33
5'CU3' 3'GA5'	−2.08
5'CA3' 3'GU5'	−2.11
5'GU3' 3'CA5'	−2.24
5'GA3' 3'CU5'	−2.35
5'CG3' 3'GC5'	−2.36
5'GG3' 3'CC5'	−3.26
5'GC3' 3'CG5'	−3.42

Xia et al. *Biochemistry* **37**, 14719-14735 (1998)

**There are also some parameters for terminal base pairs, hairpins, etc. that we are ignoring here

AUUAGCCGUAAUCGGC

((((. . . .)))) . . . .
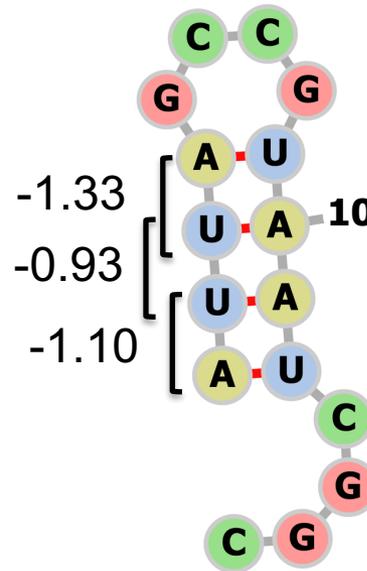
ΔG = -1.10 + -0.93 + -1.33

ΔG = -3.36 kcal/mol

Predicting RNA secondary structure

Nearest neighbor parameters

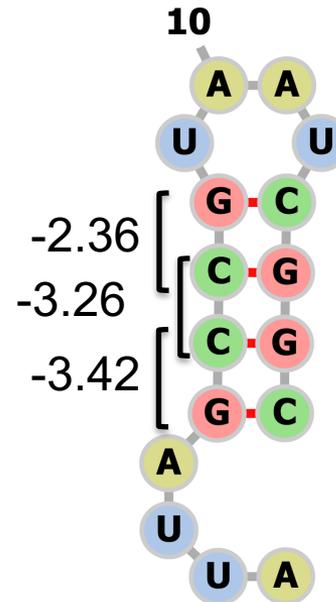Table 4: RNA Thermodynamic Parameters for INN-HB Nearest-Neighbor Model, 1 M NaCl, pH 7[a]

parameters	ΔG°_{37} (kcal/mol)
5′AA3′ 3′UU5′	−0.93
5′AU3′ 3′UA5′	−1.10
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5′GA3′ 3′CU5′	−2.35
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5′GG3′ 3′CC5′	−3.26
5′GC3′ 3′CG5′	−3.42

Xia et al. *Biochemistry* **37**, 14719-14735 (1998)

AUUAGCCGUAAUCGGC
. . . . ((((. . . .))))

ΔG = -3.42 + -3.26 + -2.36
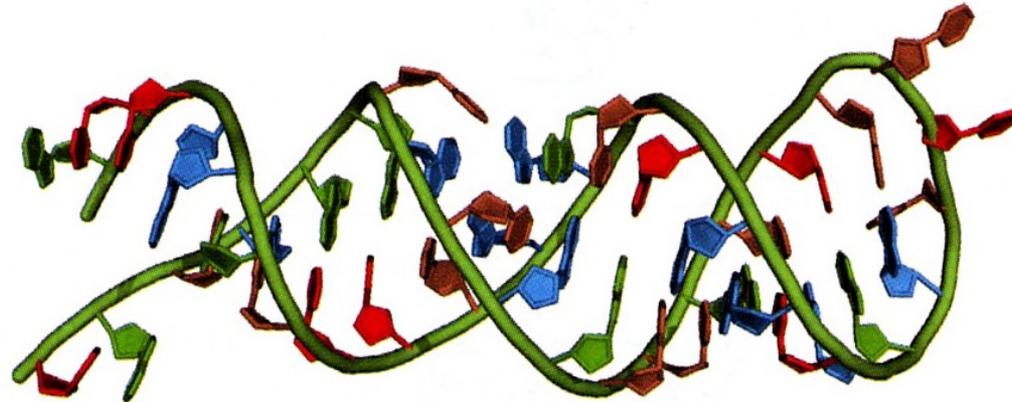
ΔG = -9.04 kcal/mol

RNAfold WebServer: http://rna.tbi.univie.ac.at/cgi-bin/RNAWebSuite/RNAfold.cgi
RNAeval WebServer: http://rna.tbi.univie.ac.at/cgi-bin/RNAWebSuite/RNAeval.cgi

Secondary and Tertiary Structure of RNA

Basic elements of Secondary Structure in RNAs:
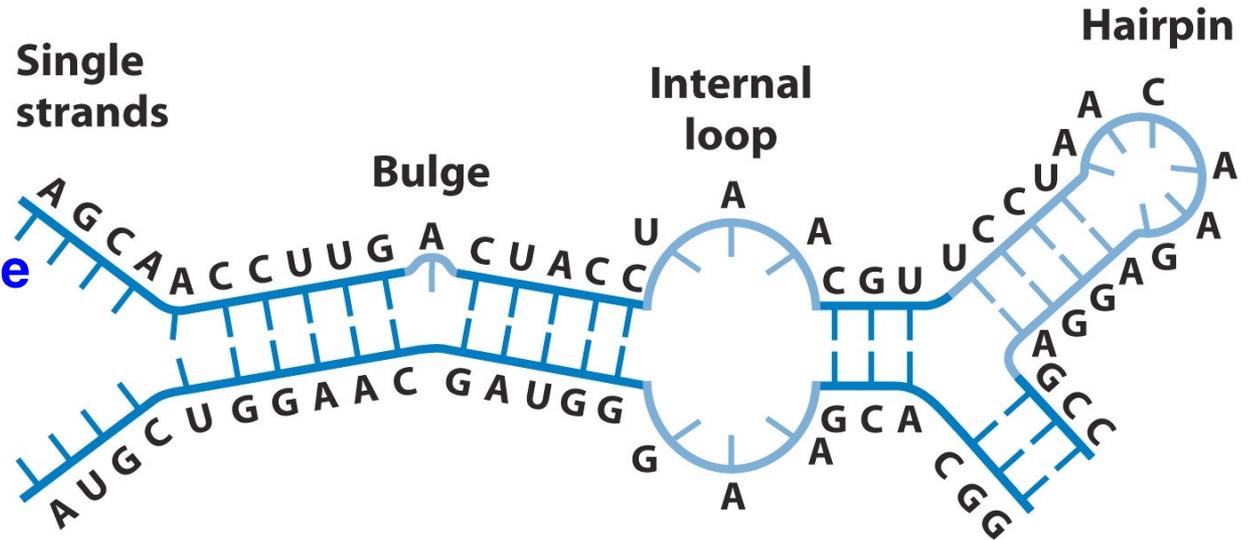
A hairpin segment in pseudo 3D:

Single strandedness nature of RNA makes it able to "fold" on itself and base-pair with complementary segments within the same molecule