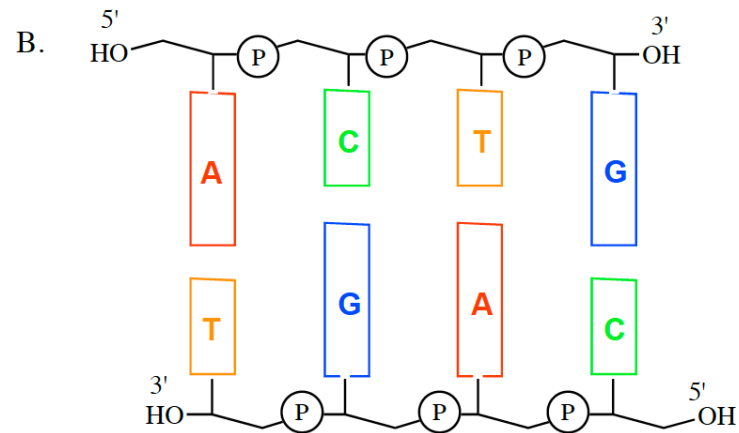
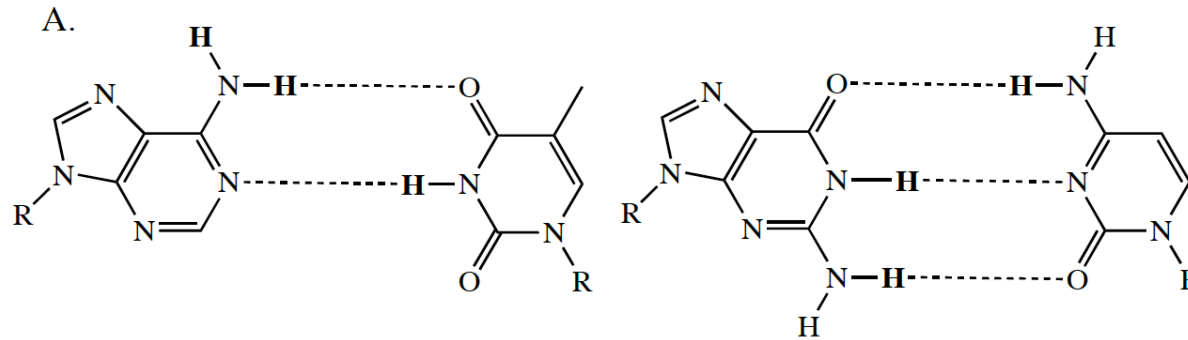
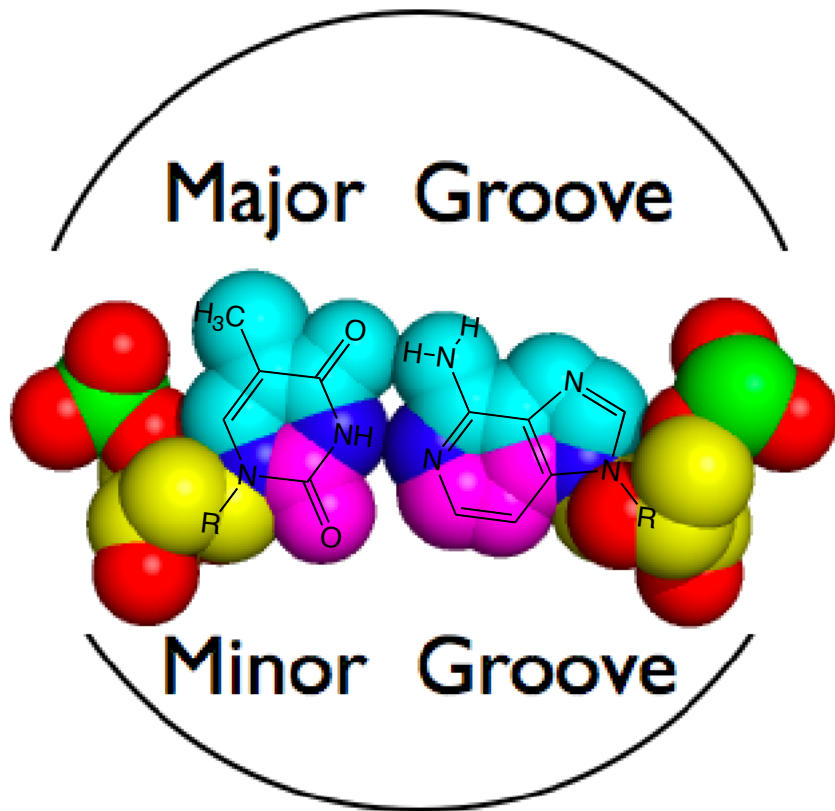


# Watson-Crick Base Pairing

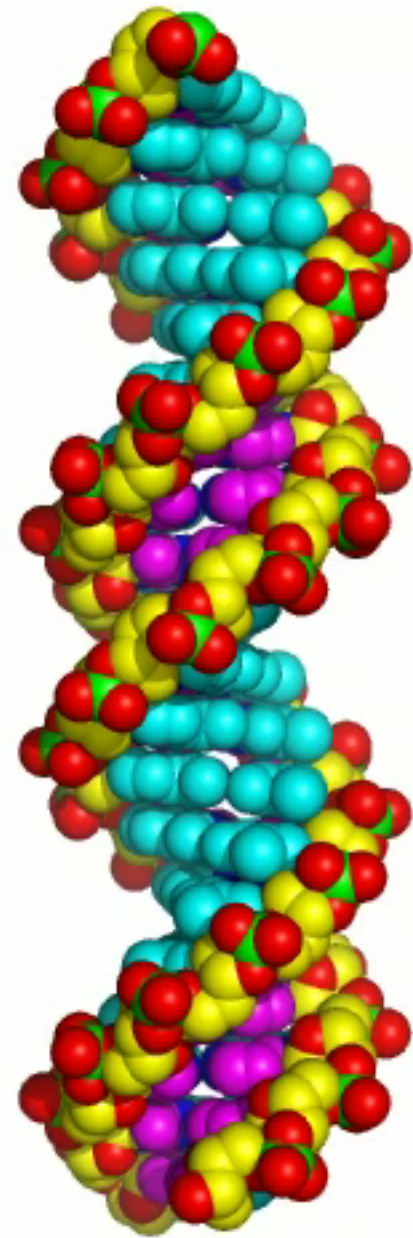


# DNA Duplex



Minor Groove

Major Groove



# Stability and Sequence

**Table N. 2.** Table<sup>a</sup> of thermodynamic data for contributions made by base pair doublets in duplex melting. Each sequence can be seen as two dinucleotides that complement each other. For example, AT/TA is 5'-AT-3'/3'-TA-5'.

	$\Delta H_{\text{melt}}$ (kcal/mol)	$\Delta S_{\text{melt}}$ (cal/molK)	$\Delta G_{\text{melt}}$ (kcal/mol)
AT/TA	7.2	20.4	1.1
TA/AT	7.2	21.3	0.9
CT/GA	7.8	21	1.5
AA/TT	7.9	22.2	1.3
GG/CC	8	19.9	2.1
GA/CT	8.2	22.2	1.6
GT/CA	8.4	22.4	1.7
CA/GT	8.5	22.7	1.7
GC/CG	9.8	24.4	2.5
CG/GC	10.6	27.2	2.5

<sup>a</sup>. SantaLucia (1998) *Proc. Natl. Acad. Sci. USA* **95**, 1460-5.

### Direct Measurements of Base Stacking Interactions in DNA by Single-Molecule Atomic-Force Spectroscopy

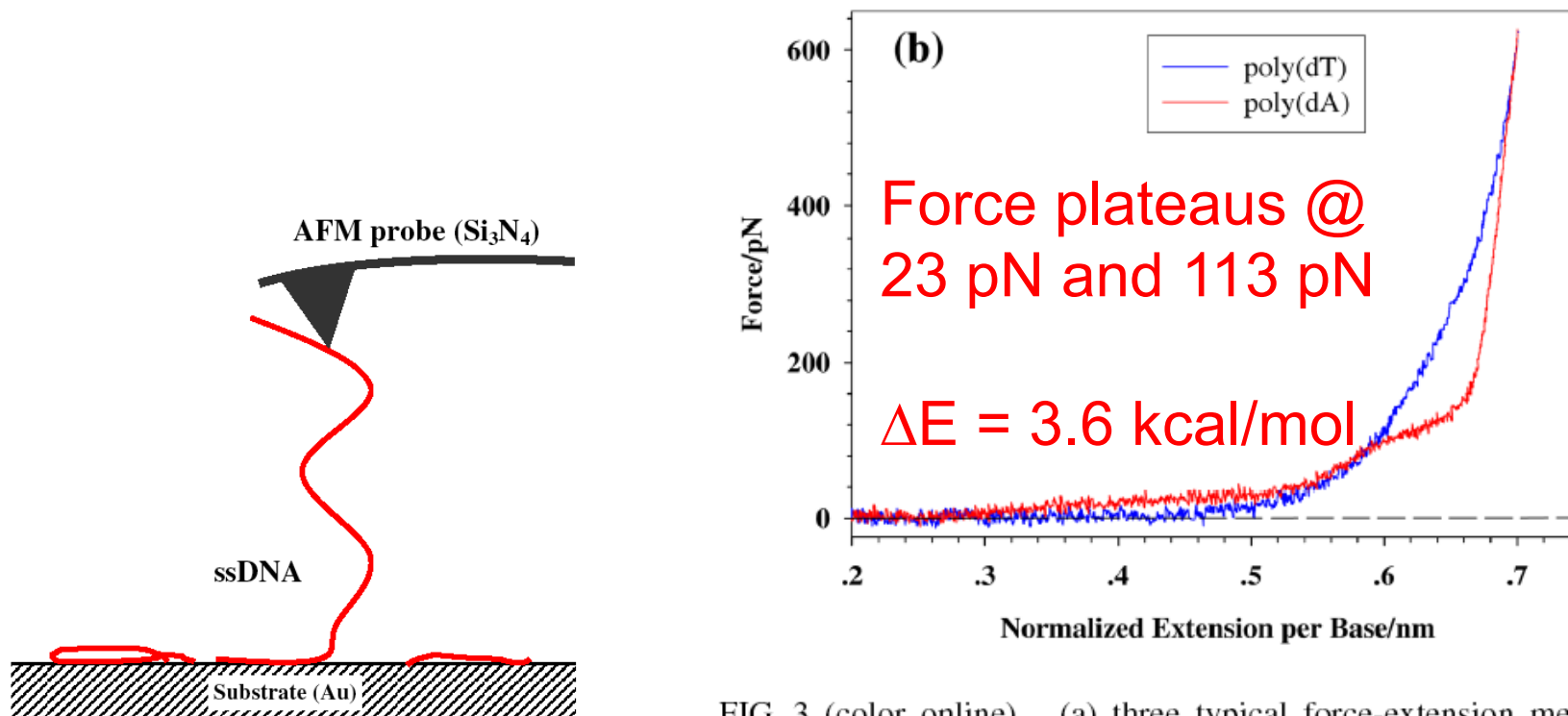
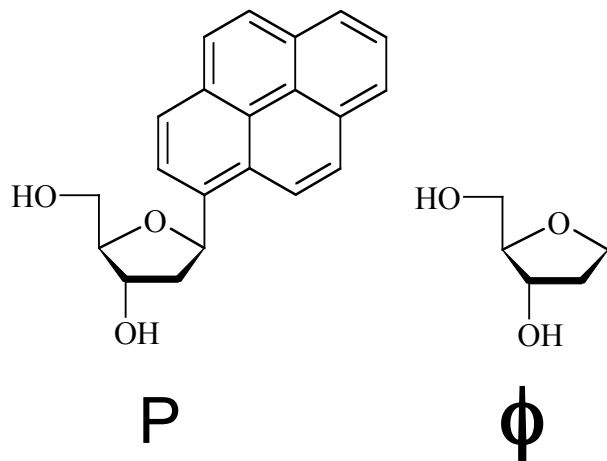


FIG. 1 (color online). Schematic of single-molecule atomic-force microscopy measurements of ssDNA molecules (the figure is not to scale).

FIG. 3 (color online). (a) three typical force-extension measurement curves for poly(dT), (b) comparison between poly(dA) and poly(dT) on a normalized extension basis. We assume that at a force of 600 pN, ssDNA is fully stretched, and the distance between two neighboring phosphates is 0.7 nm.

# Base Stacking and Stability



Duplex	$T_m$ ( $^{\circ}\text{C}$ )	$\Delta G_{\text{melt}}$ (kcal/mol)
5' CTTTTCTTTCTT 3' GAAAAGAAAGAA	43.2	12.6
5' CTTTTC $\phi$ TTCTT 3' GAAAAGAAAGAA	22.0	7.0
5' CTTTTC $\phi$ TTCTT 3' GAAAAG $P$ AAGAA	41.6	12.1

Matray and Kool (1998) *JACS* 120, 6191

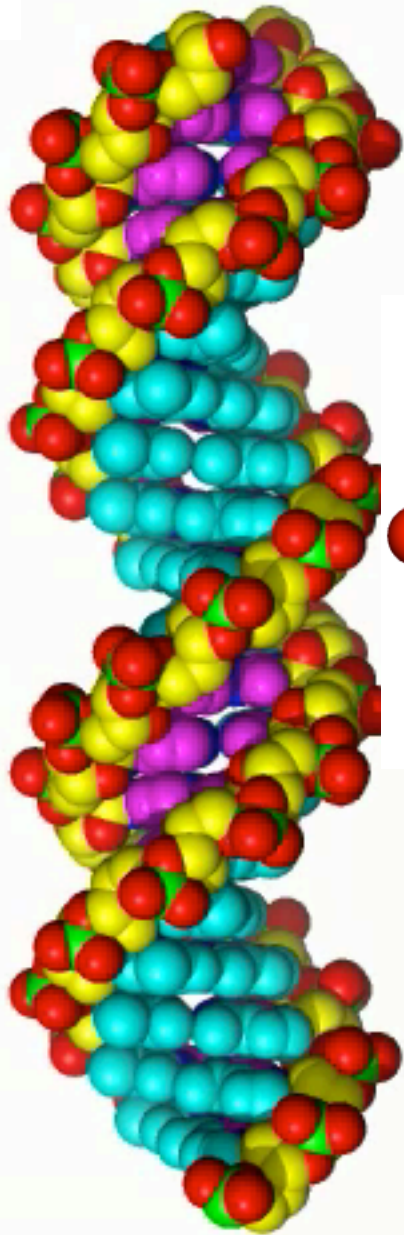
# The Overhang Experiment

5' – XCGCGCG

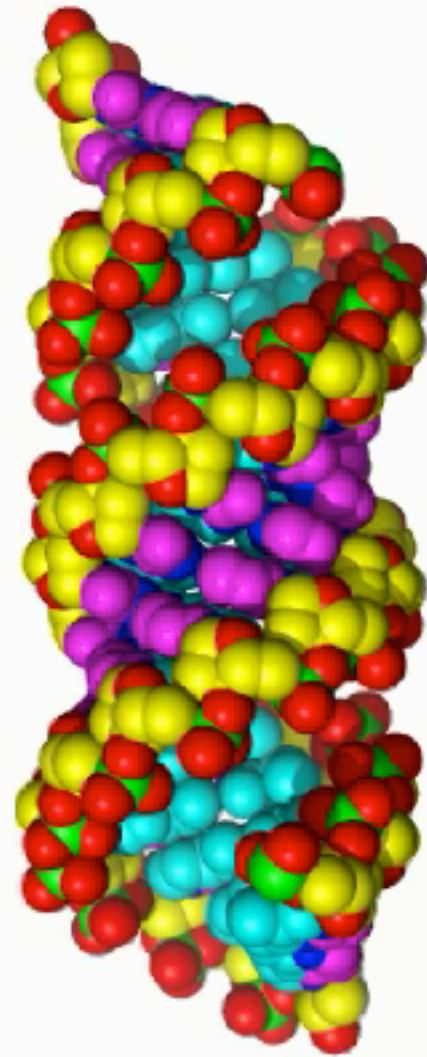
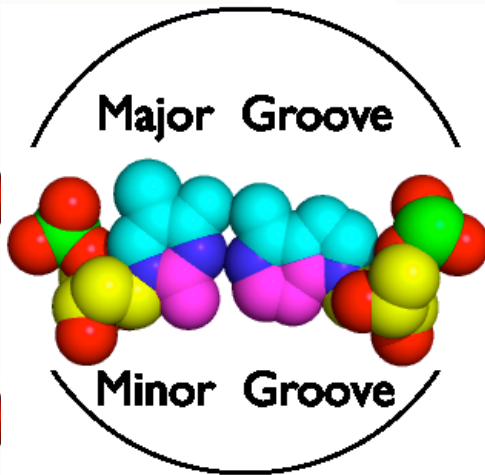
GCGCGCX – 5'

<b>X</b>	<b>T<sub>m</sub> (°C)</b>	<b>ΔH<sub>melt</sub> (kcal/mol)</b>	<b>ΔS<sub>melt</sub> (cal/molK)</b>	<b>ΔΔG<sub>melt</sub> (kcal/mol)</b>
<i>None</i>	41.7	45.9	122	-
Thymine	48.1	47.9	125	1.1
Cytosine	46.2	50.4	133	1.0
Adenine	51.6	54.7	144	2.0
Guanine	51.5	43.3	109	1.3
<b>Benzene</b>	<b>48.3</b>	<b>51.4</b>	<b>135</b>	<b>1.4</b>

J. Am. Chem. Soc. 1996, 118, 8182-8183.

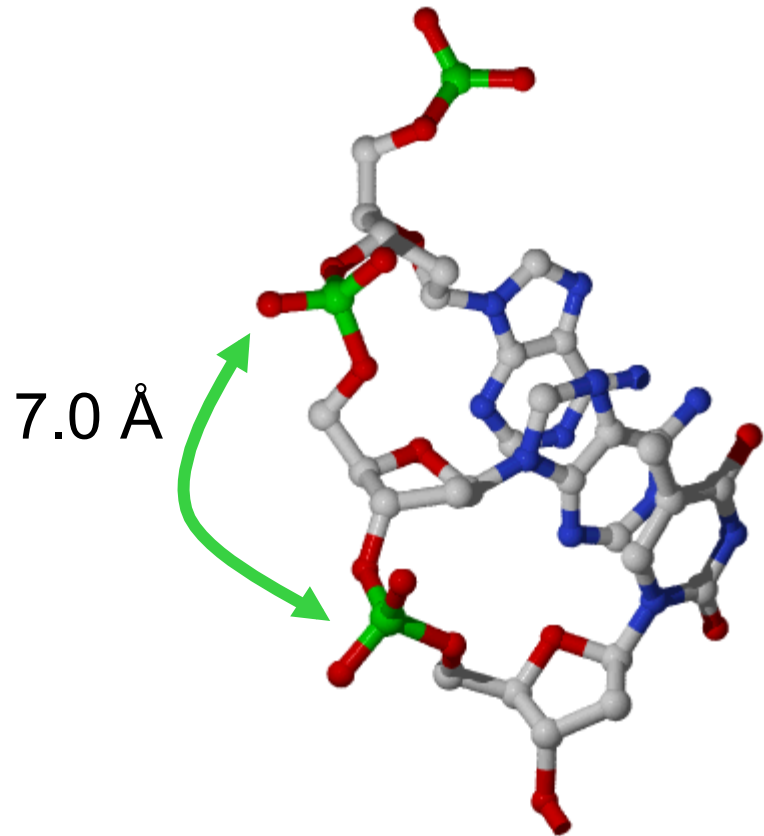


**B DNA**



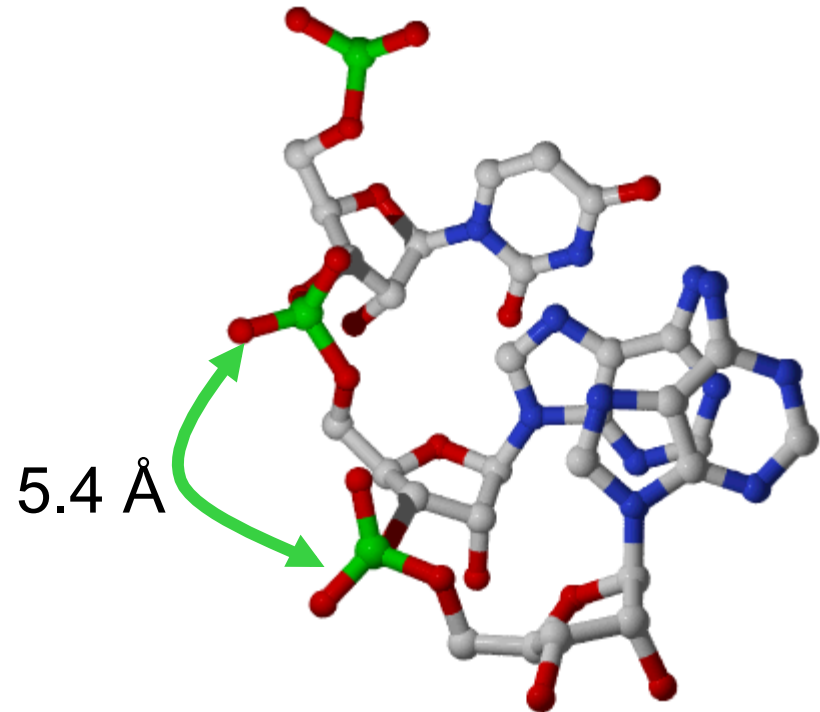
**A DNA**

# Phosphate Separation



7.0 Å

**B-conformation**

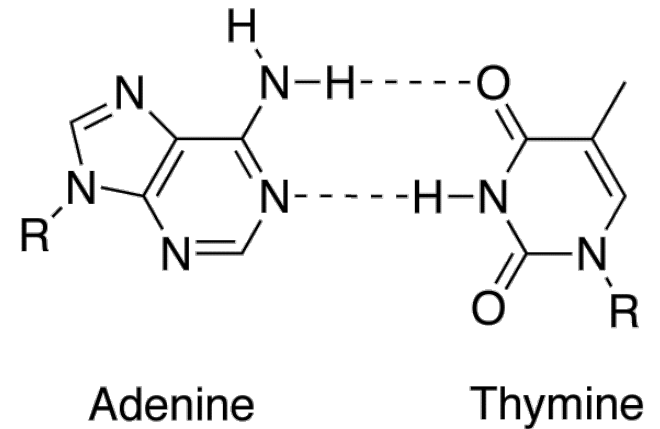
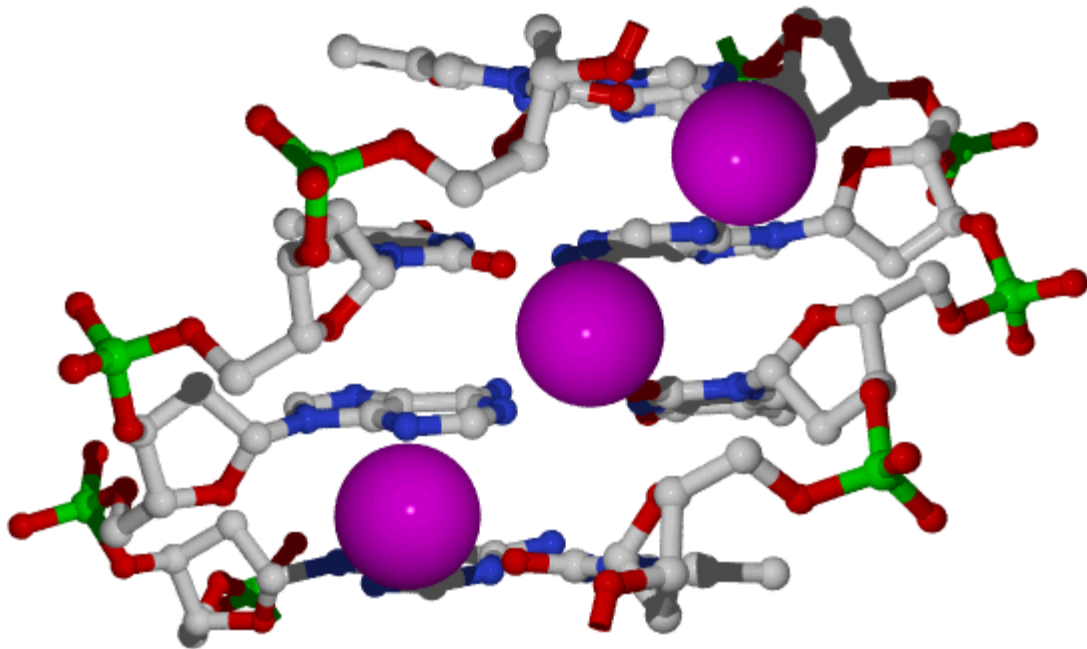


5.4 Å

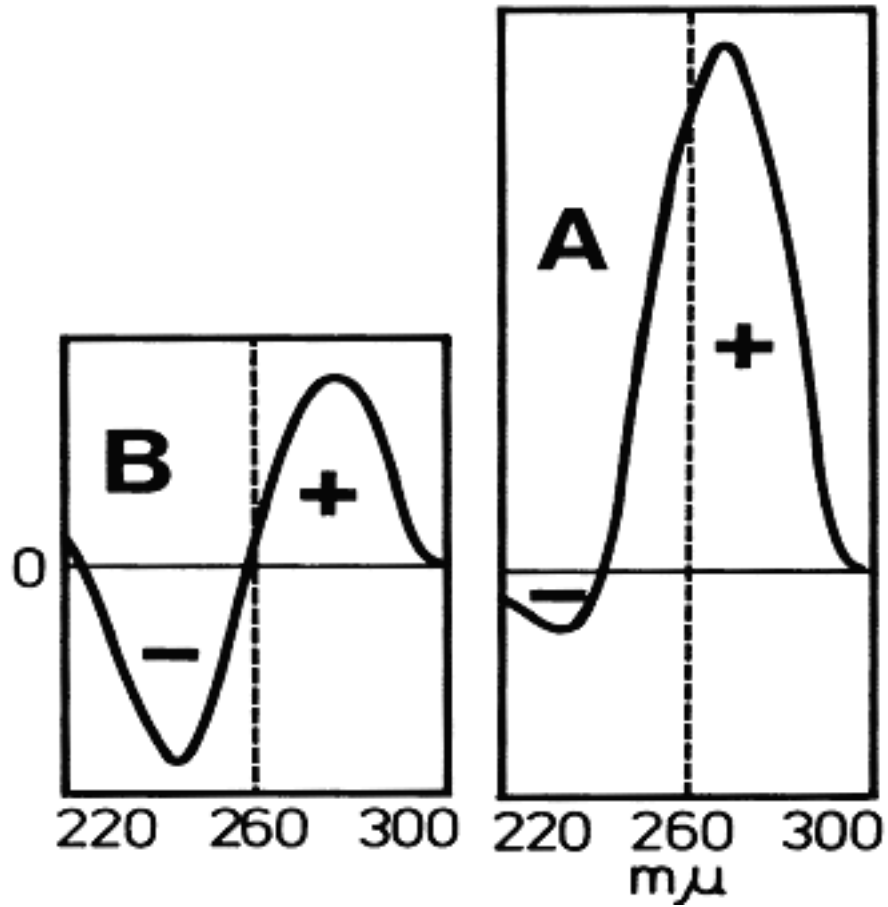
**A-conformation**



# Spine of Hydration in AT rich DNA



# CD Spectra of DNA



# An A-DNA triplet code: Thermodynamic rules for predicting A- and B-DNA

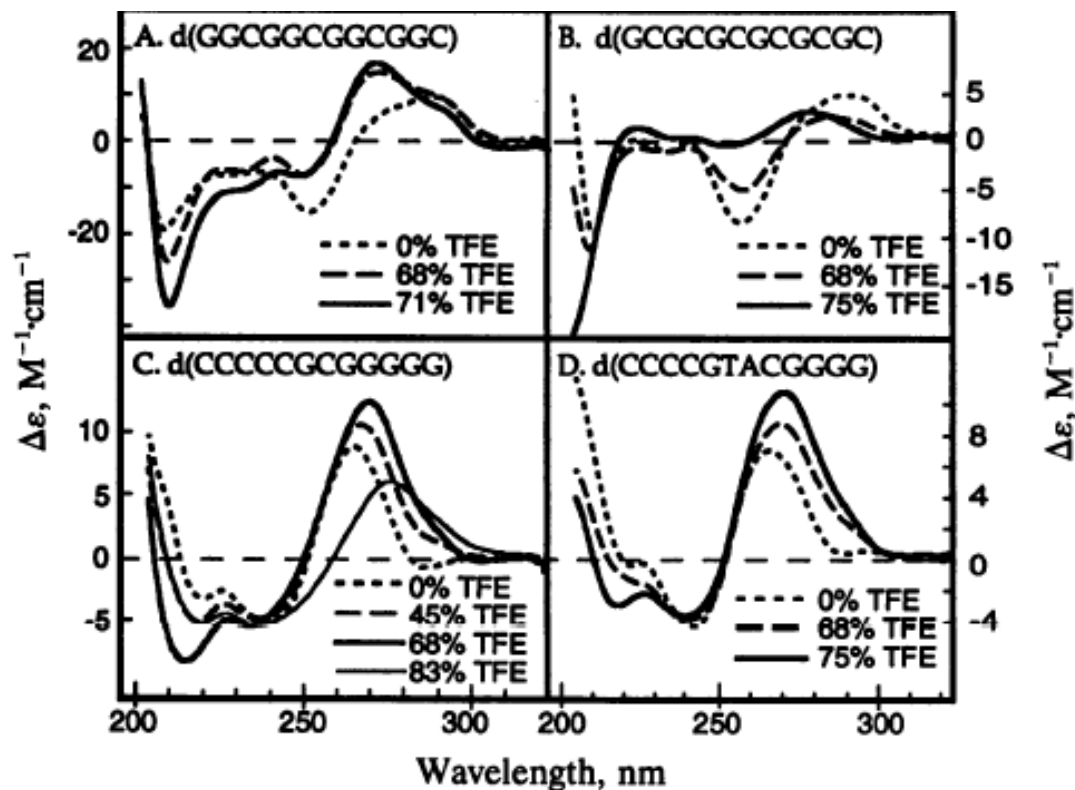
(DNA structure/structure prediction/crystallography/circular dichroism/spectroscopy)

BETH BASHAM, GARY P. SCHROTH, AND P. SHING HO\*

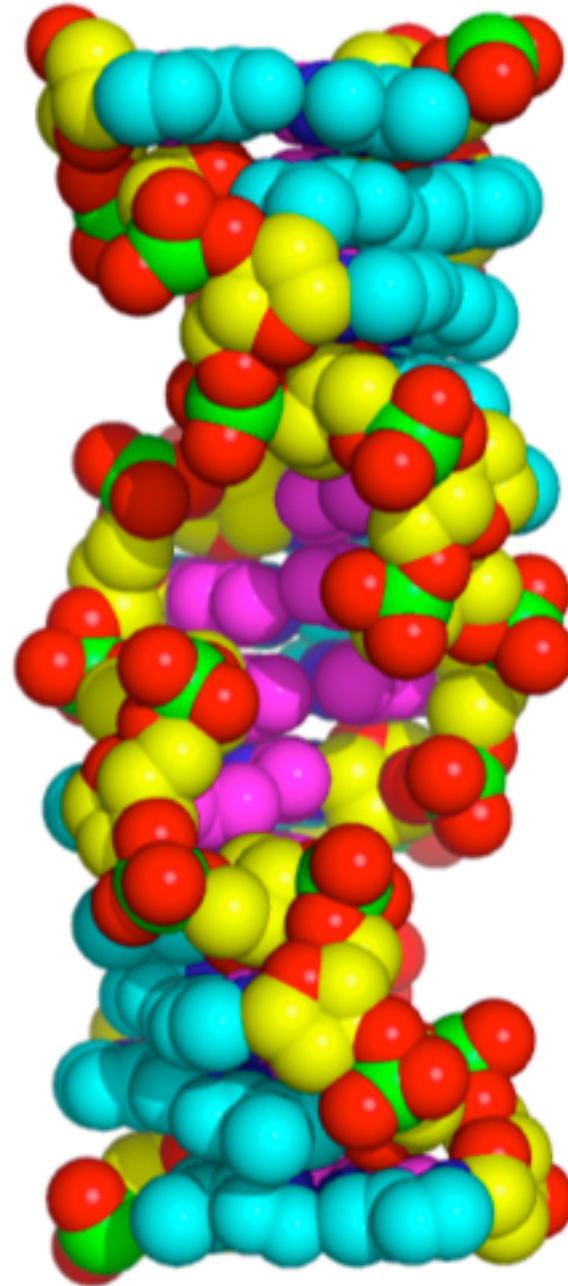
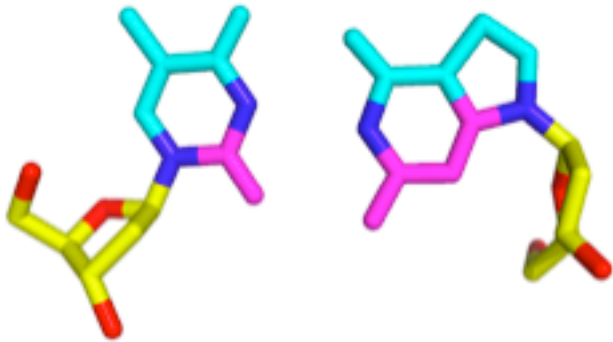
Table 5. Conformations of dodecanucleotides in aqueous solution (0% TFE) and in high concentrations of TFE (concentrations shown in parentheses)

Sequence	APE	DNA conformation		
		Predicted	0% TFE	High TFE
d(GGCGGCGGCGGC)	0.10	B	B	A (71%)
d(GCGCGCGCGCGC)	0.71	B	B	Z (75%)
d(CCCCCGCGGGG)	-0.15	A	A-like	A (68%)
d(CCCCGTACGGG)	-0.03	A	A-like	A (75%)

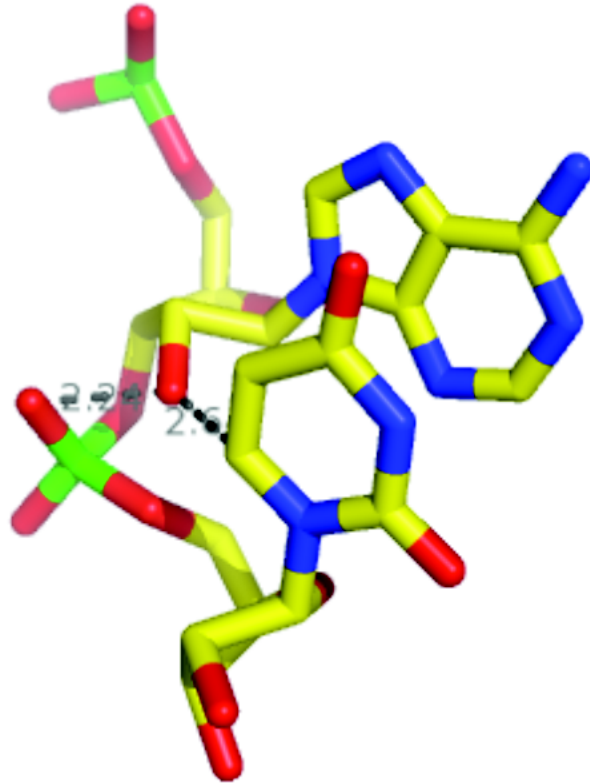
**APE=A-DNA Propensity  
 Related to  $\Delta G_{\text{solvation}}(\text{B} \rightarrow \text{A})$**



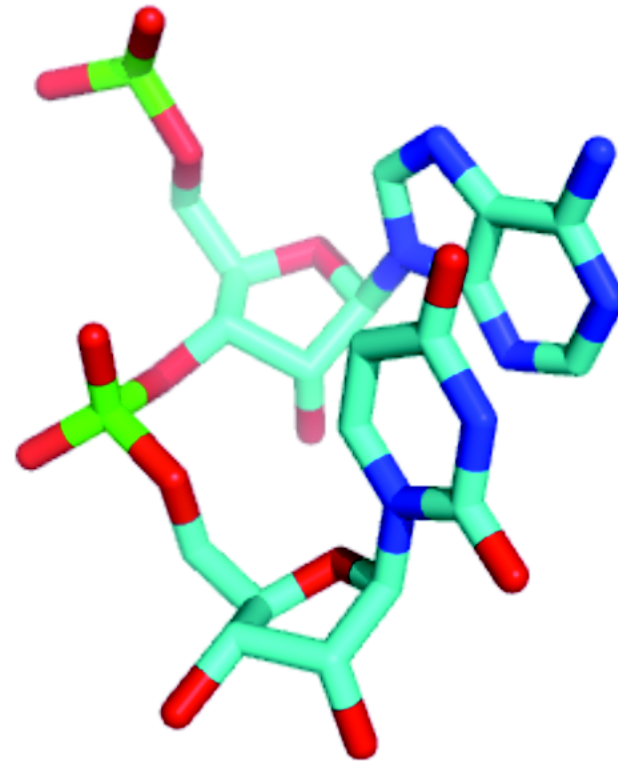
# Z DNA



# RNA is Always in A Conformation



B-RNA



A-RNA

# UUCG Tetraloop

Loop	$T_m$ ( $^{\circ}\text{C}$ )	$\Delta H^{\circ}$ (kcal/mol)	$\Delta G^{\circ}$ (kcal/mol)
G(UUCG)C	60.1	-48.6	-3.4
G(UUUG)C	51.1	-39.2	-1.7
G(UUUU)C	51.5	-38.2	-1.7
G(CUCG)C	62.4	-47.5	-3.6
deoxy - G(TTCG)C	44.7	-31.2	-1.4

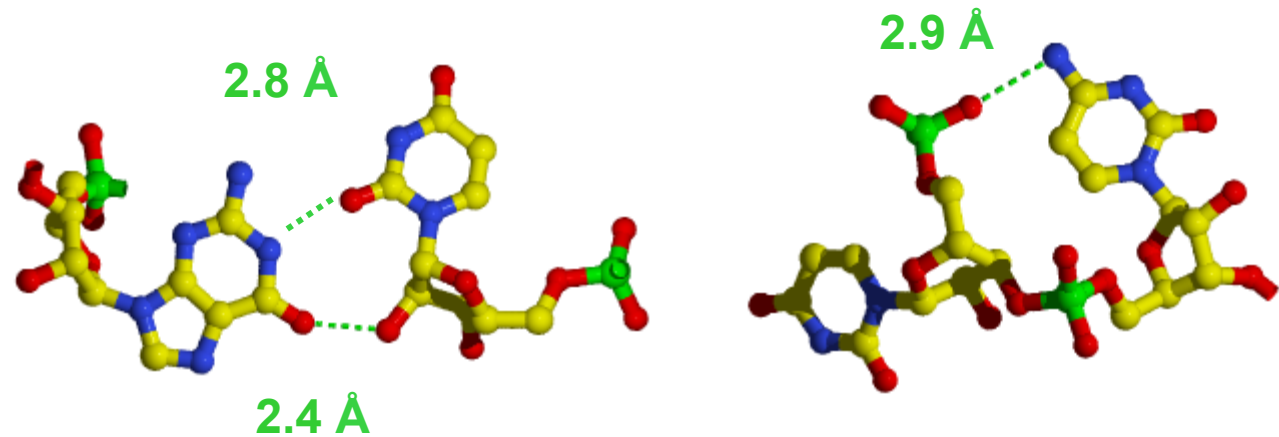
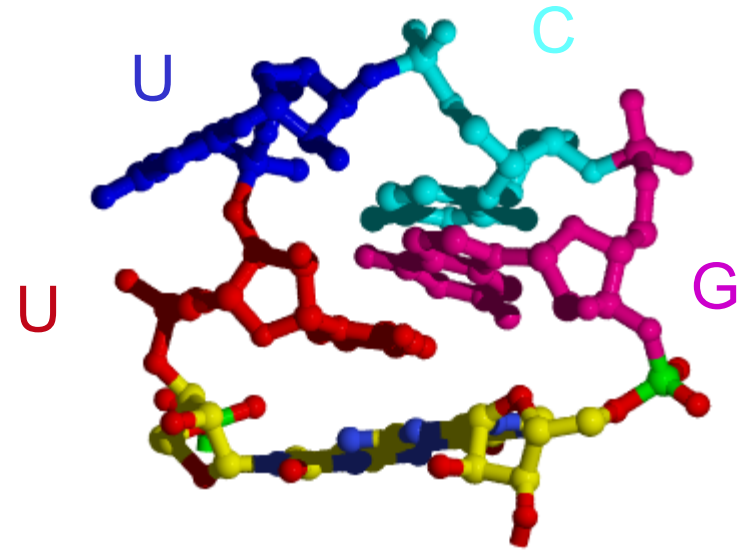
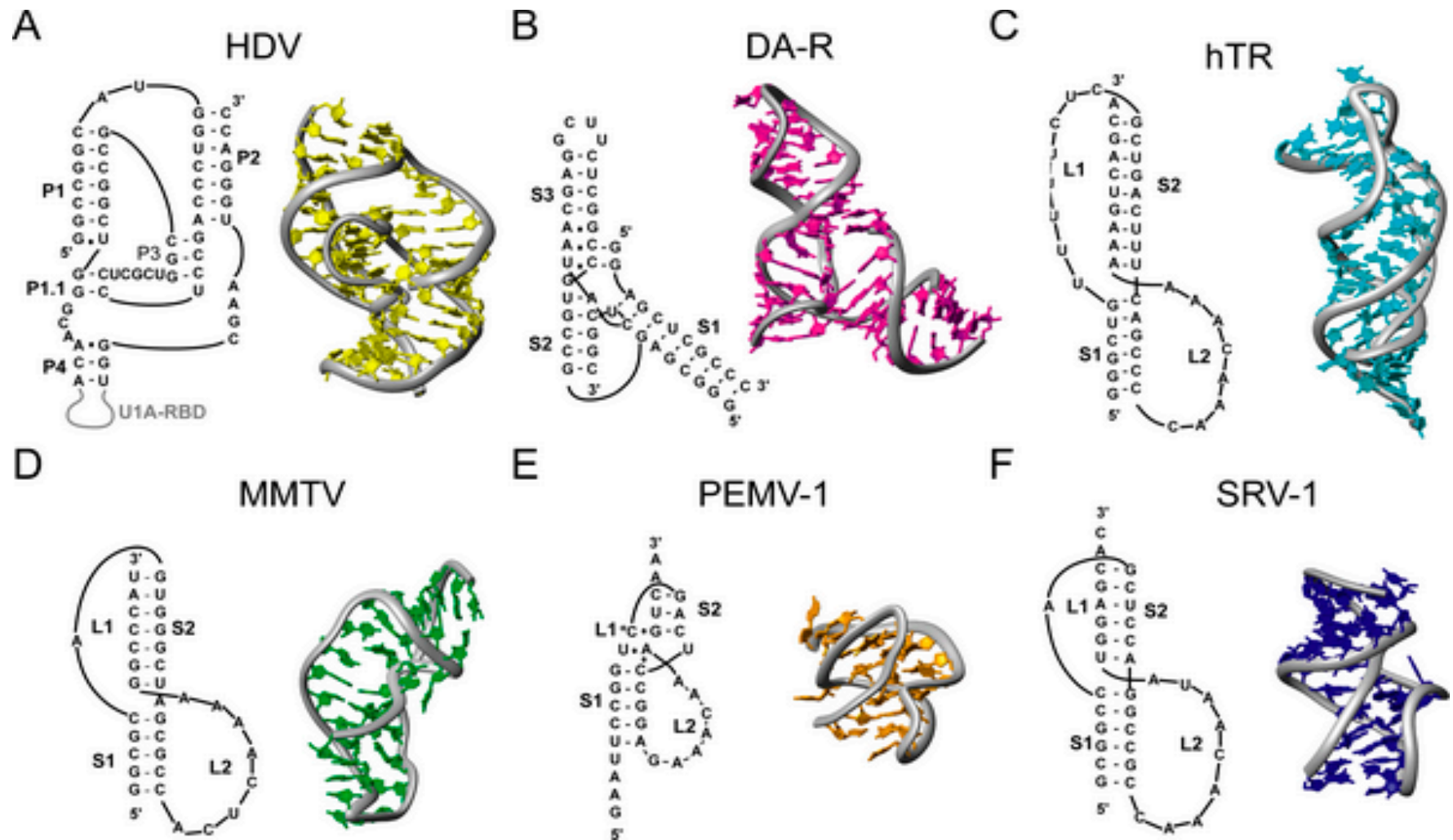


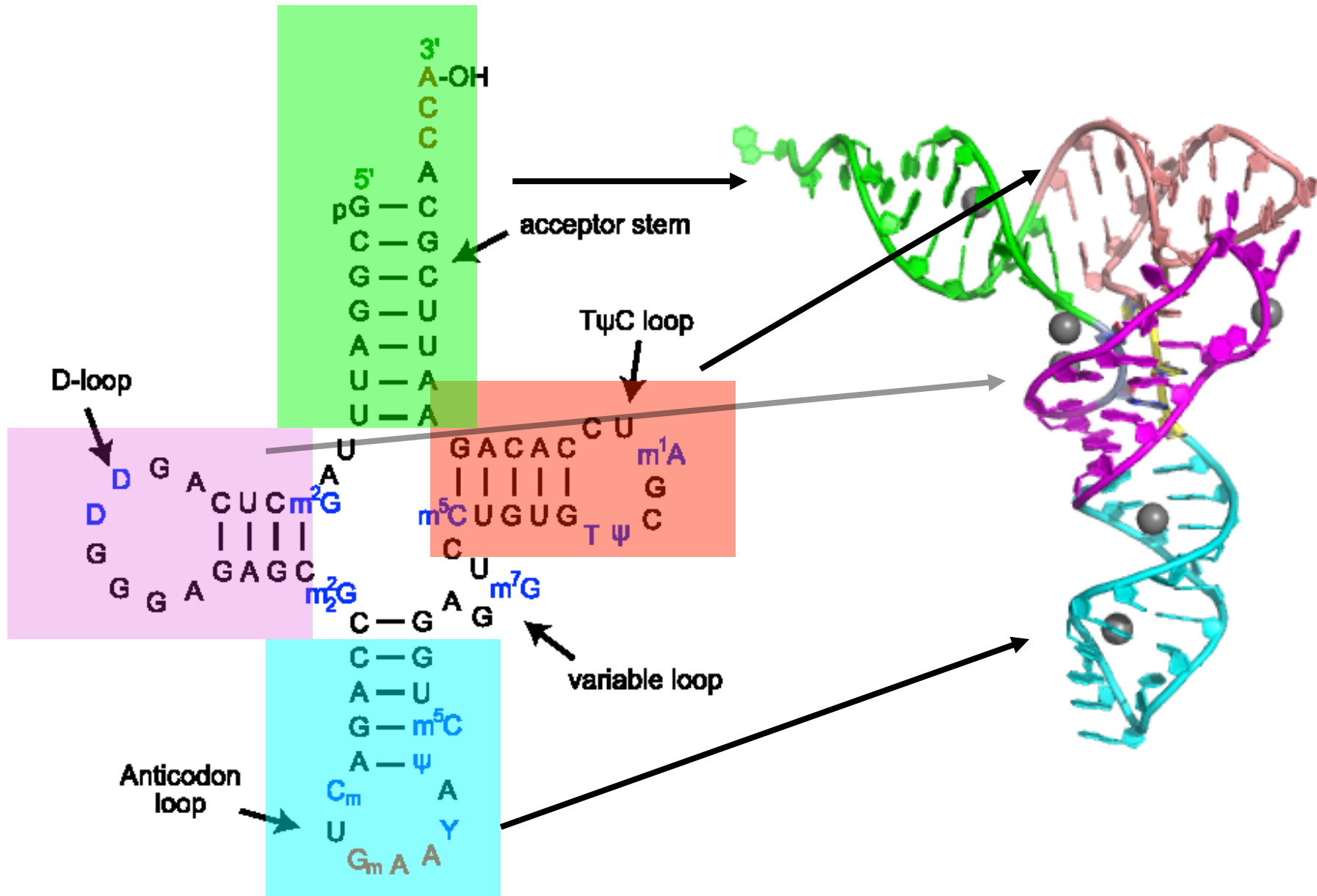
Figure 2. Sequences and Structures of RNA Pseudoknots



Staple DW, Butcher SE (2005) Pseudoknots: RNA Structures with Diverse Functions. *PLoS Biol* 3(6): e213. doi:10.1371/journal.pbio.0030213

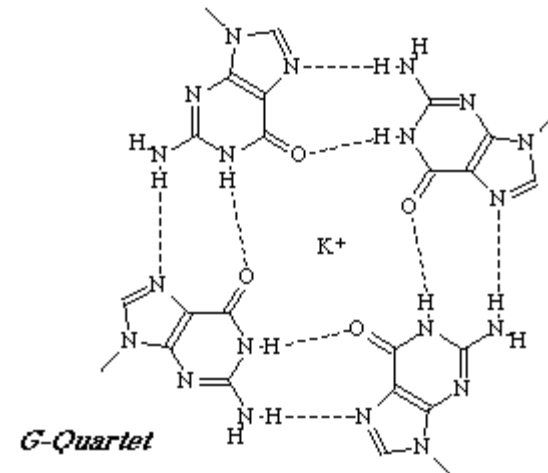
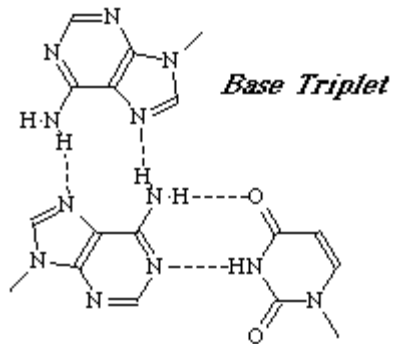
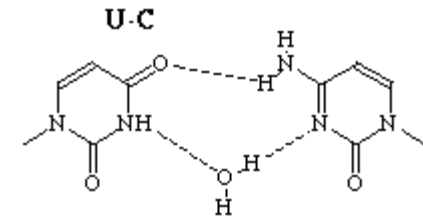
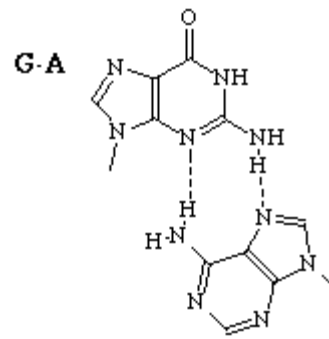
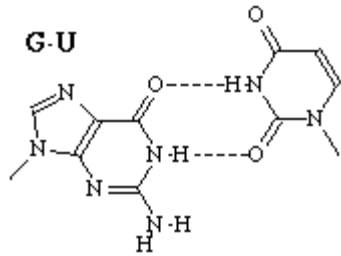
<http://www.plosbiology.org/article/info:doi/10.1371/journal.pbio.0030213>

# tRNA Structure

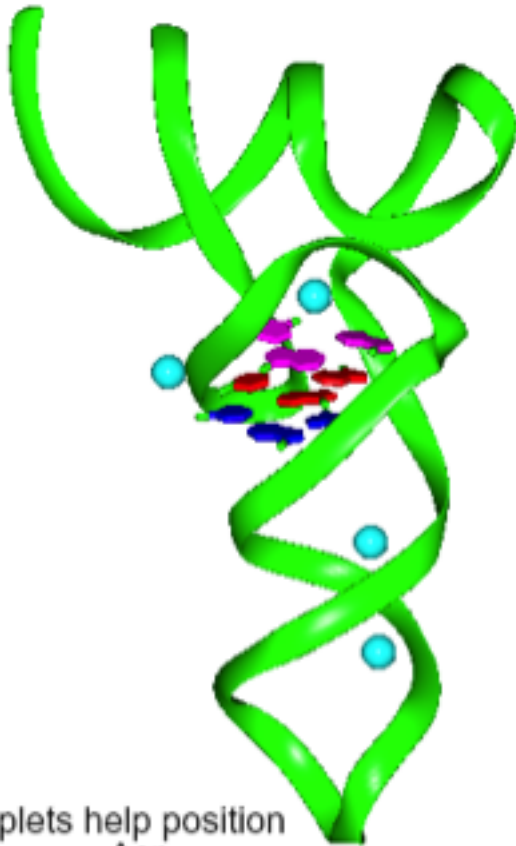




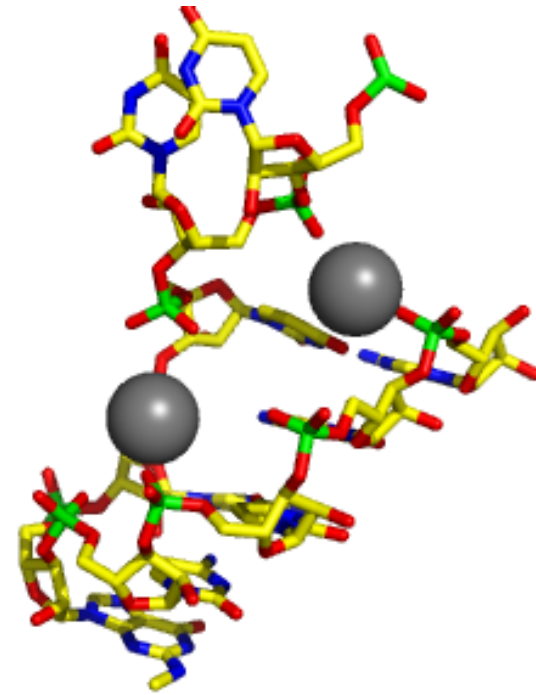
# Non Watson-Crick Base Pairs



# Tertiary Structure in RNA



Base triplets help position  
D arm of tRNA<sup>Asp</sup>.



Mg<sup>2+</sup> stabilizes dense phosphates