DNA
A look at the Chemistry
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What forces are important?

Electrostatics

Hydrogen Bonding

Burial of Hydrophobic Surface & Stacking
Base Pairing
(Donors matched to Acceptors)
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(Donors matched to Acceptors)

Good base pairing
Watson-Crick facing
but Anti-Watson-Crick orientation
Base Pairing
(Donors matched to Acceptors)

Good base pairing
WC-Hoogsteen facing
Bad Base Pairing

(Donors *not* matched to Acceptors)
Bad Base Pairing
(Donors to Acceptors with terrible angles)
Wild (but good) Base Pairing

G-quartet (Telomeres)
AT Base Pair

Ten H-Bonds

Sugar

Ten H-Bonds

Sugar
Burial of hydrophobic surface drives helix formation (hydrophobic core / stacking interactions)

Flat faces are nonpolar
Edges are very polar (can H-bond)
Other chemical constraints
Furanose Sugar Ring
Furanose Sugar Ring

endo

exo
Duplex - An Ideal Structure

- Charges outside
- H-bonders pointing outside
- Aromatic faces buried
- Result:
  - Helix
  - Twisted
  - Major/Minor Grooves
Palindromes

- Sequences reads the same 5’ to 3’ on either strand
- Yeah, so what?
Palindromes

- Palindromic DNA/RNA can adopt alternate structures
  - Stem/hairpins
    - RNA structure
Palindromes

- Palindromic DNA/RNA can adopt alternate structures
  - Holliday junctions
    - Recombination
Palindromes

- Homodimeric proteins can recognize twice the monomor binding site, easily…
RNA Secondary Structure

- Common structural features
RNA Secondary Structure

- Base stacking and pairing is maintained.
RNA Secondary Structure

- GU Pairs are “reasonable” energy
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Tertiary Structure - Polyanionic RNA

• Very water soluble
  – Charges need to be “outside”
• This limits size of folded structures
  – *Except* that Mg$^{2+}$ can neutralize charge and allow larger folded structures
Mg$^{2+}$ can “allow” otherwise unstable close approach of phosphodiester backbones.
Tertiary Structure

tRNA