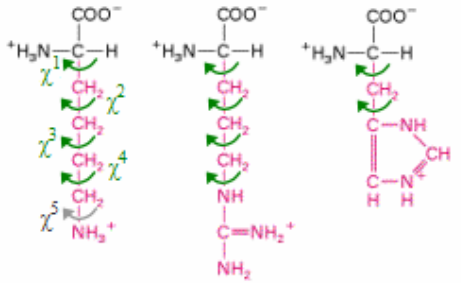
MOBILITY OF AMINO ACID SIDECHAINS AND PROTEIN BACKBONE

Modeling full flexibility in torsion (internal) coordinates

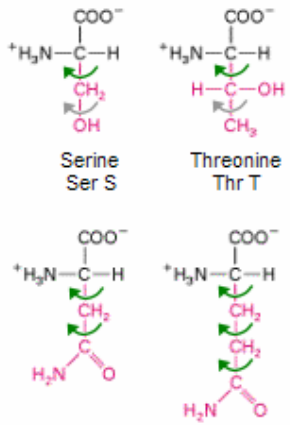
HYDROPHILIC (POLAR) AMINO ACIDS

Basic (+ charge at neutral pH)



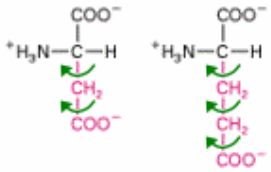
Lysine Lys K — Arginine Arg R — Histidine His H

Polar, but uncharged at neutral pH



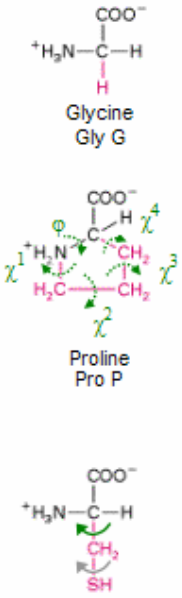
Serine Ser S — Threonine Thr T — Asparagine Asn N — Glutamine Gln Q

Acidic (- charge at neutral pH)



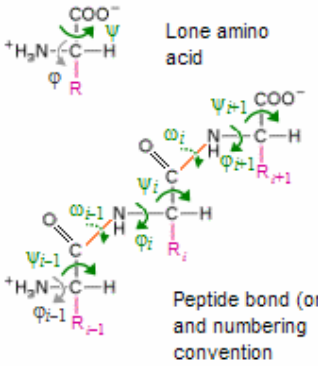
Aspartic acid Asp D — Glutamic acid Glu E

SPECIAL AMINO ACIDS



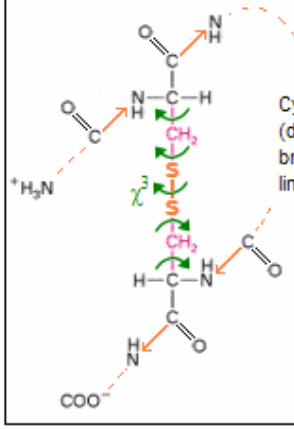
Glycine Gly G — Proline Pro P — Cysteine Cys C

BACKBONE



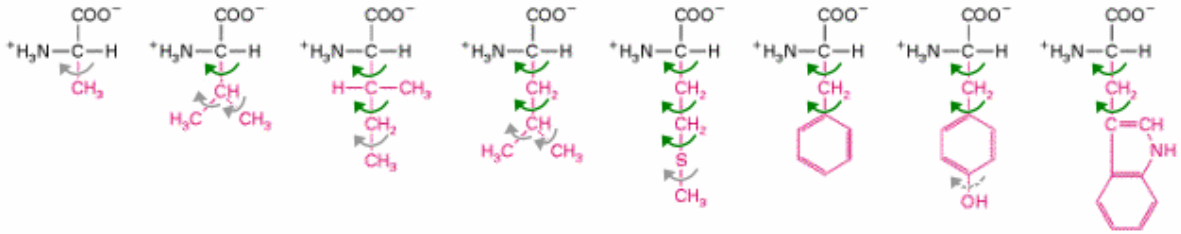
Lone amino acid

Peptide bond (orange) and numbering convention



Cys-Cys bond (disulphide bridge) cross-links backbone

HYDROPHOBIC (NON-POLAR) AMINO ACIDS



Alanine Ala A — Valine Val V — Isoleucine Ile I — Leucine Leu L — Methionine Met M — Phenylalanine Phe F — Tyrosine Tyr Y — Tryptophan Trp W

LEGEND

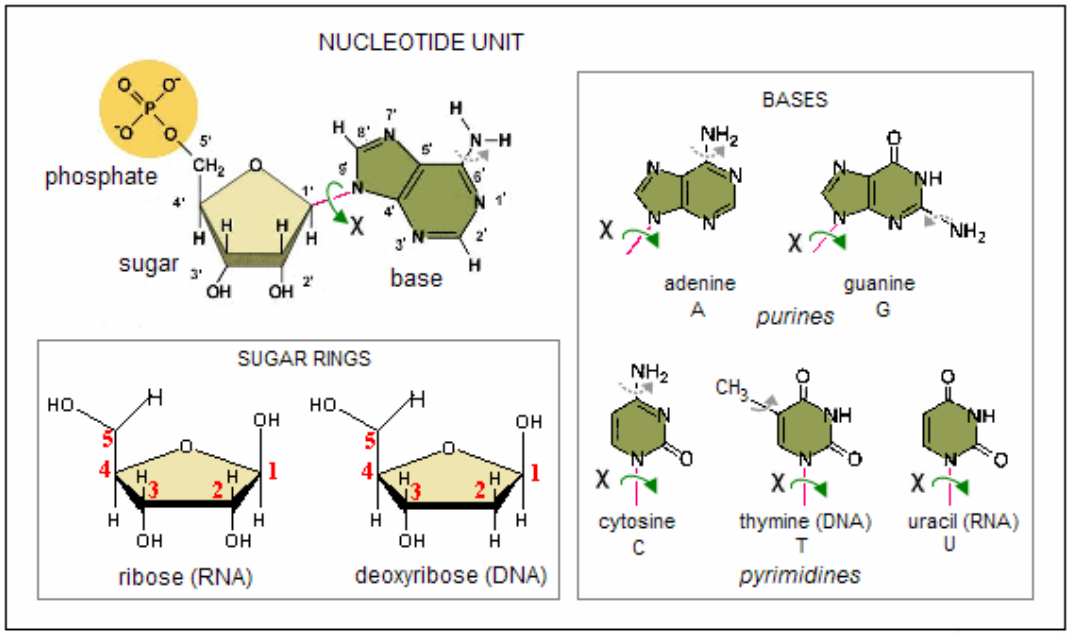
- "Heavy" degree of freedom
- "Light" DOF moves H only -- consider leaving out of model
- Limited range of motion -- consider treating as rigid
  - stiff peptide bond limits omega to about +/-10 degrees about nominal
  - proline forms near-rigid loop to backbone and locks its phi angle

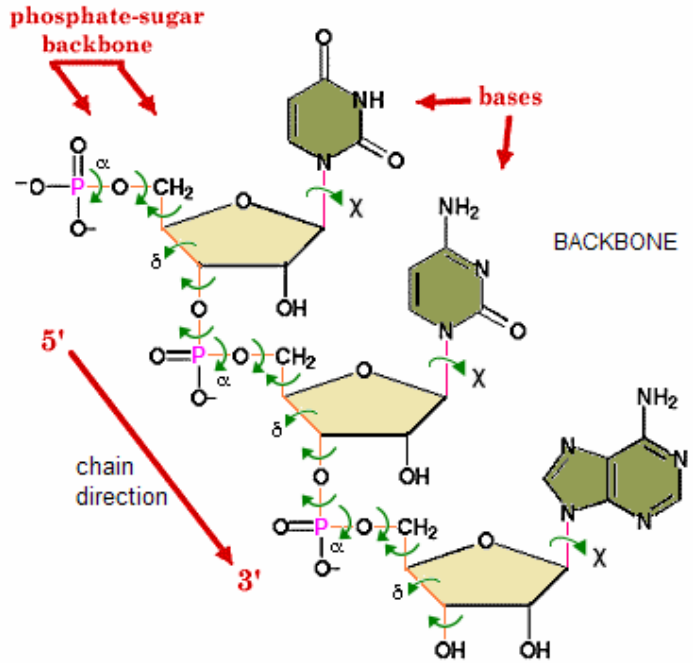
Michael Sherman
May, 2007

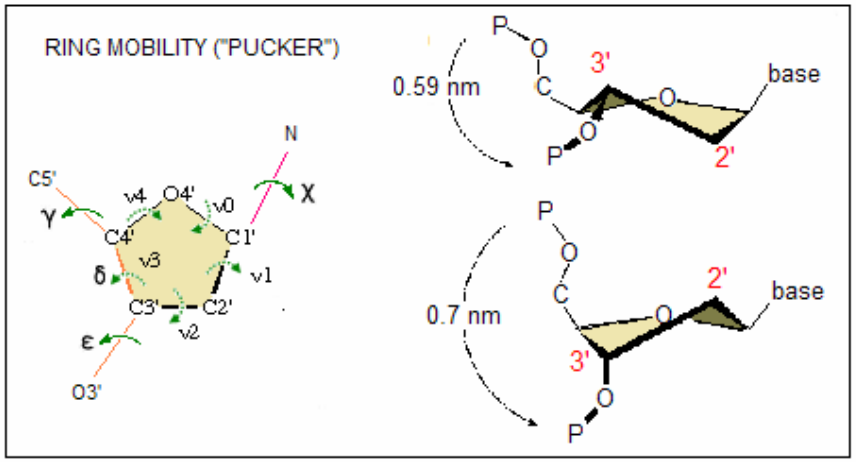
See other side for nucleic acids.

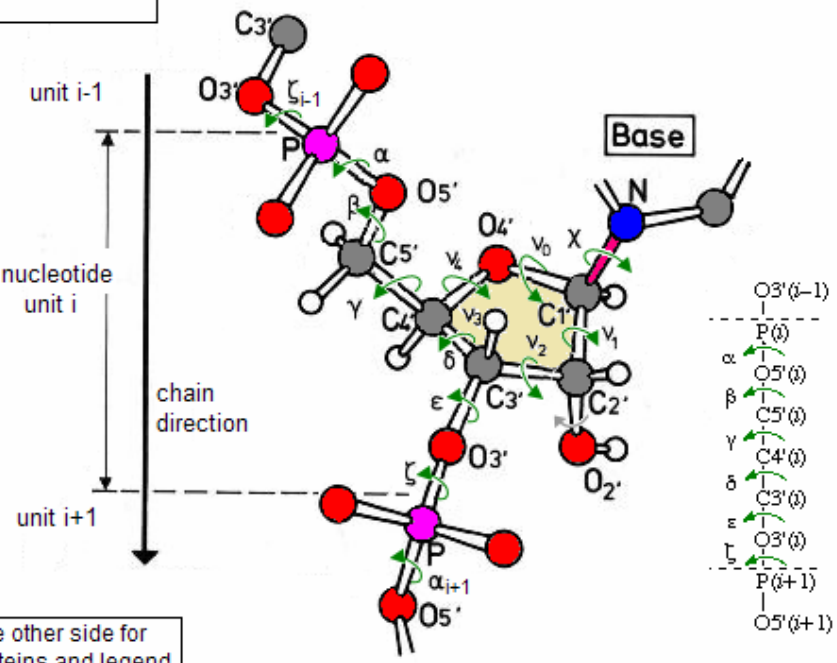
MOBILITY OF NUCLEIC ACID BACKBONE, SUGAR RING, AND BASE

Modeling full flexibility in torsion (internal) coordinates









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May, 2007
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See other side for proteins and legend.