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)

- Acidic (- charge at neutral pH)
  - Aspartic acid (Asp D)
  - Glutamic acid (Glu E)

- Polar, but uncharged at neutral pH
  - Serine (Ser S)
  - Threonine (Thr T)

SPECIAL AMINO ACIDS

- Glycine (Gly G)
- Proline (Pro P)

BACKBONE

- Peptide bond (orange) and numbering convention
- Cys-Cys bond (disulfide 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

Bioengineering 215    bugs/comments to msherman@stanford.edu
See other side for nucleic acids

Michael Sherman
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MOBILITY OF NUCLEIC ACID BACKBONE, SUGAR RING, AND BASE
Modeling full flexibility in torsion (internal) coordinates

NUCLEOTIDE UNIT

phosphate
sugar
base

SUGAR RINGS

5' 4' 3' 2' 1'

ribose (RNA)
deoxyribose (DNA)

BASES

adenine
purines

guanine

pyrimidines

cytosine
thymine (DNA)
uracil (RNA)

phosphate-sugar backbone
bases

RING MOBILITY ("PUCKER")

0.59 nm

0.7 nm

unit i-1

unit i+1

See other side for proteins and legend.