

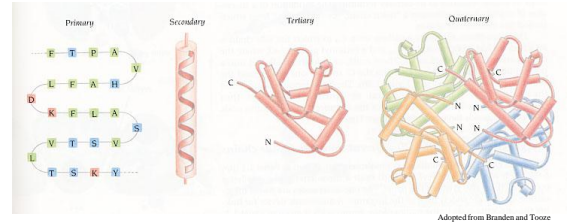
Protein Structure Analysis

<http://binf.gmu.edu/vaisman/binf731/>

Iosif Vaisman

2010

Protein Structure Hierarchy



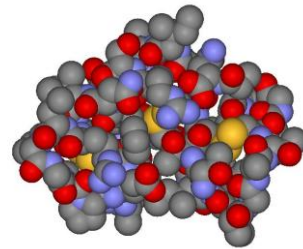
- Primary - the sequence of amino acid residues
- Secondary - ordered regions of primary sequence (helices, beta-sheets, turns)
- Tertiary - the three-dimensional fold of a protein subunit
- Quaternary - the arrangement of subunits in oligomers.

Secondary Structure: Computational Problems

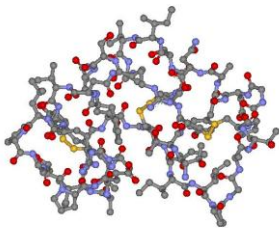
Secondary structure characterization

- Secondary structure assignment
- Secondary structure prediction
- Protein structure classification

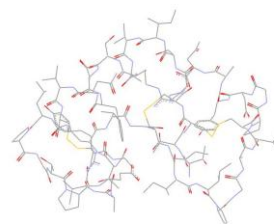
Protein representations



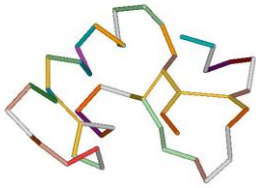
Protein representations



Protein representations



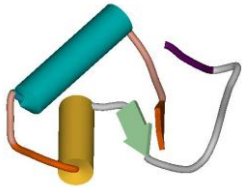
Protein representations



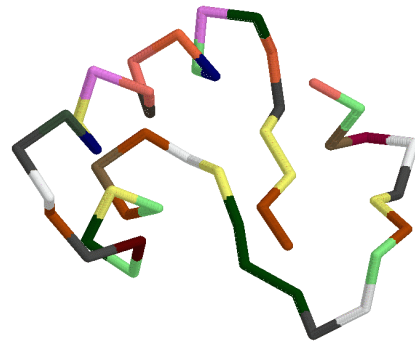
Protein representations



Protein representations

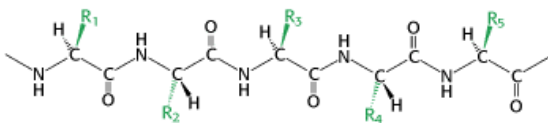


Protein backbone

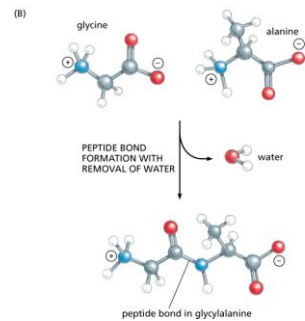
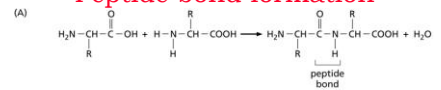


NWVLSTAADMQGVVTDGMASGLDKD

Protein backbone

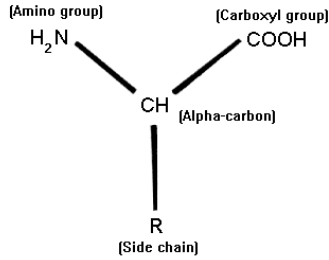


Peptide bond formation

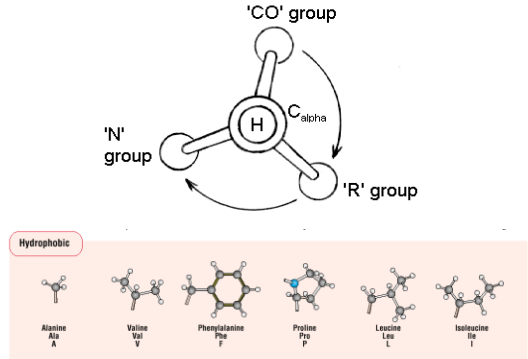


Adopted from Zvelebil, Baum, 2008

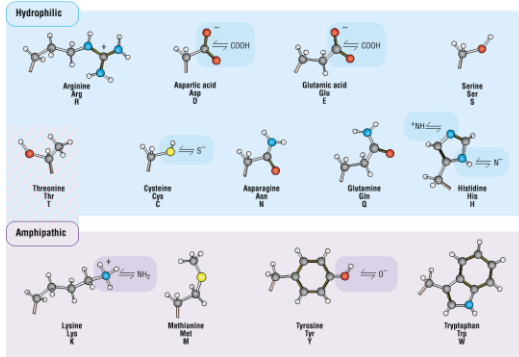
Amino Acid Residue



Amino Acid Residue

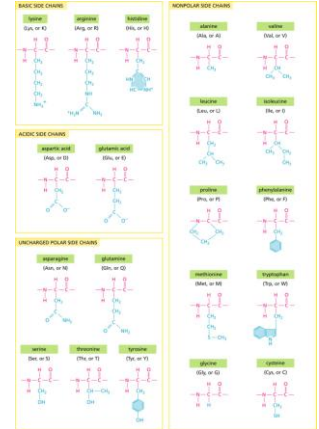


Amino Acids



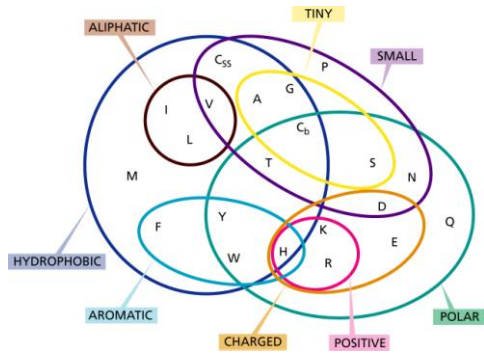
Adopted from: Gregory Pecko and Dajmar Ringe, Protein Structure and Function: From Sequence to Consequence

Amino Acids



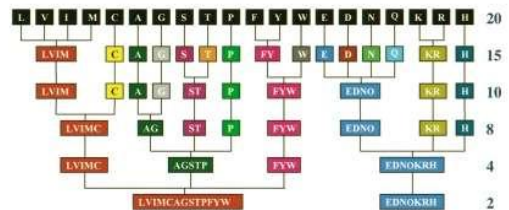
Adopted from Zvelebil, Baum, 2008

Amino Acid Residue Clustering

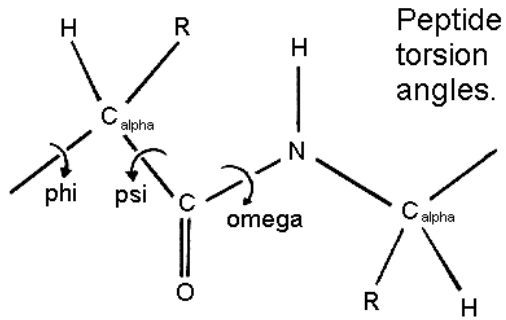


Adopted from Zvelebil, Baum, 2008

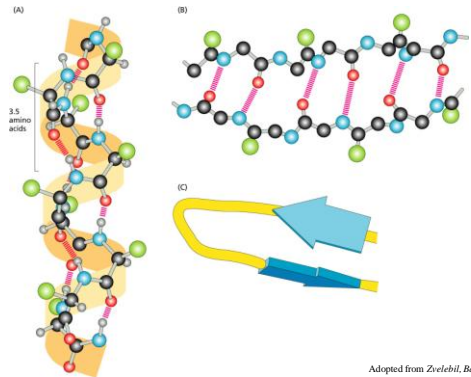
Amino Acid Residue Clustering



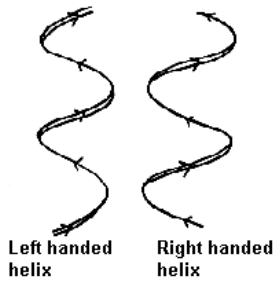
Adopted from L.R. Murphy et al., 2000



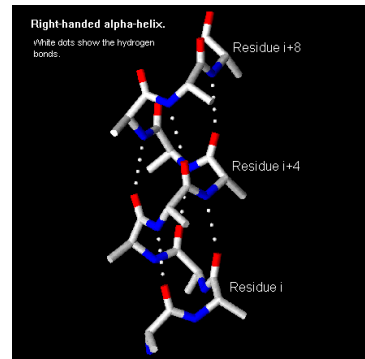
Secondary Structures



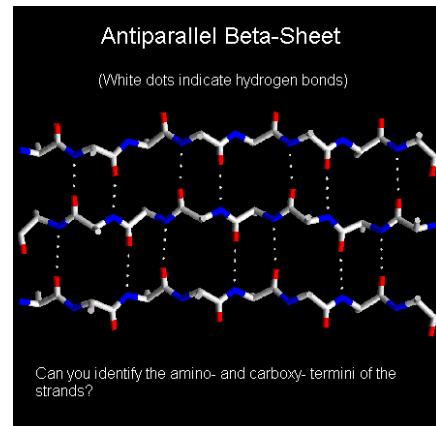
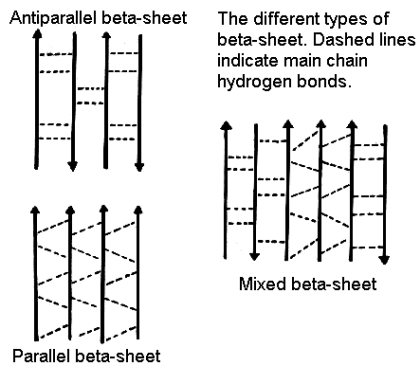
Secondary Structure (Helices)

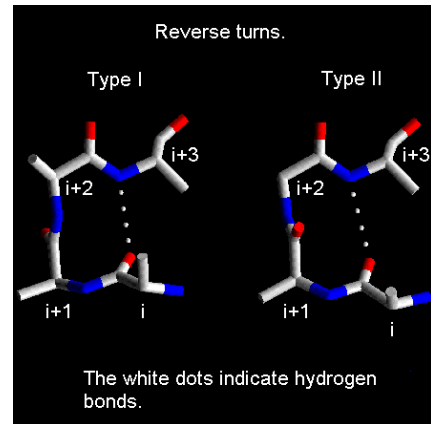
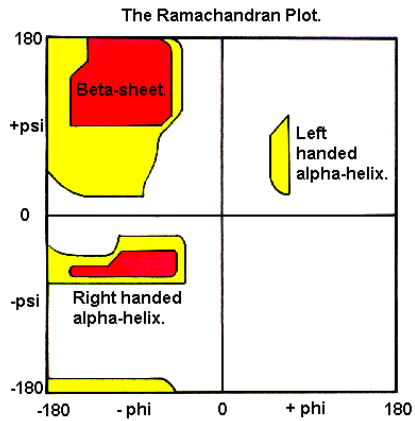


Helix

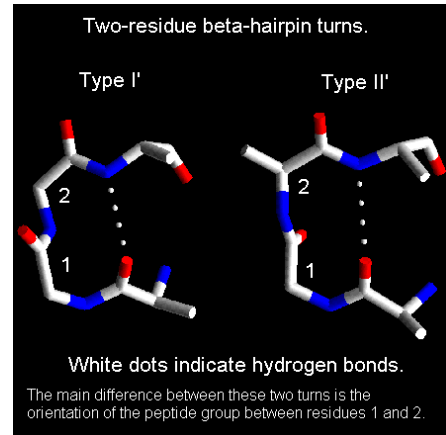
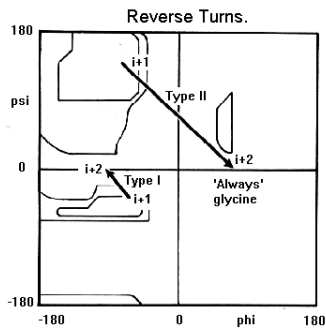


Secondary Structure (Beta-sheets)

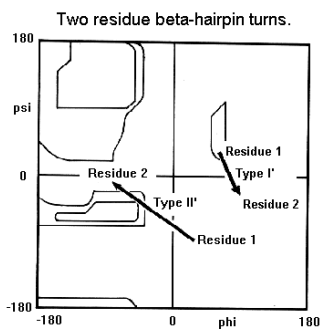




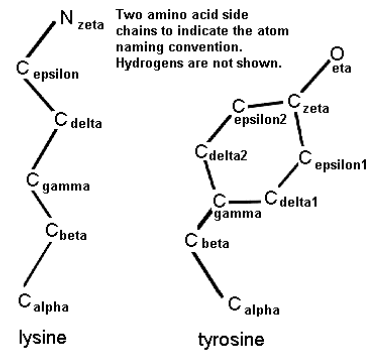
Reverse Turns on a Ramachandran Plot



Beta-hairpin Turns on a Ramachandran Plot



Side-Chain Atom Nomenclature



Side-Chain Torsional Angles

