Helices and sheets

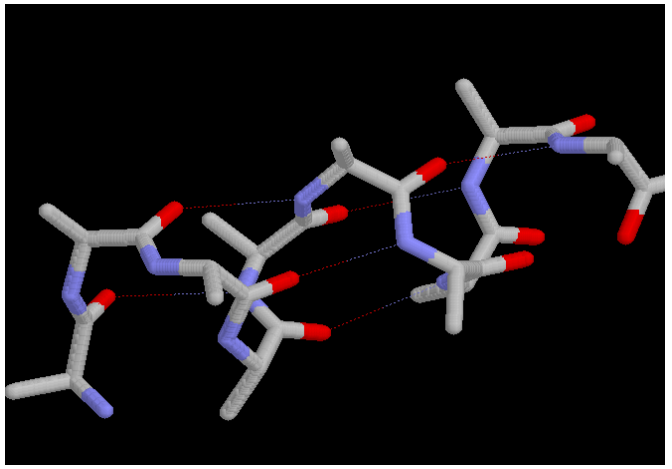
This lecture can be supplemented by the tutorial by Victoria Bragin at http://www.paccd.cc.ca.us/instadmn/physcidv/chem_dp/chemweb/protein/sec.htm, which should be reviewed in detail

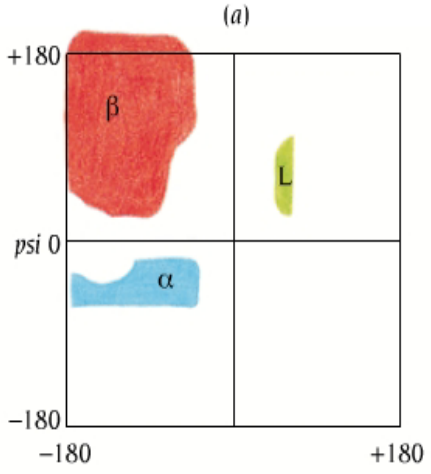
Principles of construction

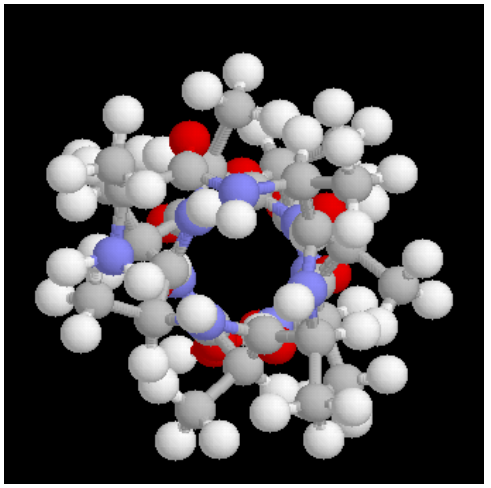
- Linus Pauling, PNAS, 37: 205 and 729 (1951)
- Planar peptide bond
- Satisfaction of backbone hydrogen bonds within structure (so features can enter into the protein interior)
- Reasonable stereochemistry at Cα
- Largely side chain independent

α - Helix

- Coiled helix
- 3.7 residues per turn
- Intrachain hydrogen bonds
- Dipole moment along helix axis (N + to C -)
- Ramachandran angles
- Residues to outside of helix

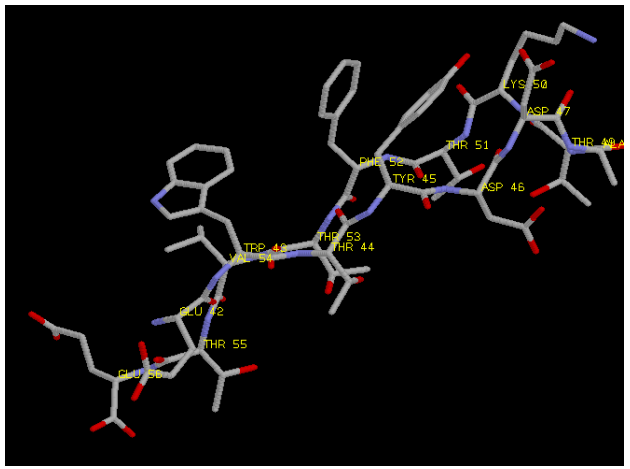


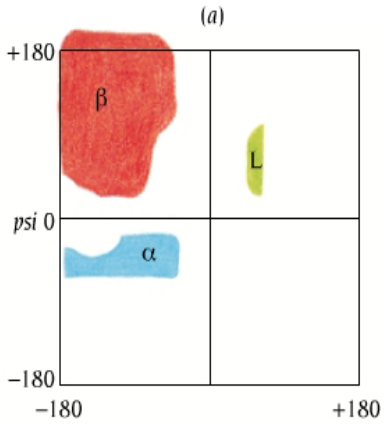




β - sheet

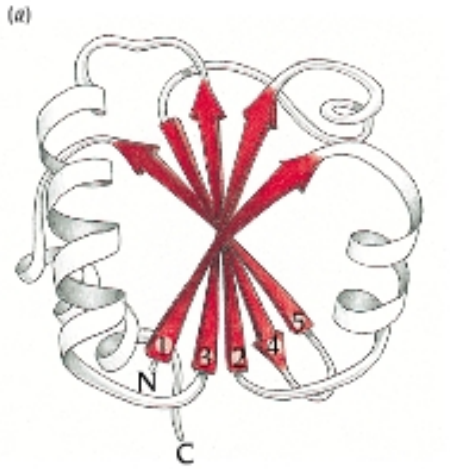
- Extended chains
- Interstrand hydrogen bonds
- Parallel or antiparallel chains
- Two surfaces
- R groups extending away from surface
- Ramachandran angles

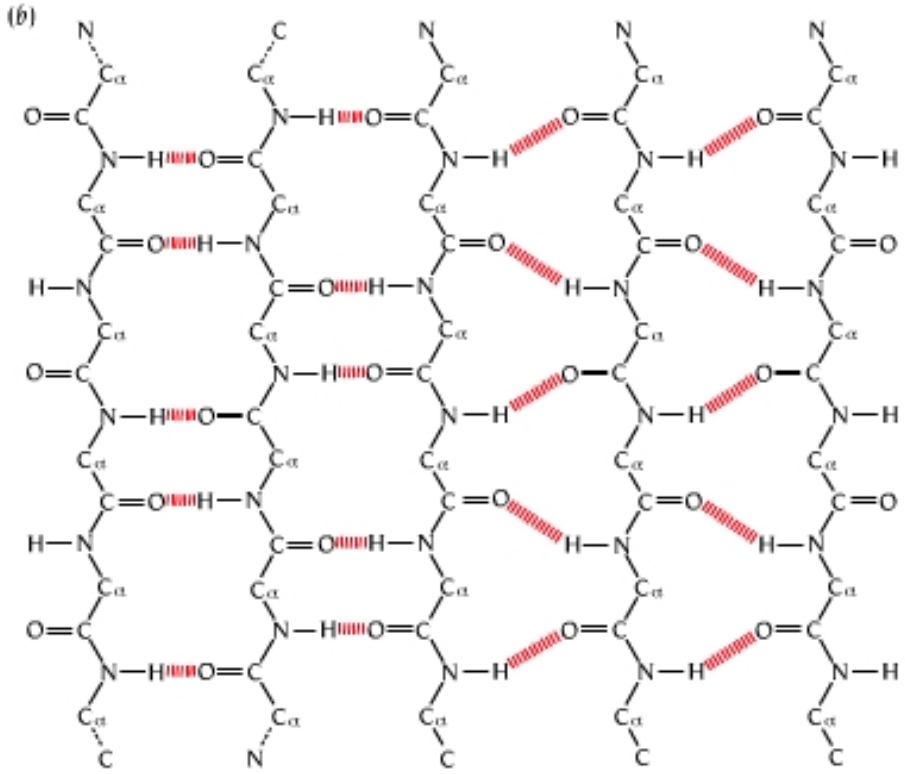




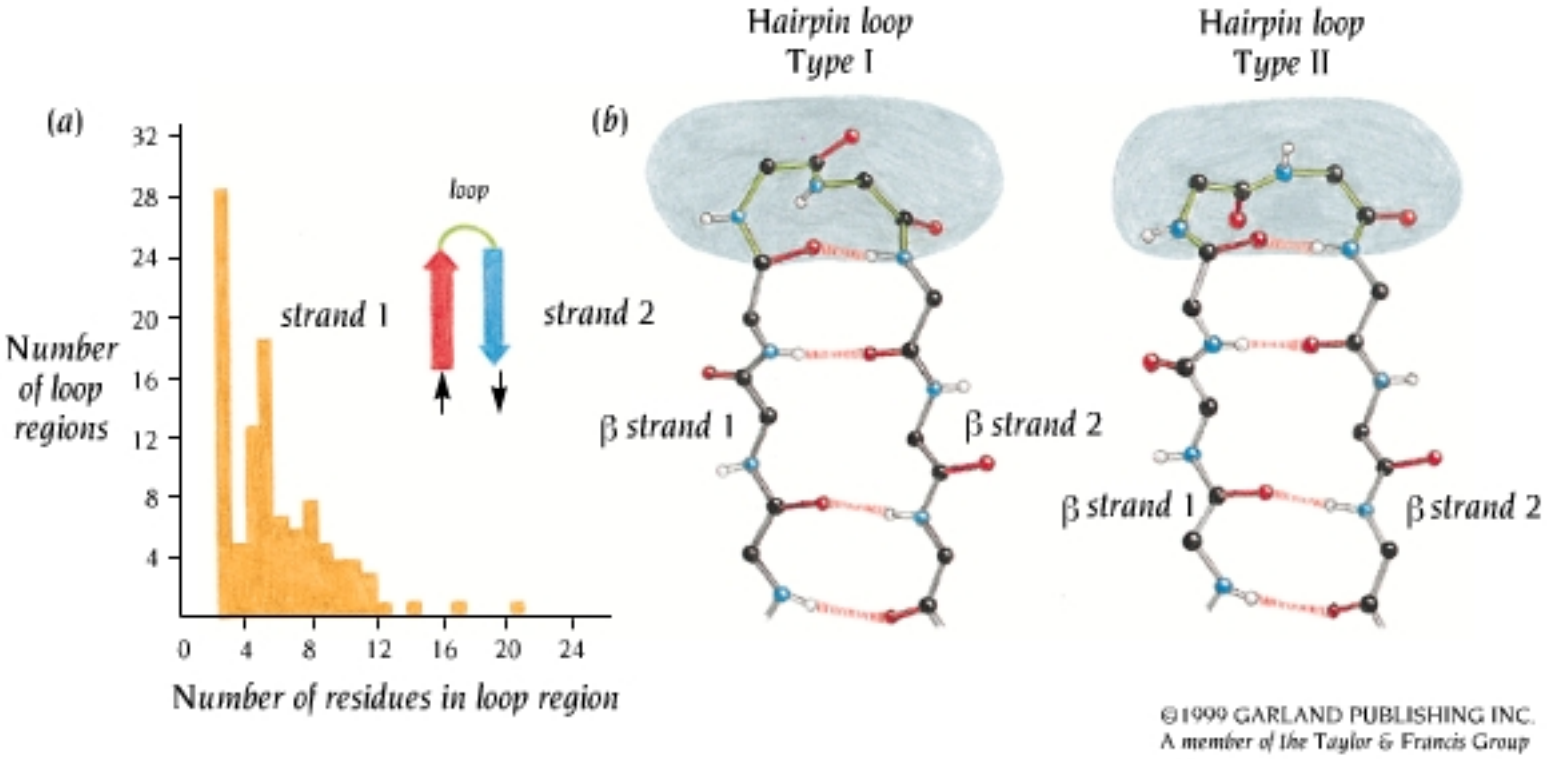
Minor variations

- Mixed parallel and antiparallel chains
- Twists



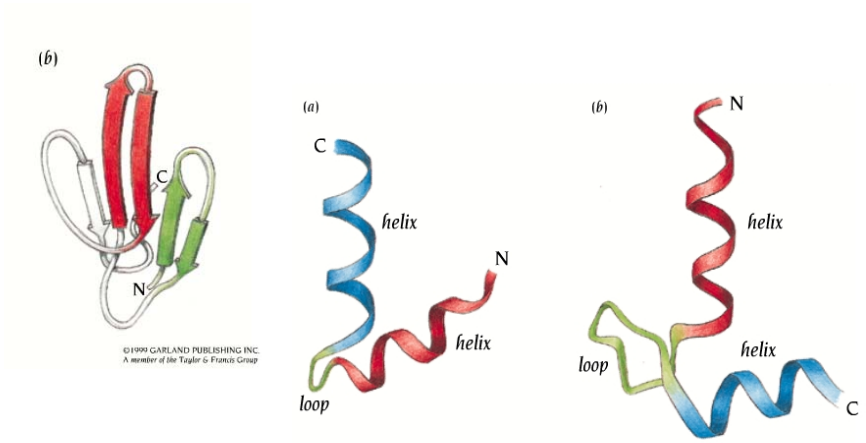


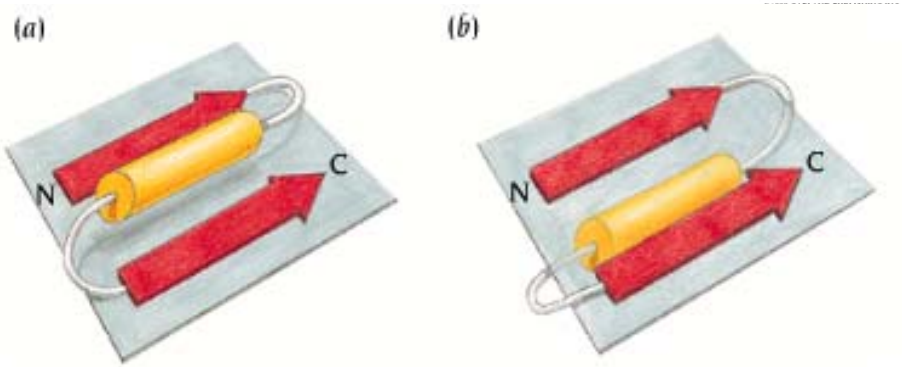
Turns



Simple assemblies

- Simple motifs (partial structures)
  - β hair pin (to give antiparallel sheet)
  - α hairpin (to give antiparallel helices)
  - βαβ to give parallel sheet
- Larger assemblies (independent structures)
  - “Perhaps the most remarkable features of the molecule are its complexity and its lack of symmetry. The arrangement seems to be almost totally lacking in the kind of regularities which one instinctively anticipates , and it is more complicated that has been predicted by any theory of protein structure” J. Kendrew, 1958, on the structure of myoglobin





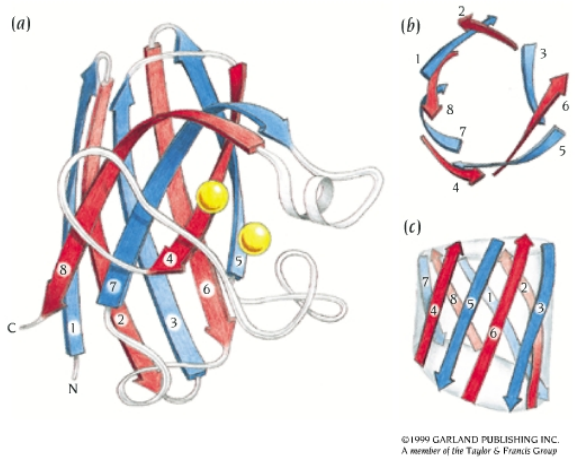
Helix motifs

- Antiparallel 4 helix bundle
  - Cytochrome b562
  - 256B
  - Cf 1bz4
- Parallel/parallel 4 helix bundle
  - Human growth hormone
  - 1HUW
- Big collection
  - Bacterial muramidase
  - 1sly
- Function specific
  - Hemoglobin
  - 1A3N
  - 246 structures

- Simple Analysis
  - VAST in MMDB
  - Examine list of structural homologs (are they functionally linked?)
  - Compare structures in Cn3D (how does similarity fit into overall structure?)

β structures

- β barrels
  - Retinol Binding Protein
    - Up and down connections
    - 1RLB
    - Select Chain E Only
  - Prealbumin
    - Greek key connections
    - 1TTA
    - Select Chain A Only
- Propellors
  - Neuraminidase
  - 7NN9



strand no.	residue no.	amino acid sequence
2	41–48	– Ile – Val – Ala – Glu – Phe – Ser – Val – Asp –
3	53–60	– Met – Ser – Ala – Thr – Ala – Lys – Gly – Arg –
4	71–78	– Ala – Asp – Met – Val – Gly – Thr – Phe – Thr –

αβ mixed structures

- TIM barrels
  - Triose phosphate isomerase (glycolytic enzyme)
  - Hydrophobic sheet strands, amphipathic helices
  - 1TIM
- Alpha/Beta Twists
  - Nucleotide Binding fold
  - Build out, switch back, build out in the other direction
  - 1BRM
- Twisted sheets, horseshoes (2bnh)