

Secondary structures

- Secondary structures are repeated local structural elements formed by consecutive amino acids with similar ϕ and ψ values.
- Stabilized by hydrogen bonds between backbone atoms but formation of a particular type of secondary structure is dictated by protein sequence.
- Formed in the early stages of protein folding following hydrophobic collapse.
- Formation of secondary structures allows the packing of polar backbone atoms in the hydrophobic core of protein structures.

α helix

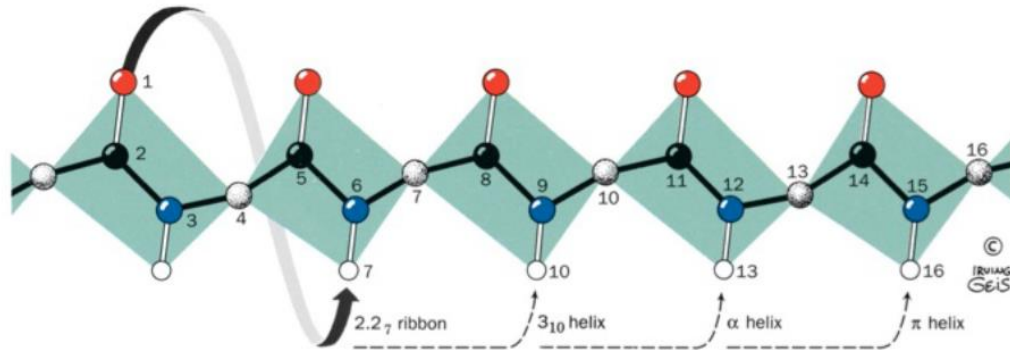
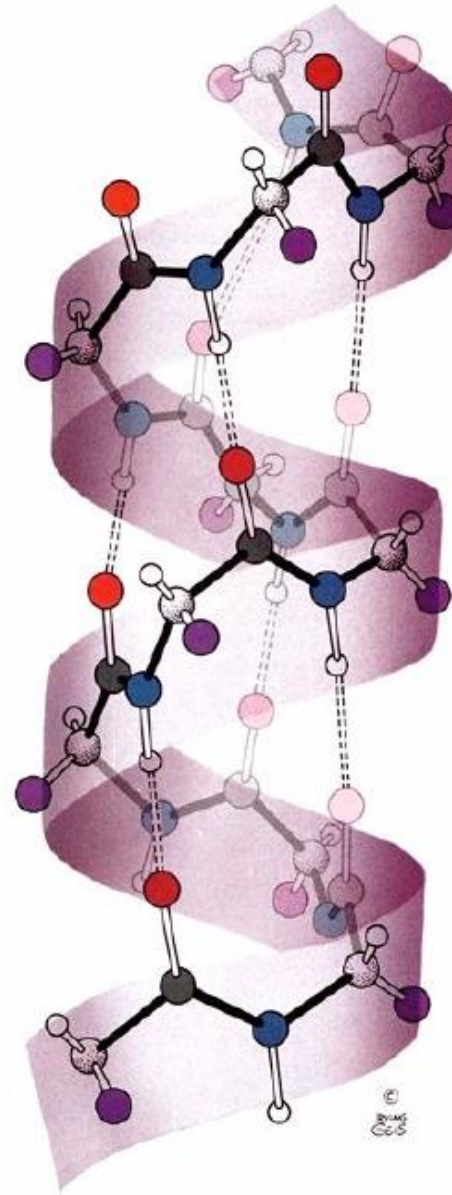
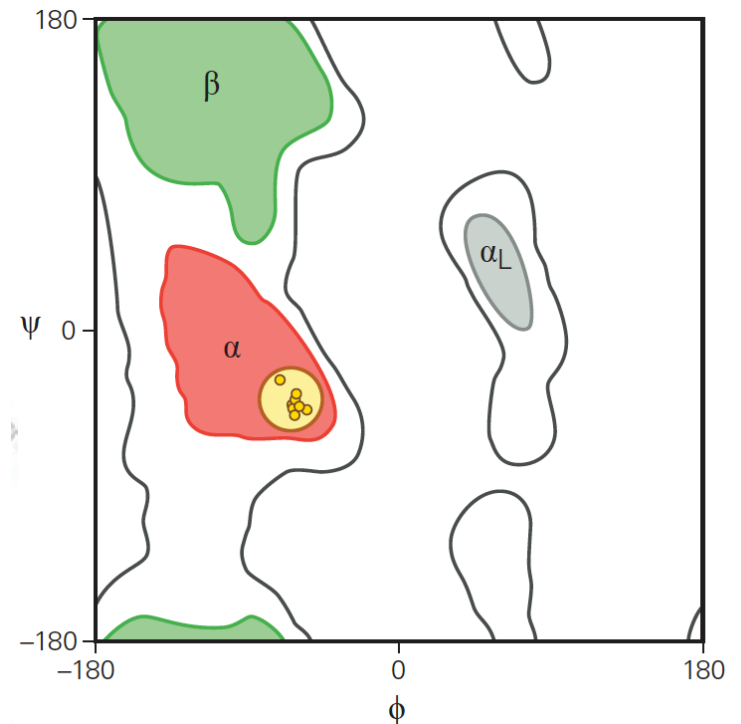
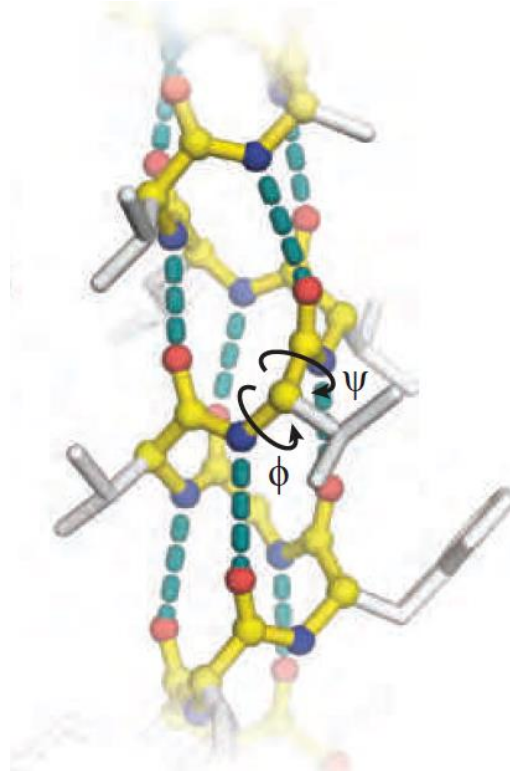


Figure 8-13
Illustration, Irving Geis. Image from the Irving Geis Collection, Howard Hughes Medical Institute. Reprinted with permission.

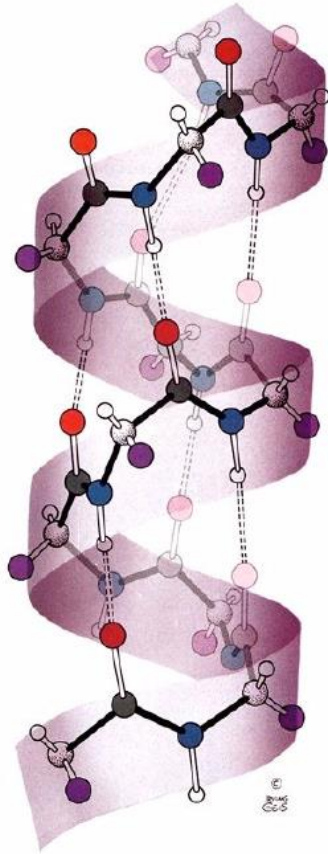


The right-handed α helix

- Hydrogen bonds form between residue n and $n + 3$
- Φ and ψ are around -60° and -50° , respectively.
- 3.6 residues per turn; 5.4 Å between turns



Helix propensity of amino acids



Ala
Leu
Met
Arg
Lys
Gln
Glu
Ile
Trp
Ser
Tyr
Phe
Val
Thr
His
Cys
Asn
Asp
⋮
Gly
Pro

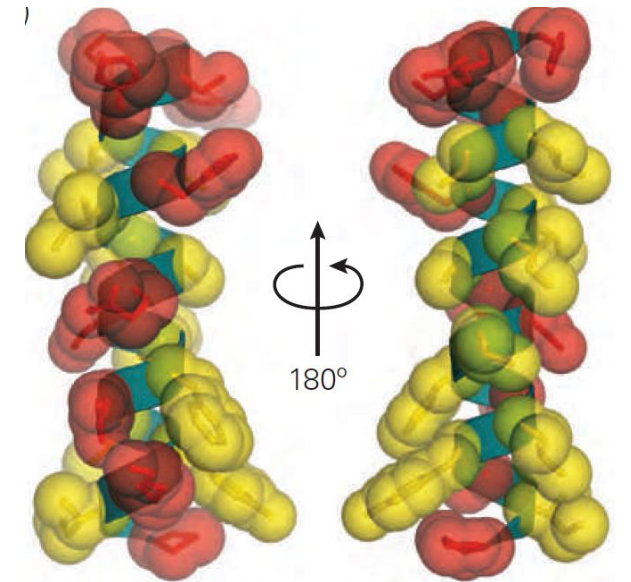
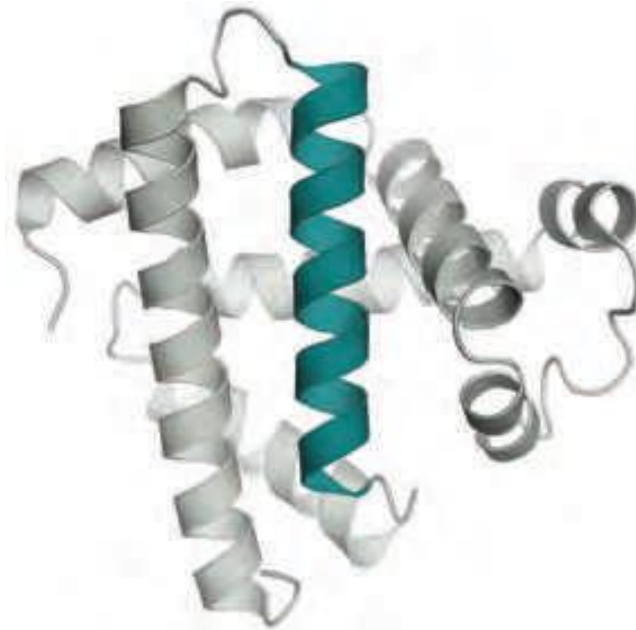
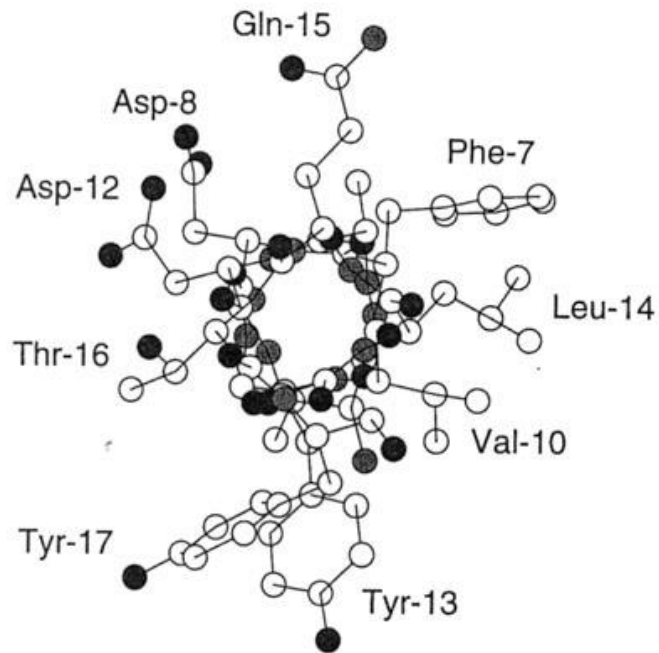


Table 5.3 *Relative Helical Tendencies of the Amino Acids Measured in One Peptide*

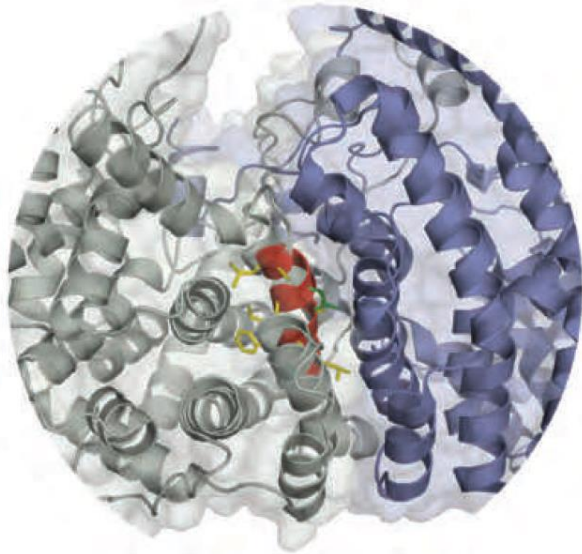
Amino acid residue	Relative stabilization of α -helical conformation ^a (kcal/mol)
Ala	-0.77
Arg	-0.68
Lys	-0.65
Leu	-0.62
Met	-0.50
Trp	-0.45
Phe	-0.41
Ser	-0.35
Gln	-0.33
Glu	-0.27
Cys	-0.23
Ile	-0.23
Tyr	-0.17
Asp	-0.15
Val	-0.14
Thr	-0.11
Asn	-0.07
His	-0.06
Gly	0
Pro	≈ 3

The helix wheel

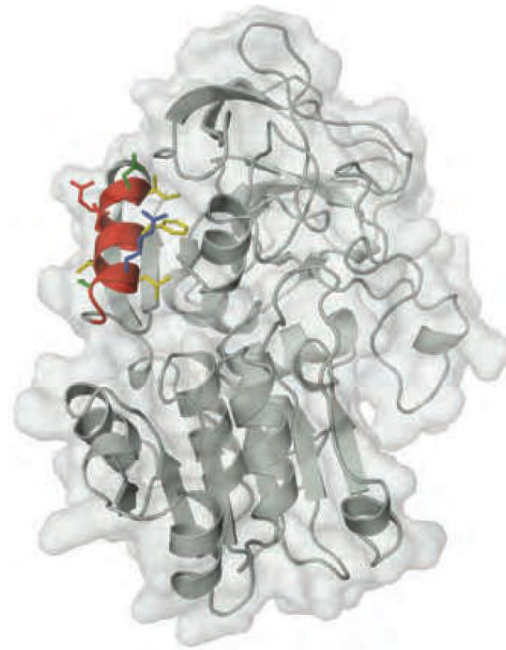
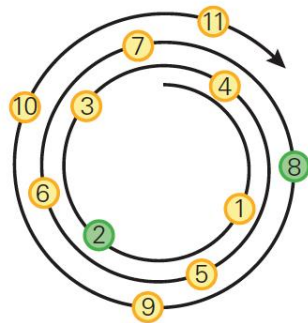
- Amphipathic: having both hydrophilic and hydrophobic parts.



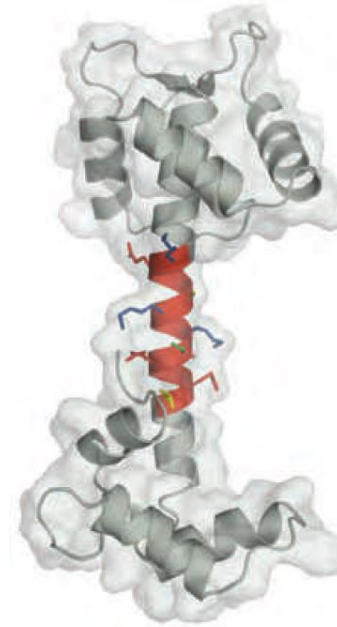
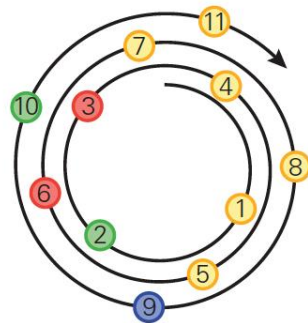
The helix wheel



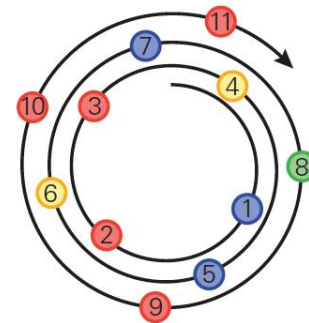
L S F A A A M N G L A



I N E G F D L L R S G

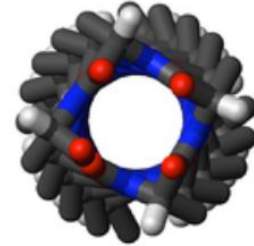
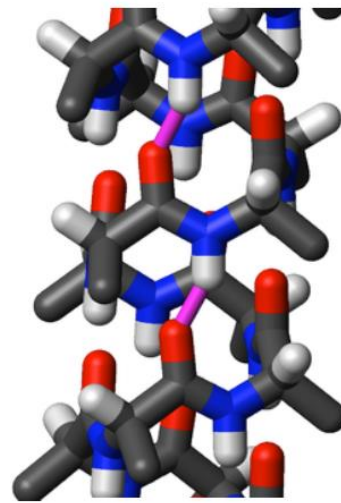
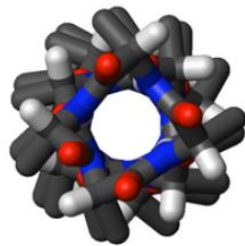
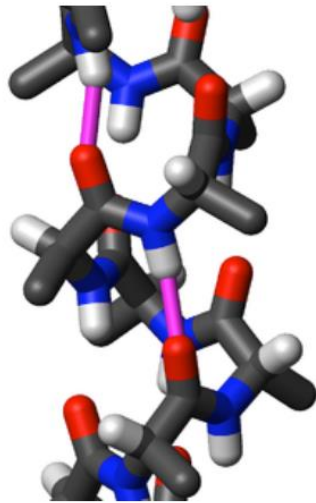
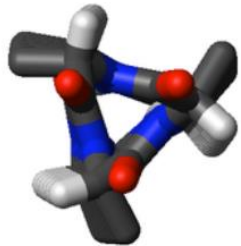
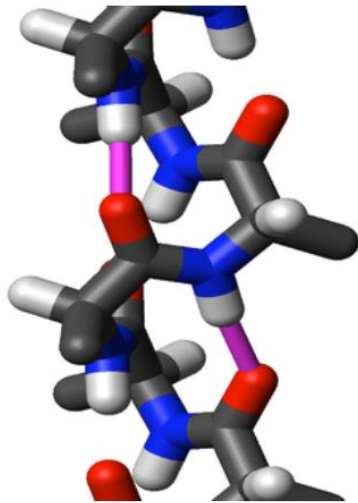


K E D A K G K S E E E

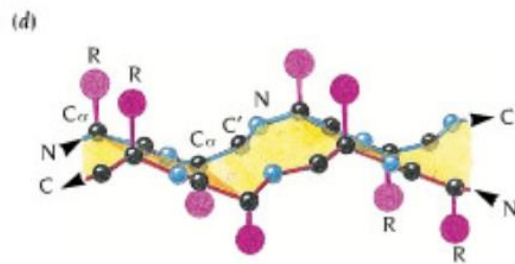
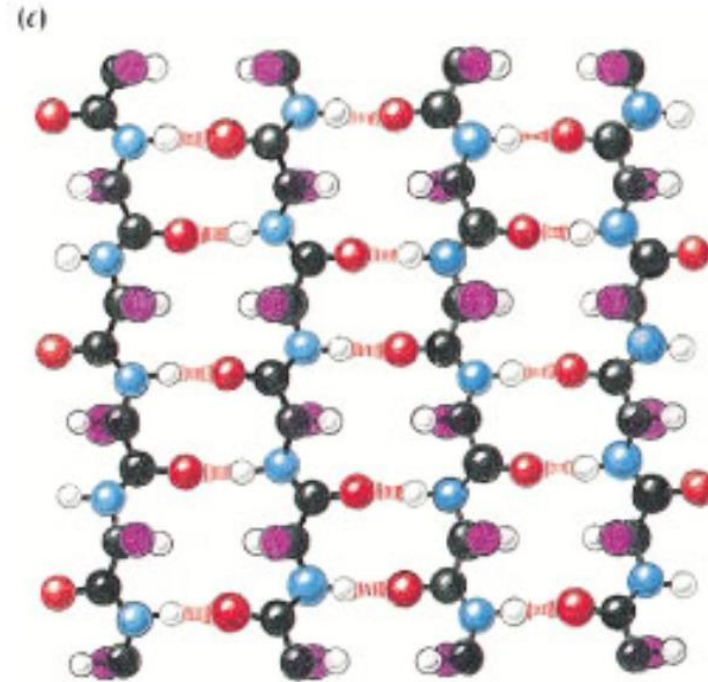
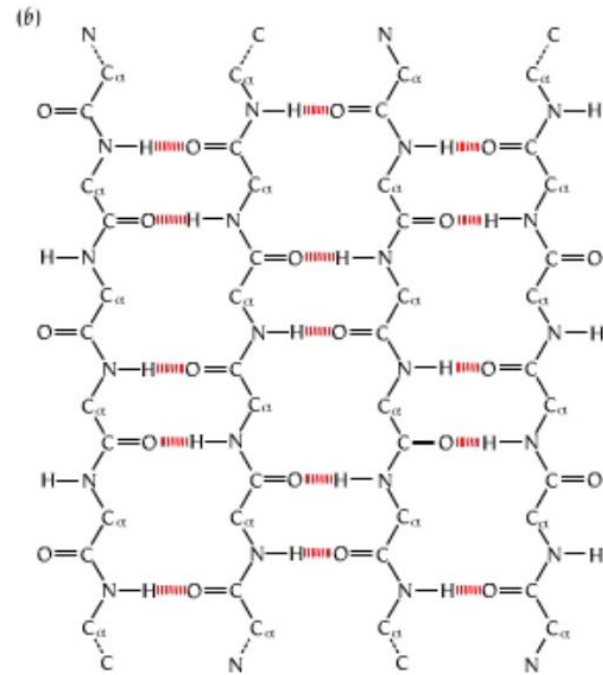
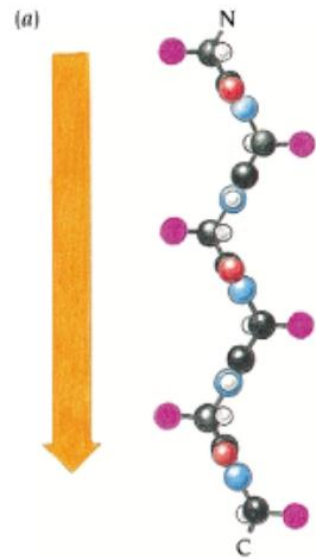


Three types of helices

- 3_{10} helix (φ : -49° , ψ : -26° , n : 3, d : 6.0\AA)
- α -helix (φ : -57° , ψ : -47° , n : 3.6, d : 5.4\AA): the most stable and common
- π -helix (φ : -57° , ψ : -70° , n : 4.4, d : 5.2\AA)

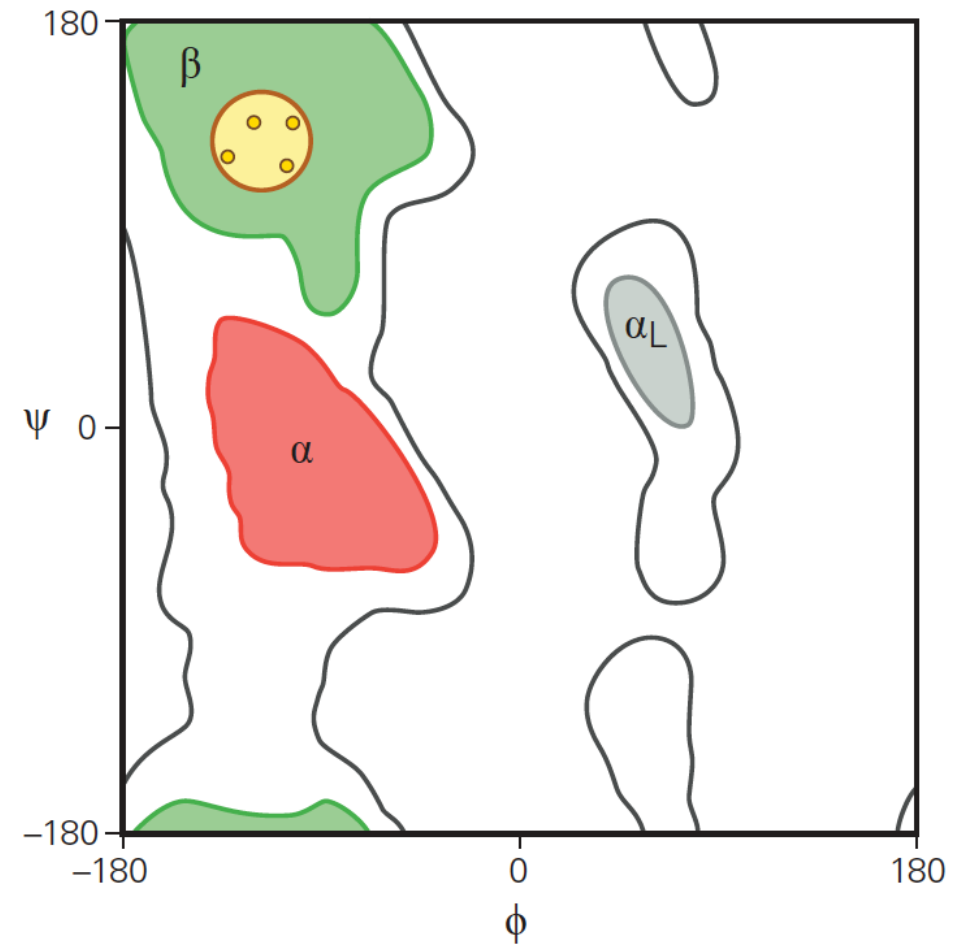
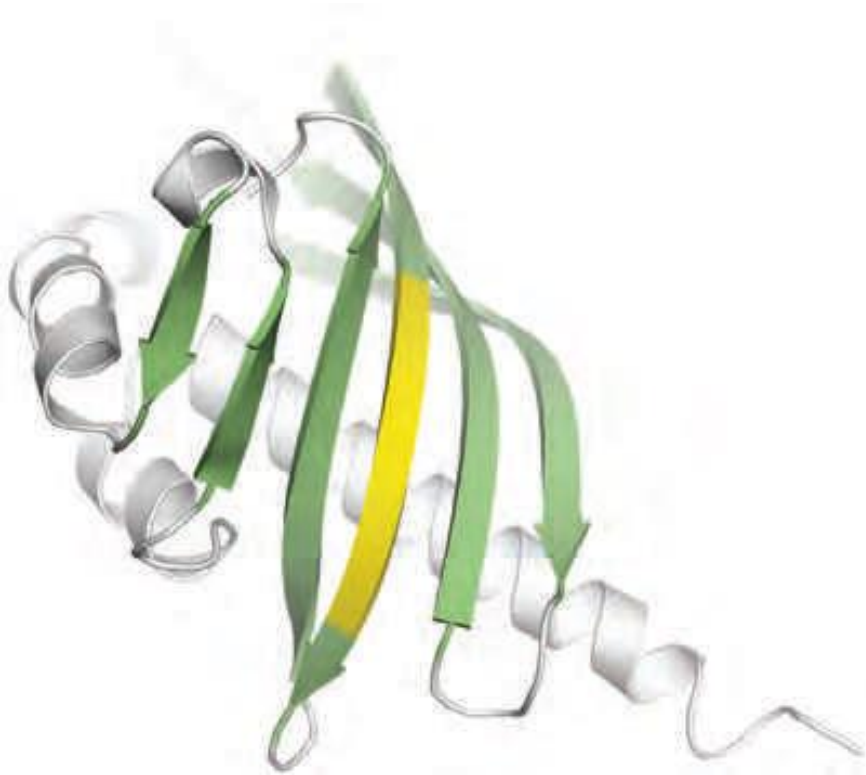


Anti-parallel β sheet ($\varphi: -139^\circ, \psi: -135^\circ$)

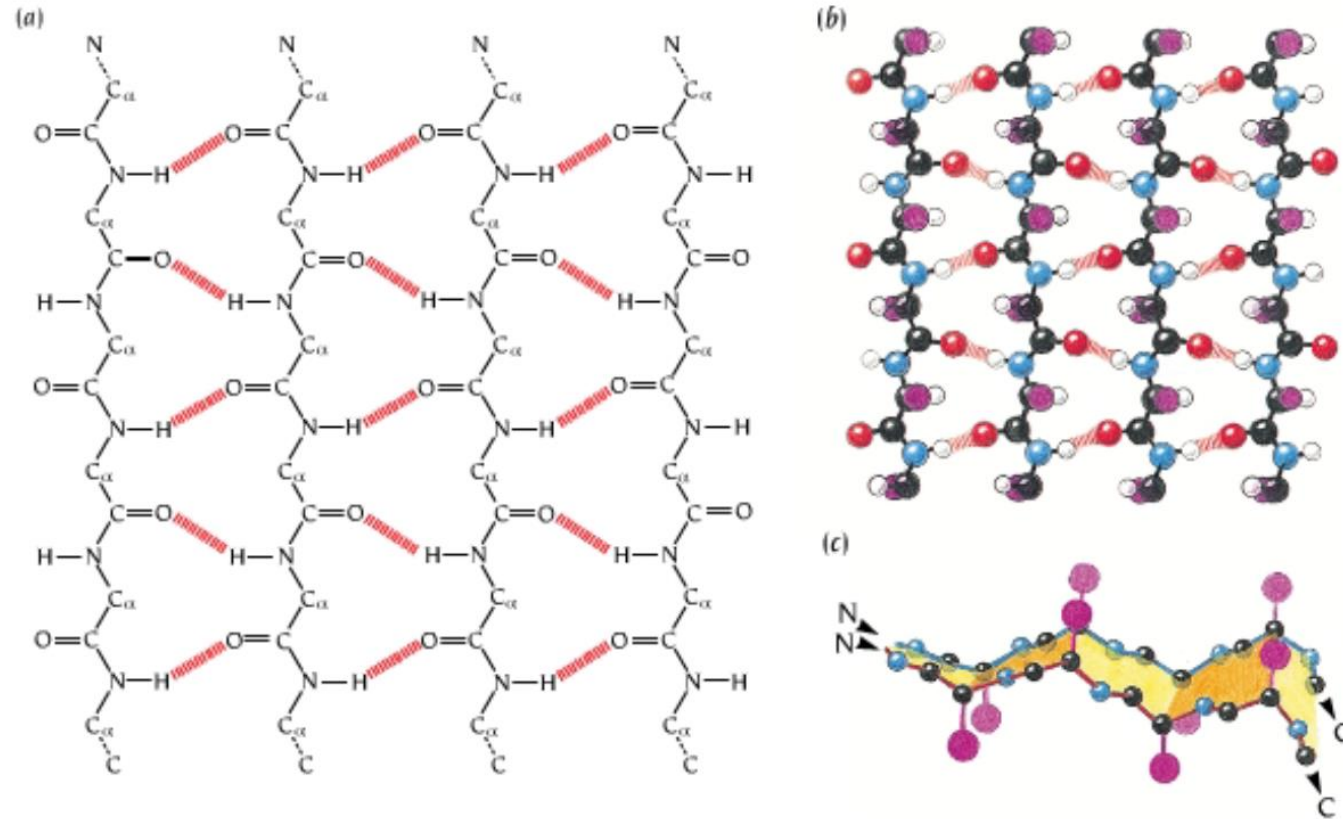


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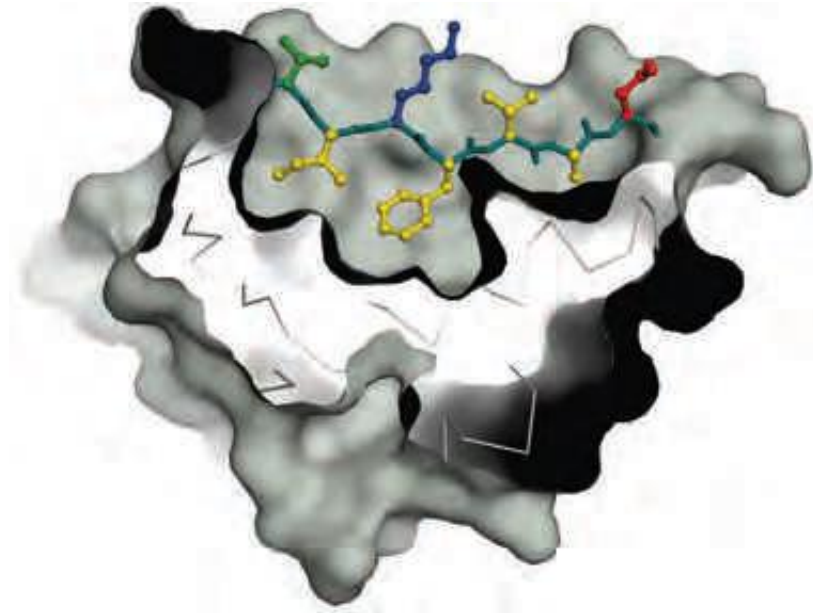
Anti-parallel β sheet (ϕ : -139° , ψ : -135°)



Parallel β sheet ($\varphi: -119^\circ, \psi: -113^\circ$)

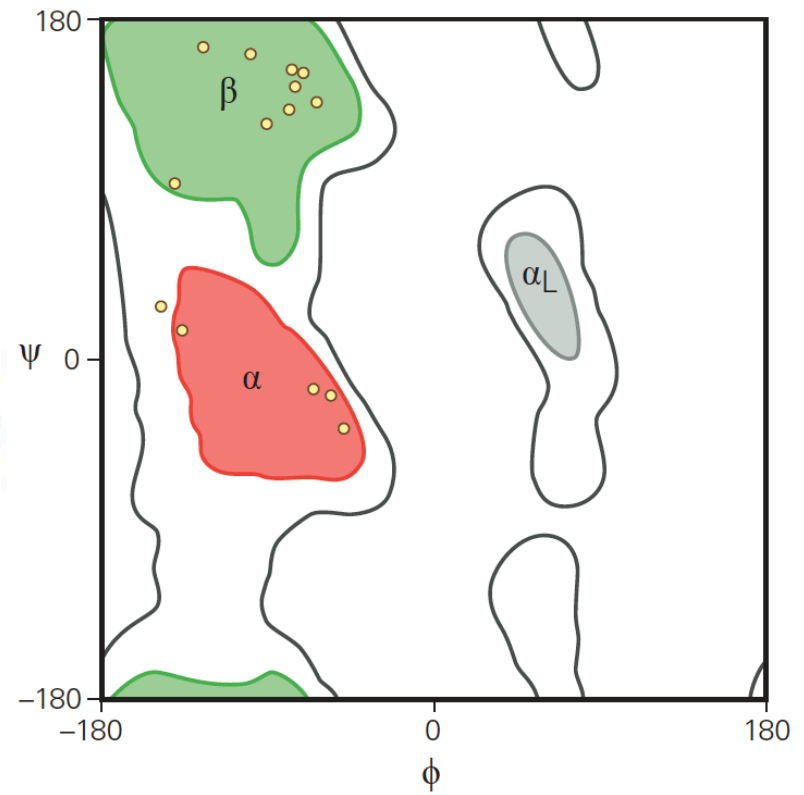
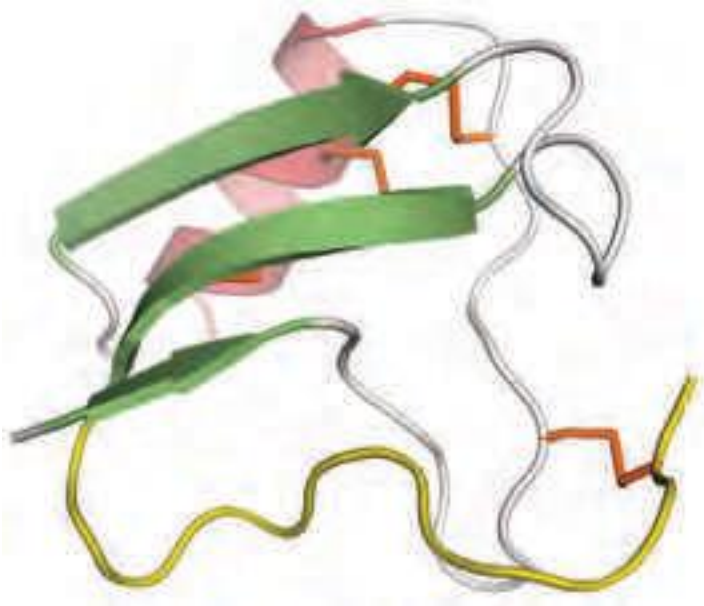


An amphipathic β sheet



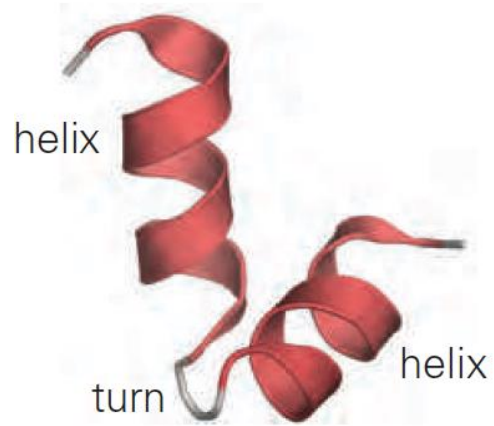
Thr - Ile - Lys - Phe - Val - Ala - Asp -

Loop

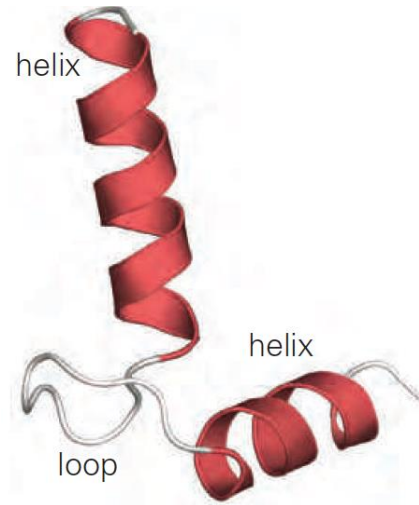


Structure motif

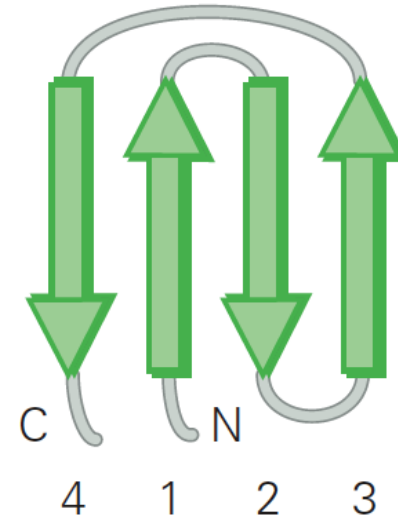
helix-turn-helix



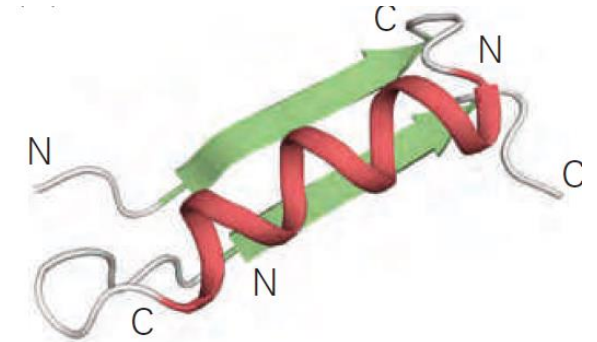
helix-loop-helix



Greek key motif

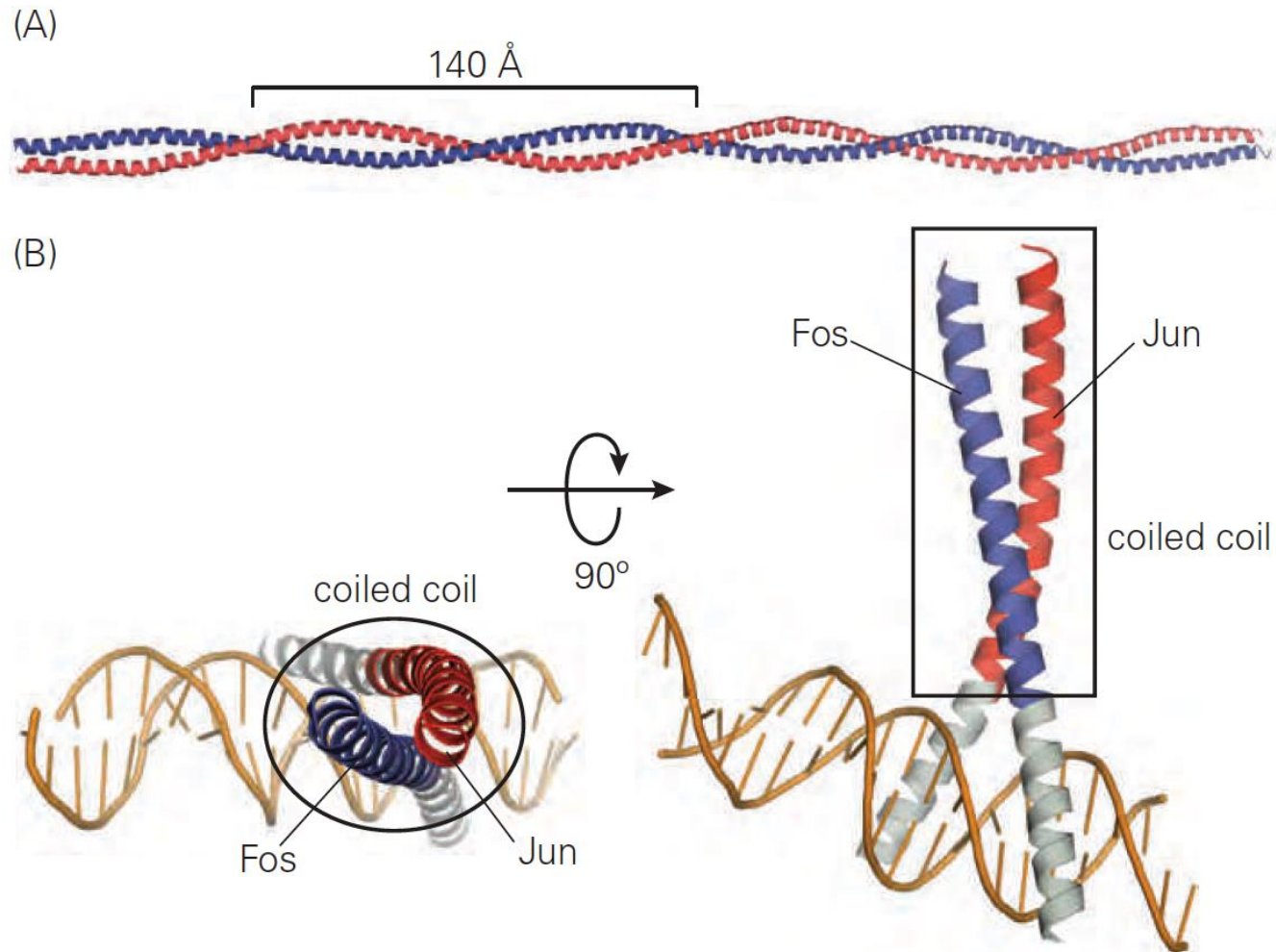


β - α - β motif



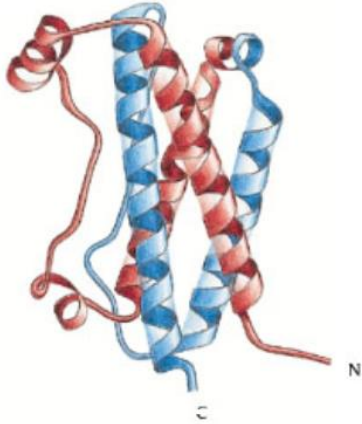
Structure motif

Coiled-coil



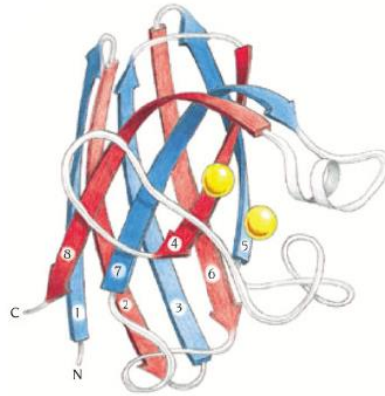
Protein domains

all- α domain



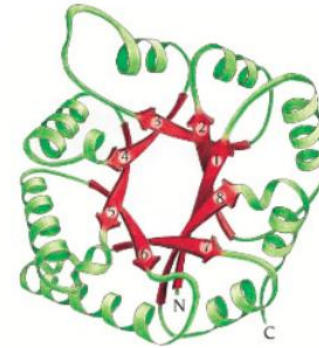
human growth hormone (3HHR)

all- β domain



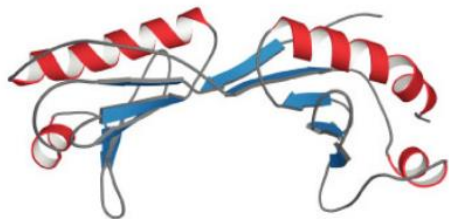
superoxide dismutase (2SOD)

α/β domain



triosephosphate isomerase (8TIM)

$\alpha+\beta$ domain



TATA-binding protein (1TBP)

small proteins



scorpion toxin (1B7D)

Where to find and visualize protein structures?

- Protein Data Bank: <https://www.rcsb.org/>
- Visualization software:
 - Chimera
 - VMD
 - PyMol