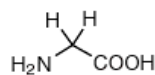


Základy molekulární biofyziky

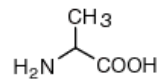
Část 4:
Struktura proteinů

Konstituční jednotky proteinů: aminokyseliny

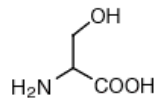
Small



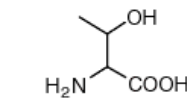
Glycine (Gly, G)
MW: 57.05



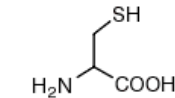
Alanine (Ala, A)
MW: 71.09



Serine (Ser, S)
MW: 87.08, pK_a ~ 16

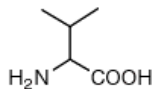


Threonine (Thr, T)
MW: 101.11, pK_a ~ 16

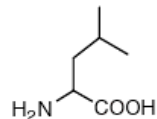


Cysteine (Cys, C)
MW: 103.15, pK_a = 8.35

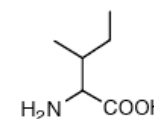
Hydrophobic



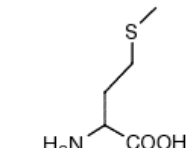
Valine (Val, V)
MW: 99.14



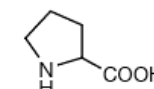
Leucine (Leu, L)
MW: 113.16



Isoleucine (Ile, I)
MW: 113.16

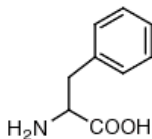


Methionine (Met, M)
MW: 131.19

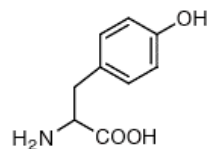


Proline (Pro, P)
MW: 97.12

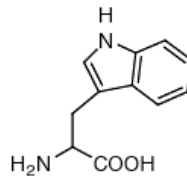
Aromatic



Phenylalanine (Phe, F)
MW: 147.18

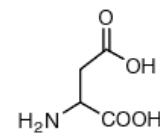


Tyrosine (Tyr, Y)
MW: 163.18

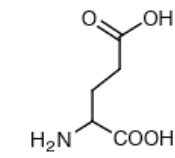


Tryptophan (Trp, W)
MW: 186.21

Acidic

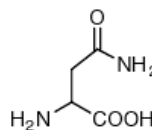


Aspartic Acid (Asp, D)
MW: 115.09, pK_a = 3.9

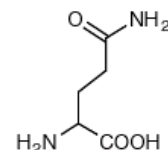


Glutamic Acid (Glu, E)
MW: 129.12, pK_a = 4.07

Amide

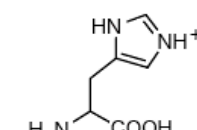


Asparagine (Asn, N)
MW: 114.11

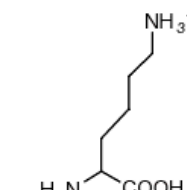


Glutamine (Gln, Q)
MW: 128.14

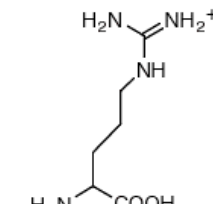
Basic



Histidine (His, H)
MW: 137.14, pK_a = 6.04

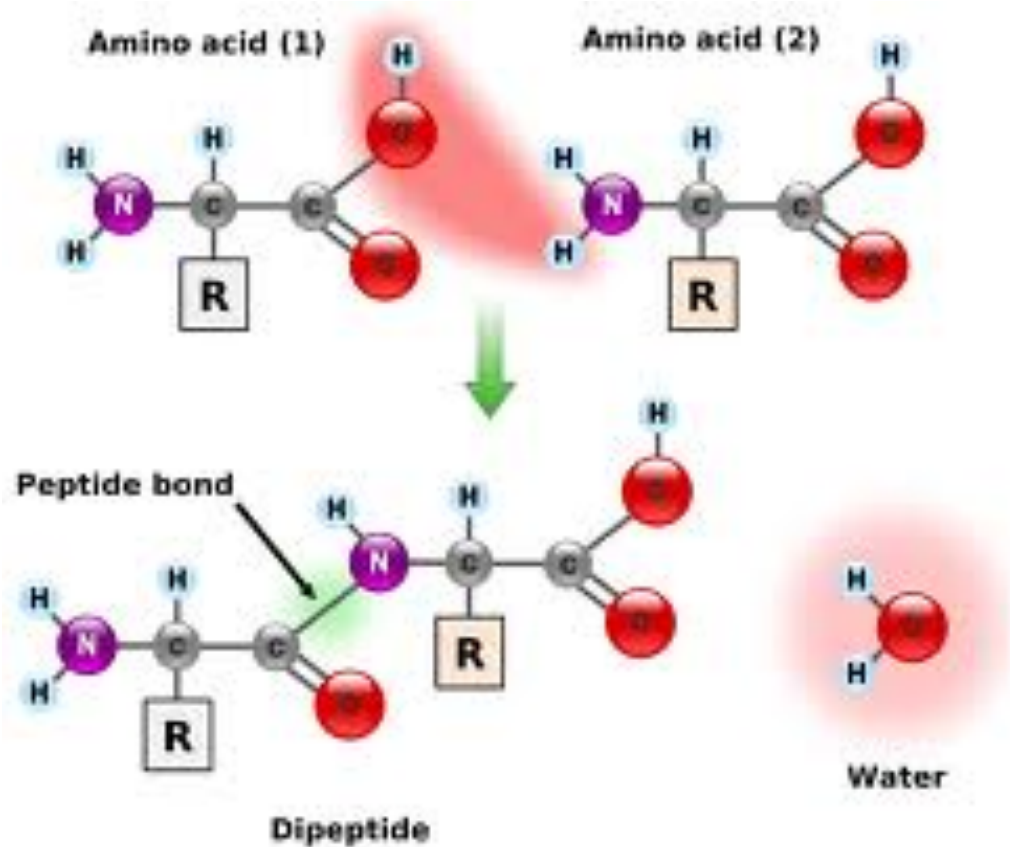


Lysine (Lys, K)
MW: 128.17, pK_a = 10.79

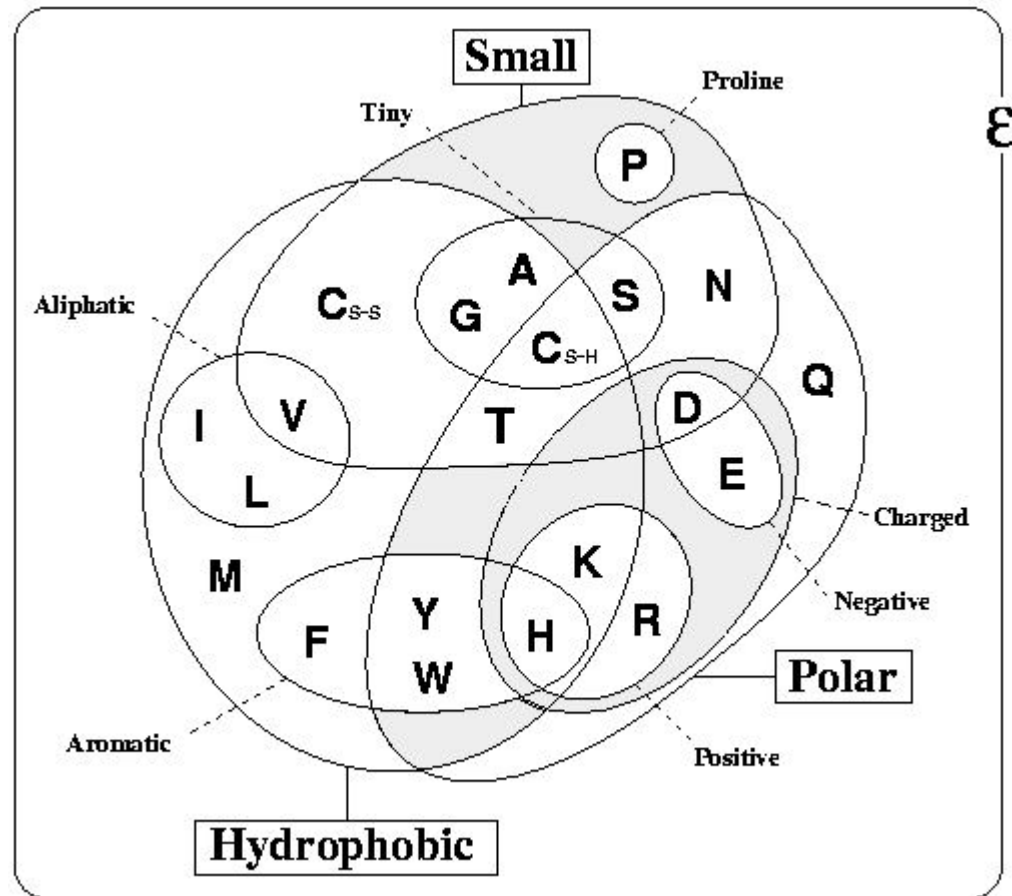


Arginine (Arg, R)
MW: 156.19, pK_a = 12.48

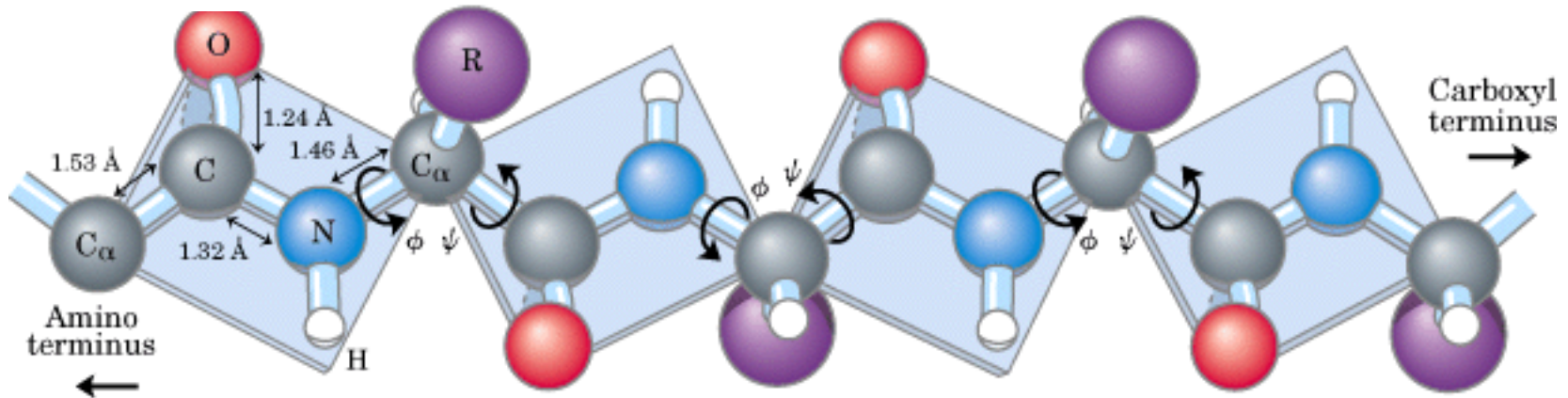
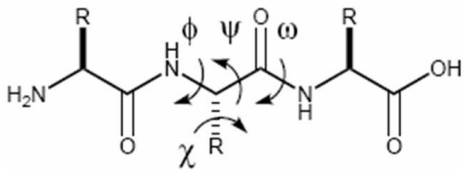
Peptidická vazba



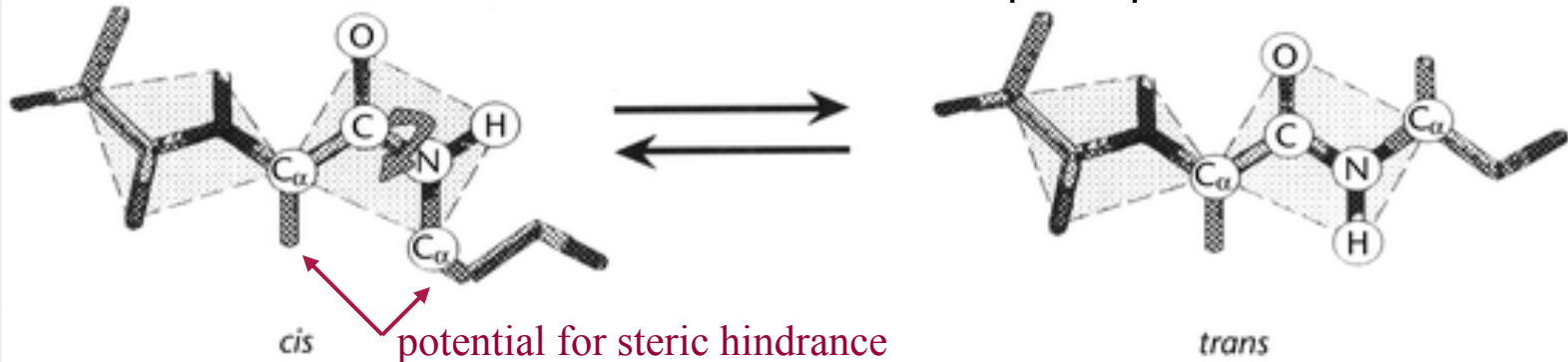
Peptidická vazba



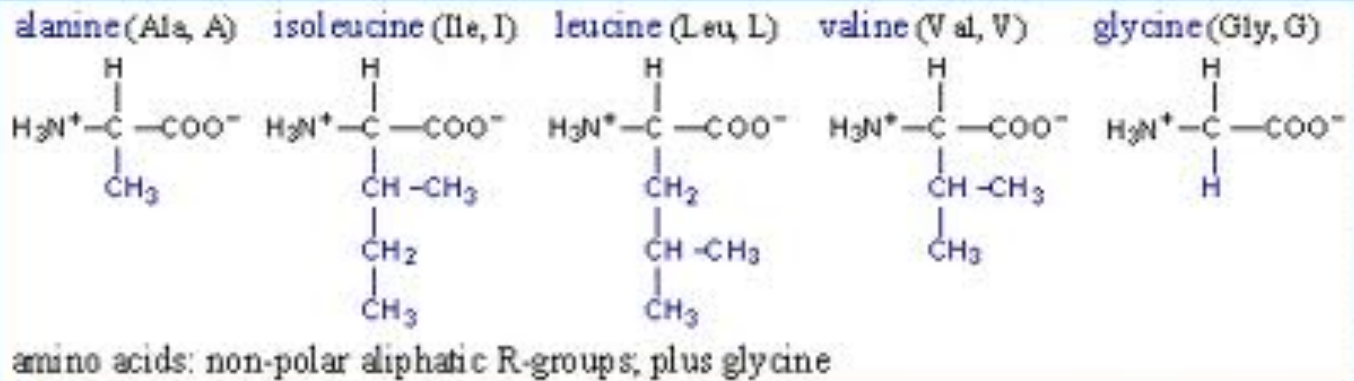
Peptidická vazba – popis geometrie



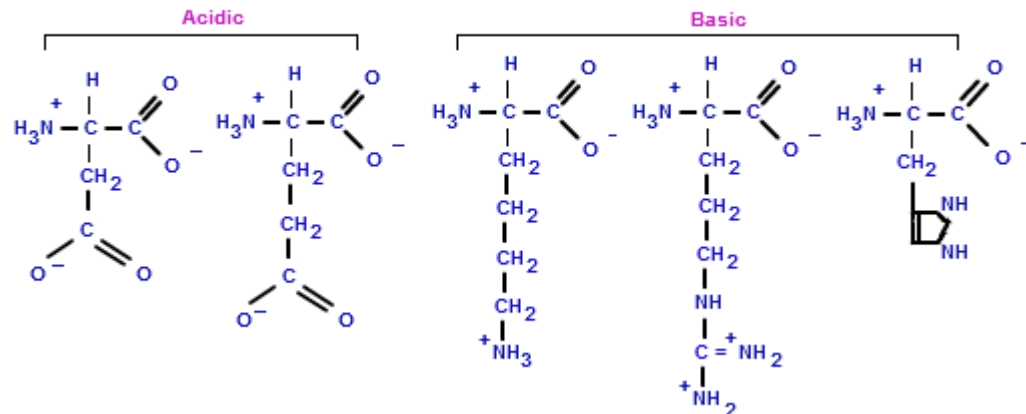
◆ *cis* conformation is rare except for proline



Postraní řetězce – určují vlastnosti



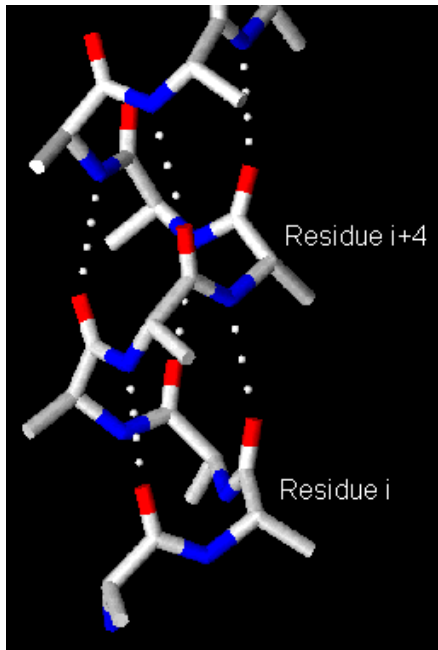
Electrically charged side chains



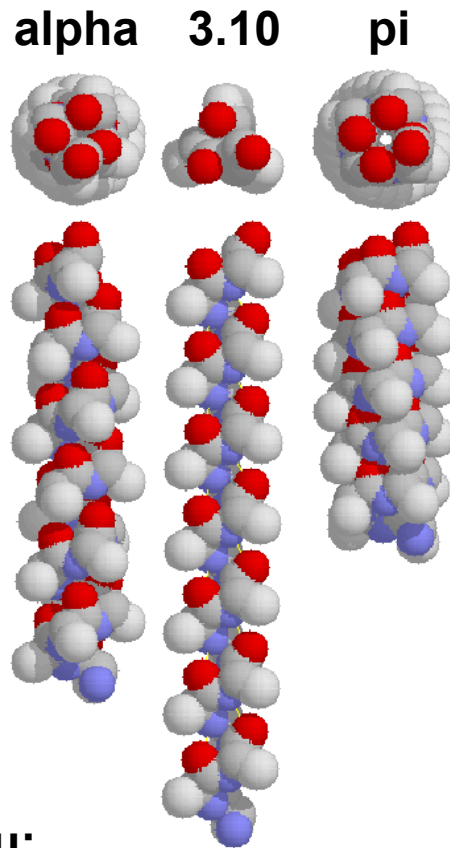
Architektura proteinů

Strukturní element	Popis
■ primární struktura	aminokyselinová sekvence
■ sekundární struktura	helixy, sheety, smyčky
■ super-sekundární struktura	asociované prvky 2° struktury
■ doména	self-contained structural unit
■ terciální struktura	poskládaná struktura celého proteinu (S-S vazby)
■ kvaterní struktura	organizace proteiného komplexu (homo/hetero-oligomery)

Architektura proteinů- helixy



H-bonding



- Alfa helixy mají kolem 10 aa

Počet aa na otáčku helixu:

3.6

3.0

4.4

Frekvence výskytu:

~97%

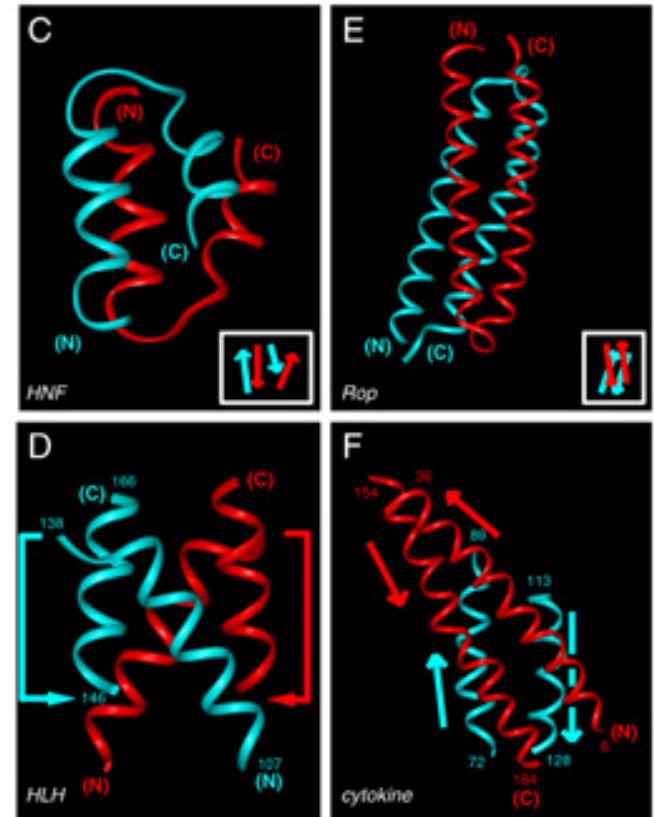
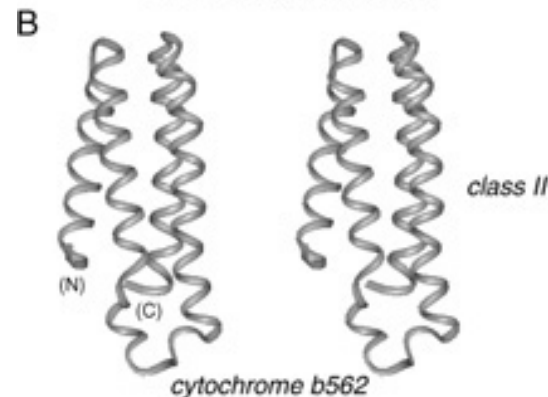
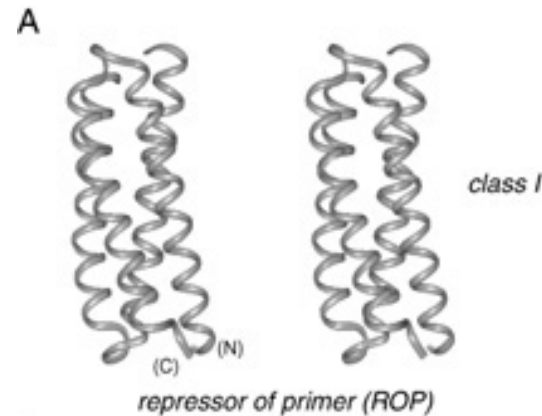
~3%

vzácné

super-sekundární struktura

Coil-coil:

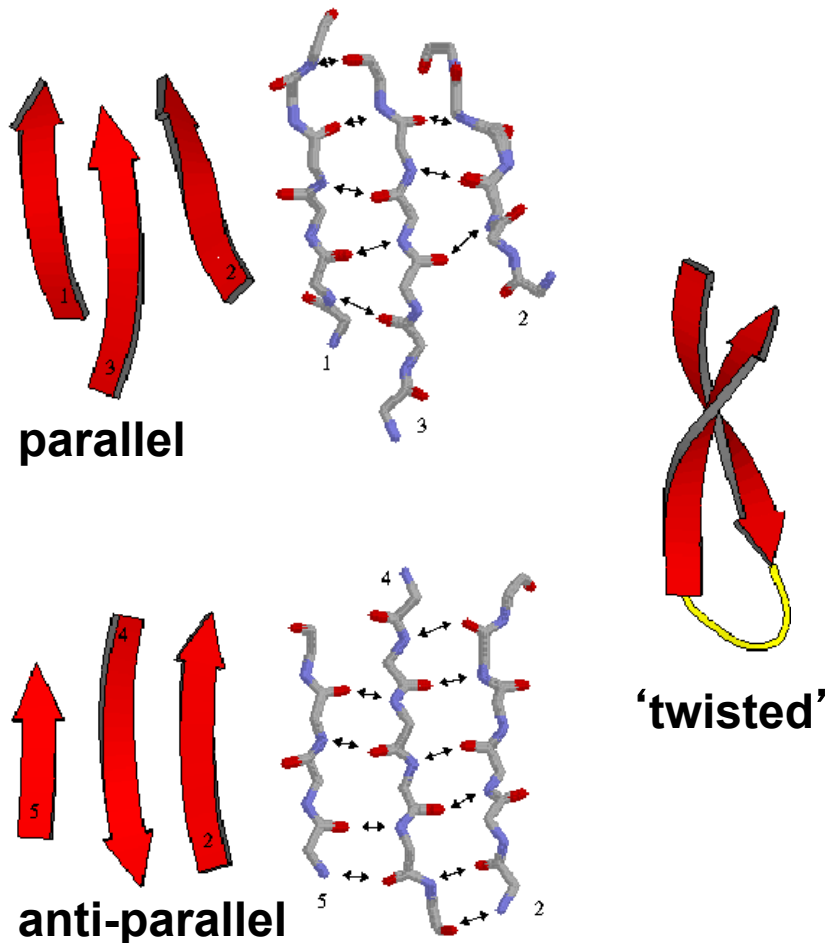
společný alfa helix
(proteinový folding,
protein-proteinové
interakce)



Helix bundle:

stále prostorové
uspořádání tří a více
helixů

Architektura proteinů- skládaný list

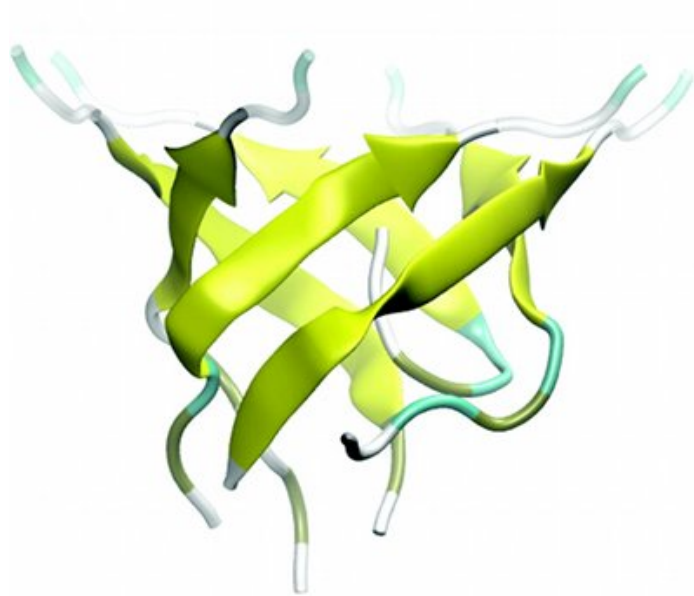


- Základní jednotkou skládaného listu je tzv. beta-strand

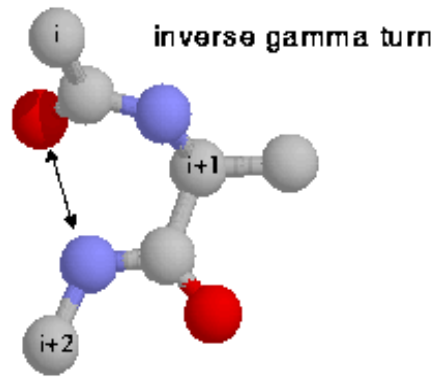
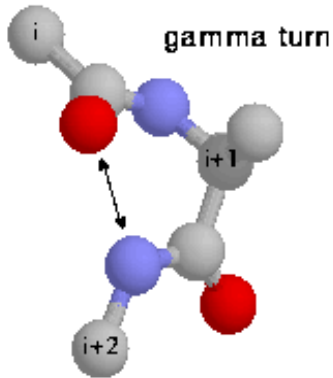
- Narozdíl o helixu, skládaný list může být tvořen z diskontinuálních řetězců

super-sekundární struktura

- např. beta-barel



Architektura proteinů- turns/loops



- Existují různé typy “turns” které se liší počtem aminokyselin a HB

- “loops” jsou většinou delší (často jsou označvány jako “coils”) Nemají regulární, opakující se strukturu

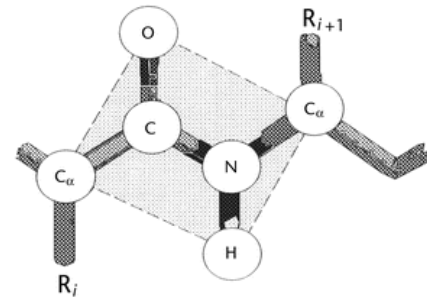
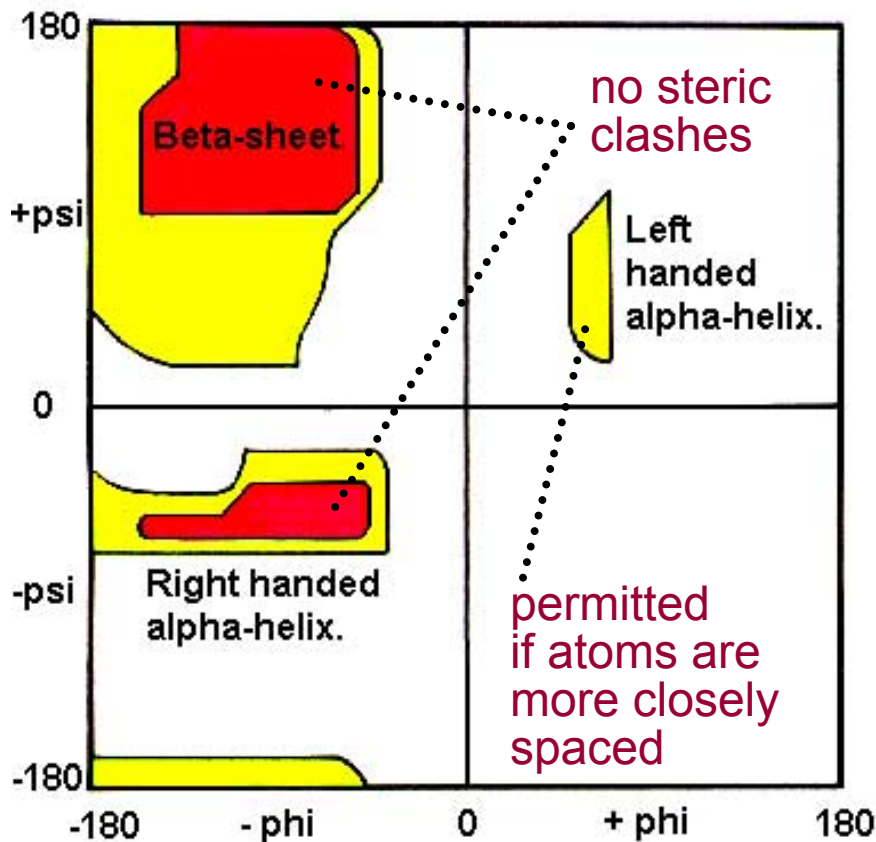


Architektura proteinů- super-sekundární organizace skládaného listu



Ramachandran plot

The Ramachandran Plot.

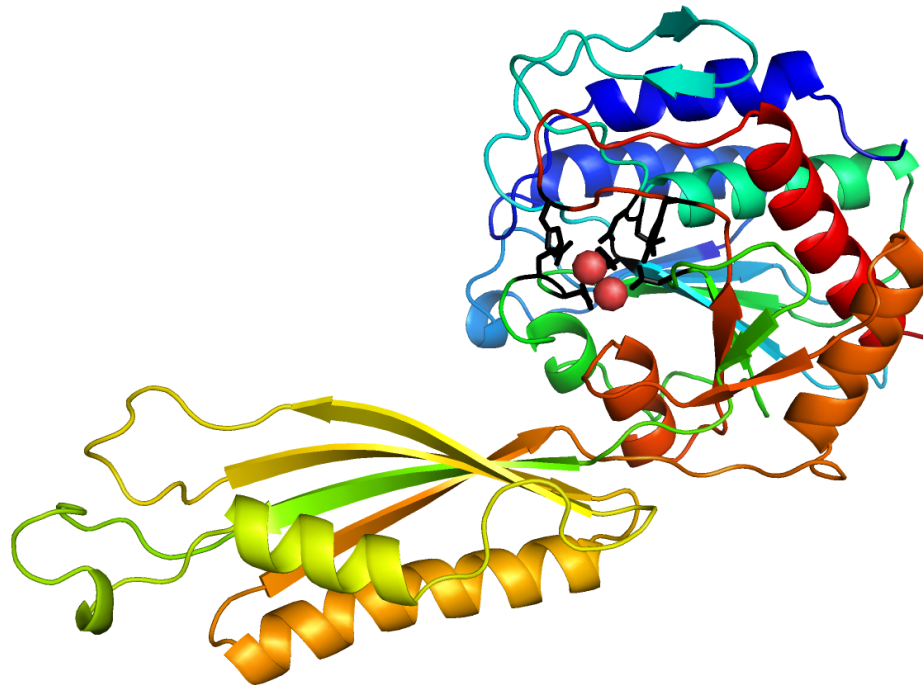


Nekovalentní interakce v proteinech

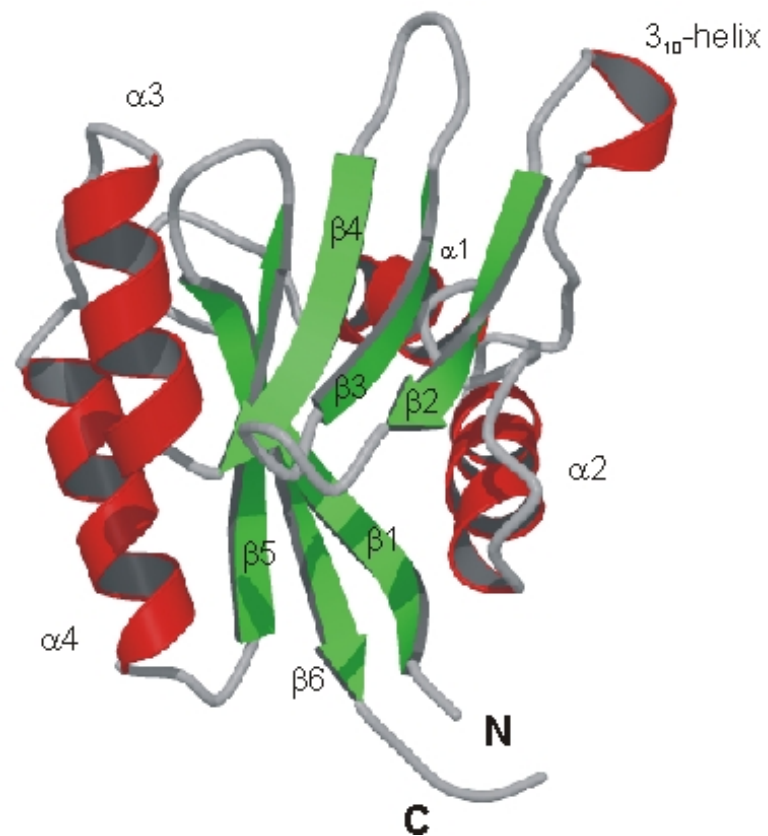
interaction	nature	bond length	“bond” strength	example
ionic (salt bridge)	electrostatic	1.8-4.0 Å (3.0-10 Å for like charges)	1-6 kcal/ mol	positive: K, R, H, N-terminus negative: D, E, C-terminus
hydrophobic	entropy	-	2-3	hydrophobic side chains (M,I,L,V,F,W,Y,A,C,P)
H-bond	H-bonding	2.6-3.5	2-10	H donor, O acceptor
van der Waals	attraction/ repulsion	2.8-4.0	<1	closely-spaced atoms; if too close, repulsion
aromatic- aromatic	π - π	4.5-7.0	1-2	F,W,Y (stacked)
aromatic- amino group	H-bonding	2.9-3.6	2.7-4.9	N-H donor to F,W,Y

Doména

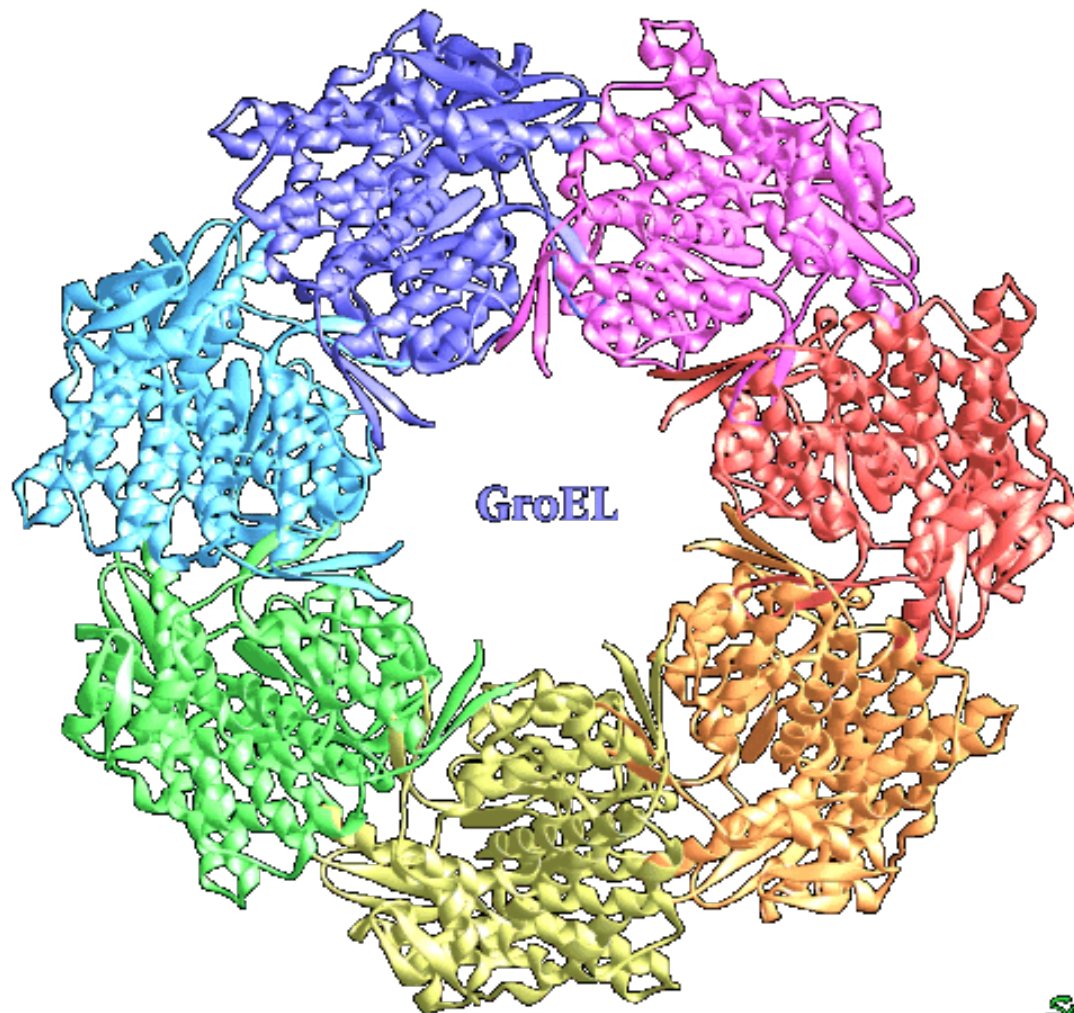
**Kompaktní jednotka uvnitř poskládaného jednořetězce
která se může vyvíjet, fungovat a existovat bez zbytku
proteinu**



Terciální struktura



Kvarterní struktura



Struktura a klasifikace proteinů (PDB), proteomické nástroje (expasy)

www.pdb.org

www.expasy.org