

LECTURE 3

POLYPEPTIDE SYNTAX

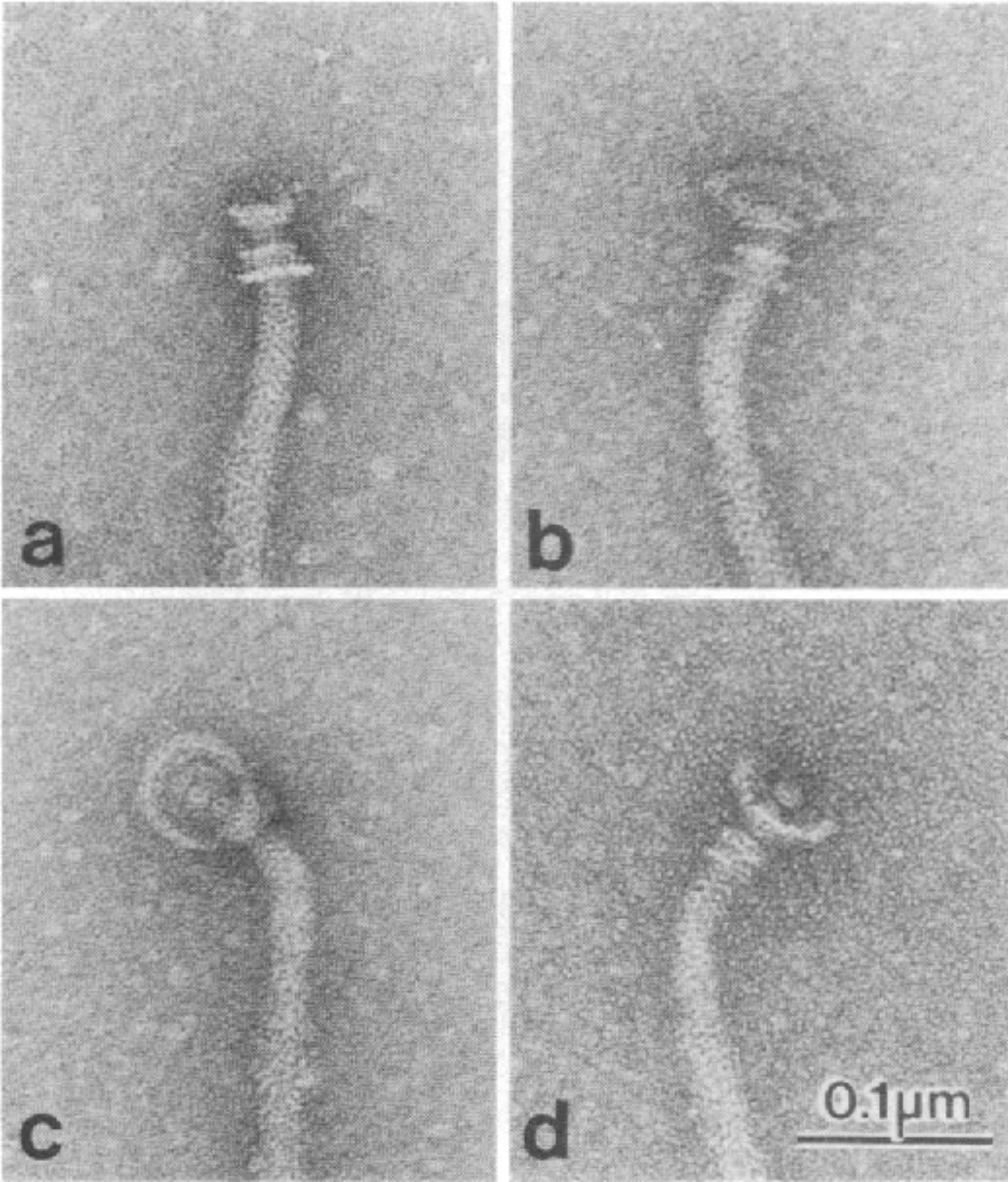
Amino acid structures
C1, Calpha carbons
hydrophobic - AGILPV
aromatic - FWY
neg charge - DE
pos charge - RHK
hydroxyllic - ST
sulfur containing - CM
polar - NQ

protein structure
peptide bond
dihedral angles
phi (N-Ca)
psi (Ca-C1)
omega (C1-N) = 180deg unless proline (0deg)
protein folding
bond forces
stretching, bending, rotating
short range forces
Pauli repulsion, van der Waals' interactions
Electrostatic forces
Coulomb's law
interaction with solvent
Motif's
alpha helix
3.6 residues per turn
each residue 100deg, 1.5A
beta sheet
planar
isoelectric point
molecular weight

protein domains
binding domain - leucine zipper, TALEN
PTM domain
phosphorylation
methylation
ubiquitination
enzymatic domains
protease
kinase
targeting domains
NLS
signal peptide
anchoring sequence

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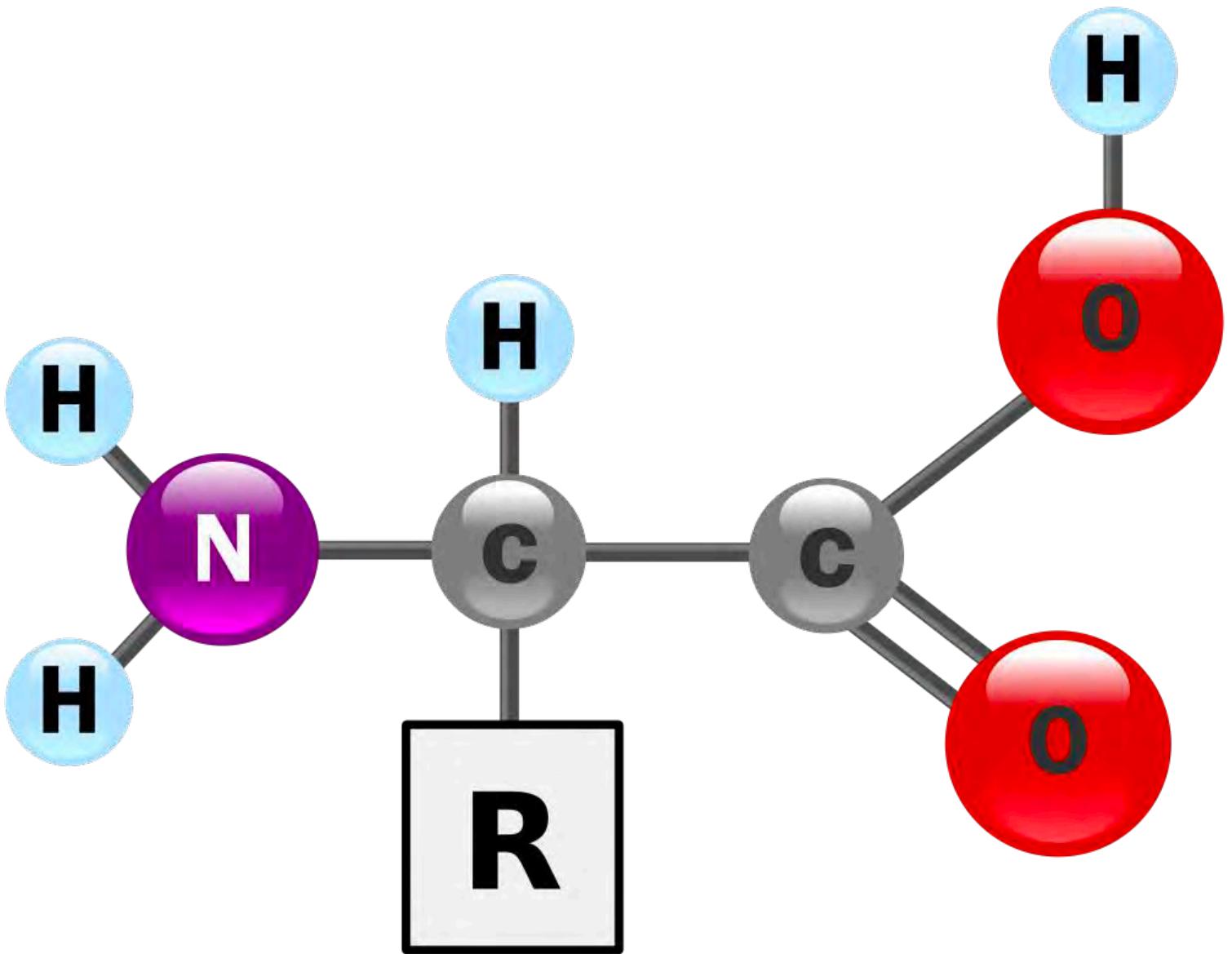


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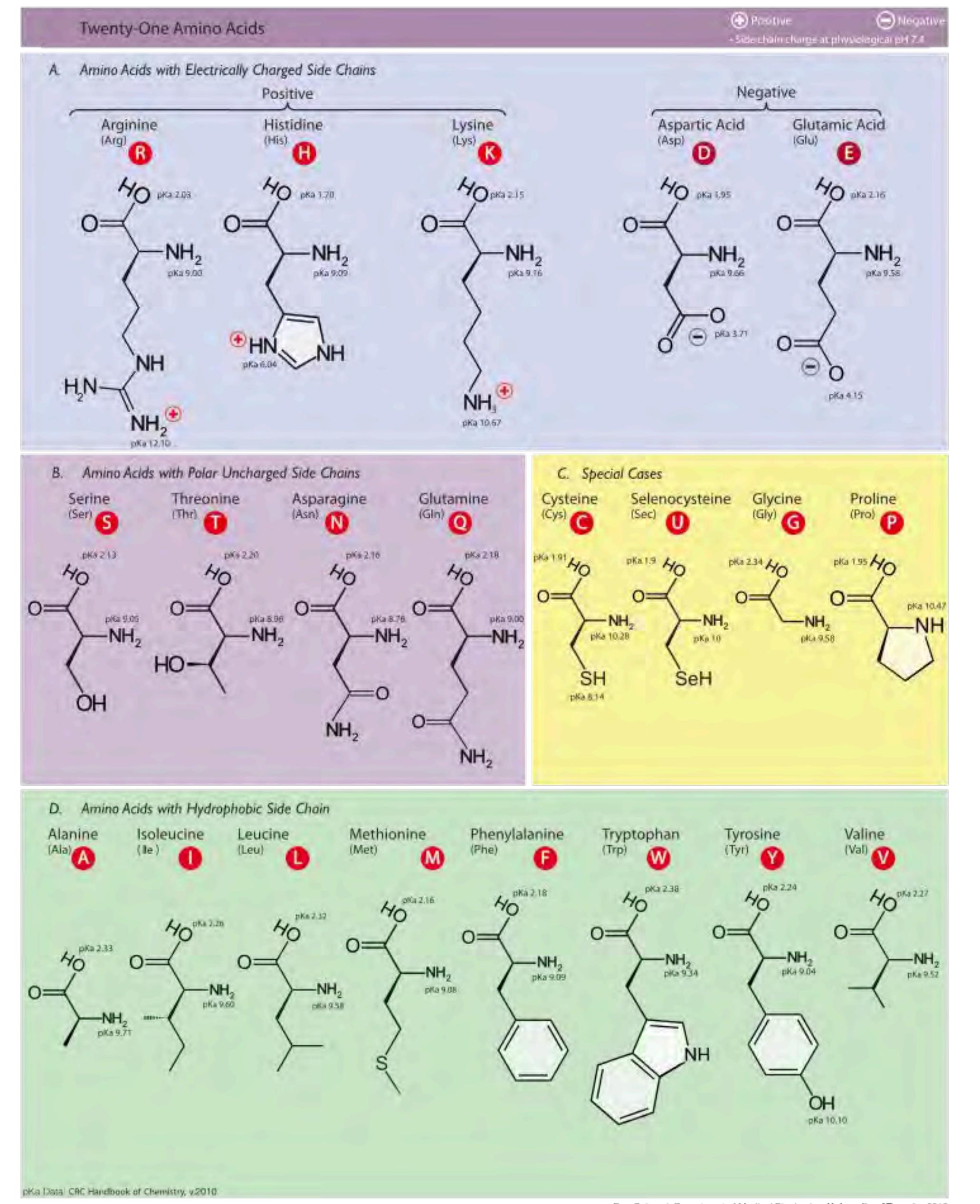
20 different variants or this organic group in essential amino acids

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essential amino acids

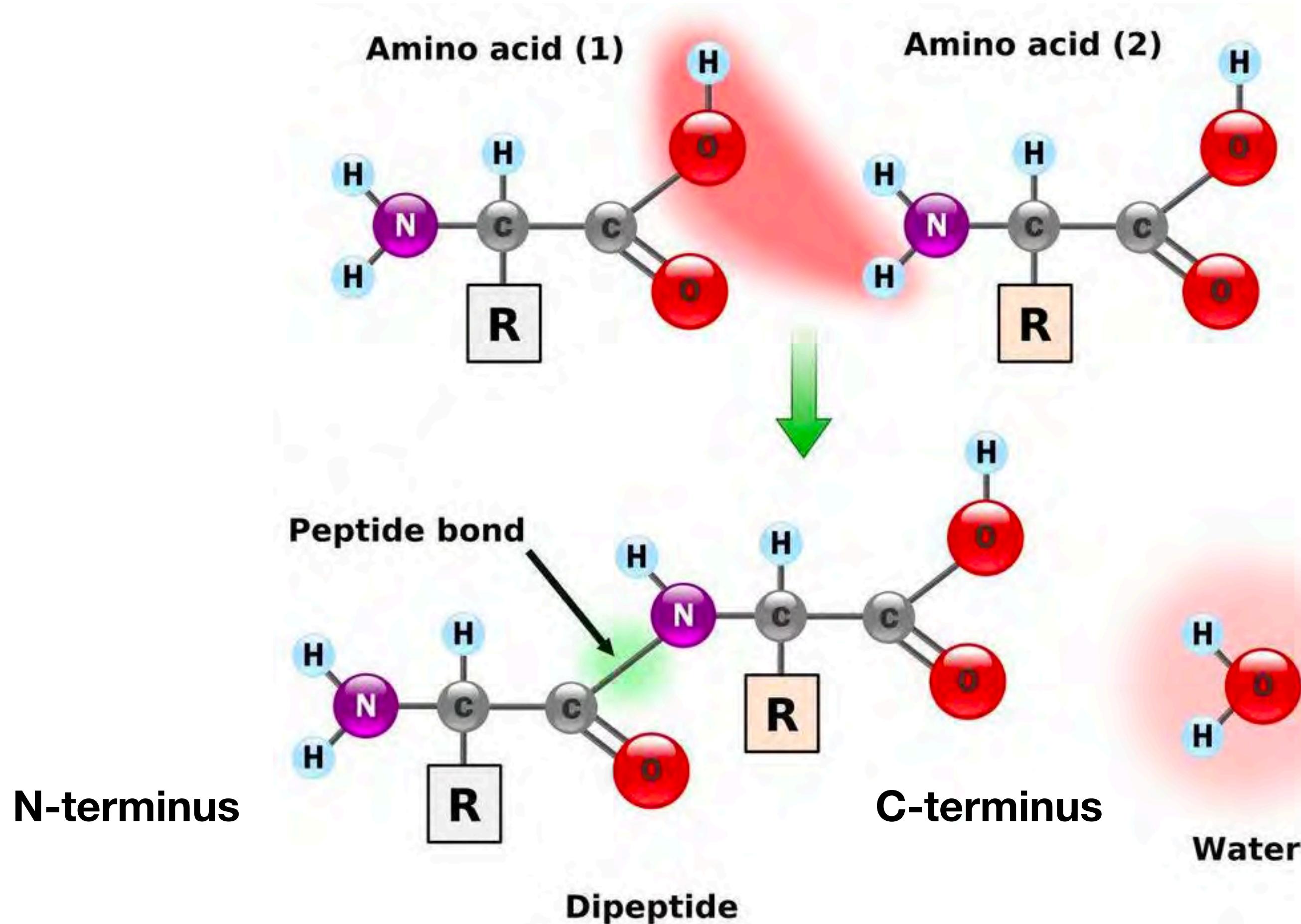


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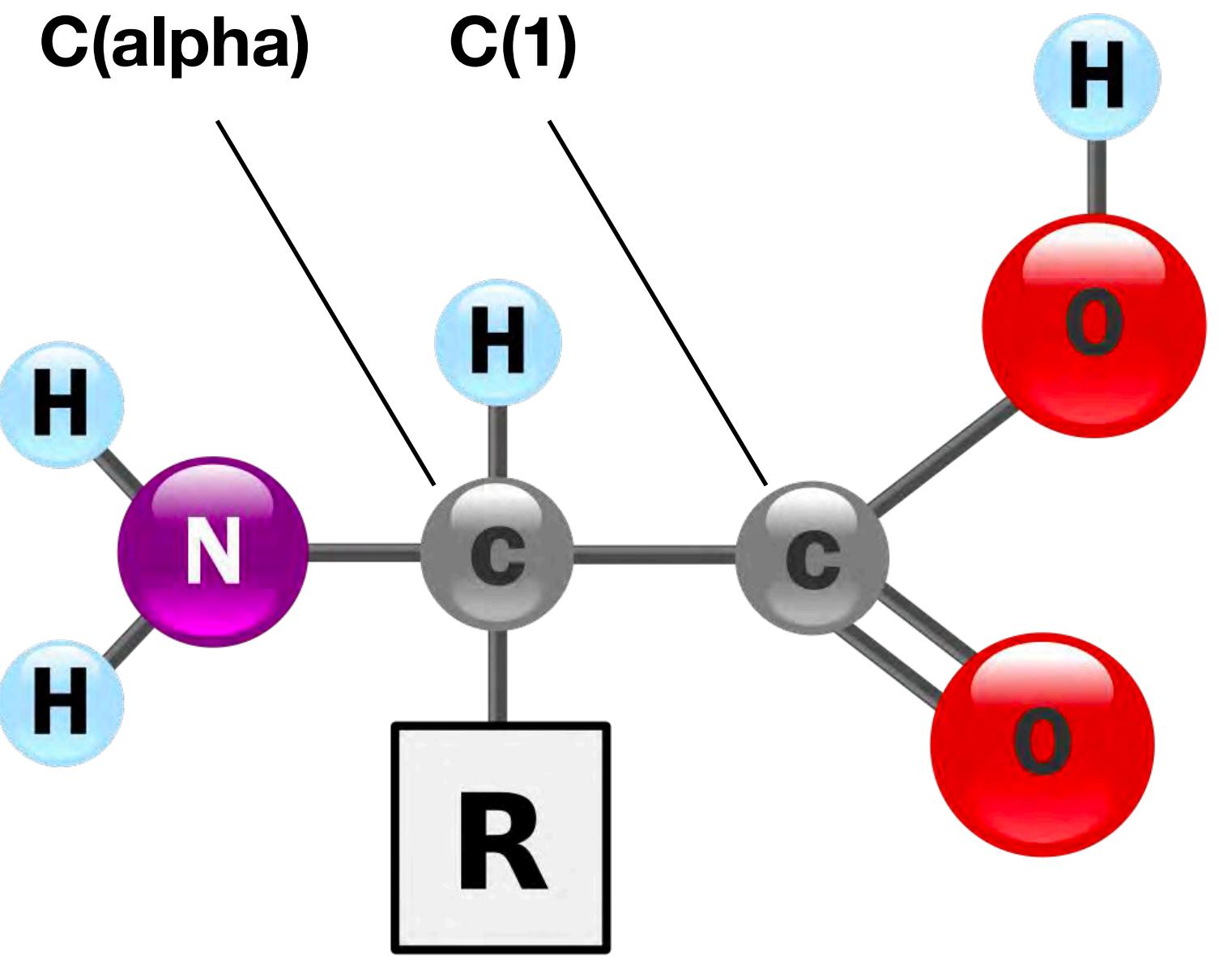
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polypeptide carbons

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polypeptide angles

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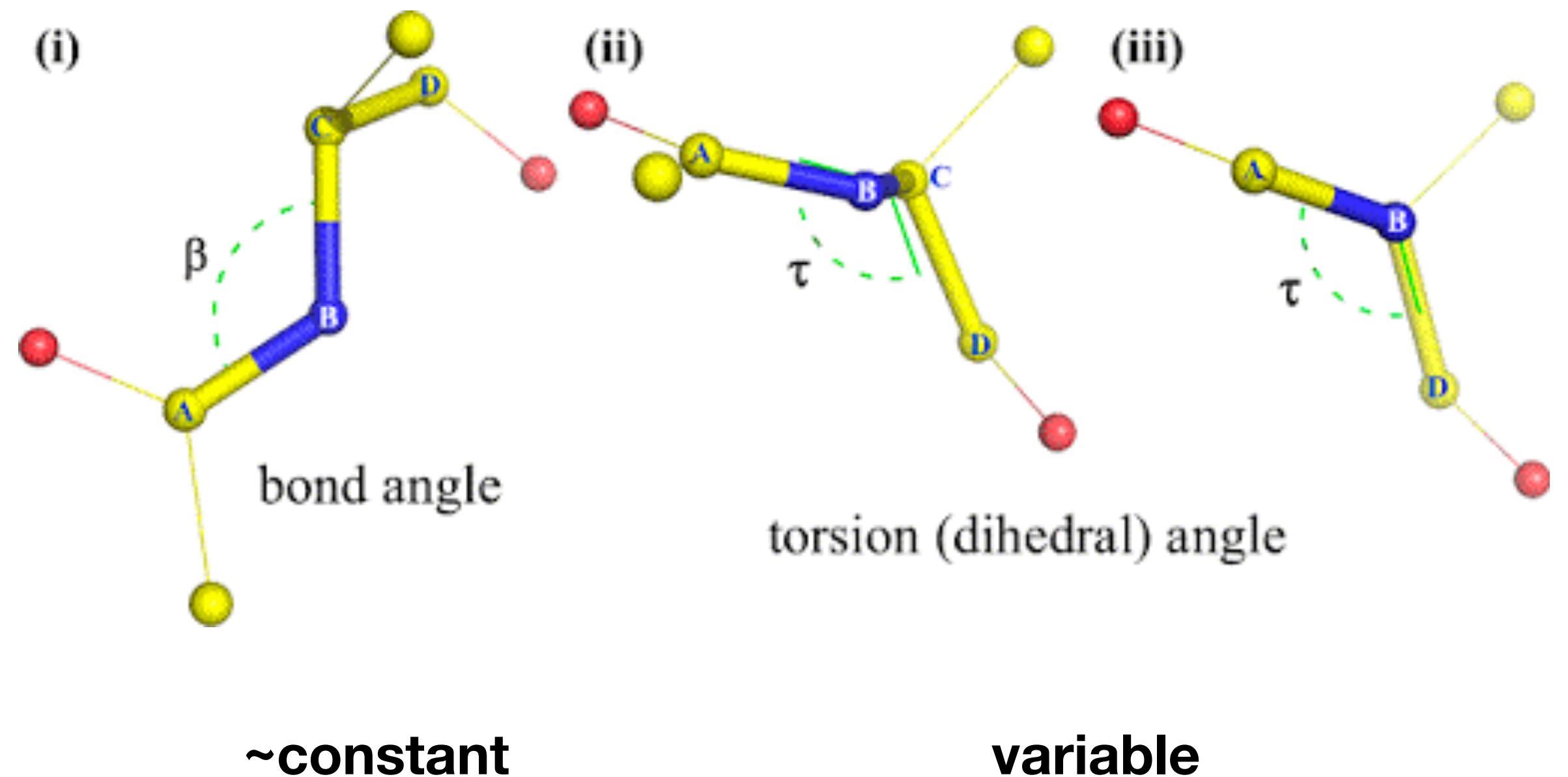
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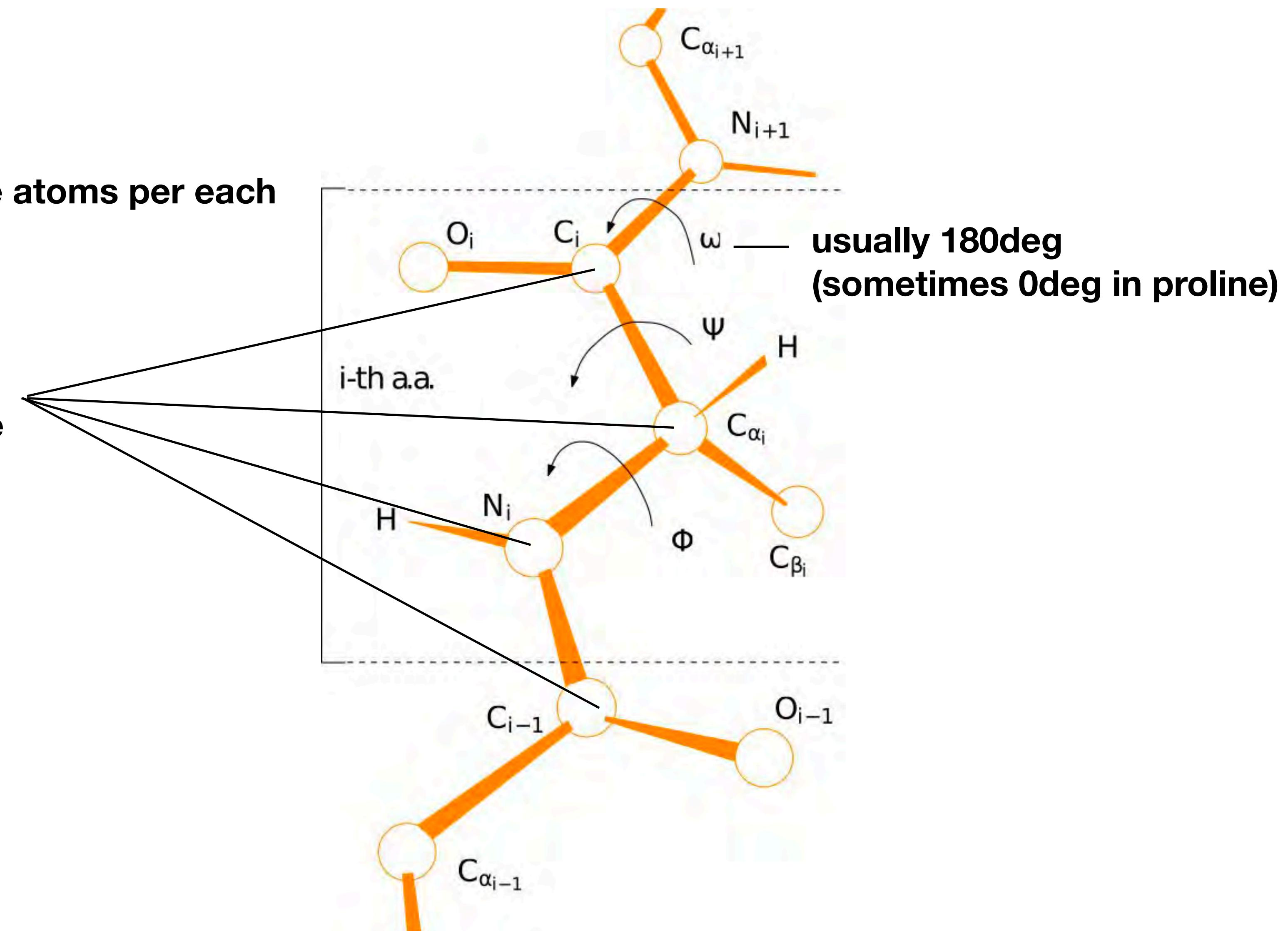


dihedral angles

LECTURE 3 POLYPEPTIDE SYNTAX

four backbone atoms per each dihedral angle

atoms used to measure phi

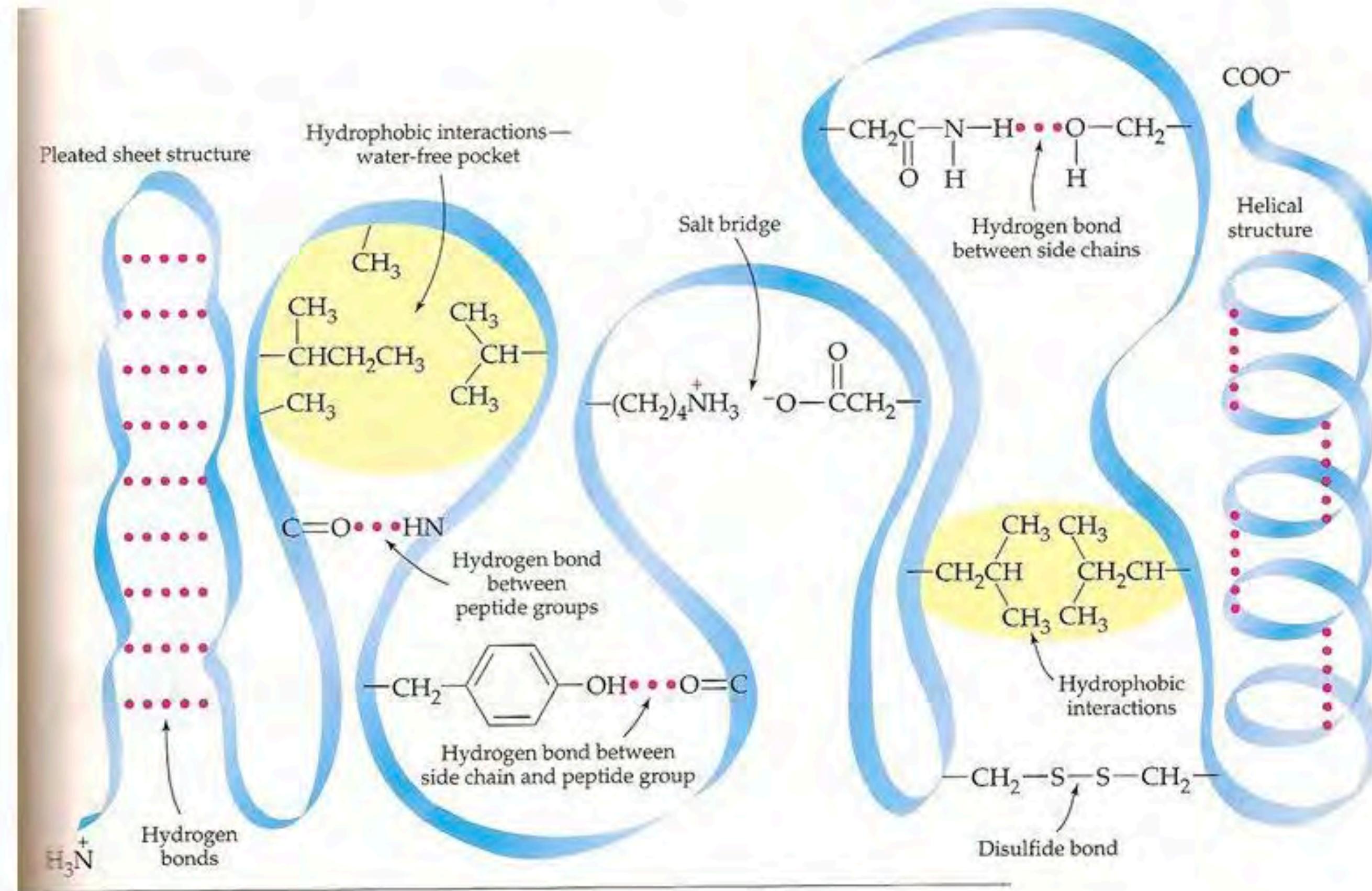


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Forces involved in protein folding



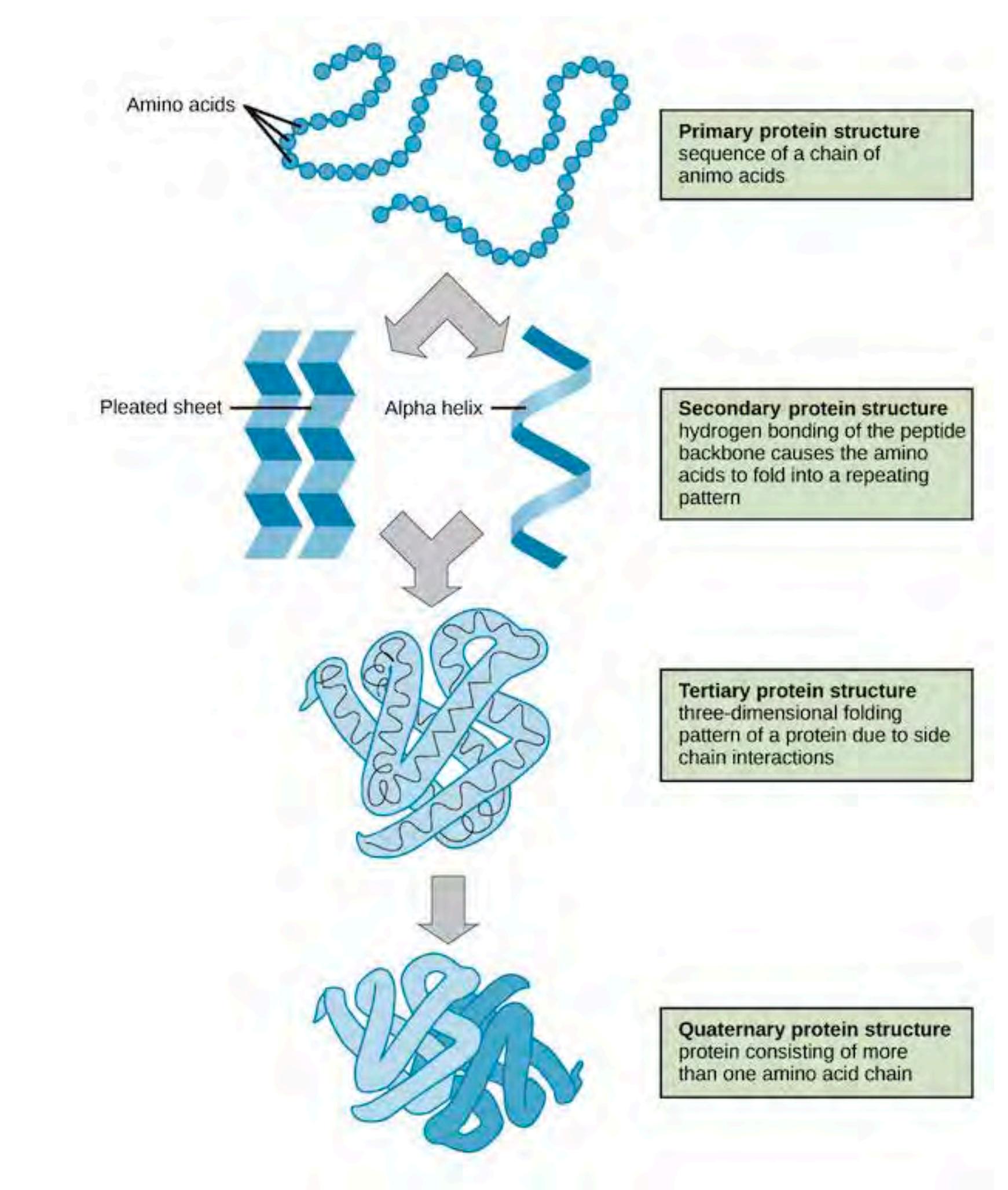
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alpha helix secondary structure

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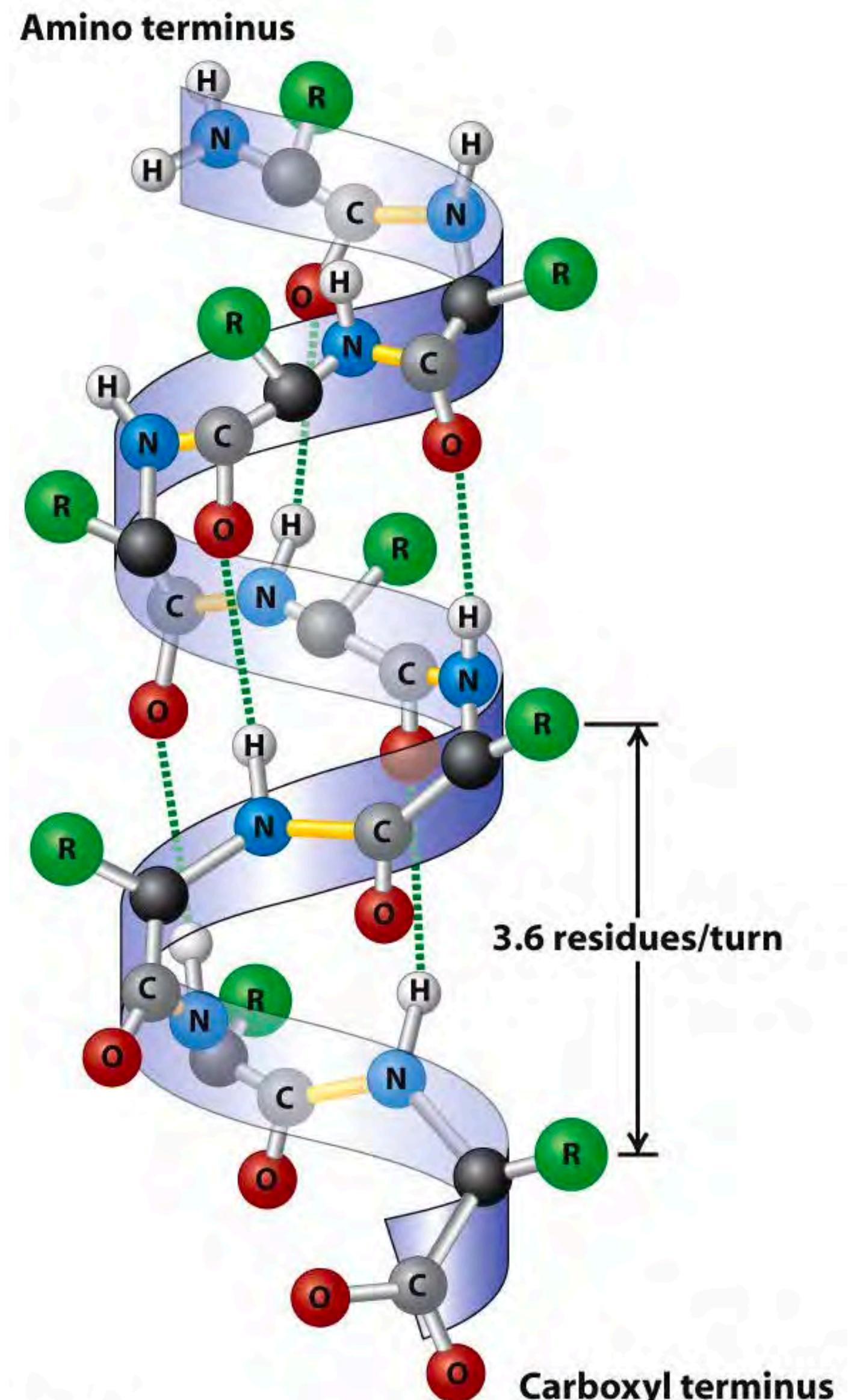


Figure 3-4
Molecular Cell Biology, Sixth Edition
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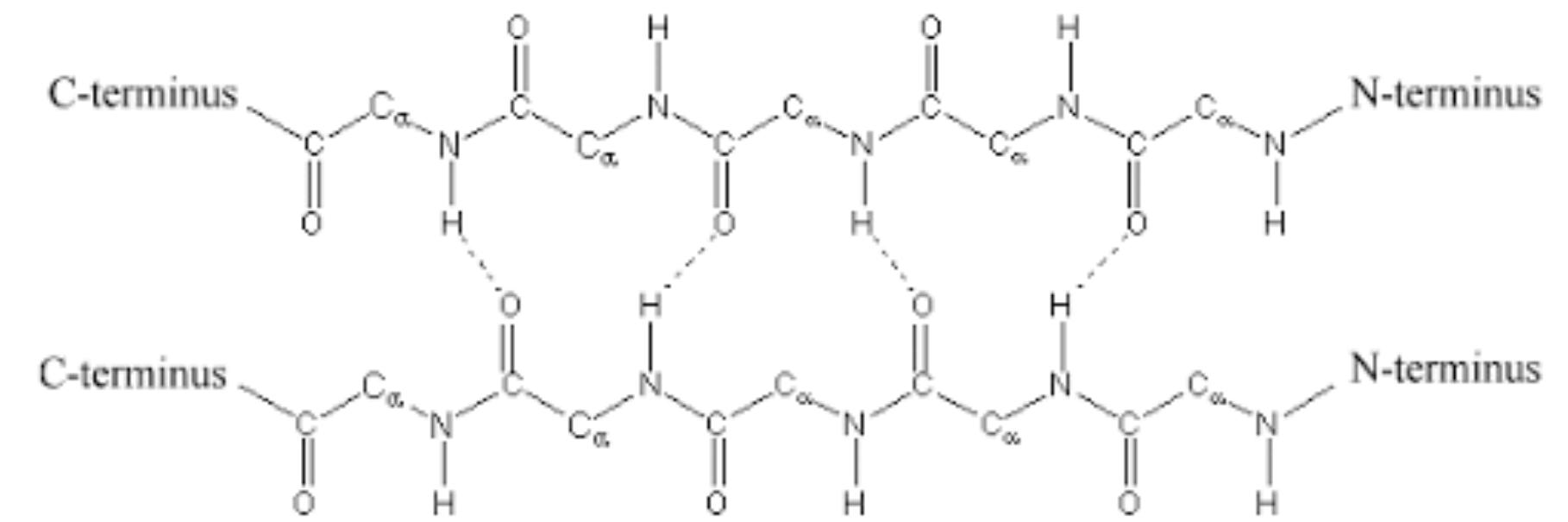
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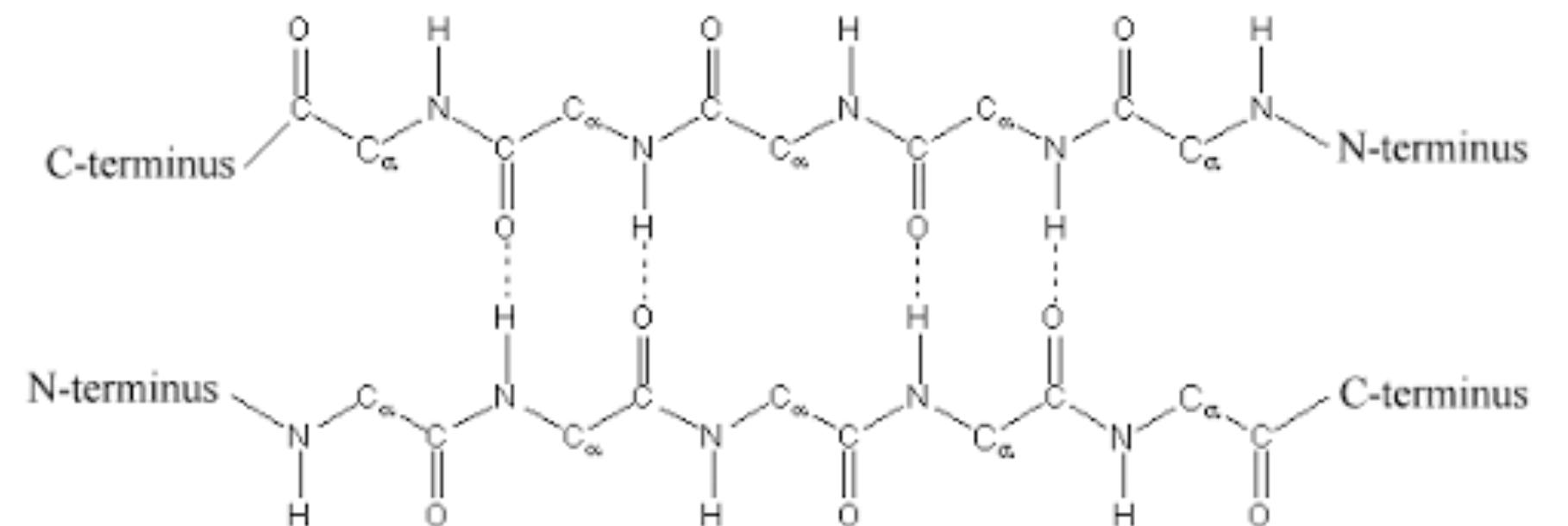
beta sheet secondary structure

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Parallel β Sheet



Antiparallel β Sheet



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secondary structure annotation

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ribbon representation tertiary + secondary

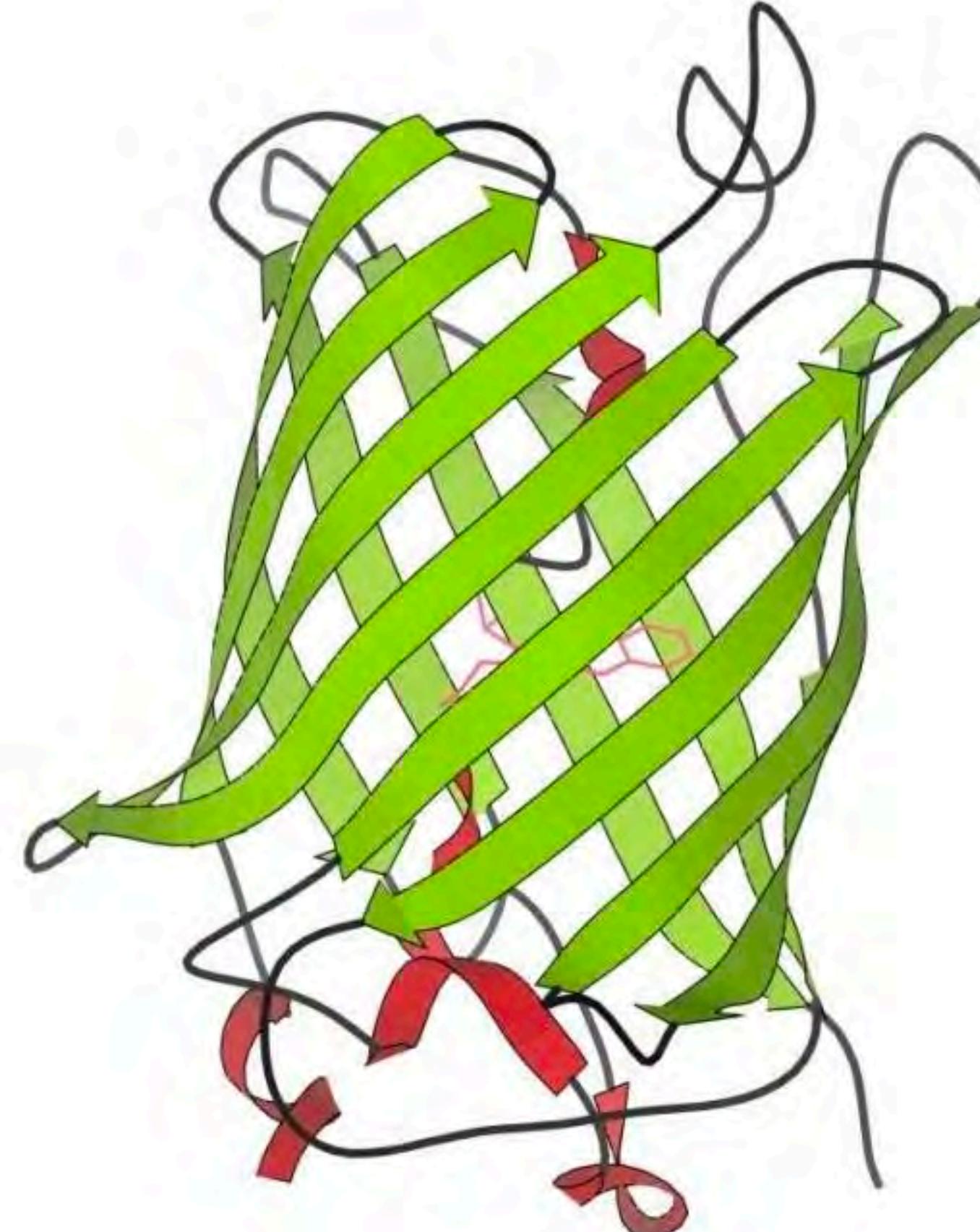
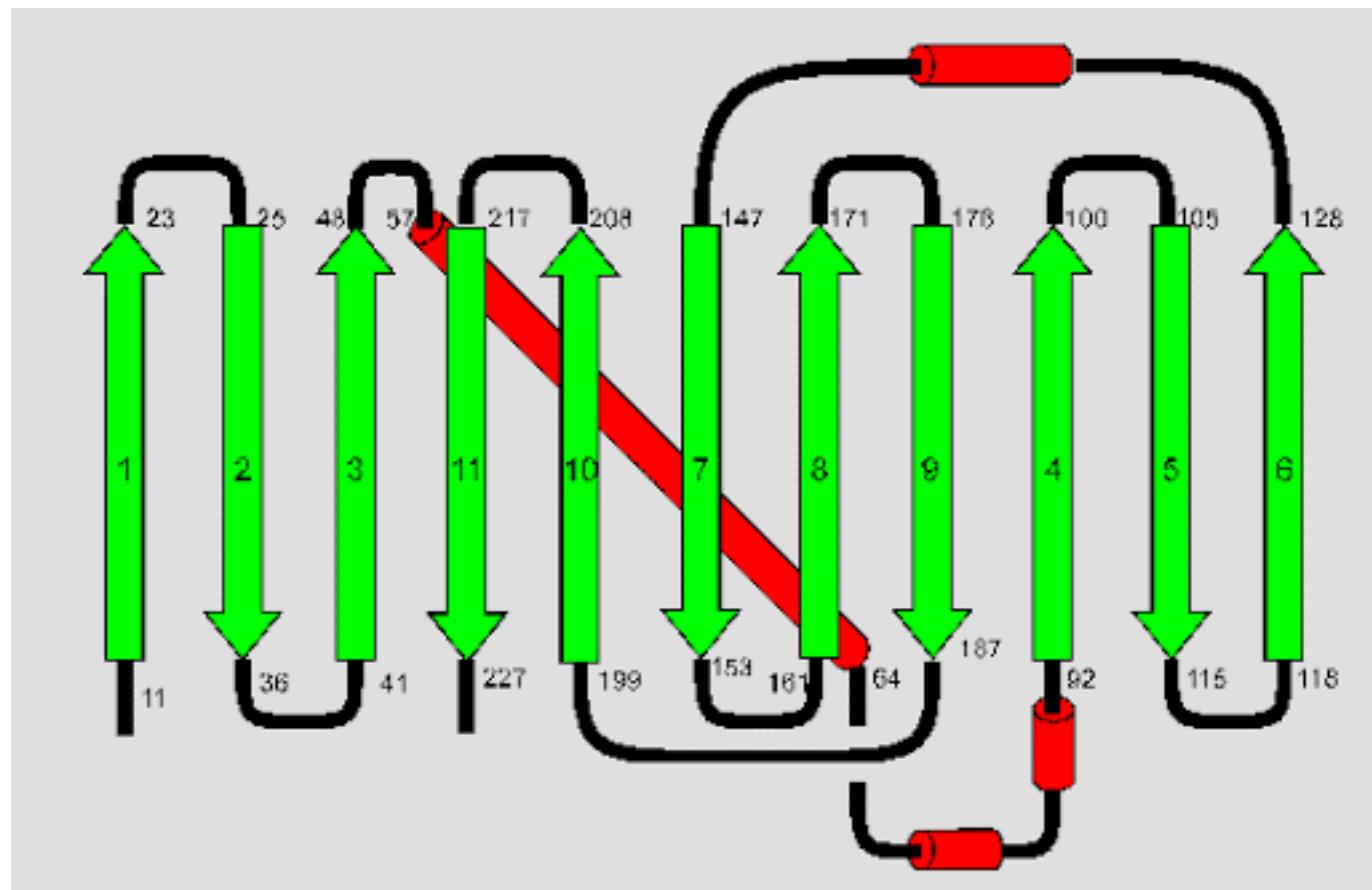
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protein jewelry



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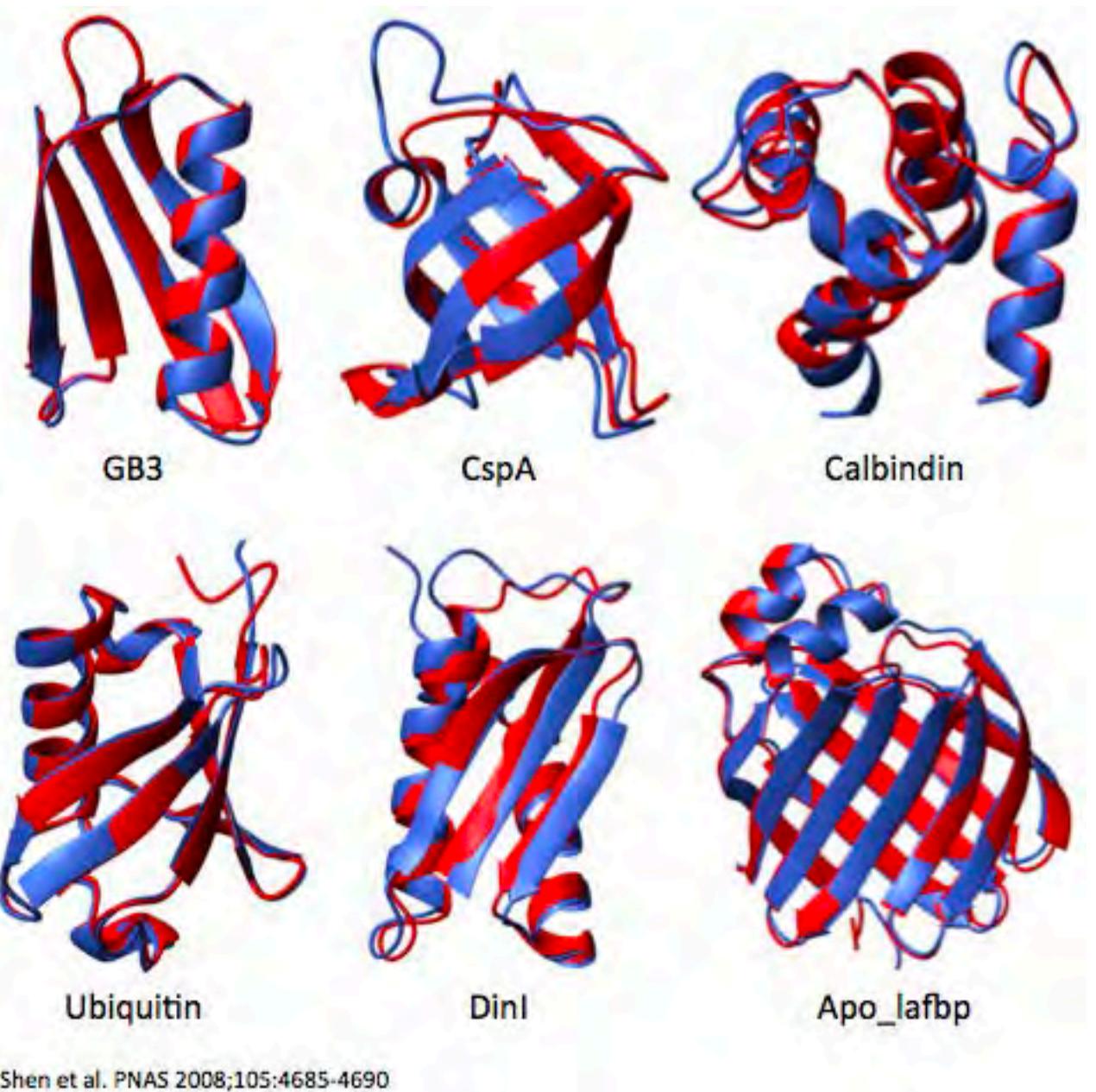
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tertiary structure stochasticity

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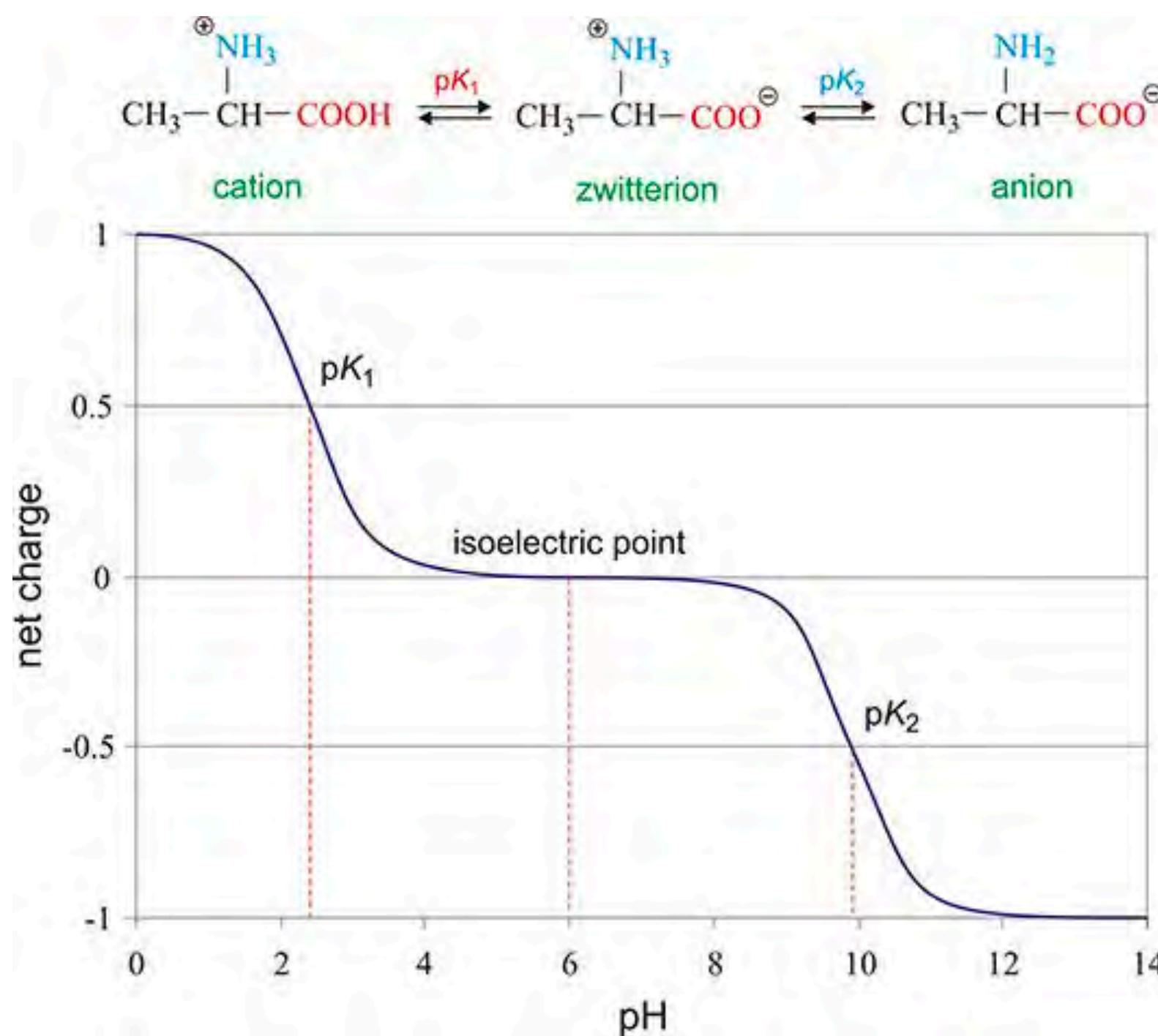
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Table 6–1 Molecular data on some proteins

	Molecular weight	Number of residues	Number of polypeptide chains
Insulin (bovine)	5,733	51	2
Cytochrome c (human)	13,000	104	1
Ribonuclease A (bovine pancreas)	13,700	124	1
Lysozyme (egg white)	13,930	129	1
Myoglobin (equine heart)	16,890	153	1
Chymotrypsin (bovine pancreas)	21,600	241	3
Chymotrypsinogen (bovine)	22,000	245	1
Hemoglobin (human)	64,500	574	4
Serum albumin (human)	68,500	~550	1
Hexokinase (yeast)	102,000	~800	2
Immunoglobulin G (human)	145,000	~1,320	4
RNA polymerase (<i>E. coli</i>)	450,000	~4,100	5
Apolipoprotein B (human)	513,000	4,536	1
Glutamate dehydrogenase (bovine liver)	1,000,000	~8,300	~40

molecular properties isoelectric point

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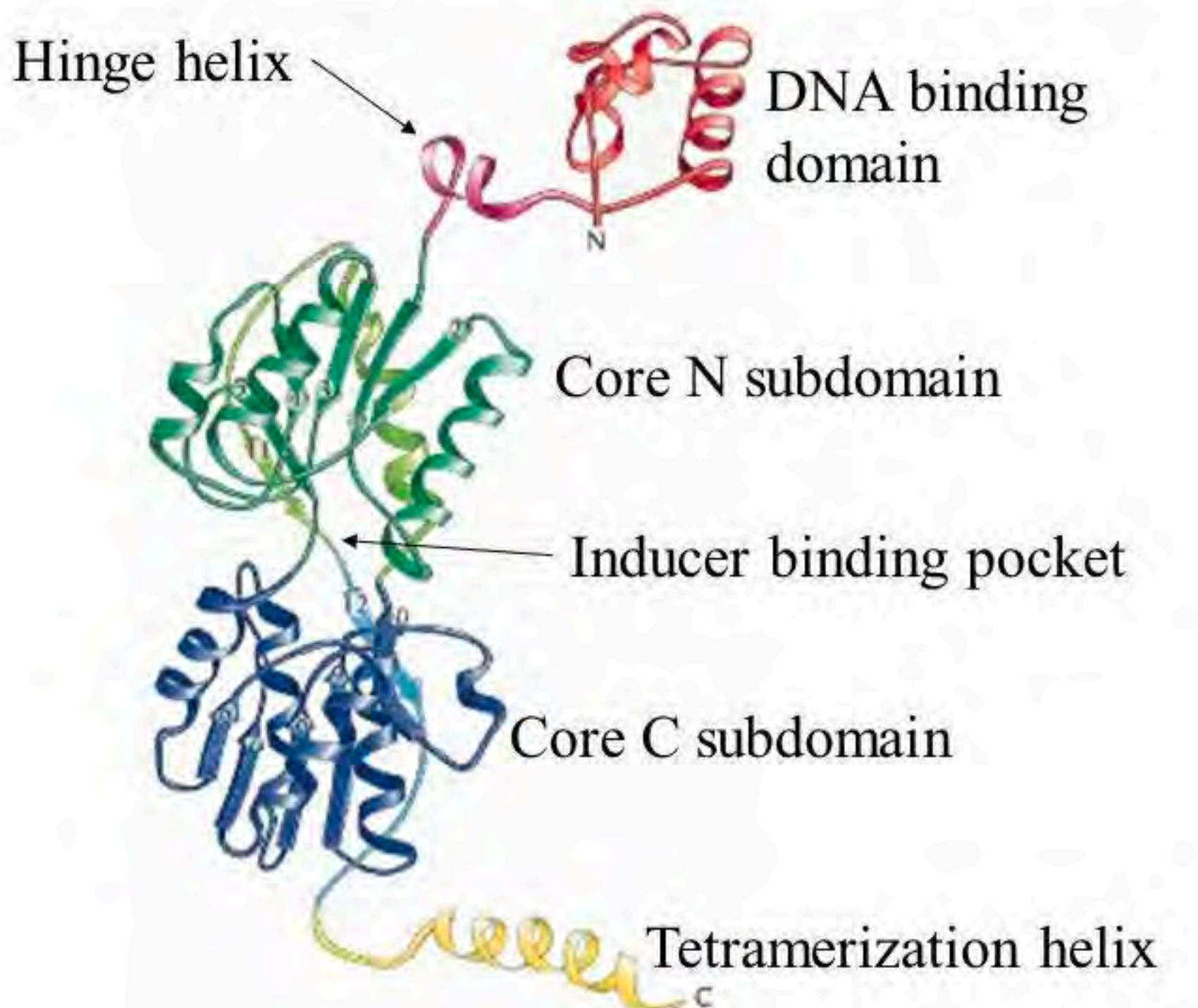


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The structure of lac repressor monomer



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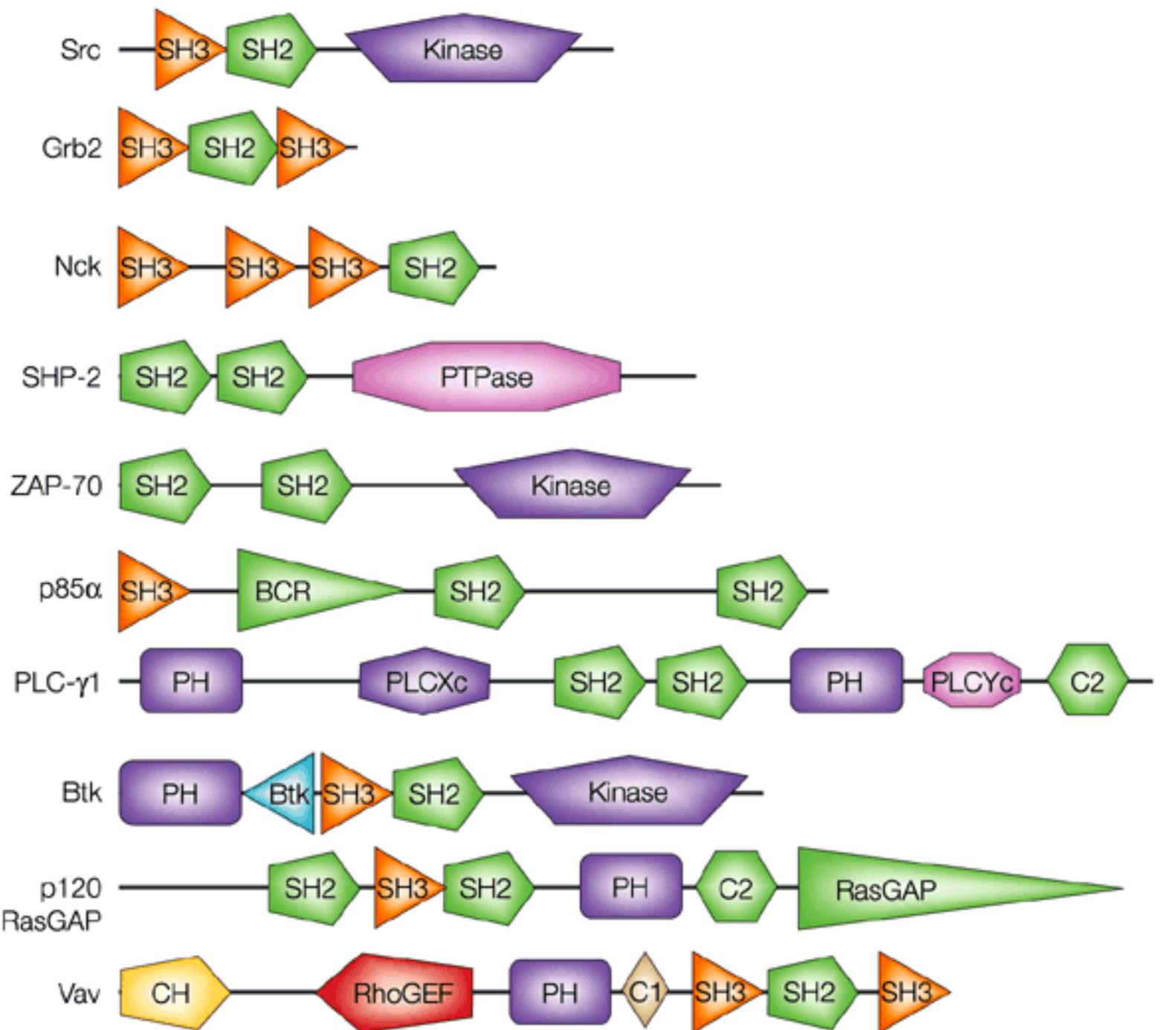
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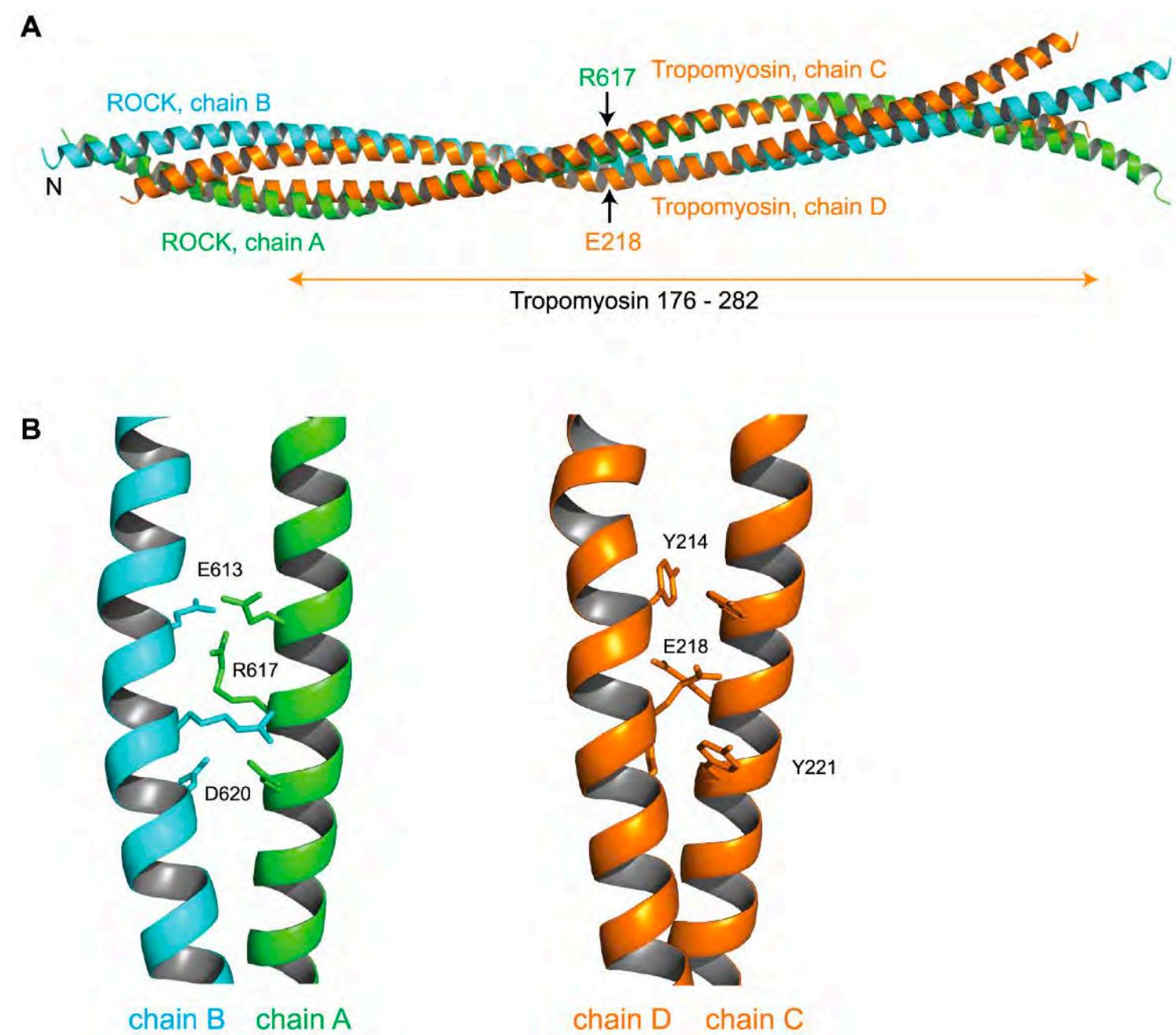
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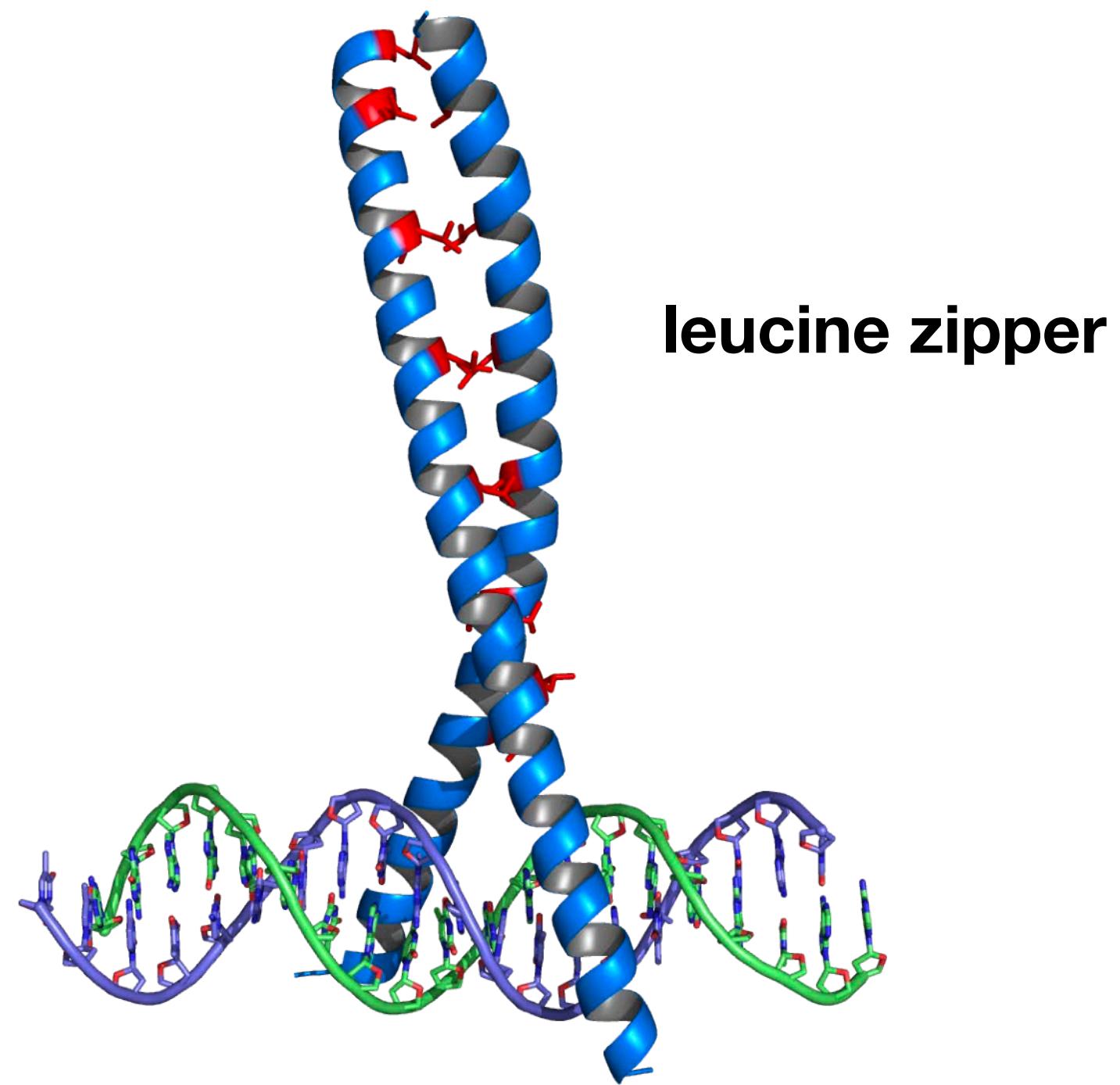
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binding domain

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coiled coil domain



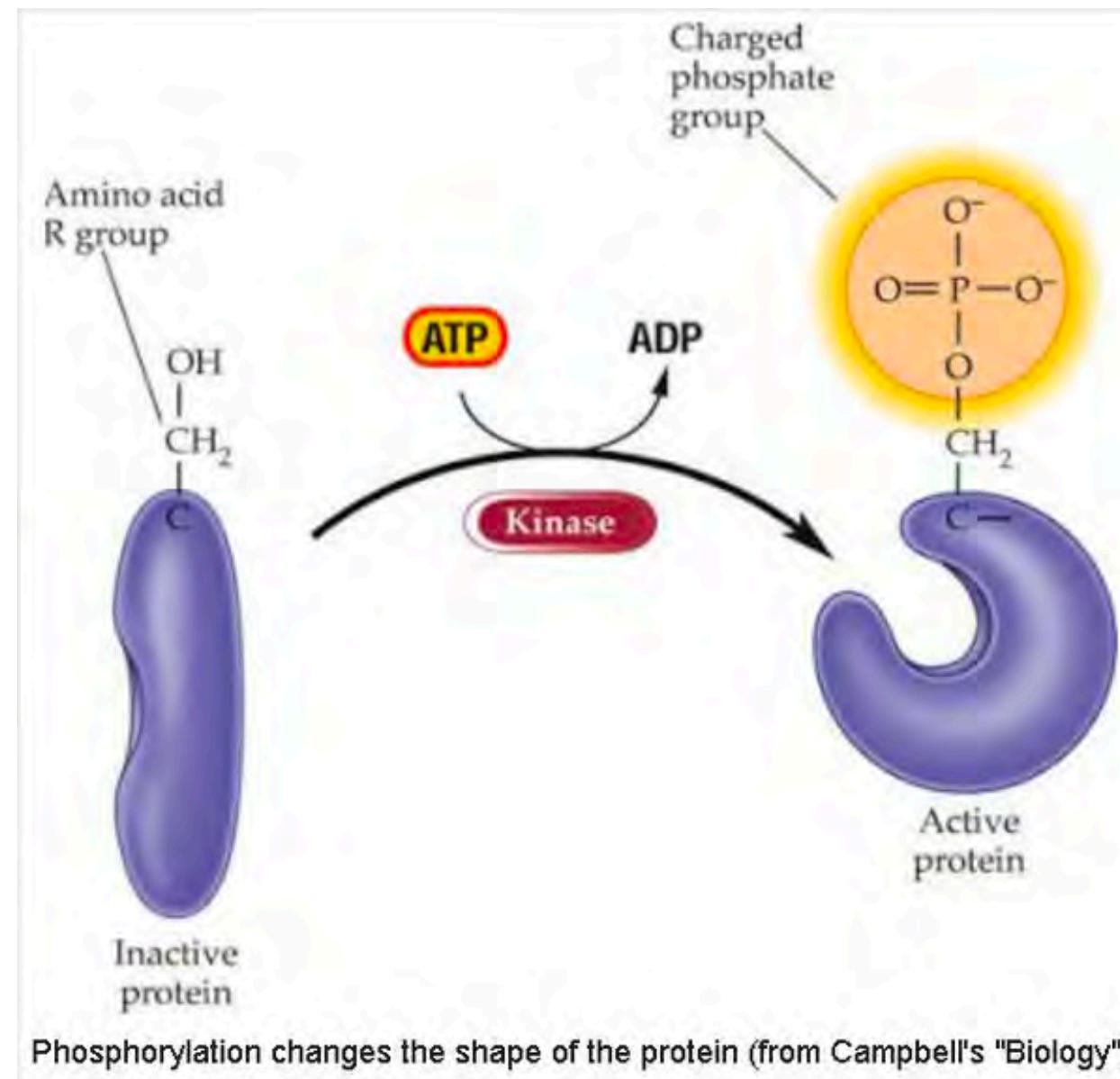
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Coulomb's law
interaction with solvent
Motif's
alpha helix
3.6 residues per turn
each residue 100deg, 1.5A
beta sheet
planar
isoelectric point
molecular weight

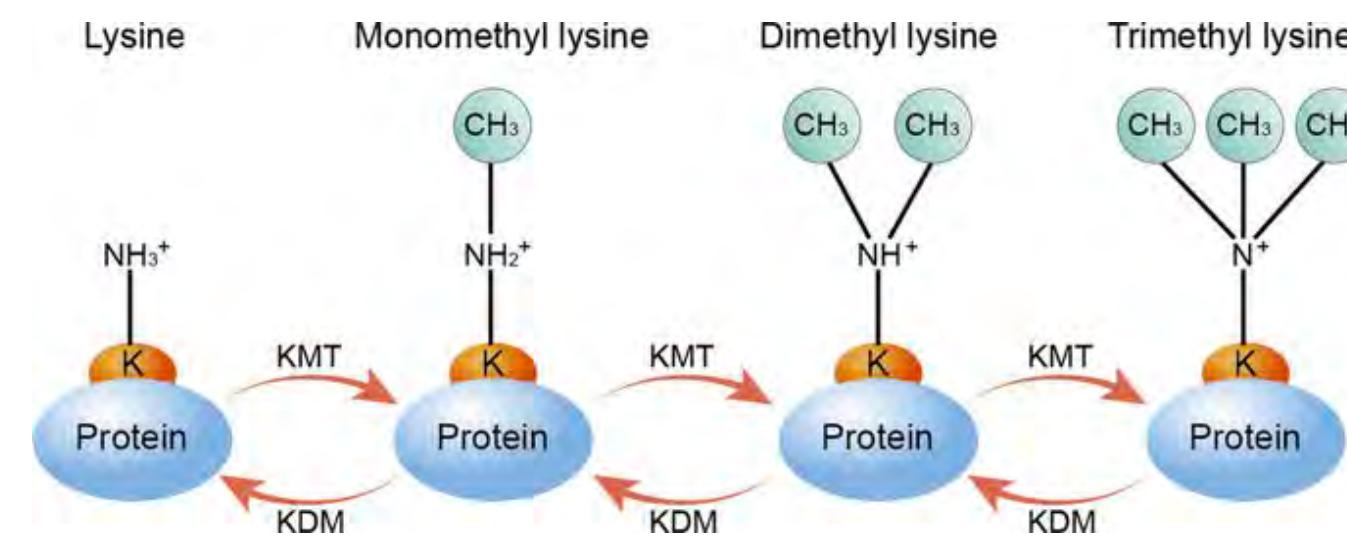
protein domains
binding domain - leucine zipper, TALEN
PTM domain
phosphorylation
methylation
ubiquitination
enzymatic domains
protease
kinase
targeting domains
NLS
signal peptide
anchoring sequence

post-translational modification addition of small groups

LECTURE 3 POLYPEPTIDE SYNTAX



phosphorylation
Y/R/H/K/S/T



methylation
R/K/termini

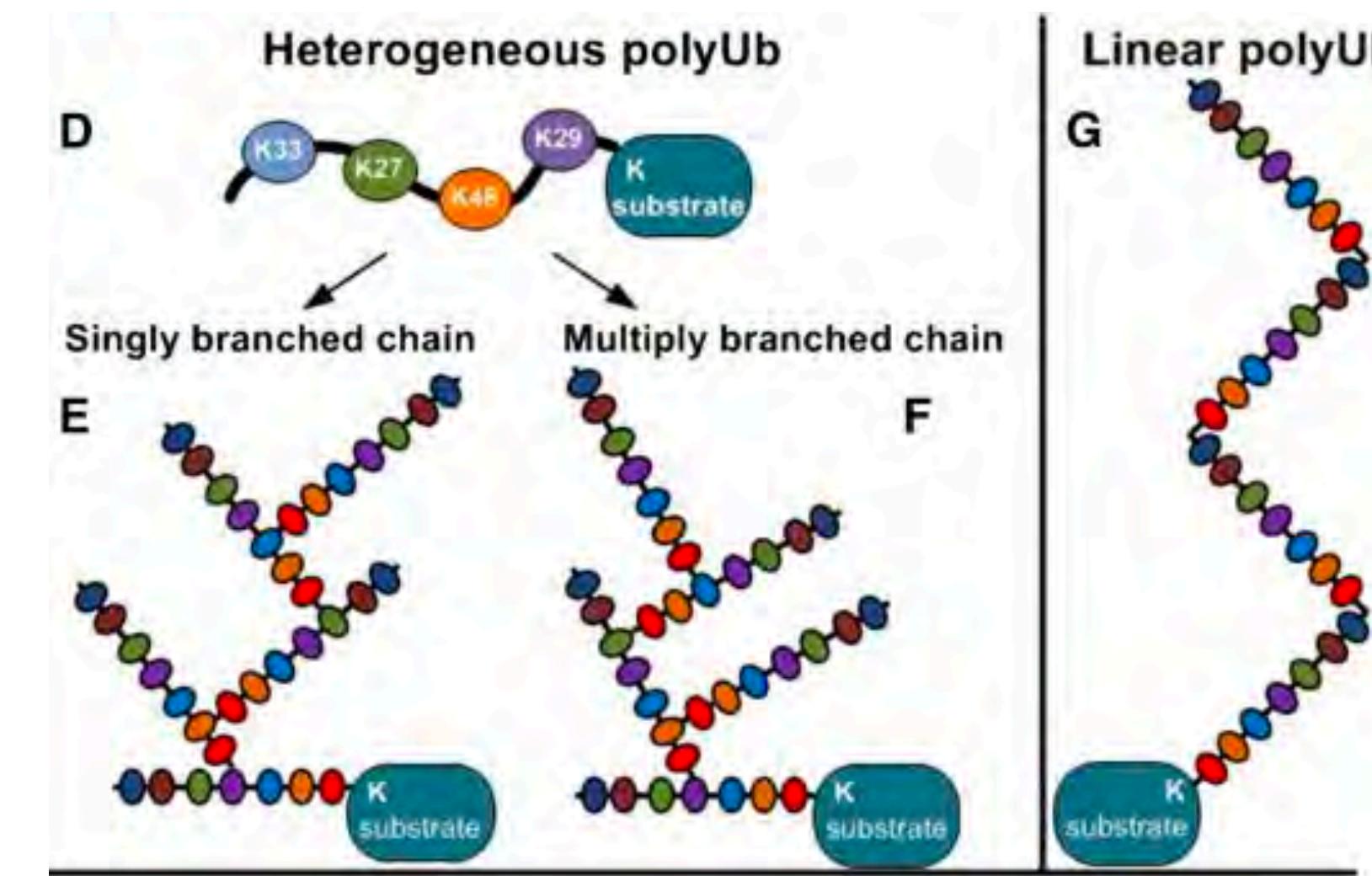
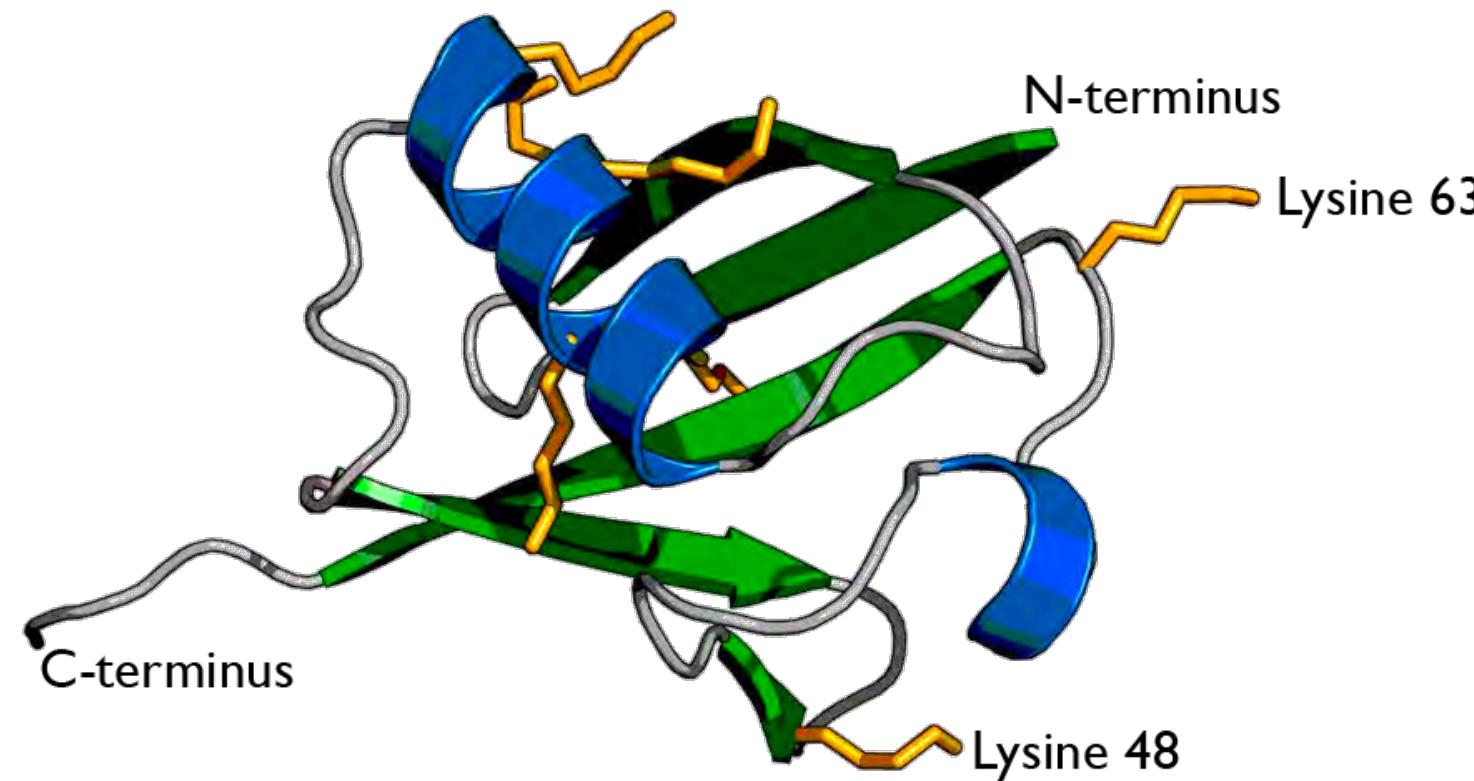
Amino acid structures
C1, Calpha carbons
hydrophobic - AGILPV
aromatic - FWY
neg charge - DE
pos charge - RHK
hydroxyllic - ST
sulfur containing - CM
polar - NQ

protein structure
peptide bond
dihedral angles
phi (N-Ca)
psi (Ca-C1)
omega (C1-N) = 180deg unless proline (0deg)
protein folding
bond forces
stretching, bending, rotating
short range forces
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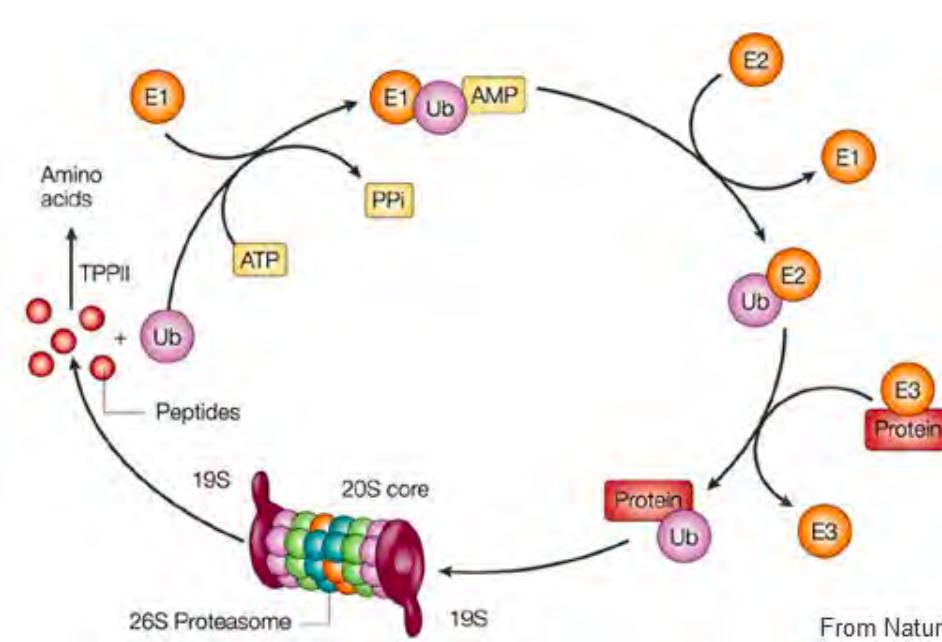
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PTM domain
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ubiquitination
enzymatic domains
protease
kinase
targeting domains
NLS
signal peptide
anchoring sequence

post-translational modification addition of bigger groups

LECTURE 3 POLYPEPTIDE SYNTAX



ubiquitination K



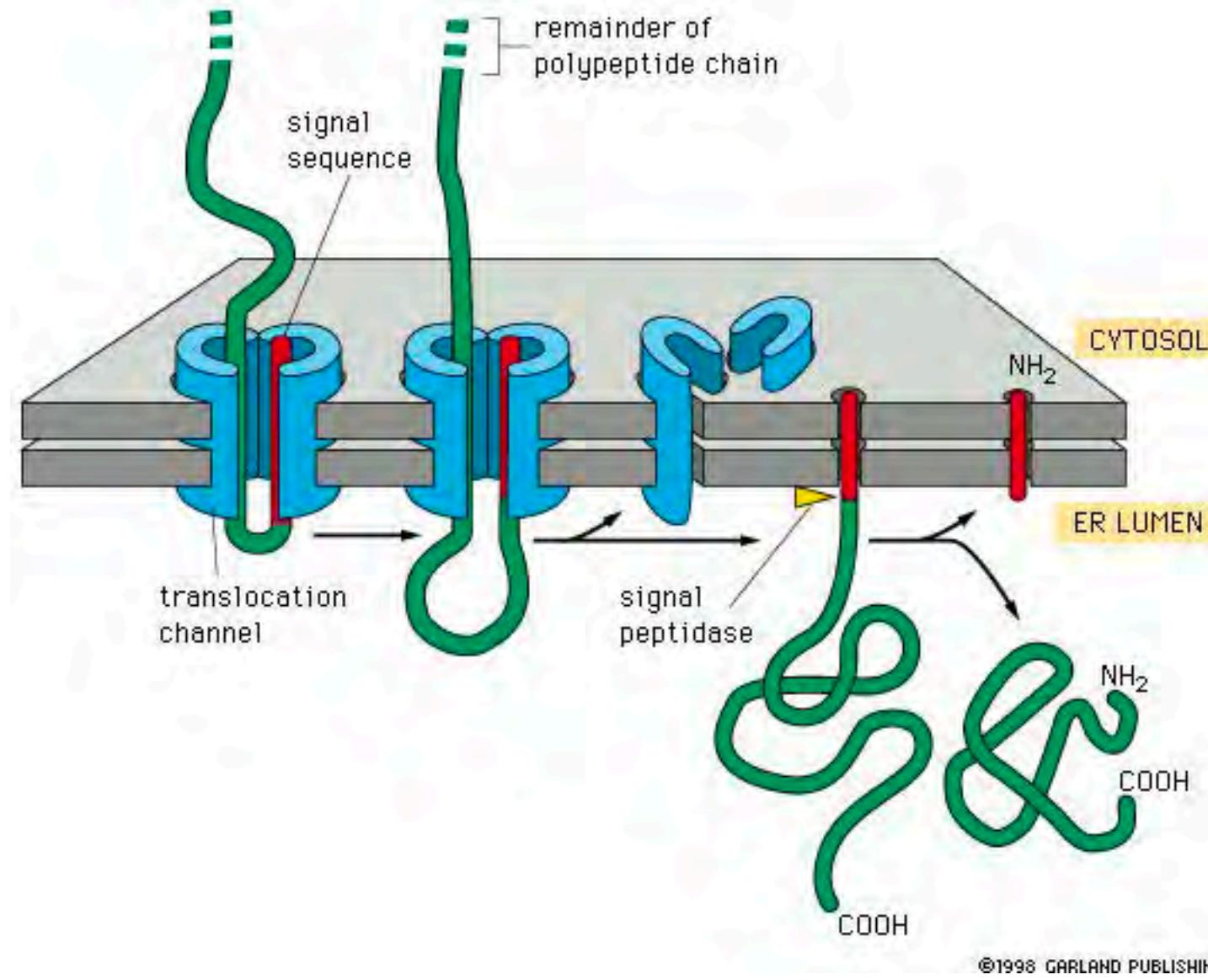
protein targeting to proteasome

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neg charge - DE
pos charge - RHK
hydroxyllic - ST
sulfur containing - CM
polar - NQ

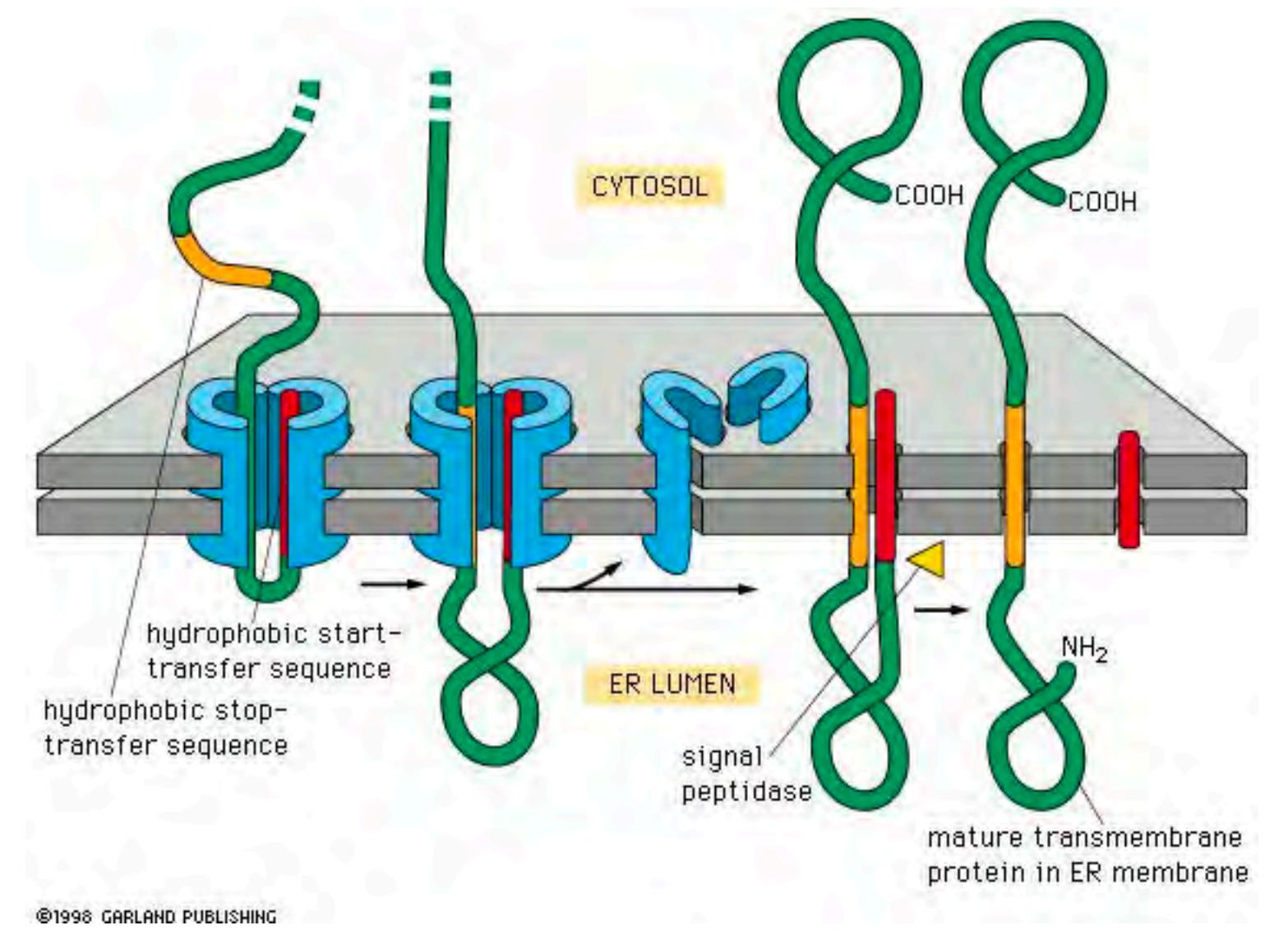
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targeting domains



**protein targeting
endoplasmic reticulum**



**protein targeting
membrane proteins**

LECTURE 3 POLYPEPTIDE SYNTAX

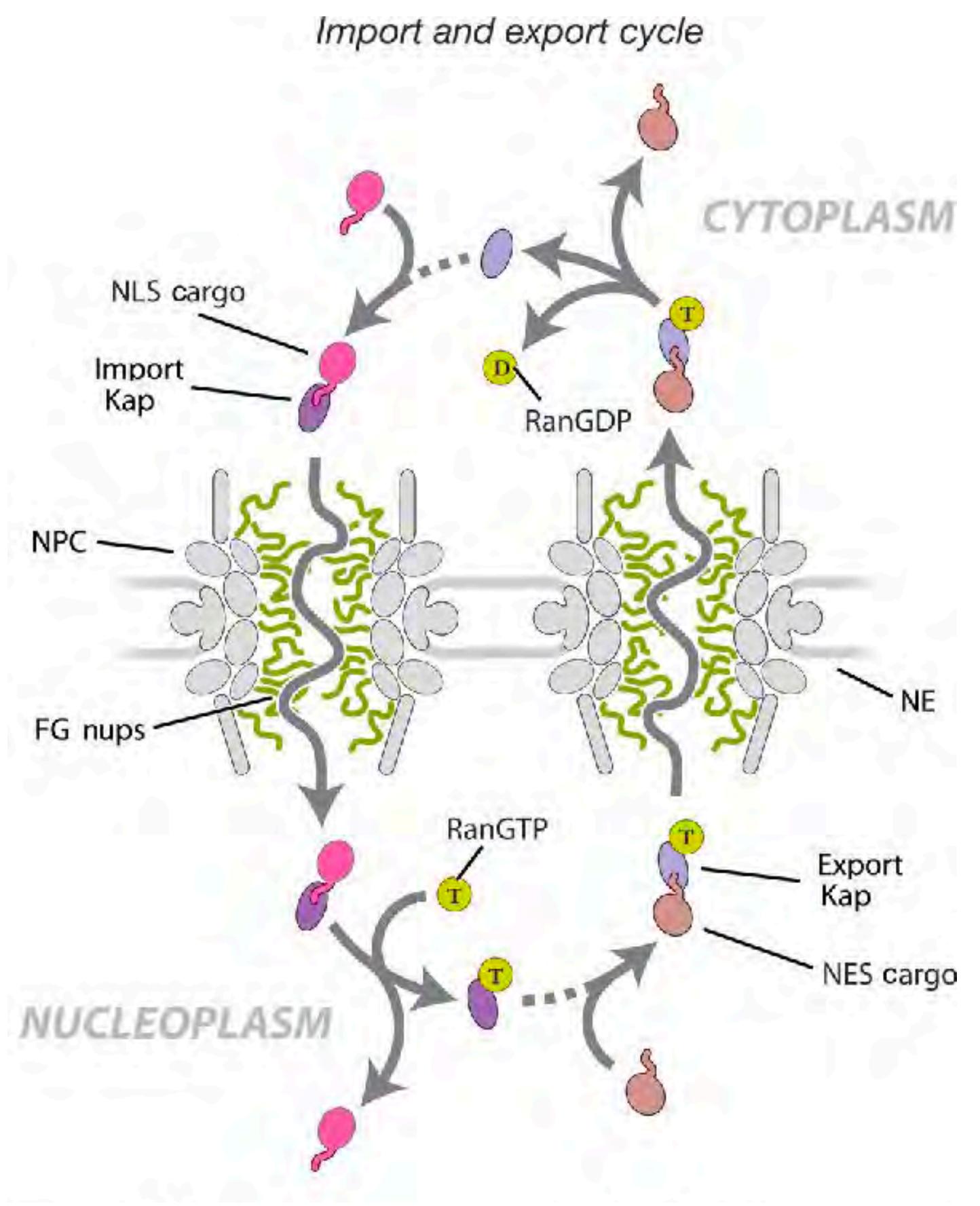
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targeting domains

LECTURE 3 POLYPEPTIDE SYNTAX



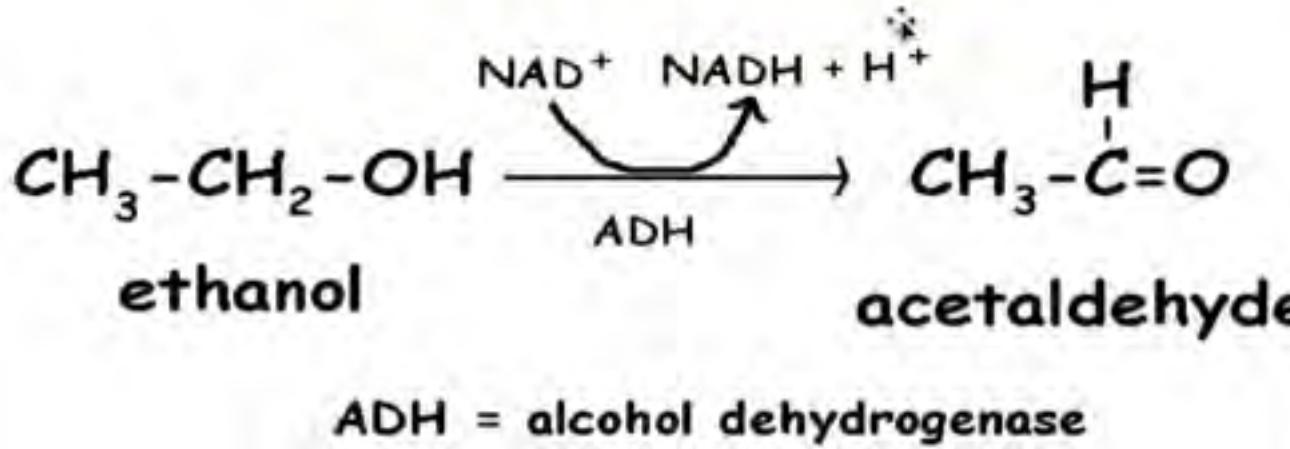
**protein targeting
nuclear localization**

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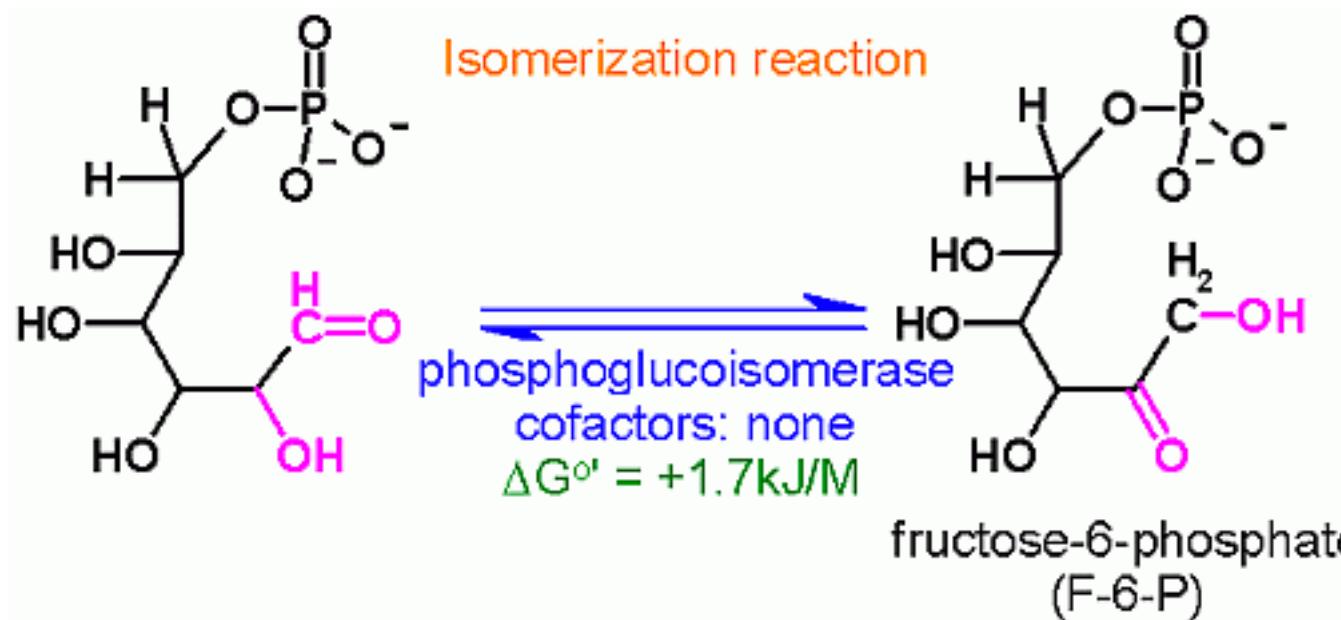
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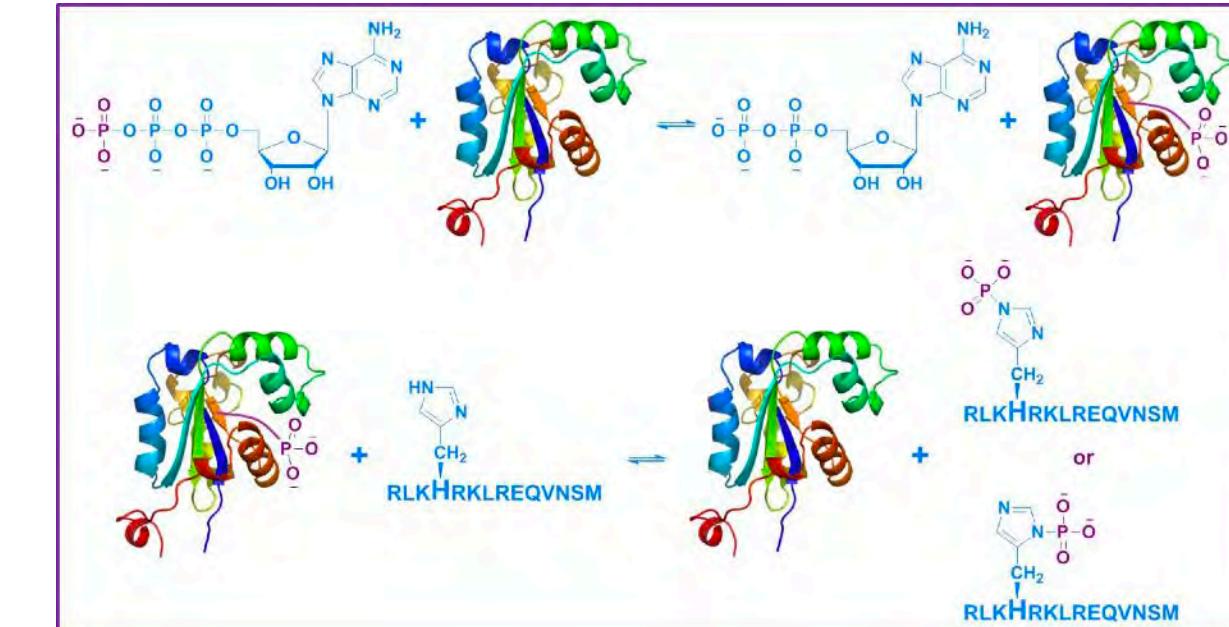
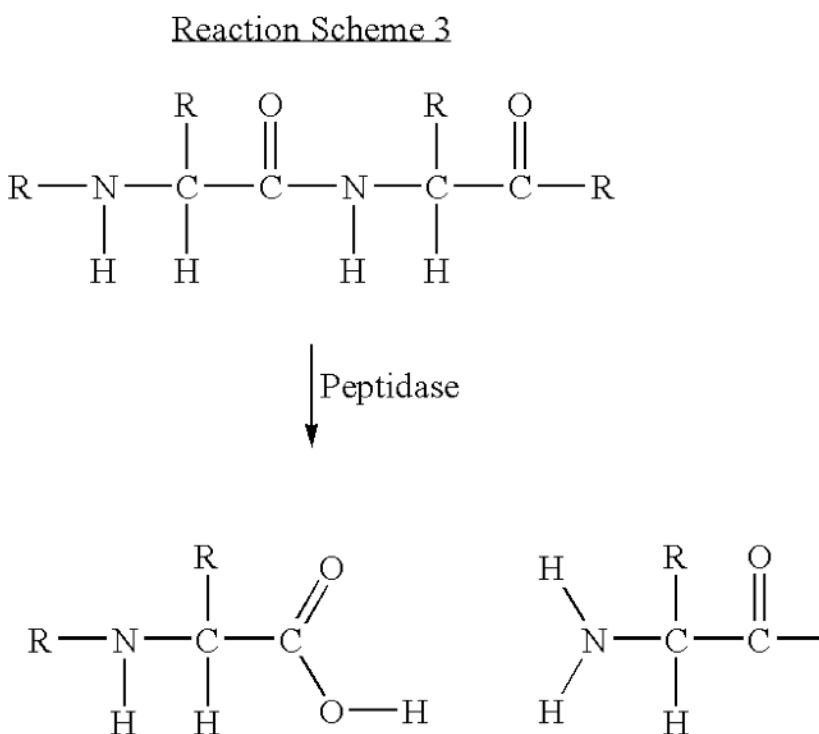
enzymatic domains



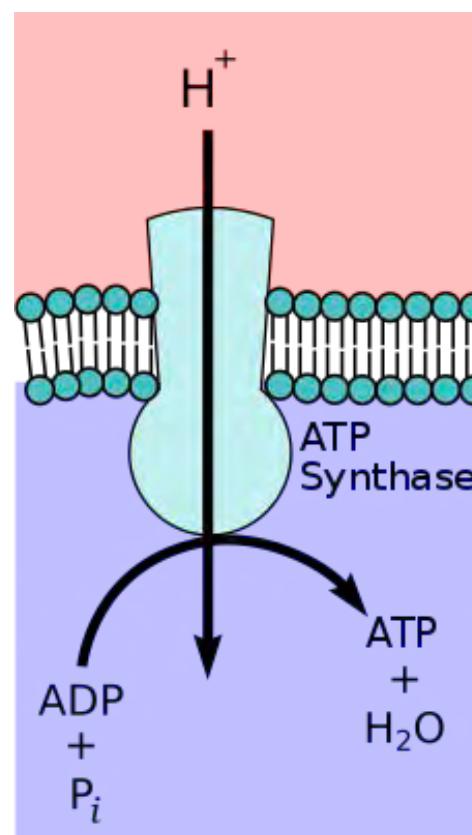
**oxidoreductase
(oxidase/dehydrogenase)
changes reduction state**



**isomerase
(PGI)
same chemical formula**

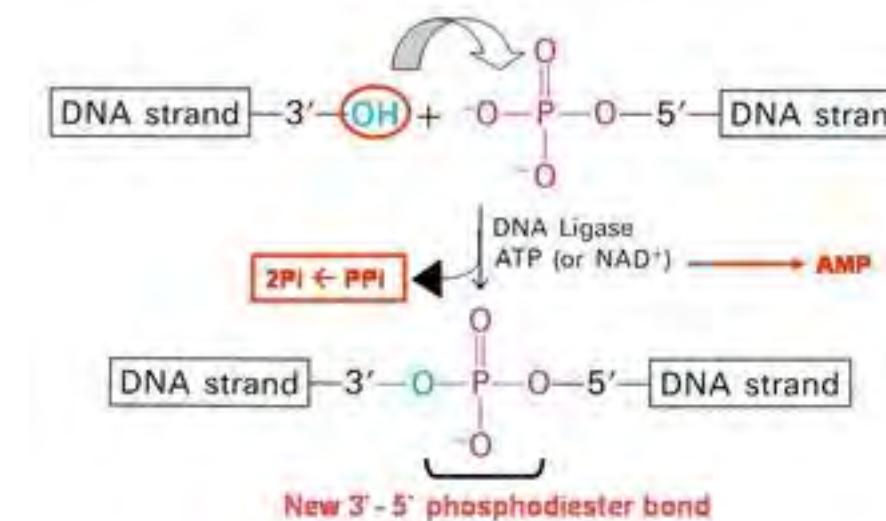


**hydrolase
(endonuclease/protease)
breakdown using H₂O**



**lyase
(synthase)
cleavage w/o H₂O**

**transferase
(kinase)
move a group**



**ligase
(synthetase)
joins by condensation**

LECTURE 3 POLYPEPTIDE SYNTAX

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LECTURE 3

POLYPEPTIDE SYNTAX

EXERCISE 2

create the following protein in benchling:

```
MEDAKNIKGPAPFYPLEDTAGEQLHKAMKRYALVPGTIAFTDAHIEVNITYAEYFEMS  
VRLAEAMKRYGLNTNHRIVVCSENSLQFFMPVLGALFIGVAVAPANDIYNERELLNSMNI  
SQPTVVVFVKKGLQKILNVQKKLPIIQKIIIMDSKTDYQGFQSMYTFVTSHLPPGFNEYD  
FVPESFDRDKTIALIMNSSGSTGLPKGVALPHRTACVRFSHARDPIFGNQIIPDTAILSV  
VPFHGFGMFTTLGYLICGFRVVLMYRFEELFLRSQDYKIQSALLVPTLFSFFAKSTL  
IDKYDLSNLHEIASGGAPLSKEVGEAVAKRFHLPGIRQGYGLTETTSAILITPEGDDKPG  
AVGKVVPPFEAKVVDLDTGKTLGVNQRGECLVRGPMIMSGYVNNPEATNALIDKDGWLHS  
GDIAYWDEDEHFFIVDRLKSLIKYKGYQVAPAELESILLQHPNIFDAGVAGLPDDAGEI  
PAAVVVLEHGKTMTKEIVDYVASQVTAKLRGGVVFDEVPKGLTGKLDARKIREILI  
KAKKGGKSKL
```

use benchling to calculate the molecular mass and the isoelectric point of the sequence

will the protein be positively or negatively charged at neutral pH?

use <http://www.compbio.dundee.ac.uk/jpred4/index.html> to predict the protein secondary structure

use <https://www.ebi.ac.uk/Tools/hmmer/search/hmmSCAN> to predict the protein functional domains

use <https://www.uniprot.org/> to BLAST the sequence and compare the domains identified

locate the PDB identifier number in uniprot and download the PDB file from <https://www.rcsb.org/>

predict the 3D structure using AlphaFold2 available in colab:

<https://colab.research.google.com/github/sokrypton/ColabFold/blob/main/AlphaFold2.ipynb>

open both PDB files in Chimera and align the structures

select three residues where the structures are not in exact alignment and calculate the distances between the Calpha carbons

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