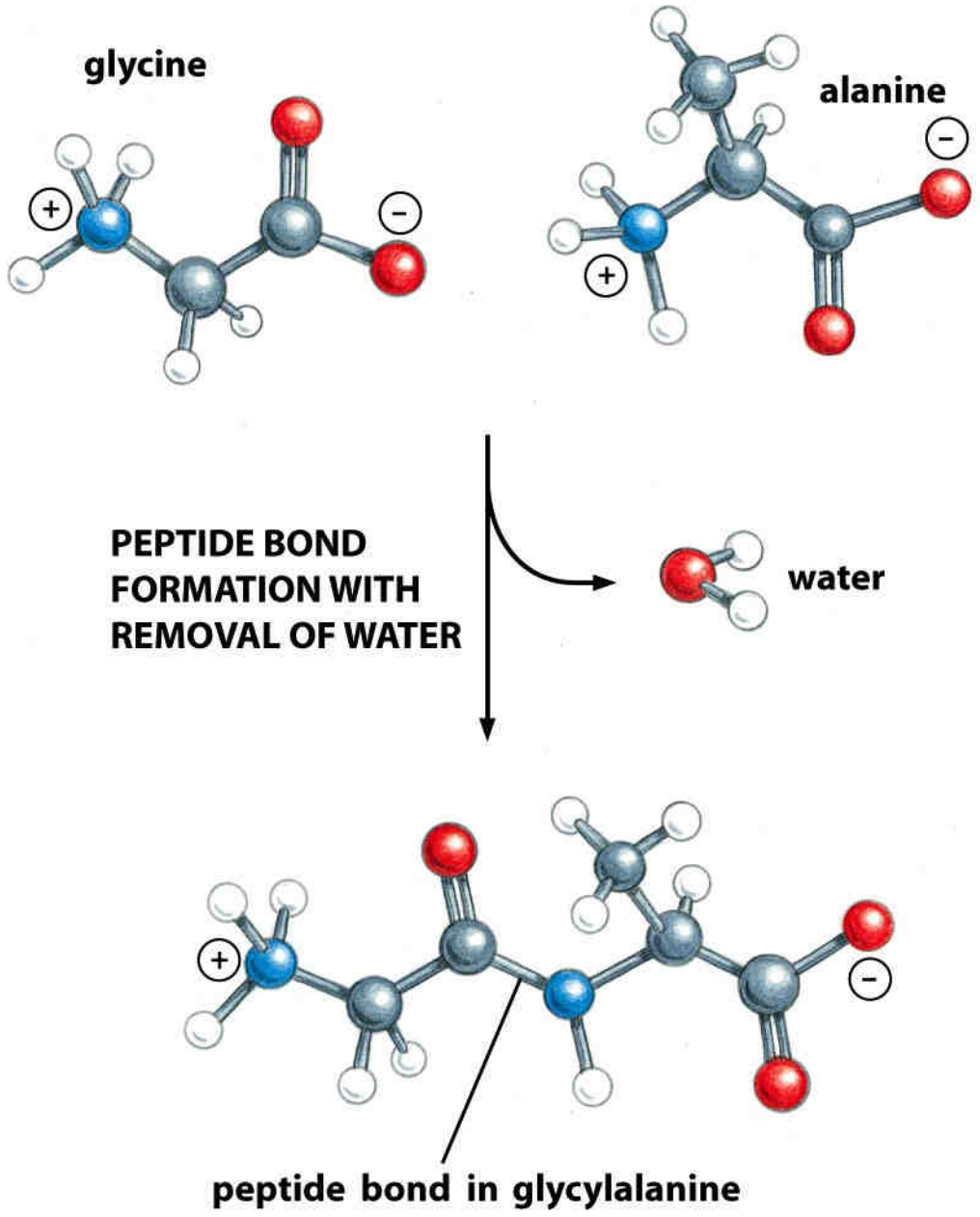
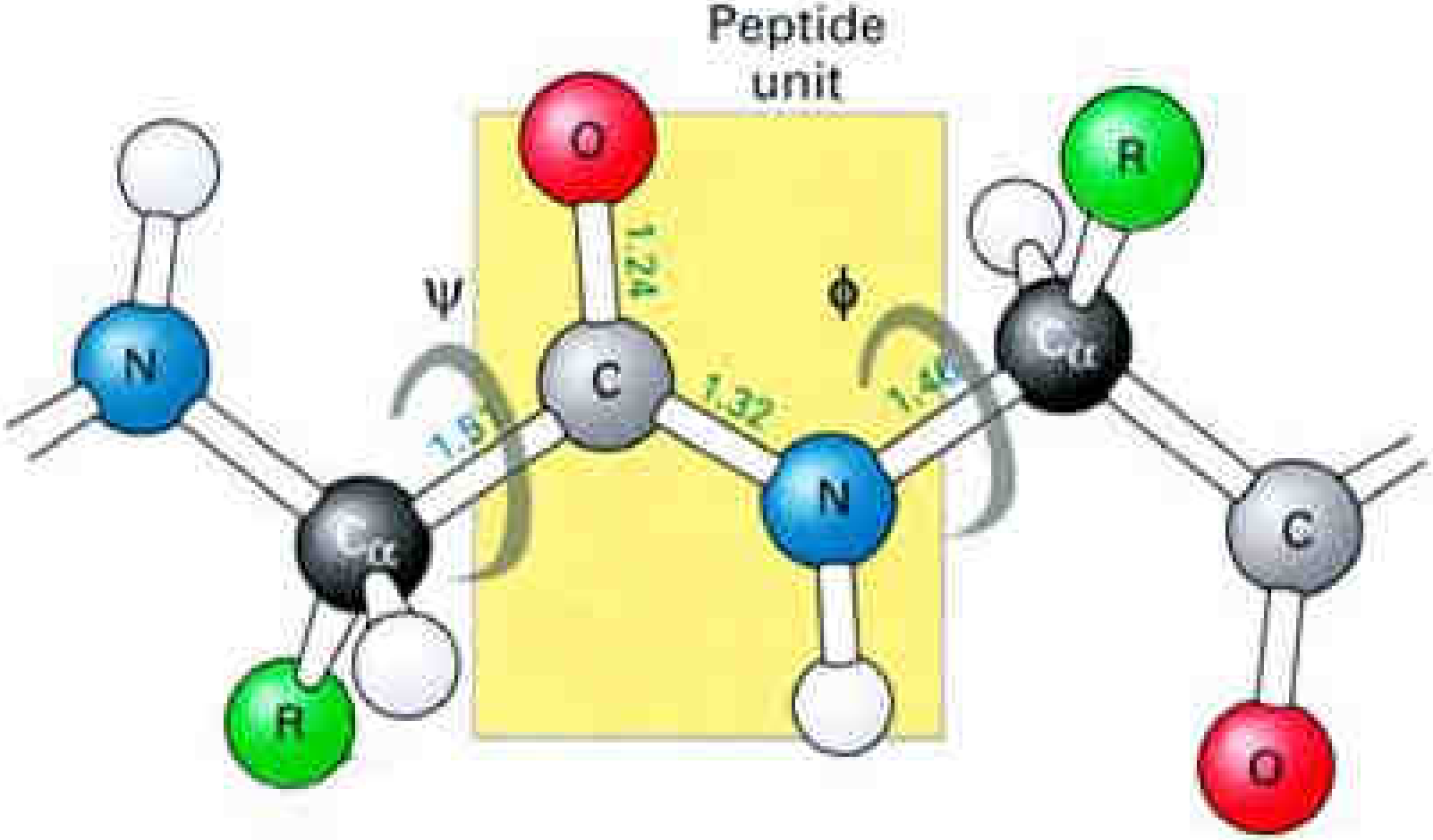
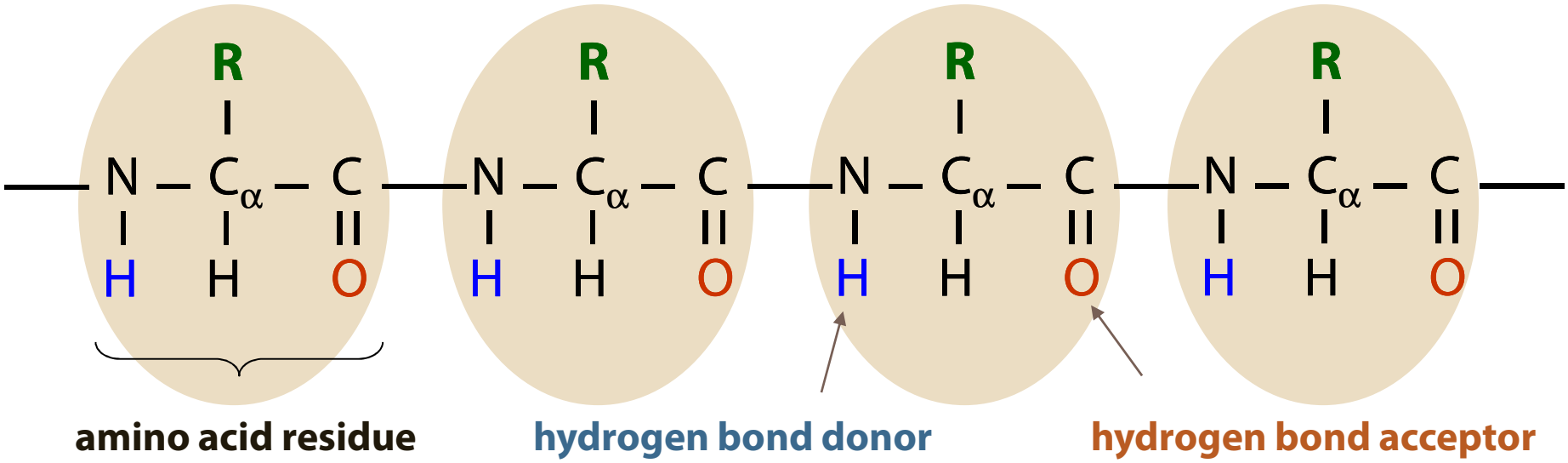


Figure 4-1 *Essential Cell Biology* (© Garland Science 2010)


Peptide
unit
O
R
1.24
ψ
ϕ
N
C
1.32
1.45
1.51
Cα
N
Cα
C
R
O


R
N – Cα – C
H H O
amino acid residue
hydrogen bond donor
hydrogen bond acceptor

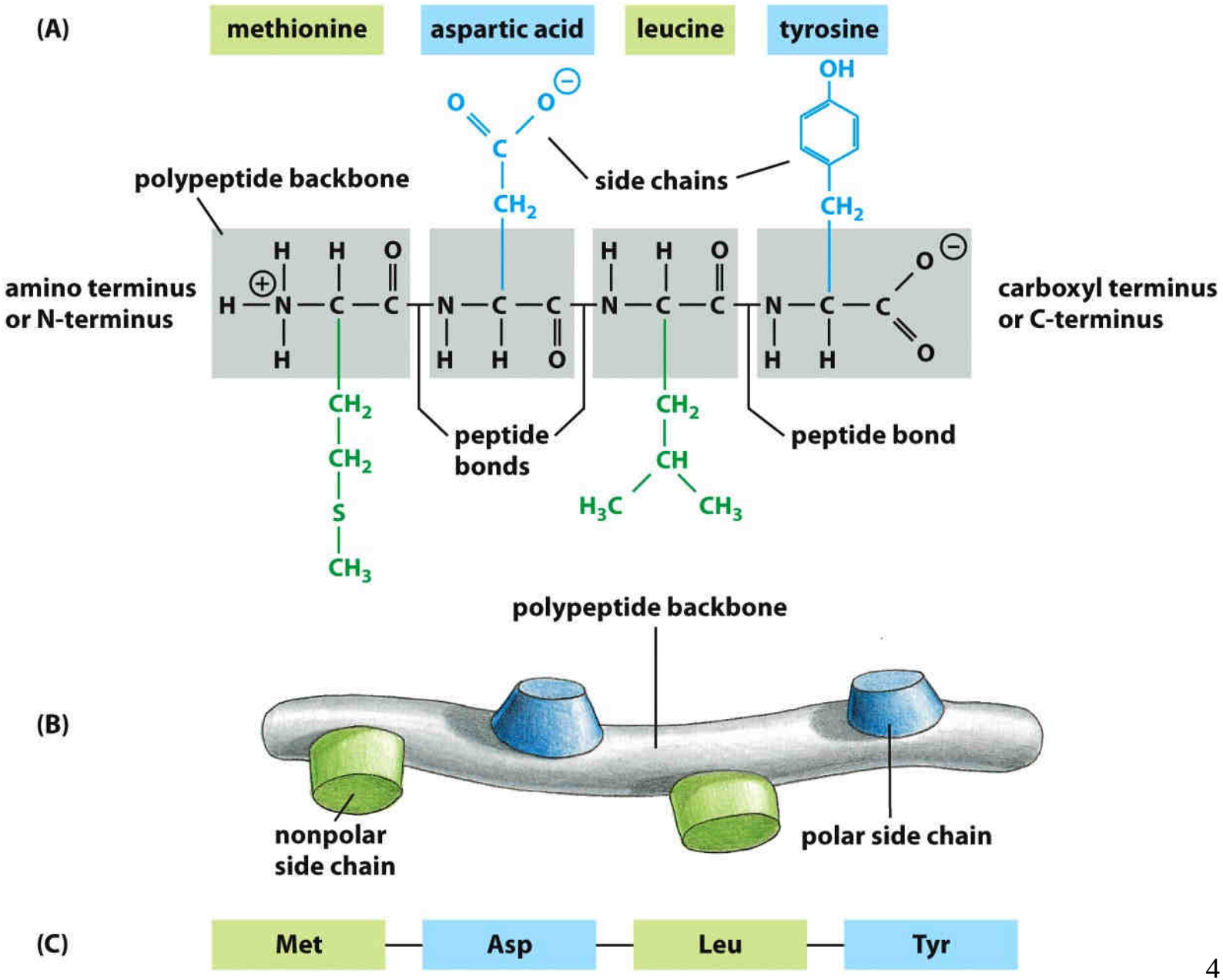


Figure 4-2 *Essential Cell Biology* (© Garland Science 2010)

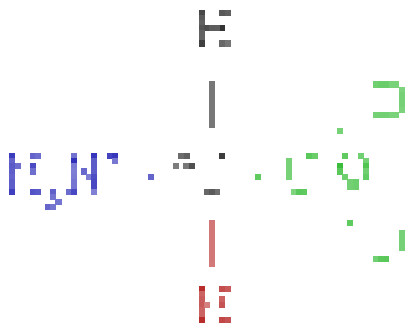
AMINO ACID			SIDE CHAIN
Aspartic acid	Asp	D	negative
Glutamic acid	Glu	E	negative
Arginine	Arg	R	positive
Lysine	Lys	K	positive
Histidine	His	H	positive
Asparagine	Asn	N	uncharged polar
Glutamine	Gln	Q	uncharged polar
Serine	Ser	S	uncharged polar
Threonine	Thr	T	uncharged polar
Tyrosine	Tyr	Y	uncharged polar

POLAR AMINO ACIDS
(hydrophilic)

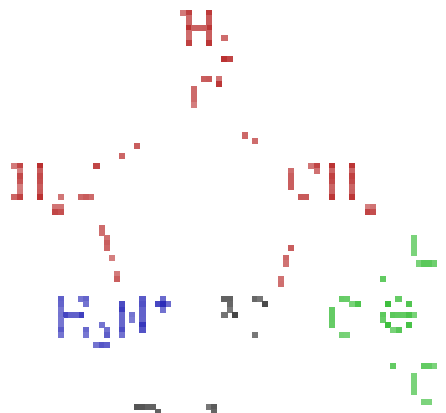
AMINO ACID			SIDE CHAIN
Alanine	Ala	A	nonpolar
Glycine	Gly	G	nonpolar
Valine	Val	V	nonpolar
Leucine	Leu	L	nonpolar
Isoleucine	Ile	I	nonpolar
Proline	Pro	P	nonpolar
Phenylalanine	Phe	F	nonpolar
Methionine	Met	M	nonpolar
Tryptophan	Trp	W	nonpolar
Cysteine	Cys	C	nonpolar

NONPOLAR AMINO ACIDS
(hydrophobic)

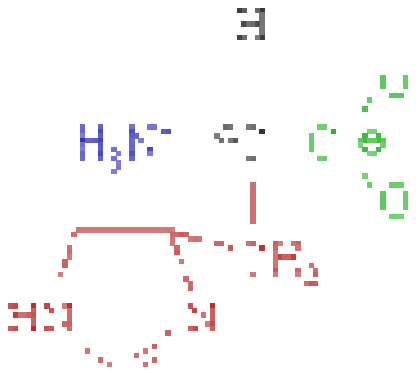
Figure 4-3 *Essential Cell Biology* (© Garland Science 2010)



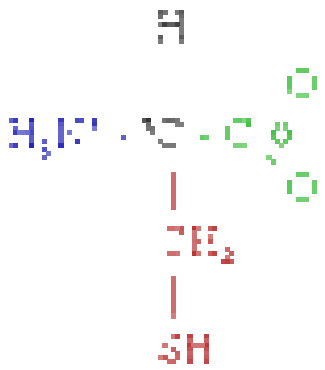
Glycine
(Gly / G)



Proline
(Pro / P)



Histidine
(His / H)



Cysteine
(Cys / C)

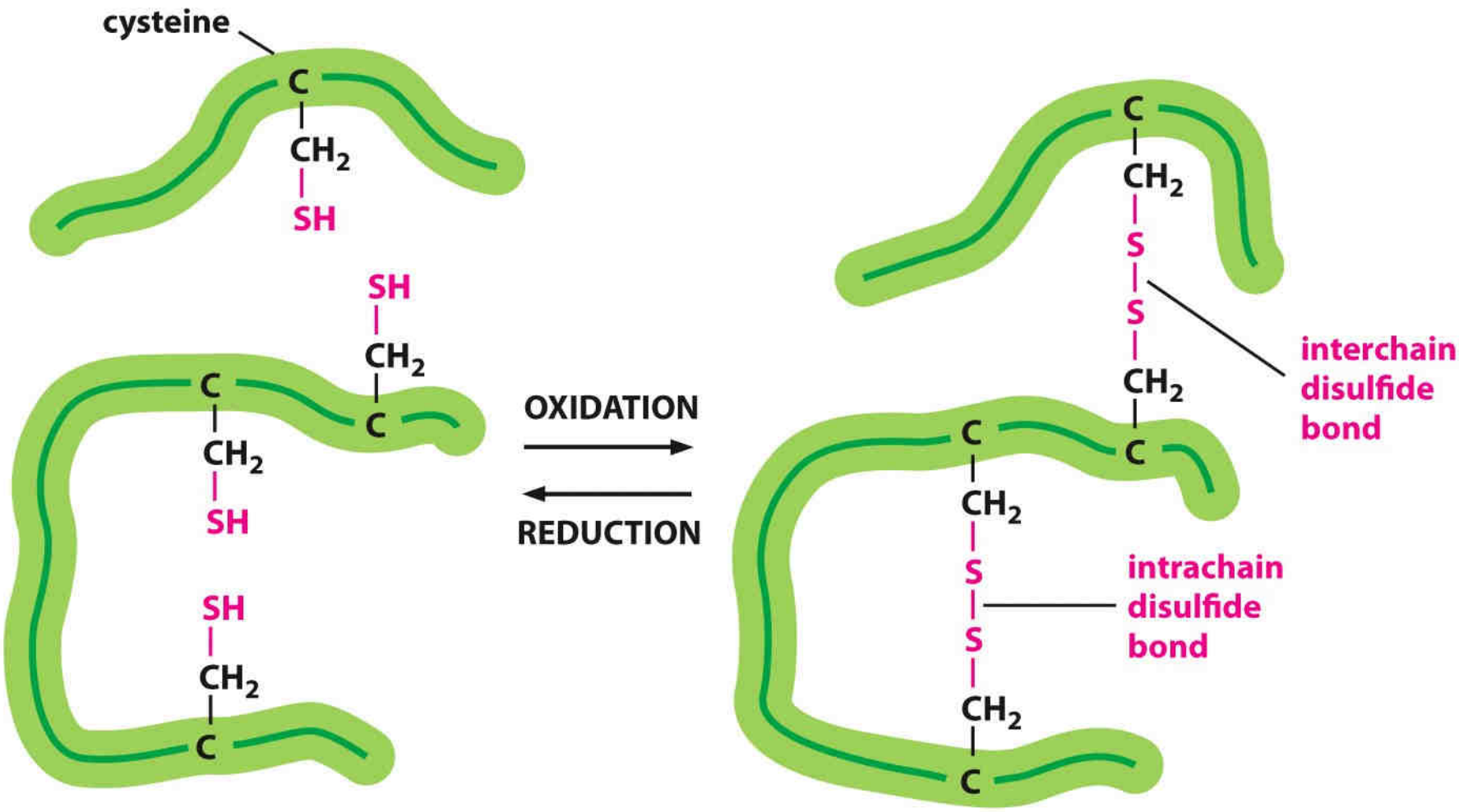


Figure 4-26 *Essential Cell Biology* (© Garland Science 2010)

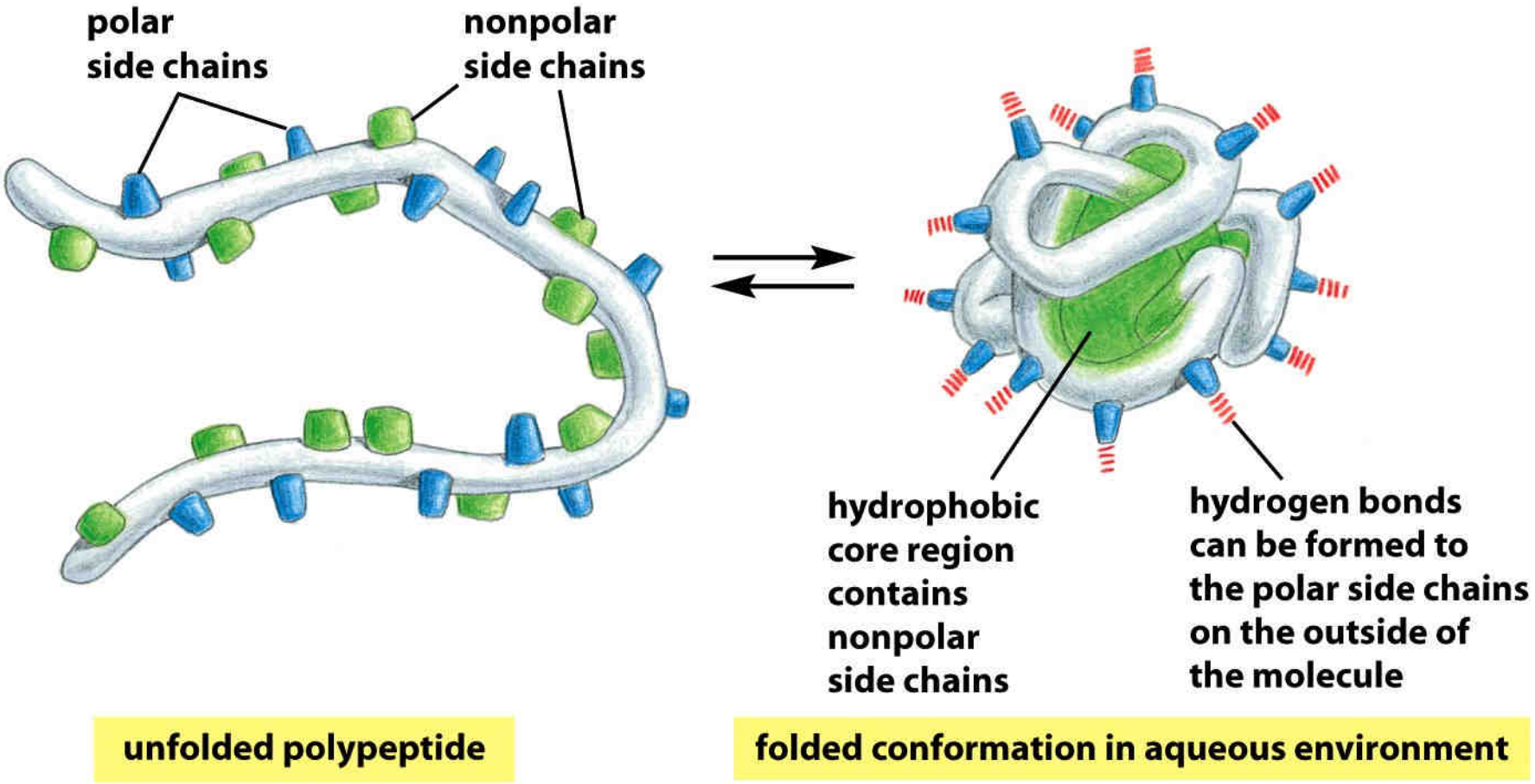


Figure 4-5 *Essential Cell Biology* (© Garland Science 2010)

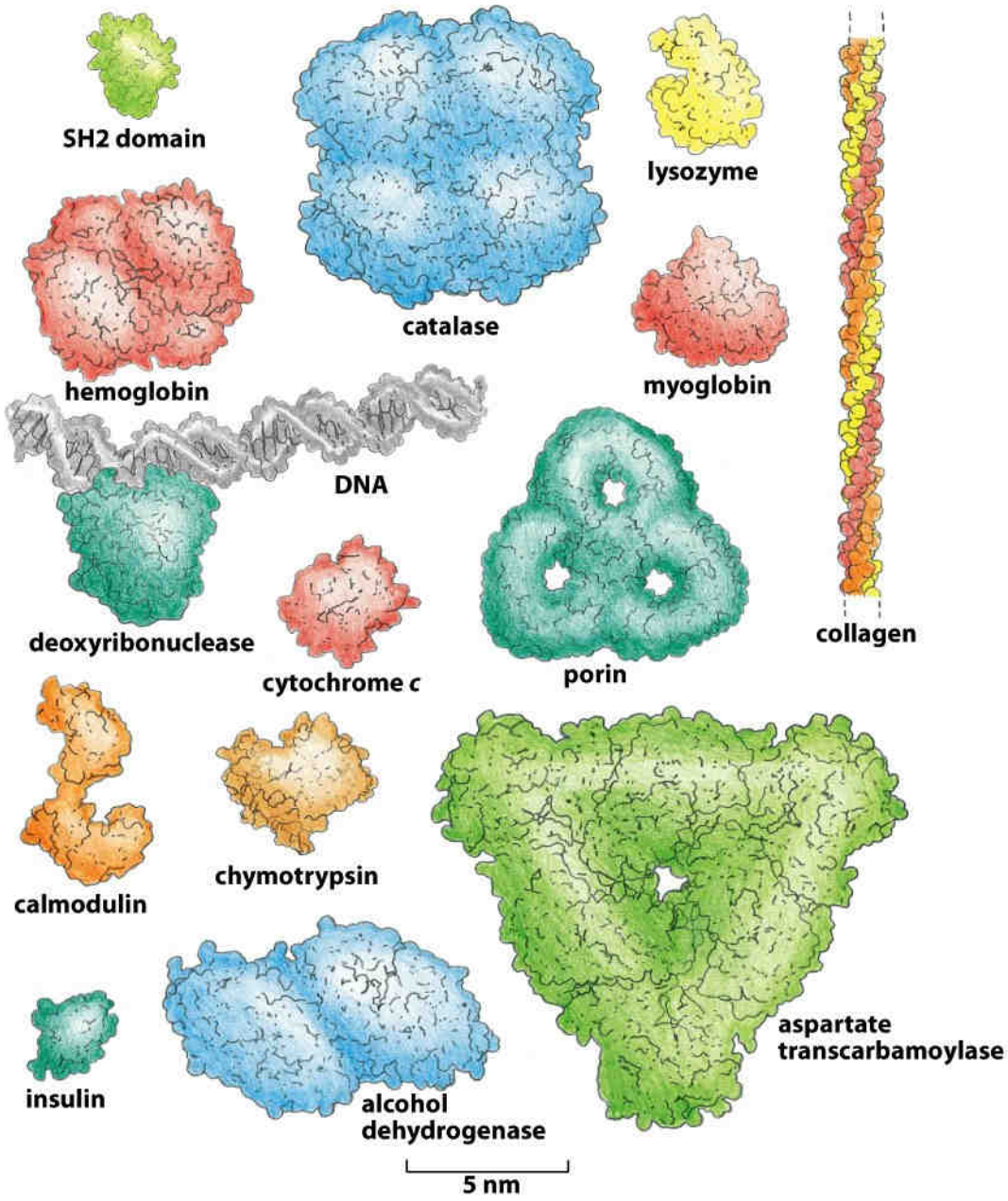


Figure 4-9 *Essential Cell Biology* (© Garland Science 2010)

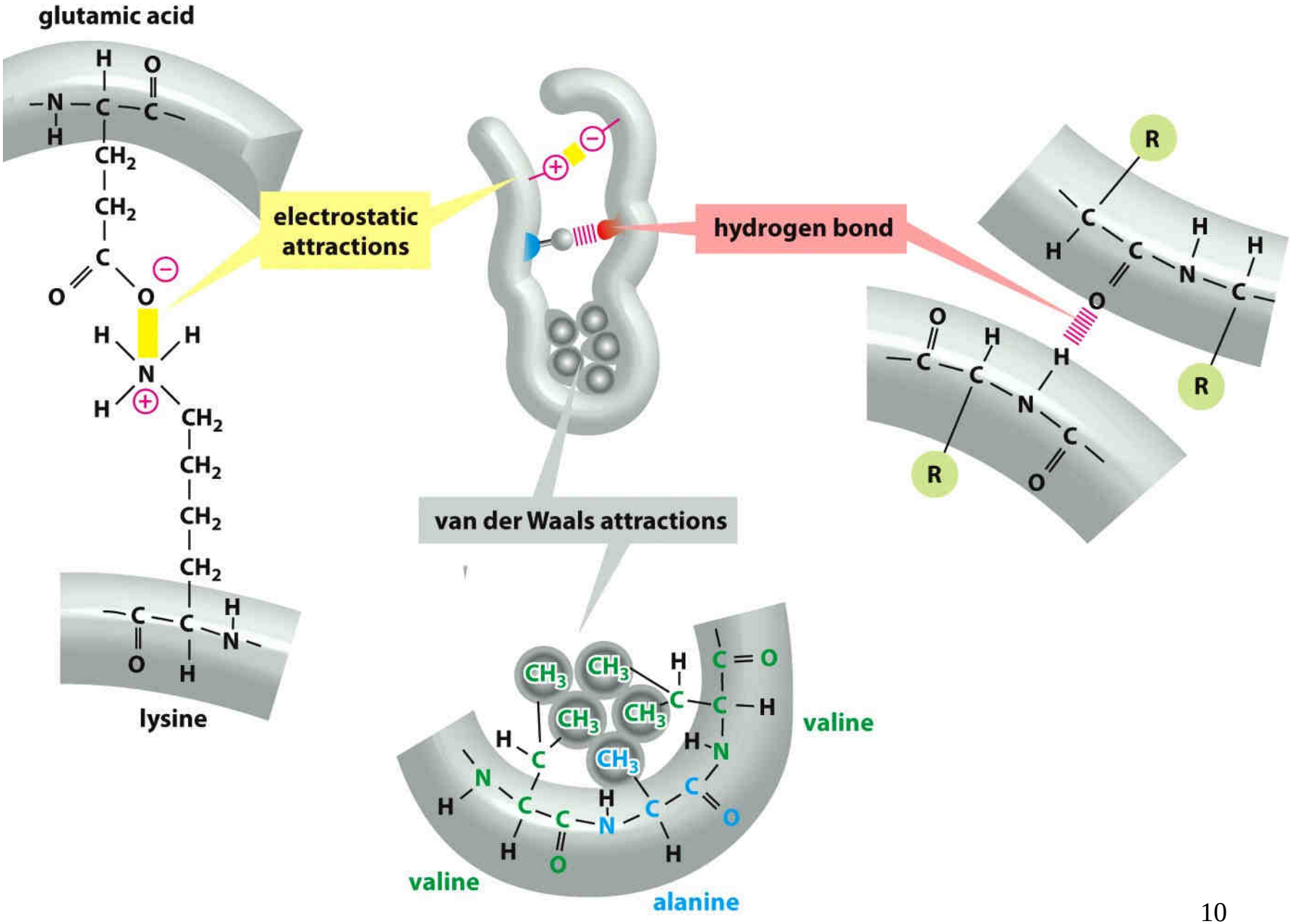
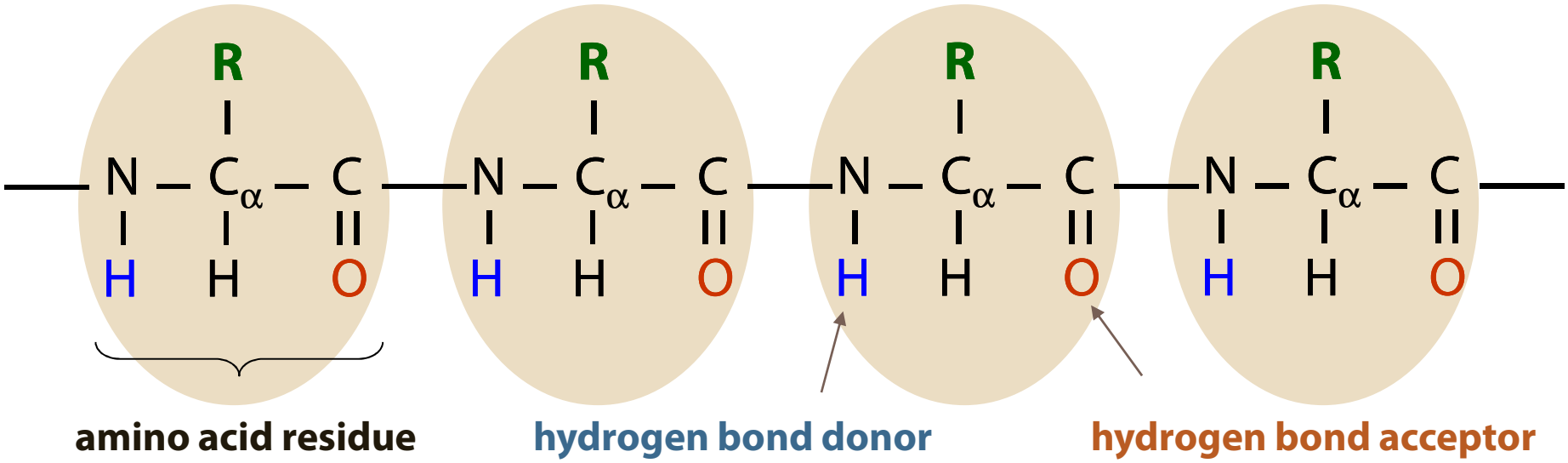


Figure 4-4 *Essential Cell Biology* (© Garland Science 2010)


R
N – Cα – C
H H O
amino acid residue
hydrogen bond donor
hydrogen bond acceptor

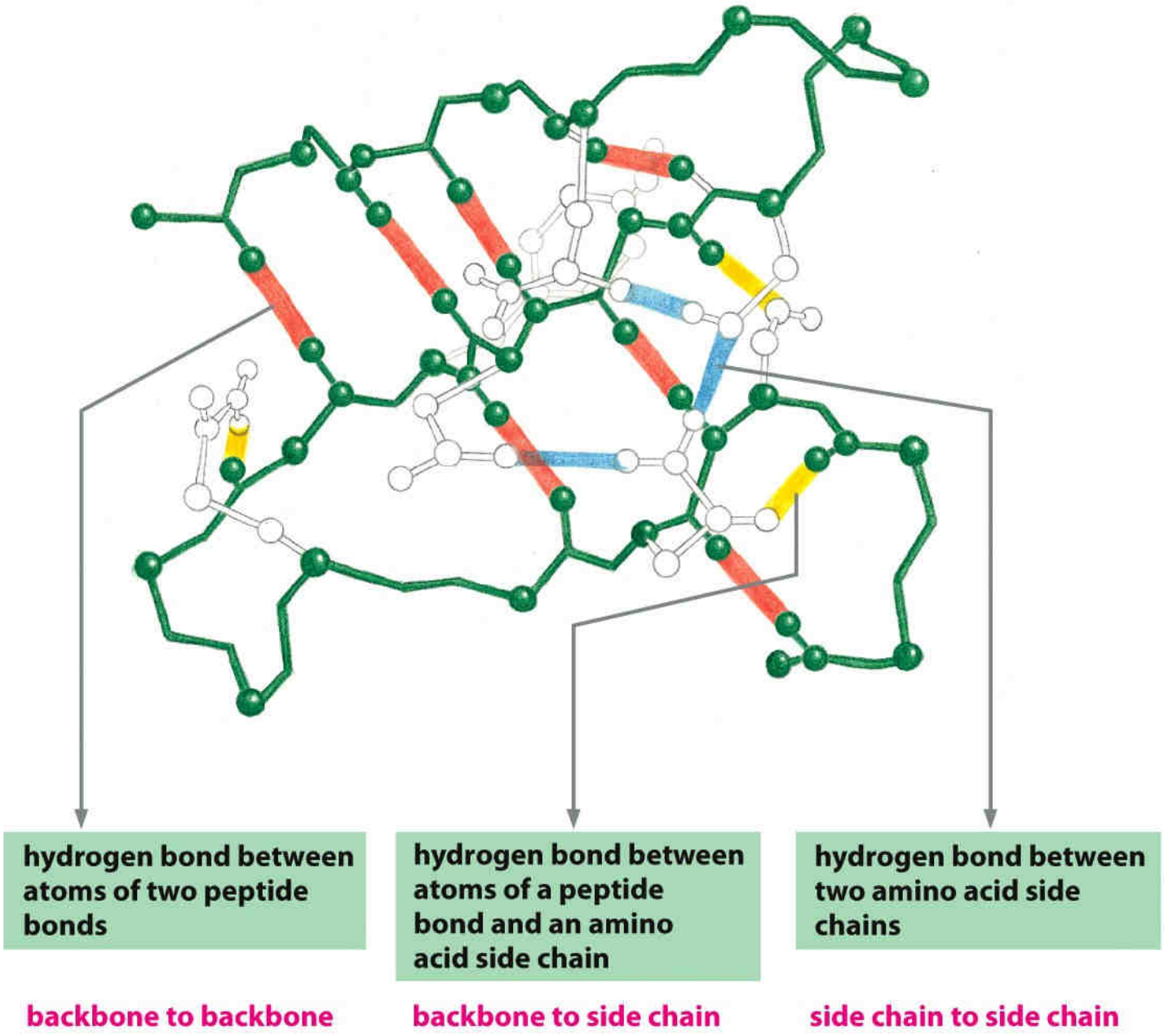
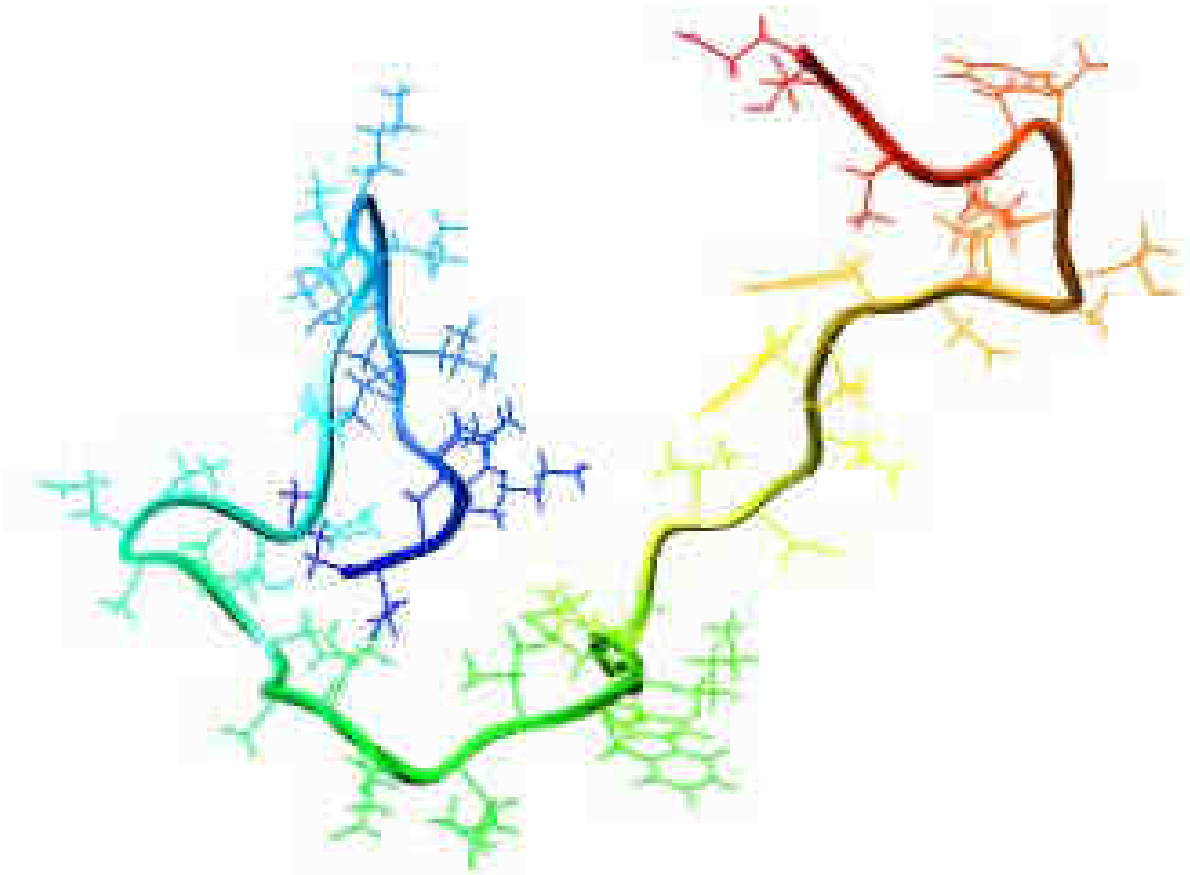
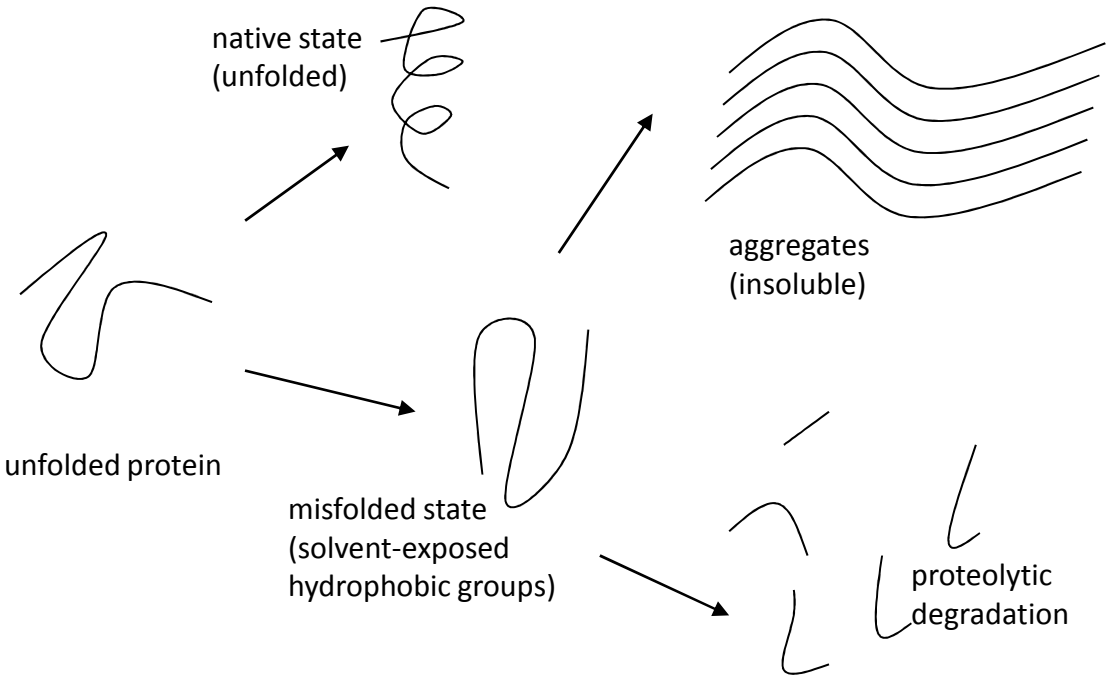


Figure 4-6 *Essential Cell Biology* (© Garland Science 2010)




native state
(unfolded)
aggregates
(insoluble)
unfolded protein
misfolded state
(solvent-exposed
hydrophobic groups)
proteolytic
degradation

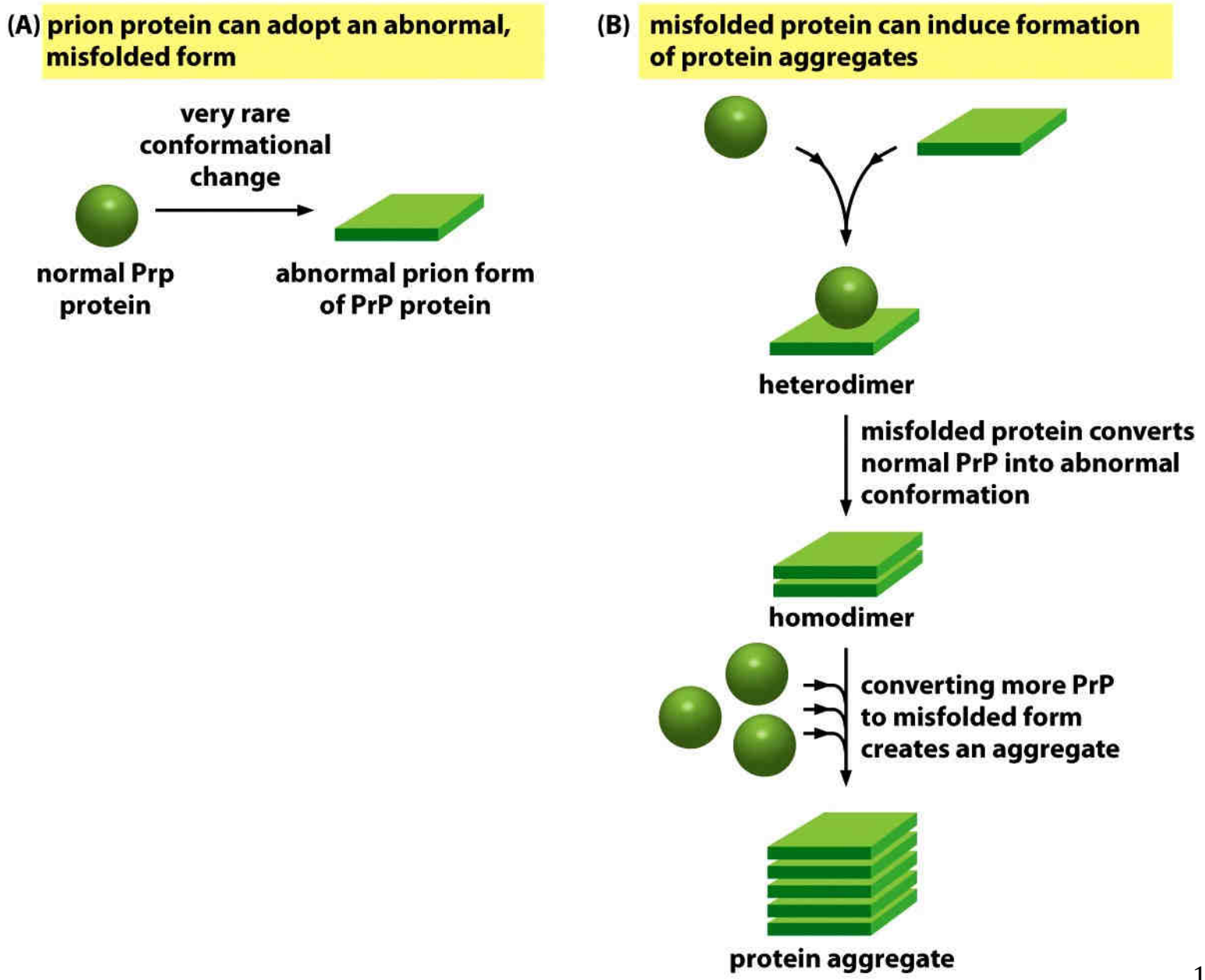


Figure 4-8 *Essential Cell Biology* (© Garland Science 2010)

secondary tertiary quartenary

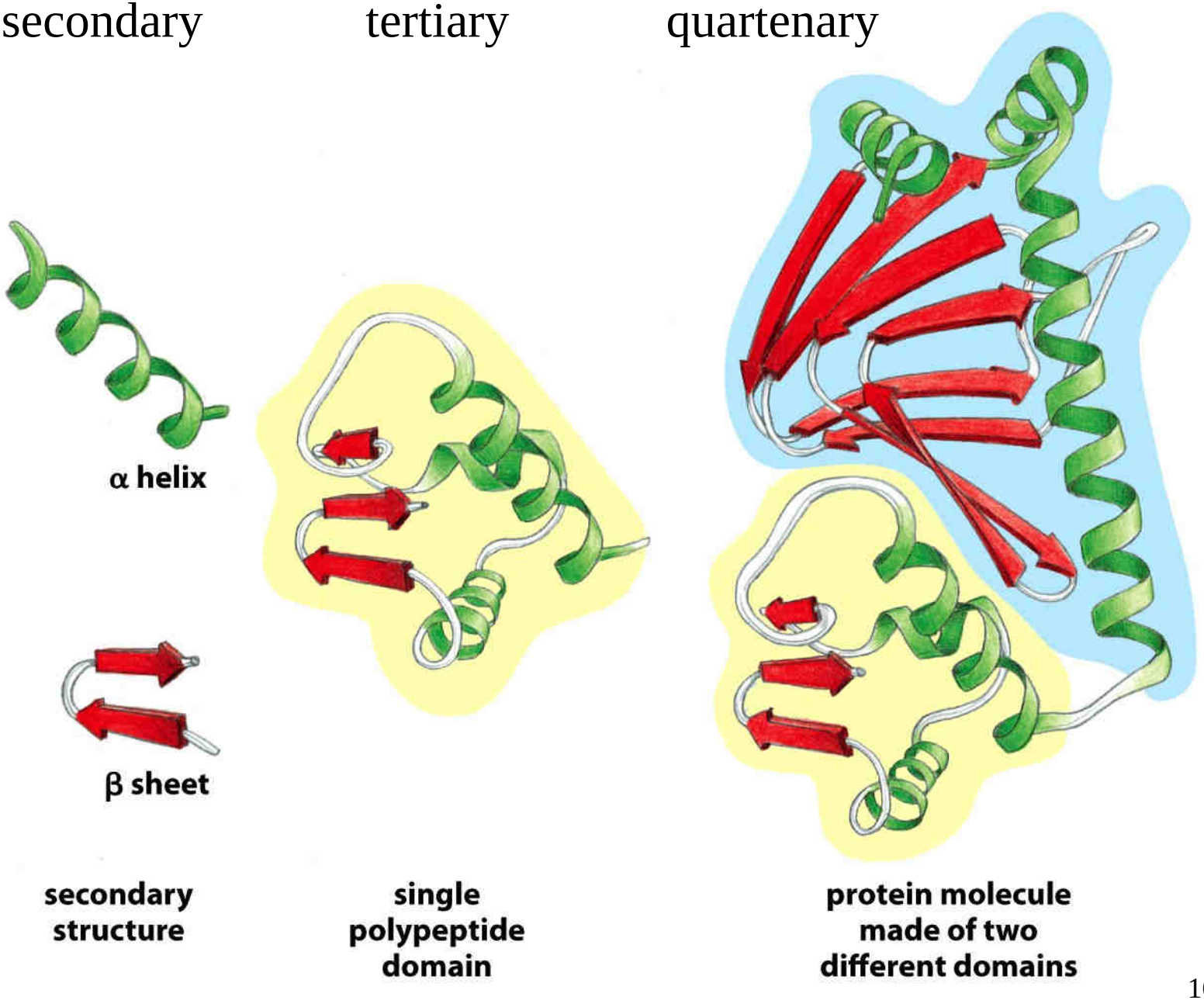
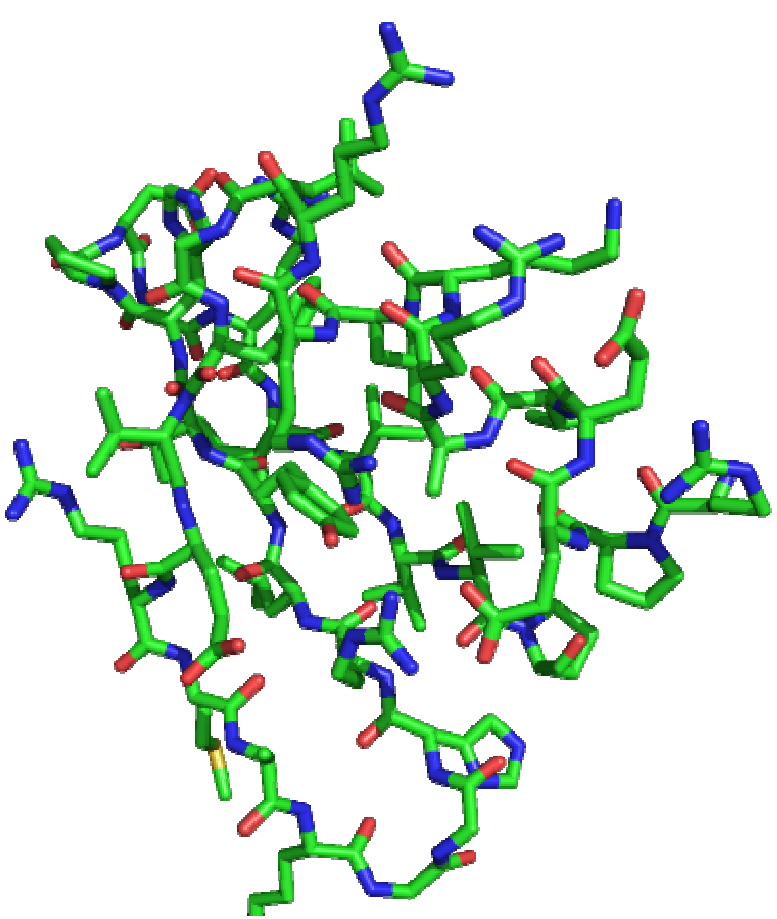
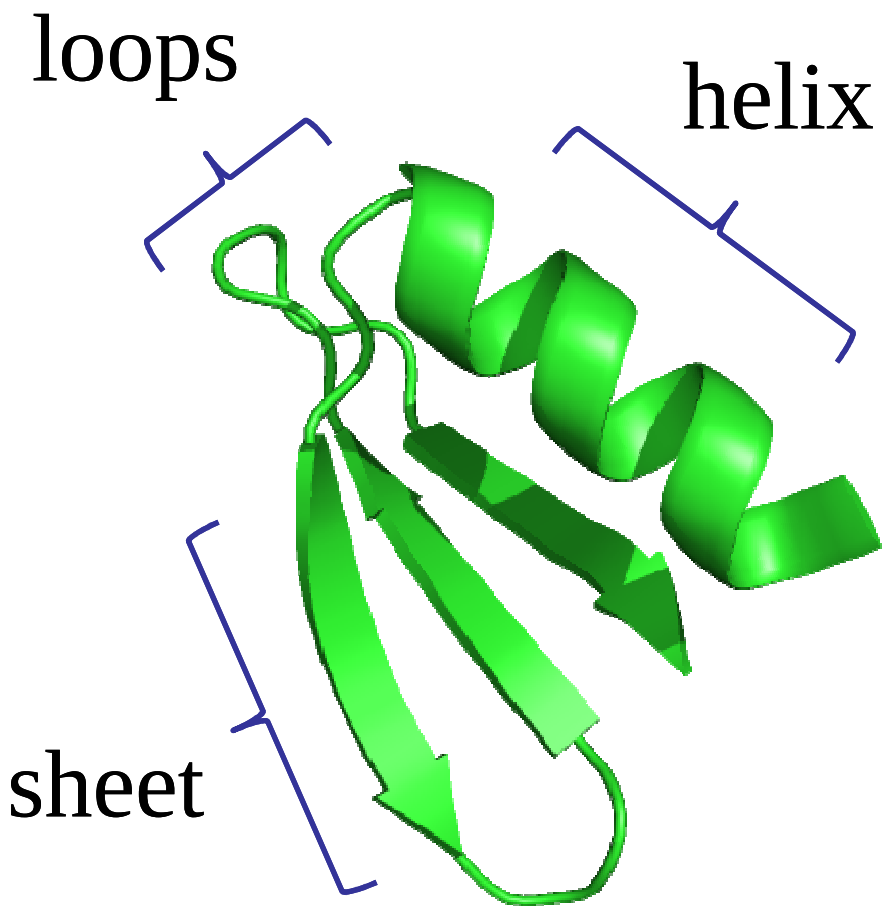


Figure 4-16 *Essential Cell Biology* (© Garland Science 2010)




loops
helix
sheet

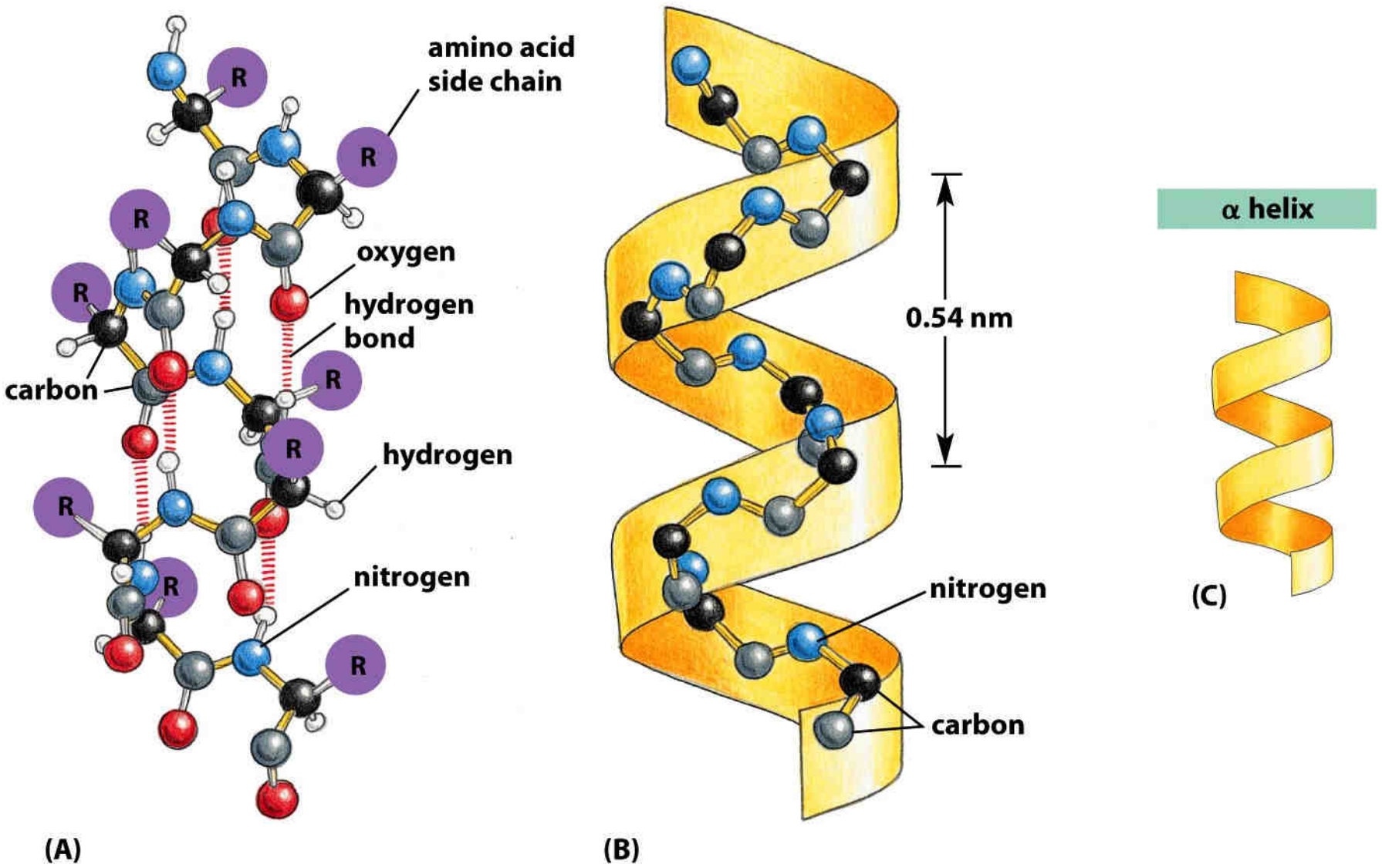


Figure 4-10a–c *Essential Cell Biology* (© Garland Science 2010)

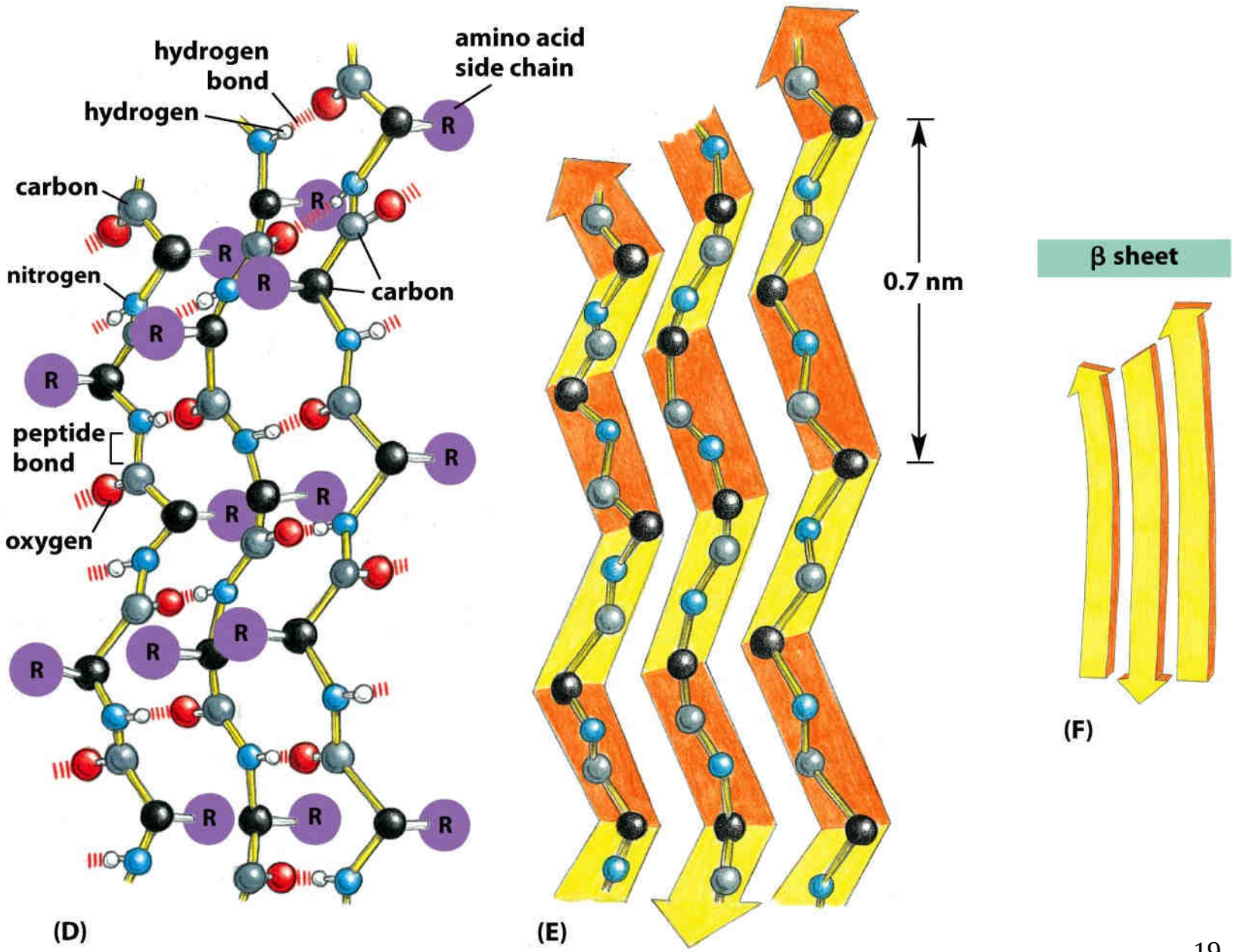


Figure 4-10d–f *Essential Cell Biology* (© Garland Science 2010)

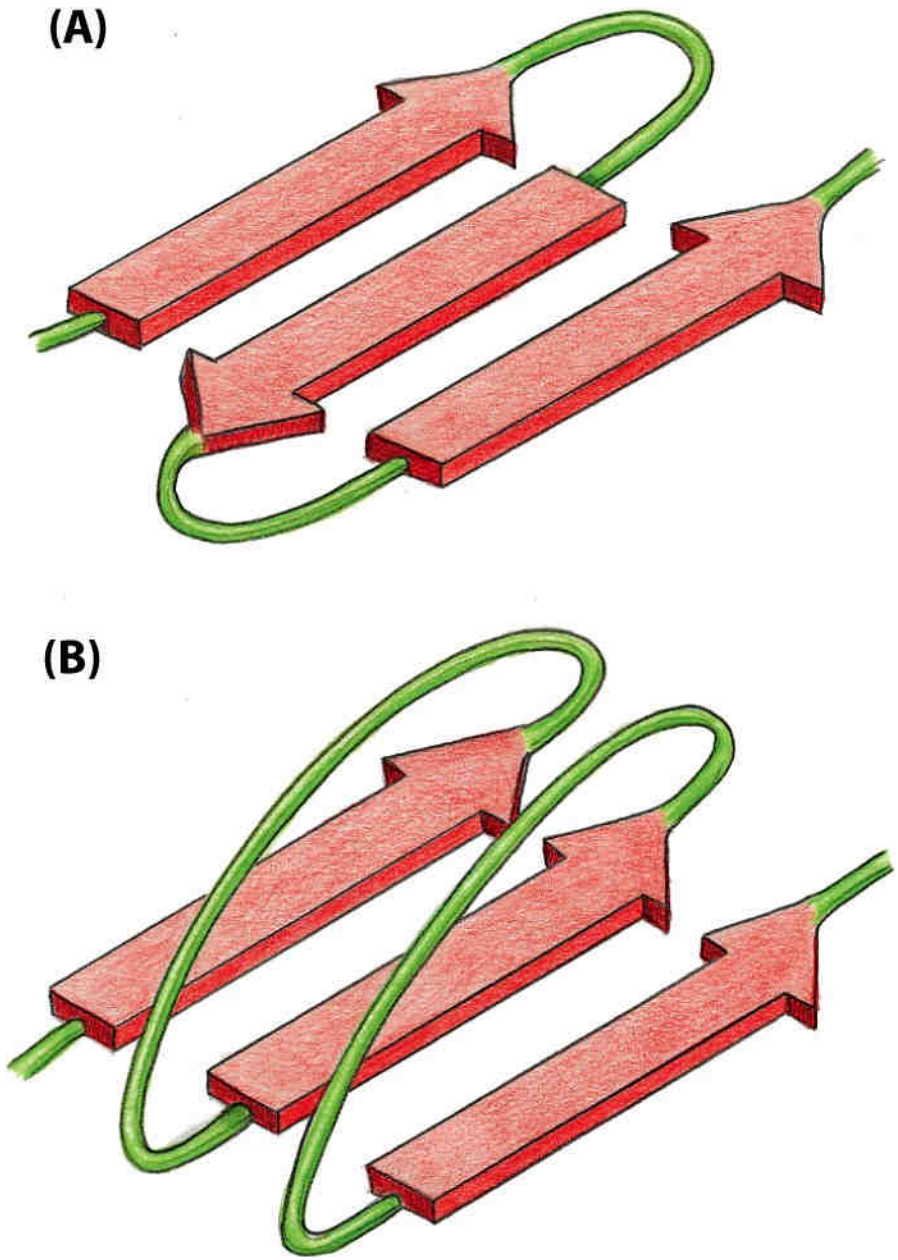


Figure 4-14 *Essential Cell Biology* (© Garland Science 2010)

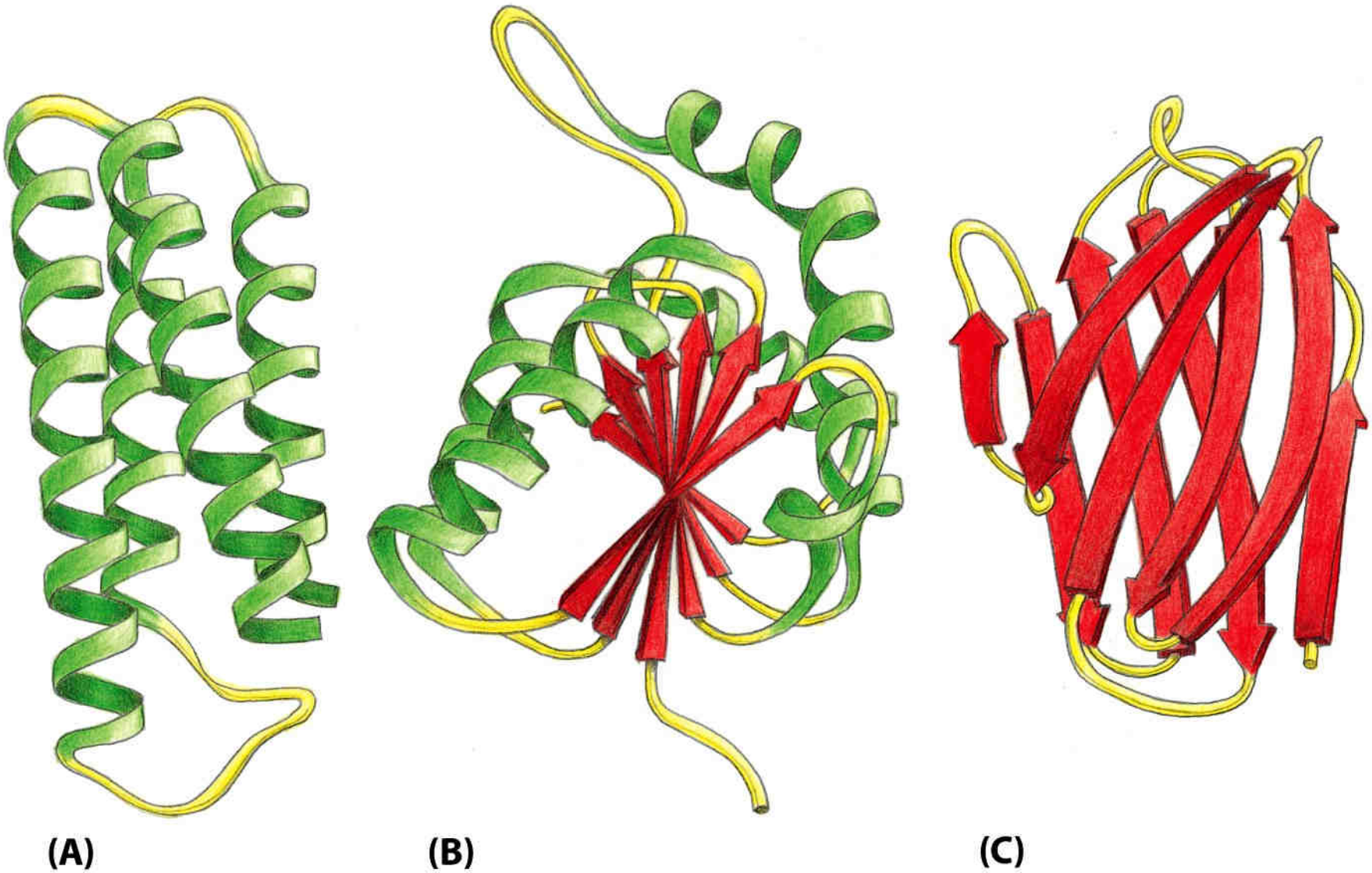


Figure 4-17 *Essential Cell Biology* (© Garland Science 2010)

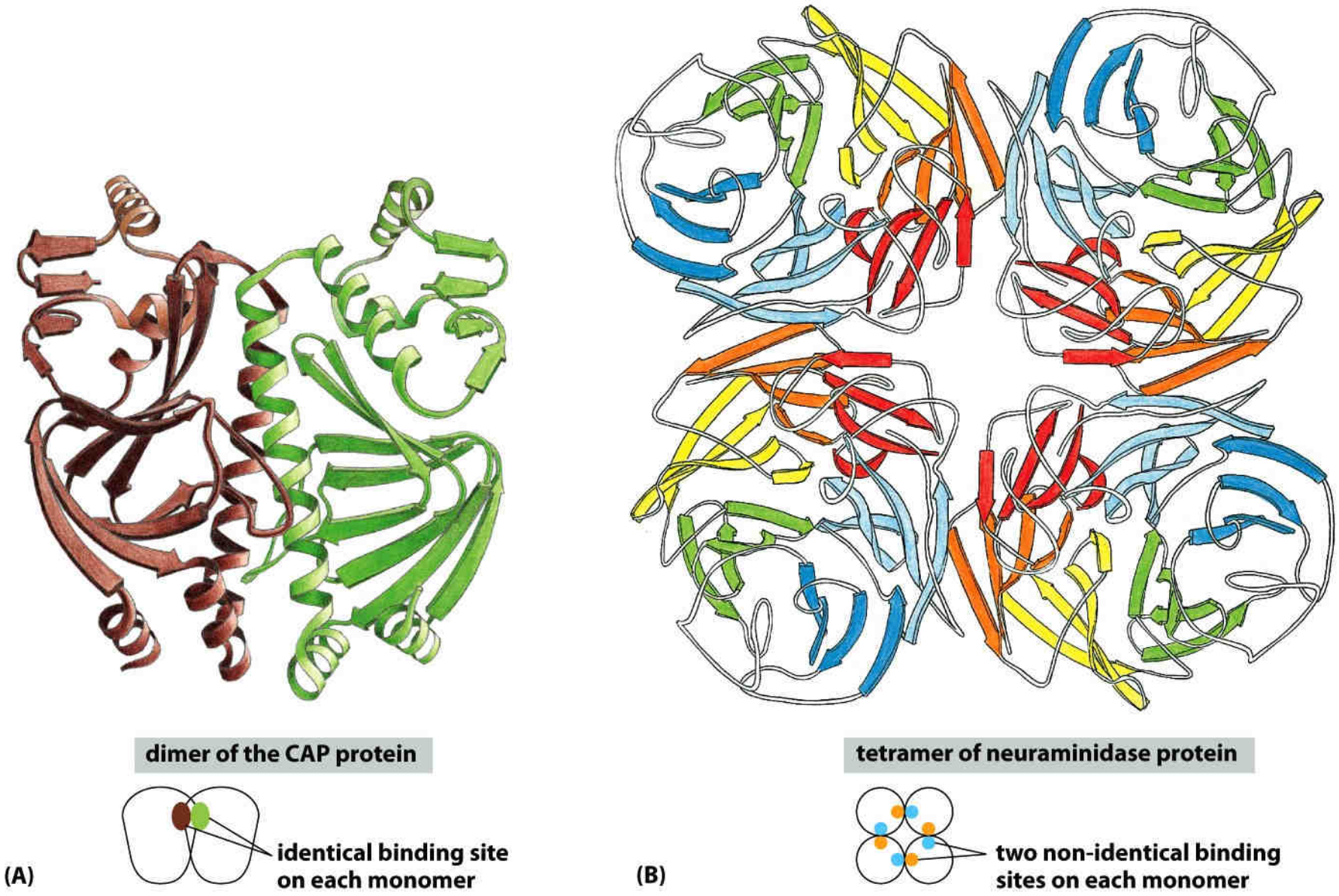


Figure 4-19 *Essential Cell Biology* (© Garland Science 2010)

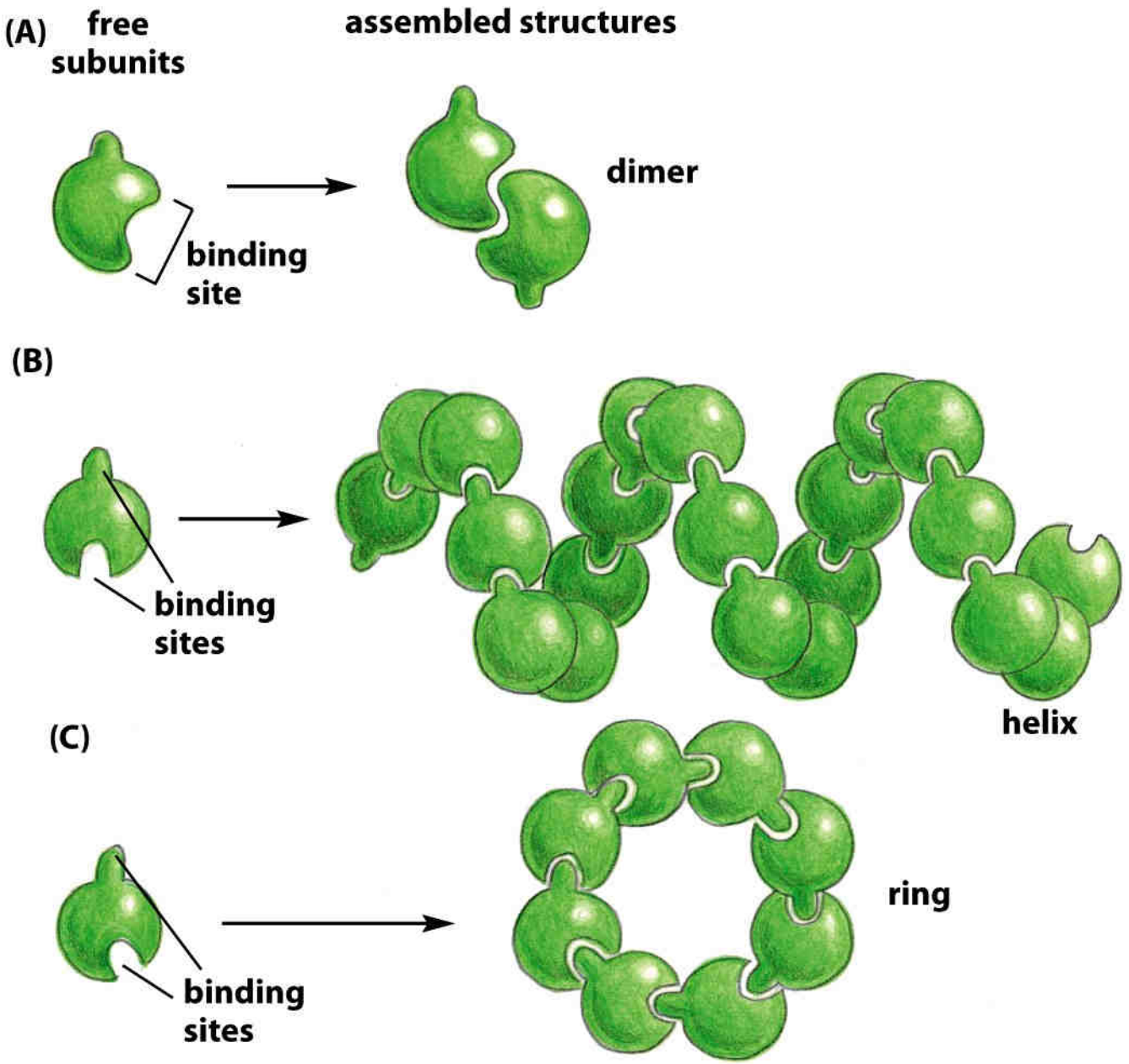


Figure 4-21 *Essential Cell Biology* (© Garland Science 2010)

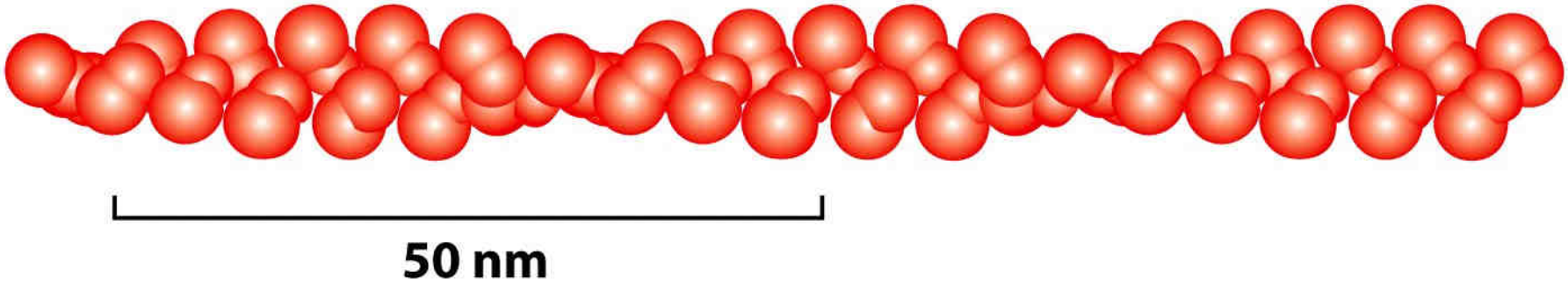


Figure 4-22 *Essential Cell Biology* (© Garland Science 2010)

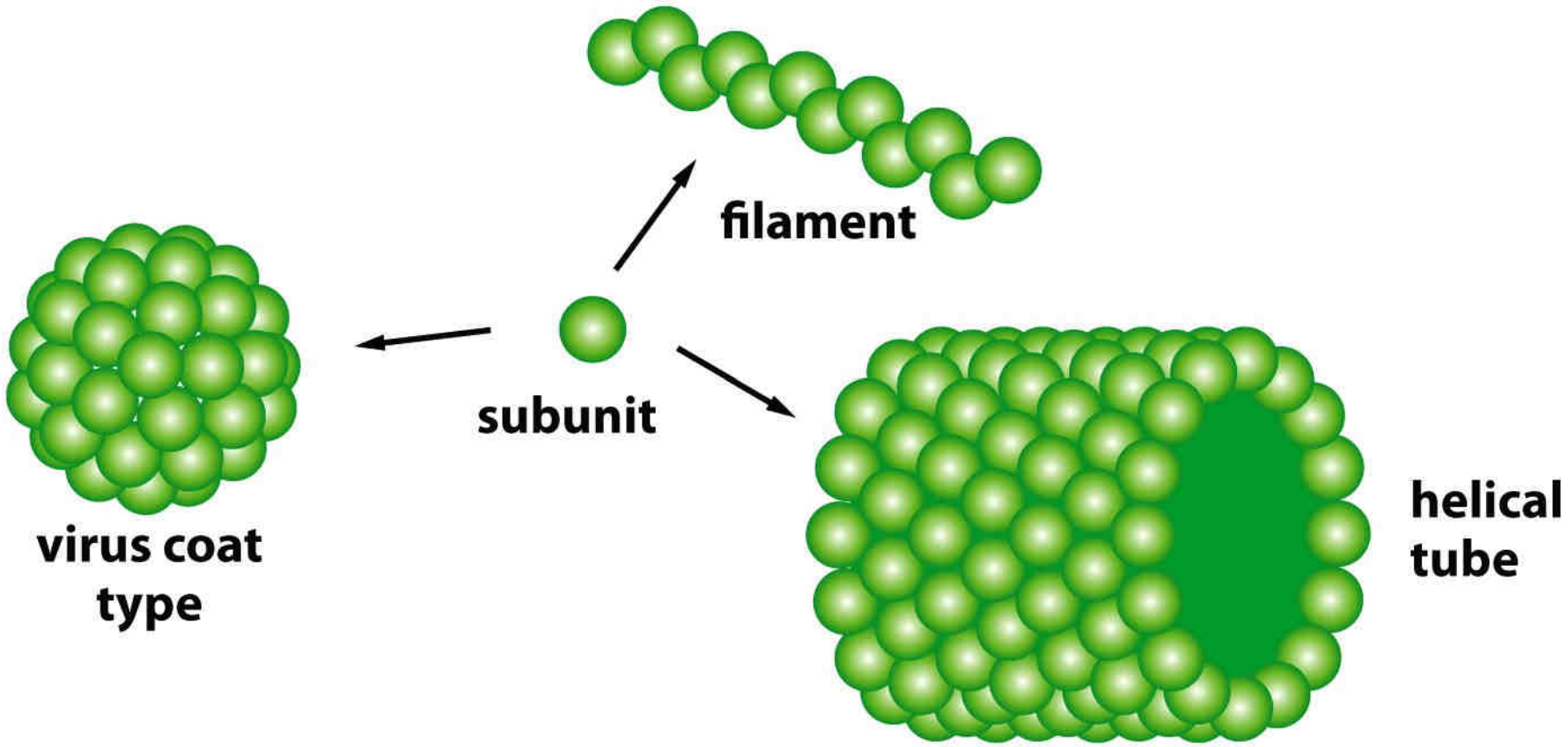


Figure 4-23 *Essential Cell Biology* (© Garland Science 2010)

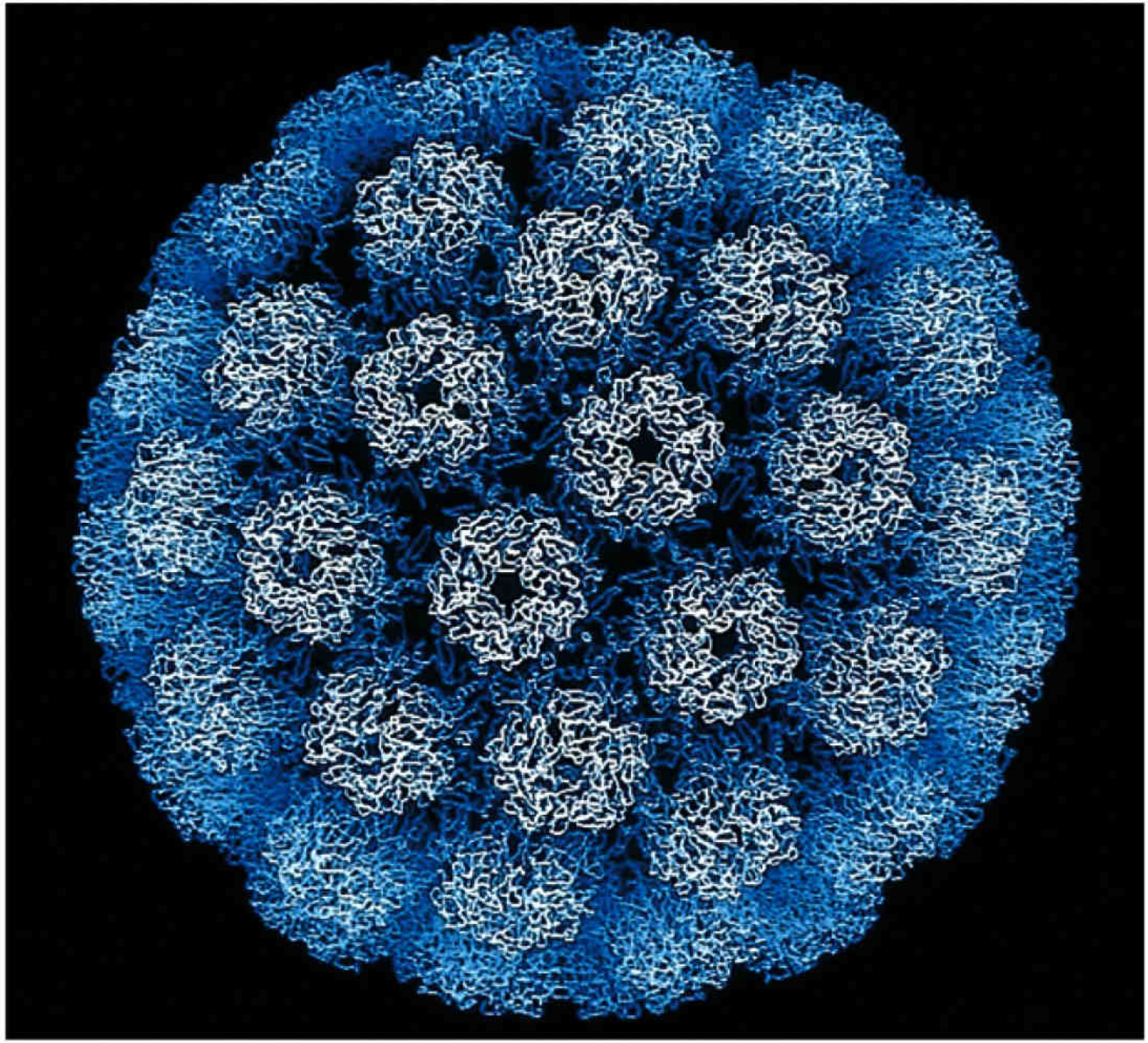


Figure 4-24 *Essential Cell Biology* (© Garland Science 2010)

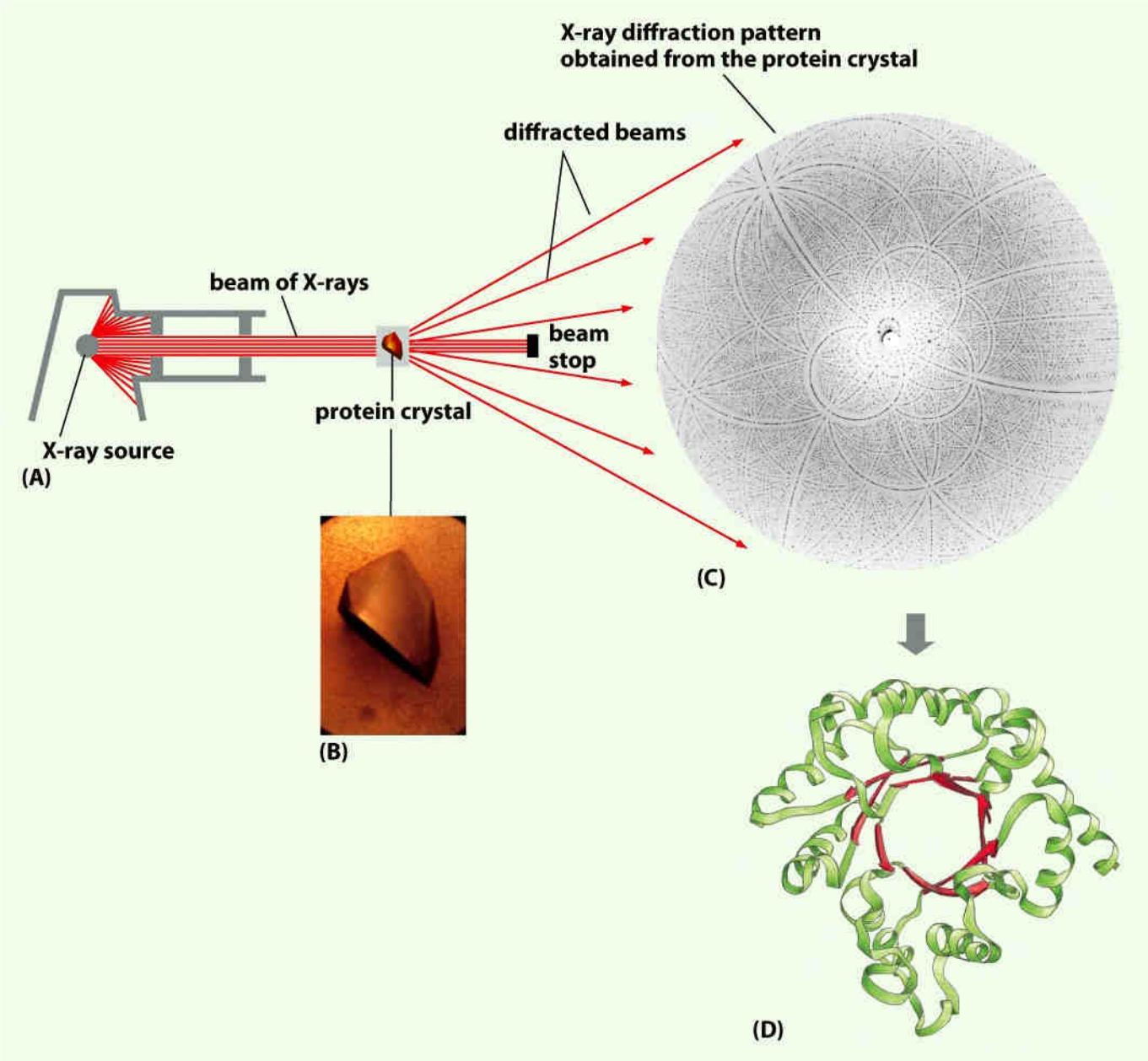


Figure 4-46 *Essential Cell Biology* (© Garland Science 2010)

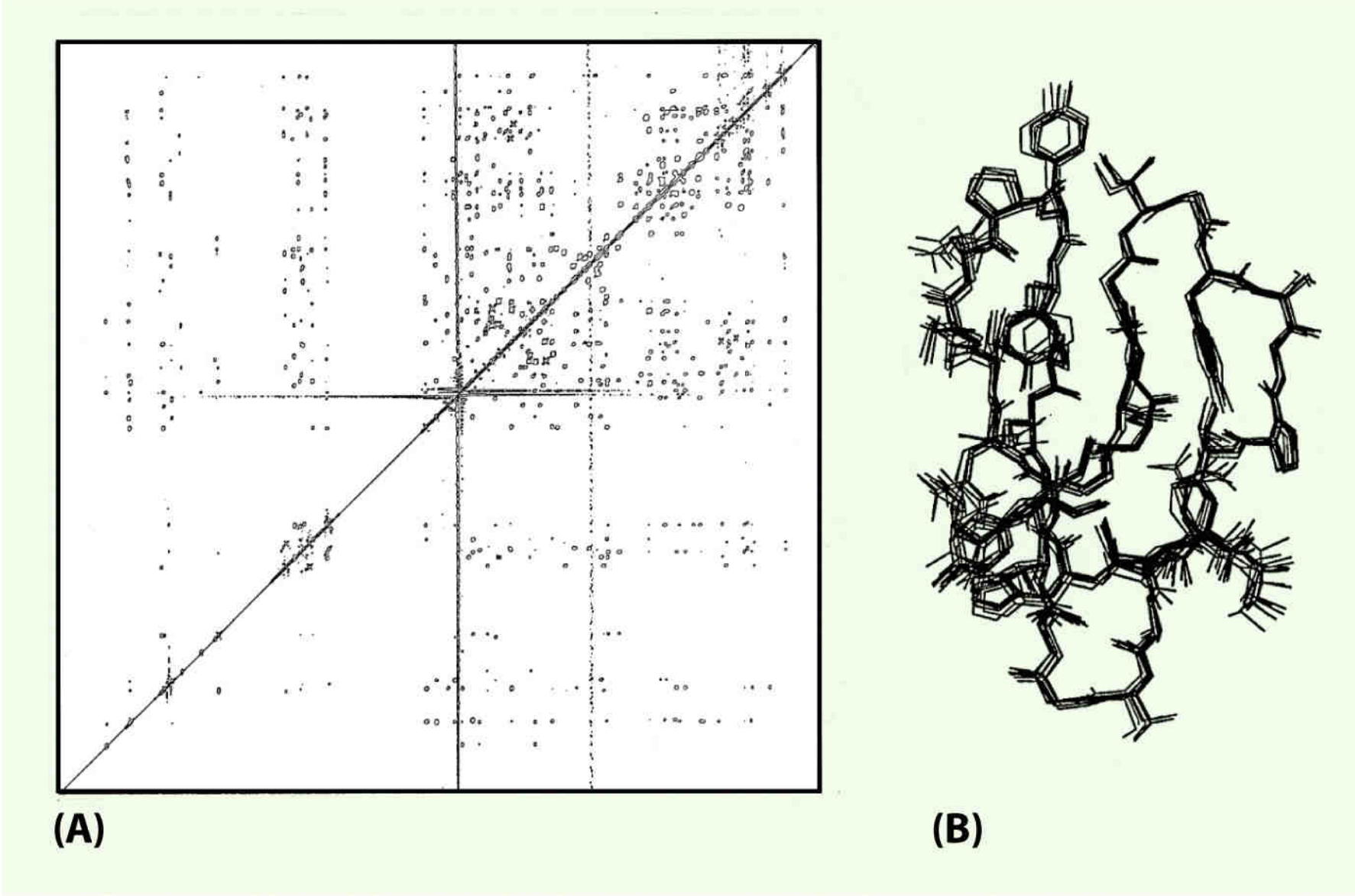
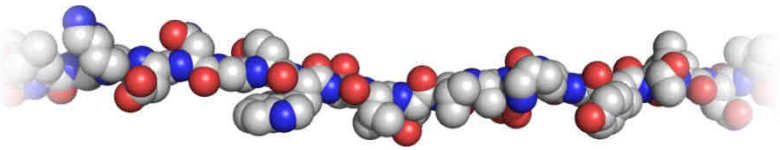


Figure 4-47 *Essential Cell Biology* (© Garland Science 2010)

Physics- versus bioinformatics-based folding

AAGHWWKGPVGEWTLMTYVAVWKHI

unknown sequence



atomically detailed representation

simulated conformational folding process guided by atomic energetics

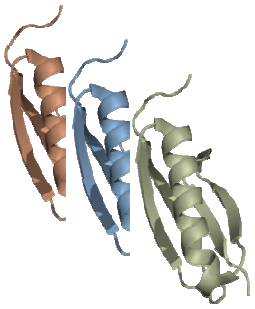
Protein Data Bank

big database of known structures

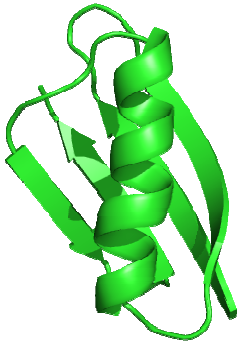
AIGHWWLRGPGAEWTLCTYVAHI

LAGHWFSGGVGEWTIMTYAAWLVEHI

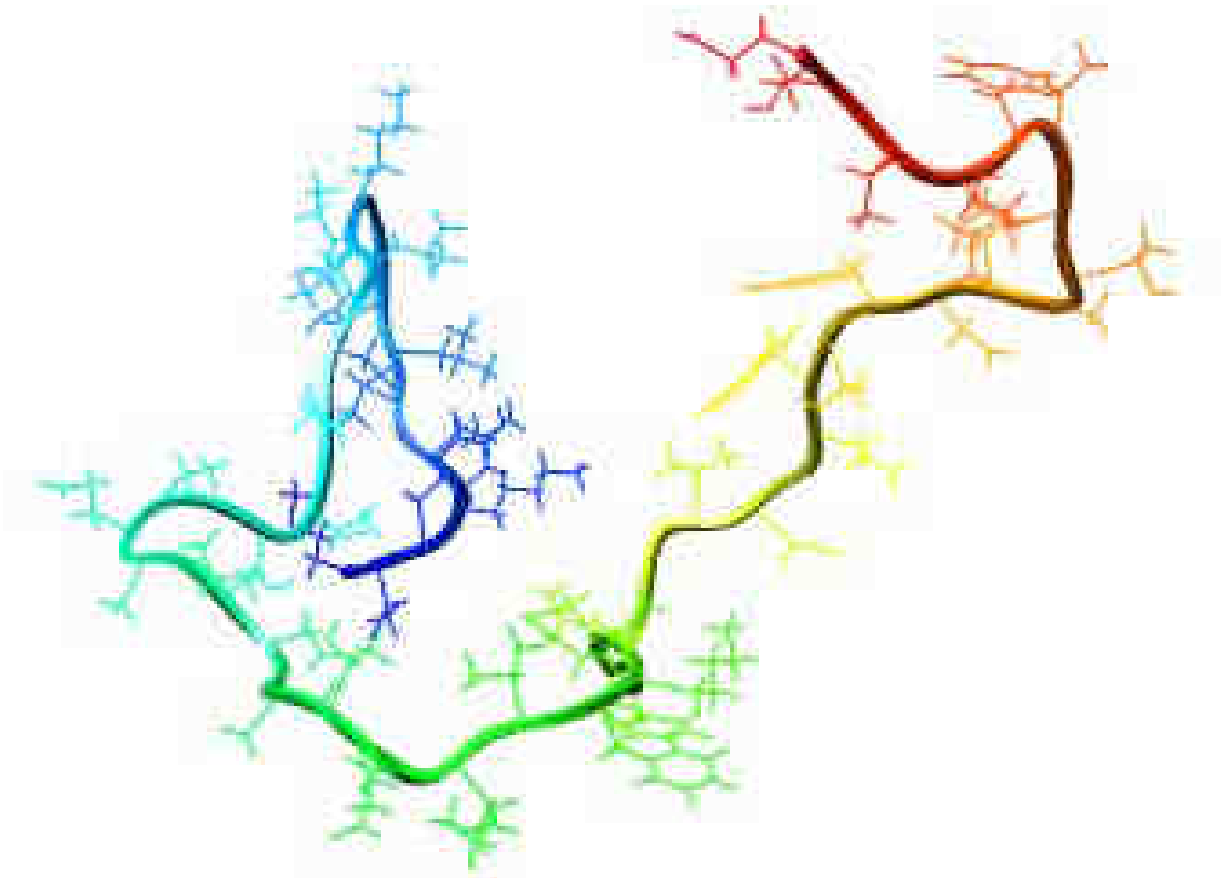
AGHWWKAAVGEYITYEKVADAVWHI



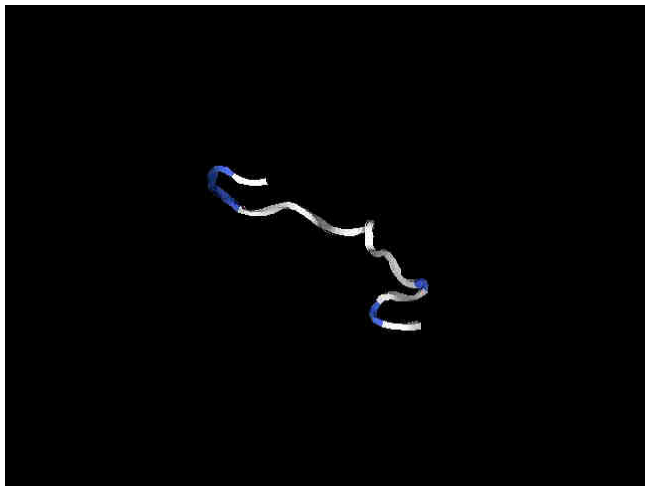
similar sequences and their structures



predicted structure



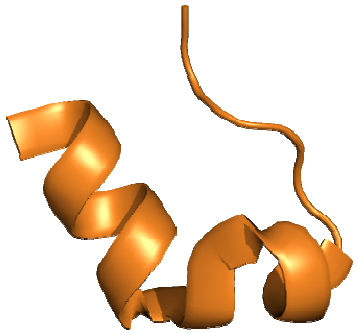
Computers can only fold tiny proteins directly



poly-alanine

20 amino acid residues

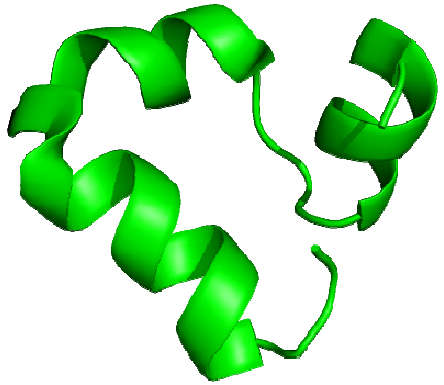
Pande et al. 2000
(movie from folding.stanford.edu)



trp cage miniprotein

20 residues

Simmerling et al. 2002
Duan et al. 2003
Pitera and Swope 2003
Pande et al. 2004



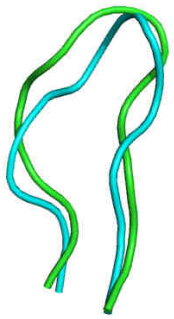
villin headpiece

35 residues

Duan and Kollman 1996
Pande et al. 2006
Duan et al. 2007

100s-1000s of CPU-years

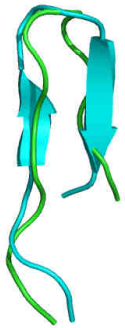
Convergence for PDB and literature peptides



1GM2
11 residues
~10 ns

C peptide
13 residues
~20 ns

EK peptide
14 residues
~10 ns



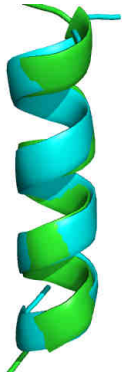
108Y
14 residues
~1 ns

15-β
15 residues
~5 ns

1E0Q
17 residues
~5 ns

native
simulated
convergence time

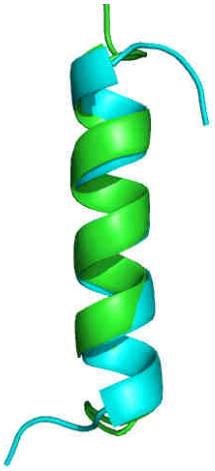
1 ns simulation time
≈ 4 CPU days
≈ 3.5 hrs real time



2I9M
17 residues
~65 ns

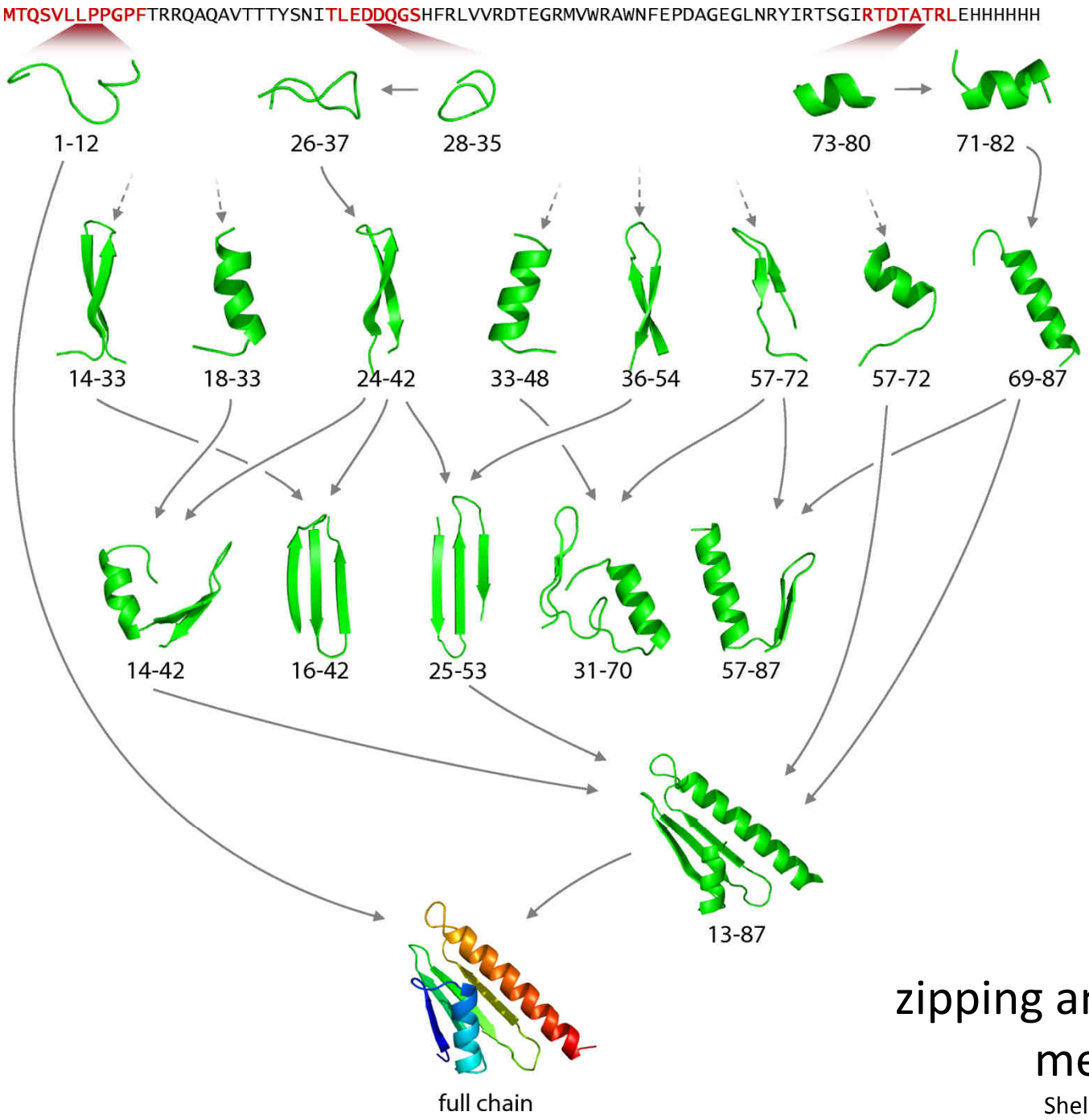
2JNI
21 residues
~40 ns

2JSB
21 residues
~25 ns



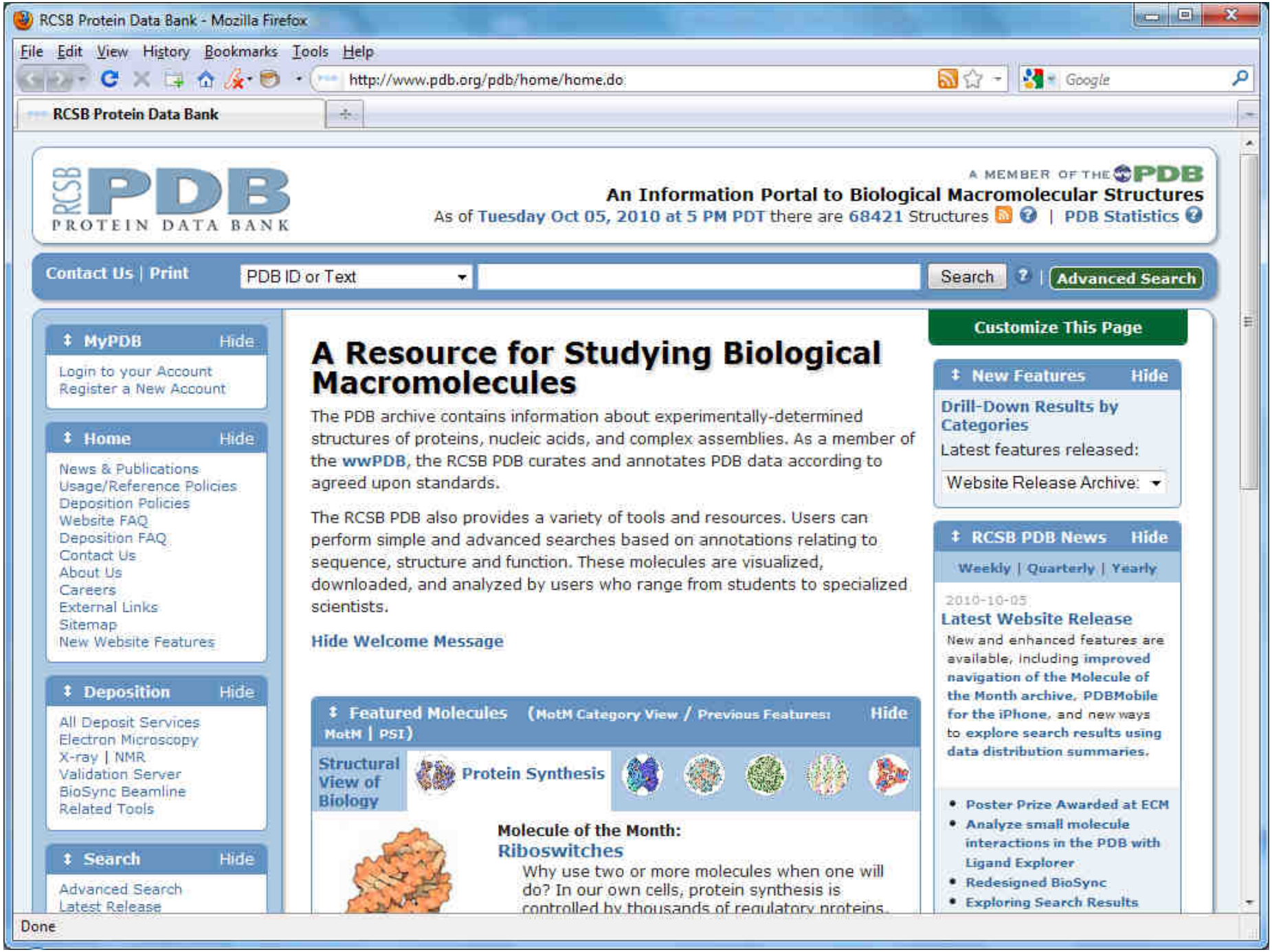
1WN8
22 residues
~30 ns

Lin and Shell, J. Comput Chem, 2009.



zipping and assembly method (ZAM)

Shell et al., Biophys. J (2008)


RCSB Protein Data Bank - Mozilla Firefox
File Edit View History Bookmarks Tools Help
http://www.pdb.org/pdb/home/home.do
Google
RCSB Protein Data Bank
RCSB PDB
PROTEIN DATA BANK
A MEMBER OF THE PDB
An Information Portal to Biological Macromolecular Structures
As of Tuesday Oct 05, 2010 at 5 PM PDT there are 68421 Structures | PDB Statistics
Contact Us | Print
PDB ID or Text
Search
Advanced Search
MyPDB Hide
Login to your Account
Register a New Account
Home Hide
News & Publications
Usage/Reference Policies
Deposition Policies
Website FAQ
Deposition FAQ
Contact Us
About Us
Careers
External Links
Sitemap
New Website Features
Deposition Hide
All Deposit Services
Electron Microscopy
X-ray | NMR
Validation Server
BioSync Beamline
Related Tools
Search Hide
Advanced Search
Latest Release
A Resource for Studying Biological Macromolecules
The PDB archive contains information about experimentally-determined structures of proteins, nucleic acids, and complex assemblies. As a member of the wwPDB, the RCSB PDB curates and annotates PDB data according to agreed upon standards.
The RCSB PDB also provides a variety of tools and resources. Users can perform simple and advanced searches based on annotations relating to sequence, structure and function. These molecules are visualized, downloaded, and analyzed by users who range from students to specialized scientists.
Hide Welcome Message
Featured Molecules (MotM Category View / Previous Features: MotM | PSI) Hide
Structural View of Biology
Protein Synthesis
Molecule of the Month:
Riboswitches
Why use two or more molecules when one will do? In our own cells, protein synthesis is controlled by thousands of regulatory proteins.
Customize This Page
New Features Hide
Drill-Down Results by Categories
Latest features released:
Website Release Archive:
RCSB PDB News Hide
Weekly | Quarterly | Yearly
2010-10-05
Latest Website Release
New and enhanced features are available, including improved navigation of the Molecule of the Month archive, PDBMobile for the iPhone, and new ways to explore search results using data distribution summaries.
Poster Prize Awarded at ECM
Analyze small molecule interactions in the PDB with Ligand Explorer
Redesigned BioSync
Exploring Search Results
Done

KLA**P**TG**I**PP**F**

RLA**G**TG**L**PP**E**

60% identity + 20% similarity

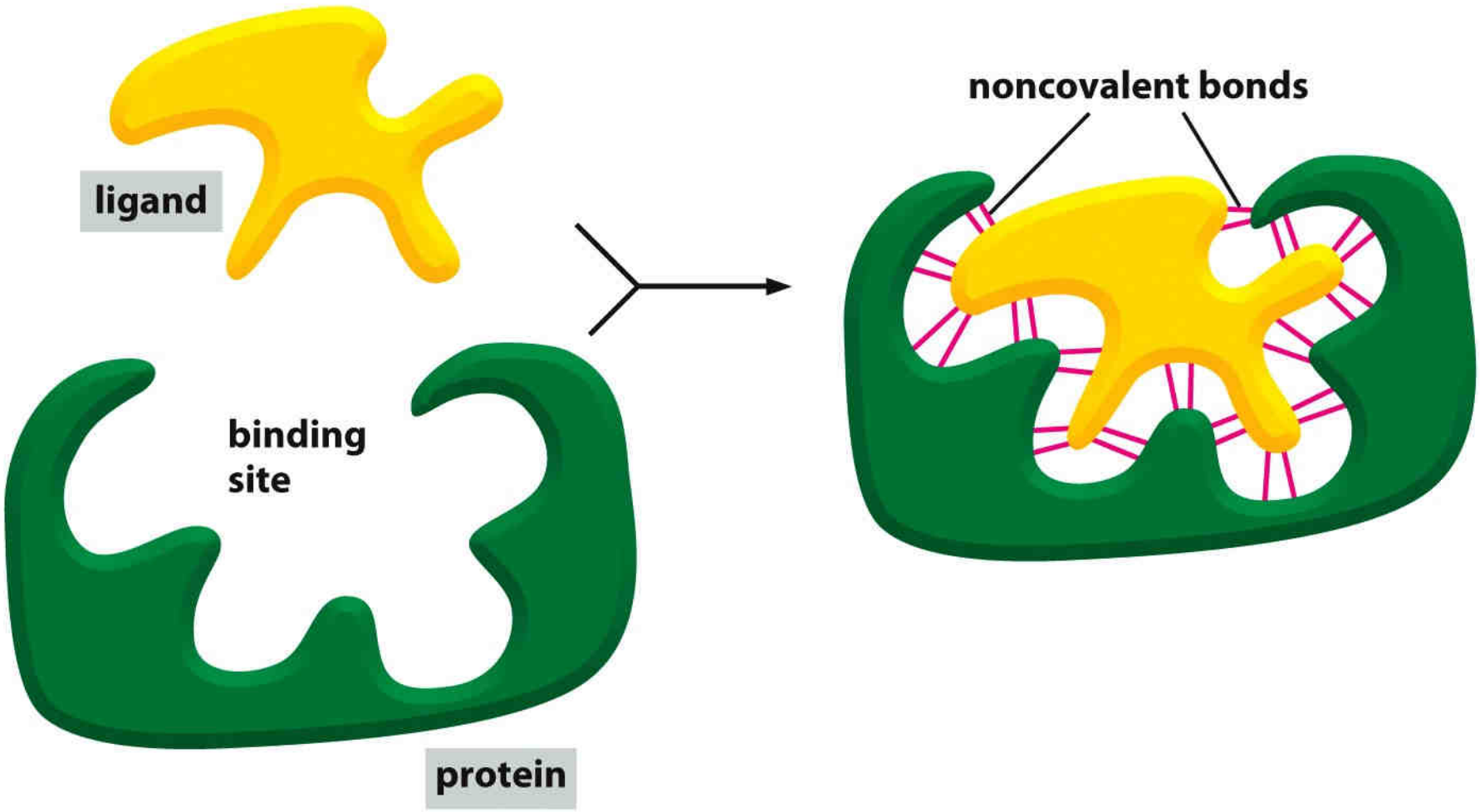


Figure 4-27 *Essential Cell Biology* (© Garland Science 2010)

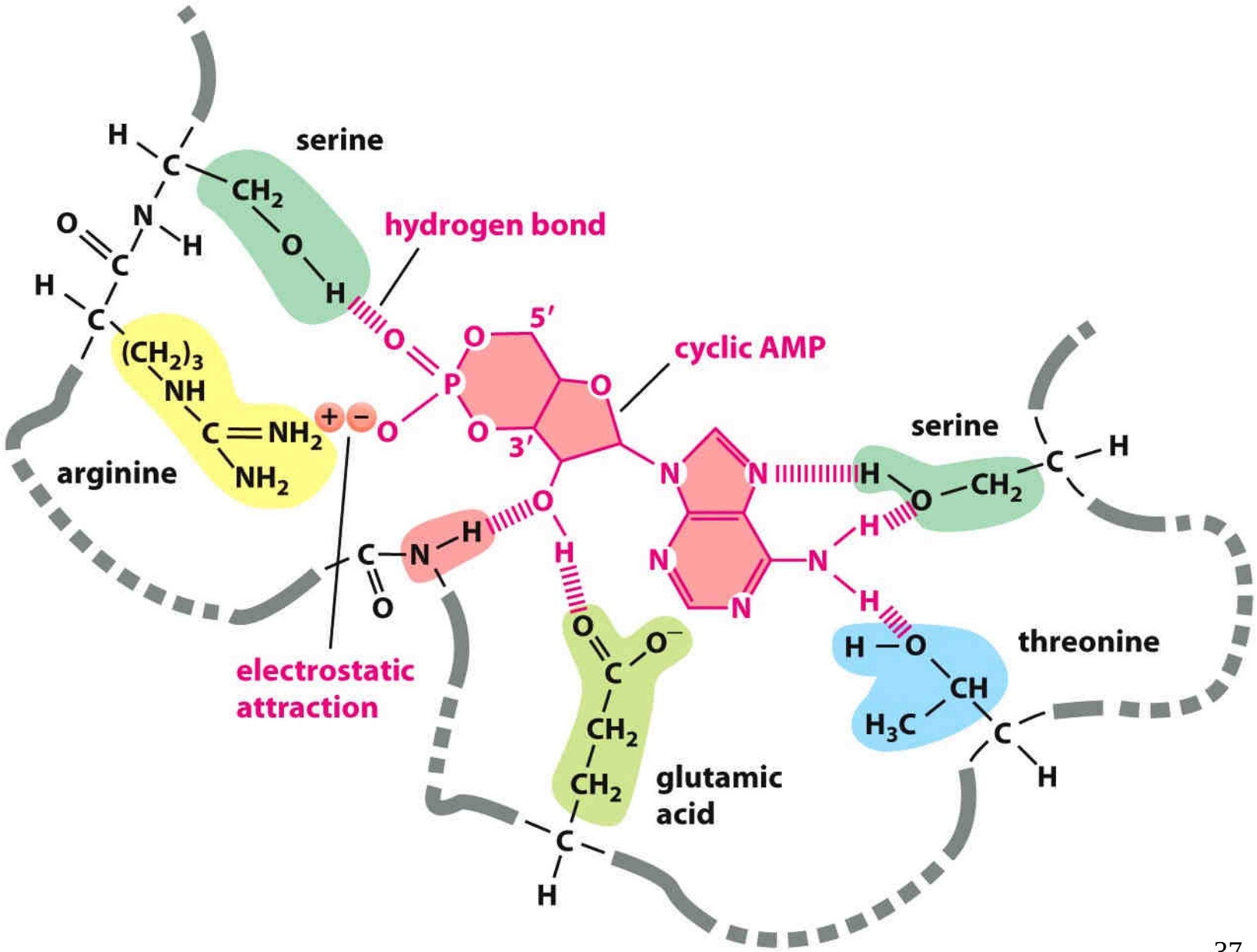


Figure 4-28b *Essential Cell Biology* (© Garland Science 2010)

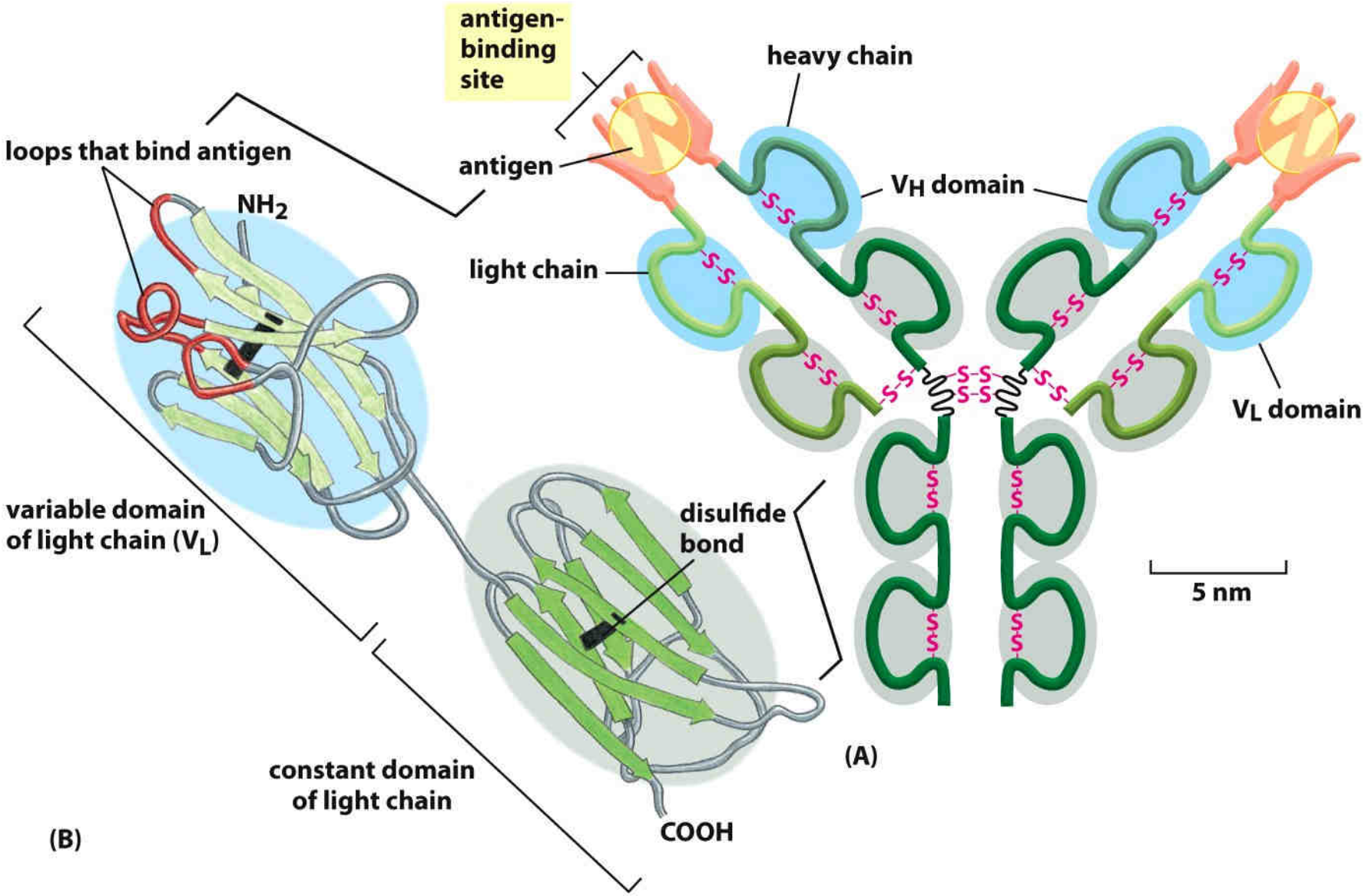


Figure 4-29 *Essential Cell Biology* (© Garland Science 2010)

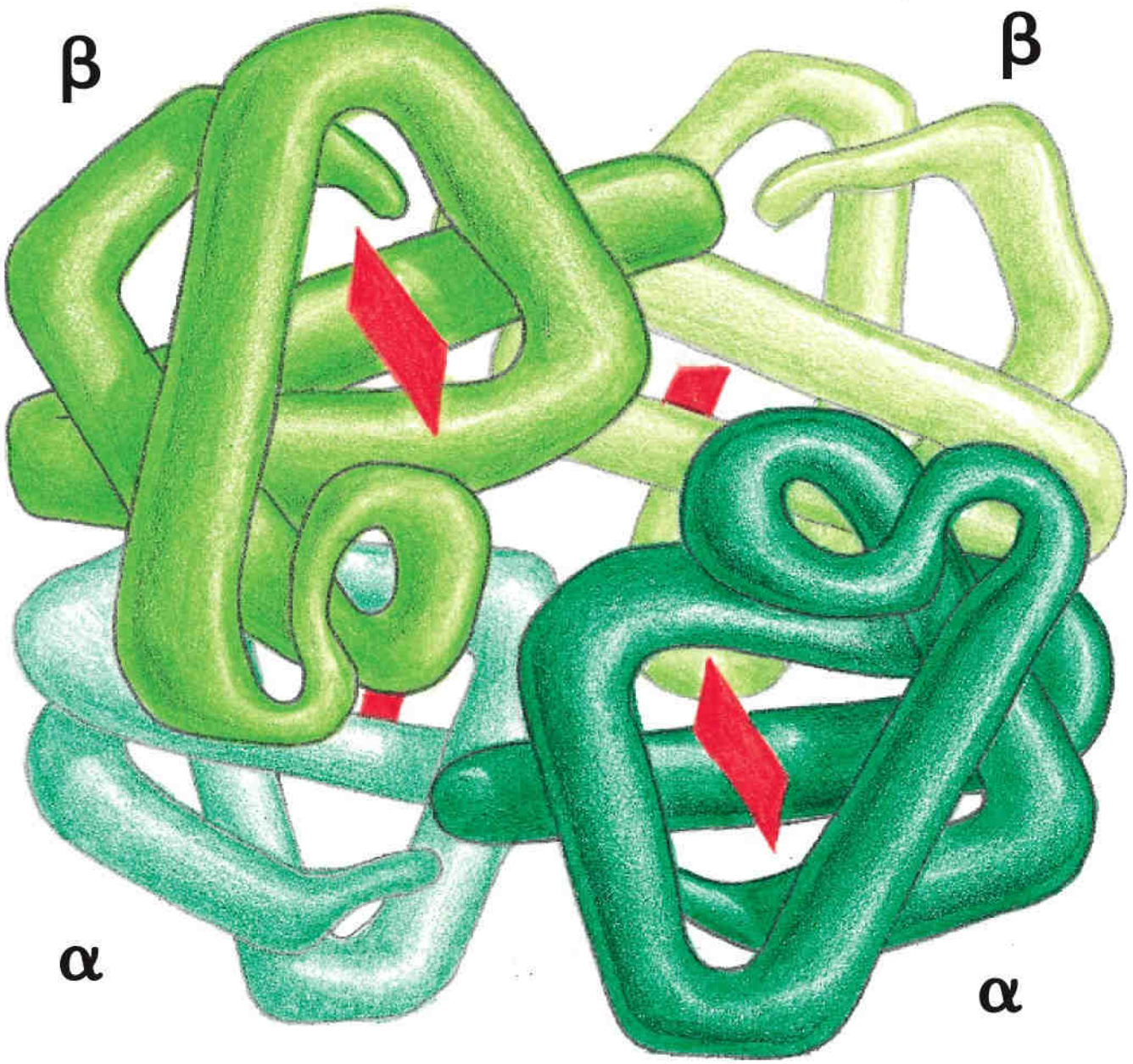
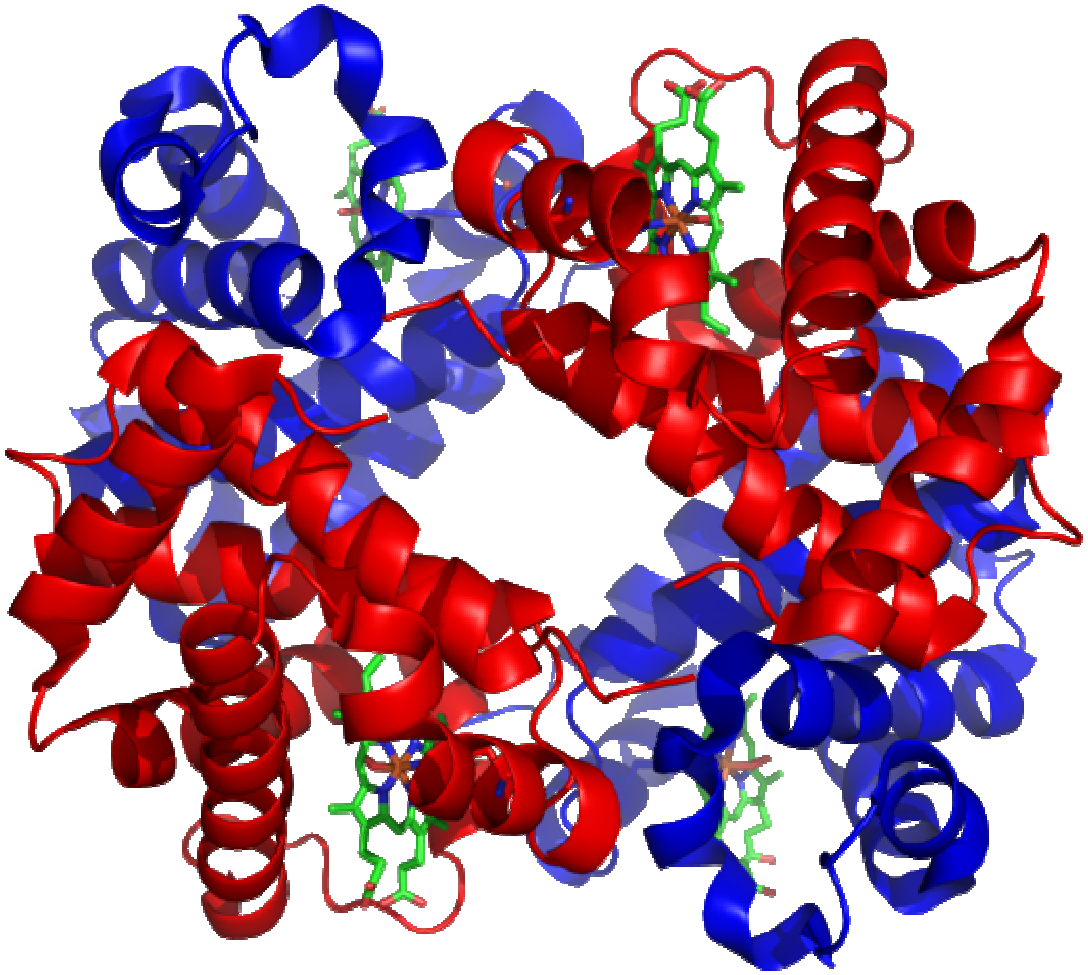
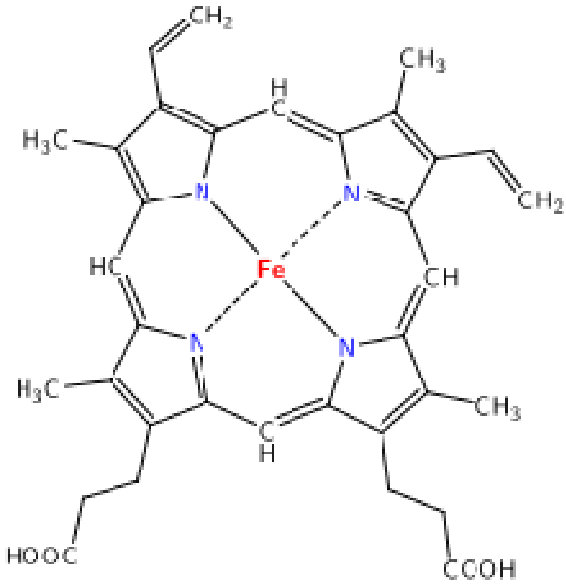


Figure 4-20 *Essential Cell Biology* (© Garland Science 2010)




CH2
CH3
H3C
H
C
N
N
CH2
HC
Fe
CH
N
N
H3C
CH3
C
H
HOOC
CCOH

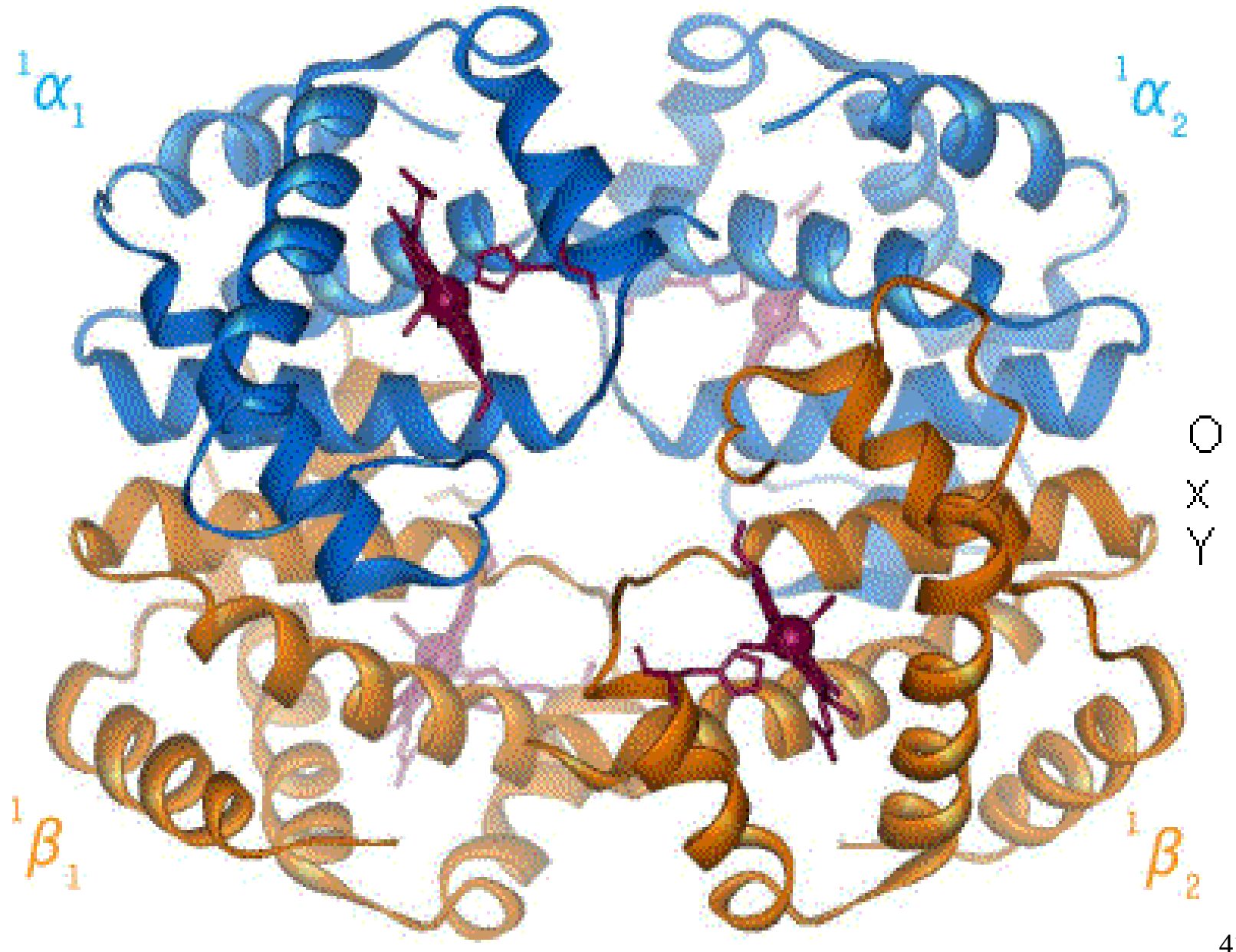

$^1\alpha_1$
$^1\alpha_2$
$^1\beta_1$
$^1\beta_2$
O
X
Y

TABLE 4–1 SOME COMMON FUNCTIONAL CLASSES OF ENZYMES

ENZYME CLASS	BIOCHEMICAL FUNCTION
Hydrolase	General term for enzymes that catalyze a hydrolytic cleavage reaction.
Nuclease	Breaks down nucleic acids by hydrolyzing bonds between nucleotides.
Protease	Breaks down proteins by hydrolyzing peptide bonds between amino acids.
Synthase	General name used for enzymes that synthesize molecules in anabolic reactions by condensing two molecules together.
Isomerase	Catalyzes the rearrangement of bonds within a single molecule.
Polymerase	Catalyzes polymerization reactions such as the synthesis of DNA and RNA.
Kinase	Catalyzes the addition of phosphate groups to molecules. Protein kinases are an important group of kinases that attach phosphate groups to proteins.
Phosphatase	Catalyzes the hydrolytic removal of a phosphate group from a molecule.
Oxido-reductase	General name for enzymes that catalyze reactions in which one molecule is oxidized while the other is reduced. Enzymes of this type are often called oxidases, reductases, or dehydrogenases.
ATPase	Hydrolyzes ATP. Many proteins with a wide range of roles have an energy-harnessing ATPase activity as part of their function, including motor proteins such as myosin and membrane transport proteins such as the sodium–potassium pump.

Enzyme names typically end in "-ase," with the exception of some enzymes, such as pepsin, trypsin, thrombin, lysozyme, and so on, which were discovered and named before the convention became generally accepted at the end of the nineteenth century. The name of an enzyme usually indicates the substrate and the nature of the reaction catalyzed. For example, citrate synthase catalyzes the synthesis of citrate by a reaction between acetyl CoA and oxaloacetate.

Table 4-1 *Essential Cell Biology* (© Garland Science 2010)

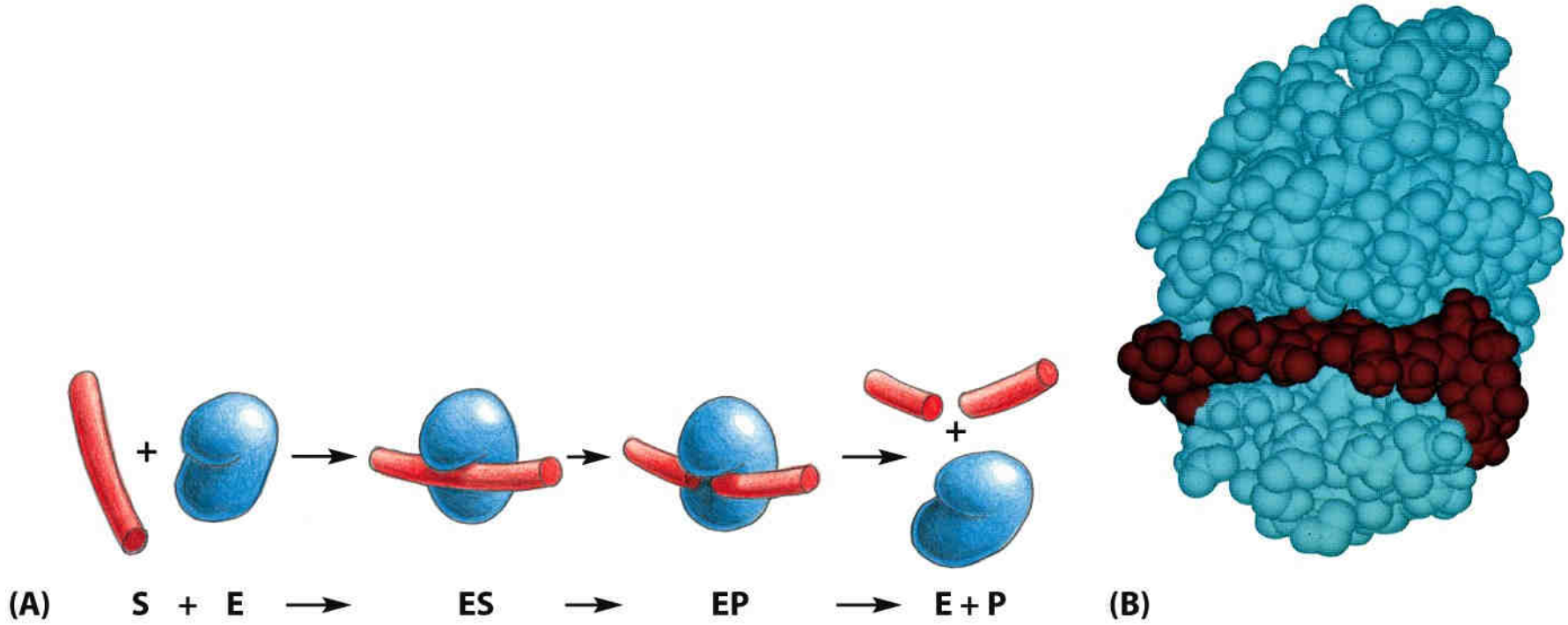


Figure 4-30 *Essential Cell Biology* (© Garland Science 2010)


zinc ion
cofactor

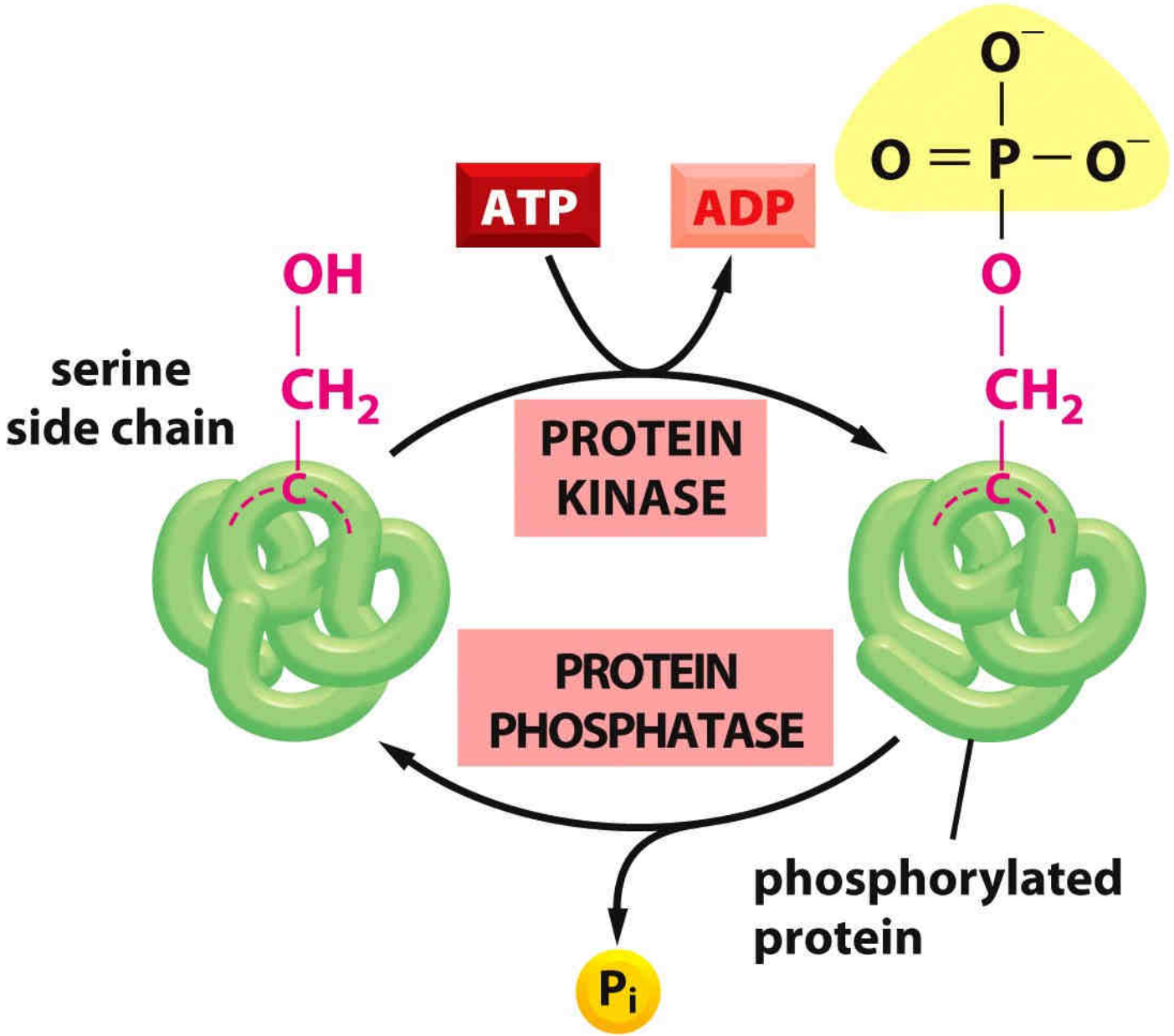


Figure 4-38a *Essential Cell Biology* (© Garland Science 2010)

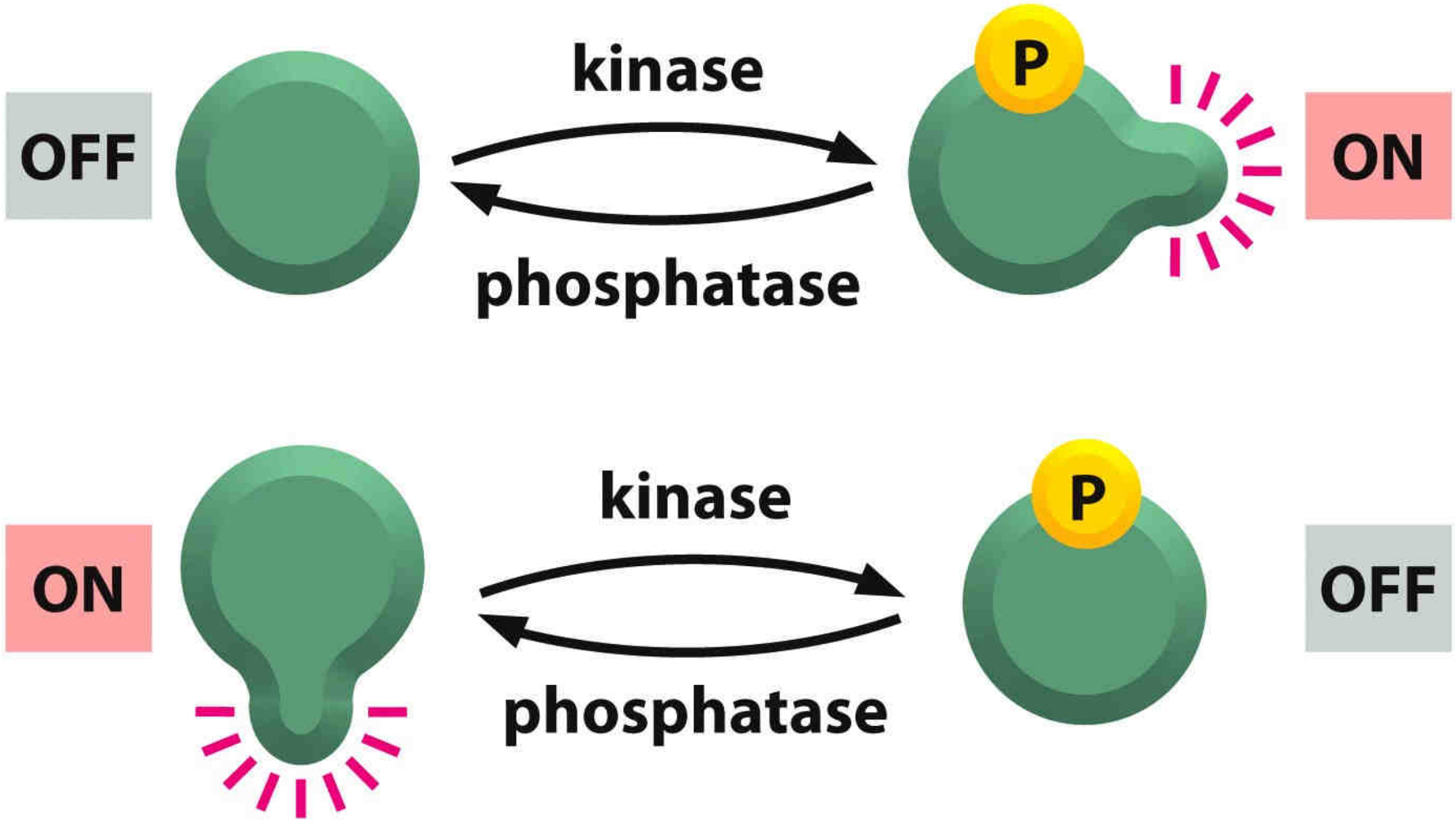


Figure 4-38b *Essential Cell Biology* (© Garland Science 2010)

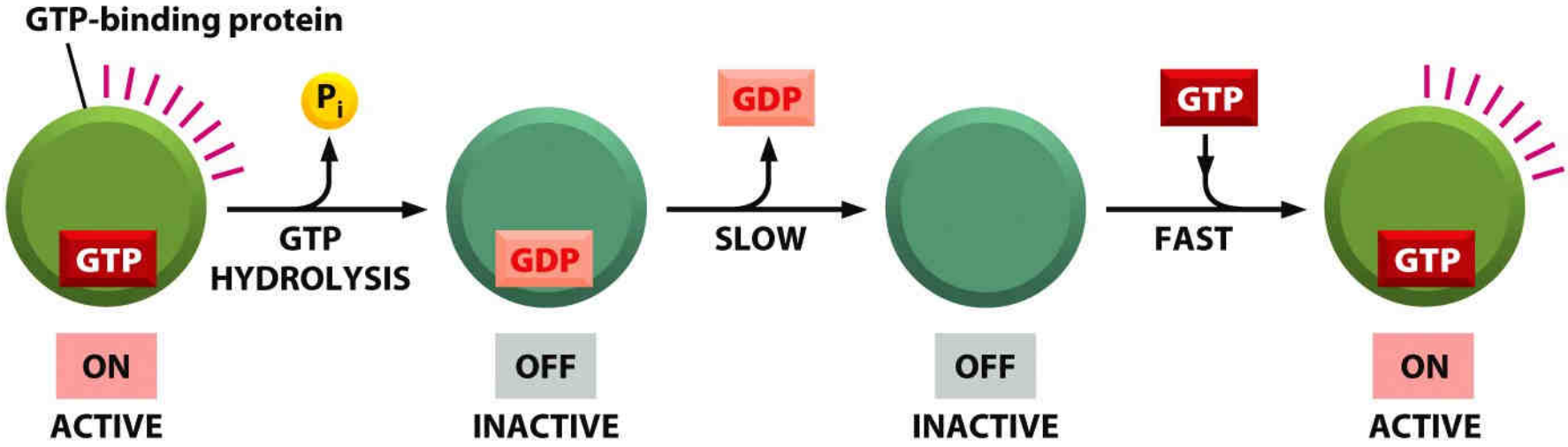


Figure 4-39 *Essential Cell Biology* (© Garland Science 2010)

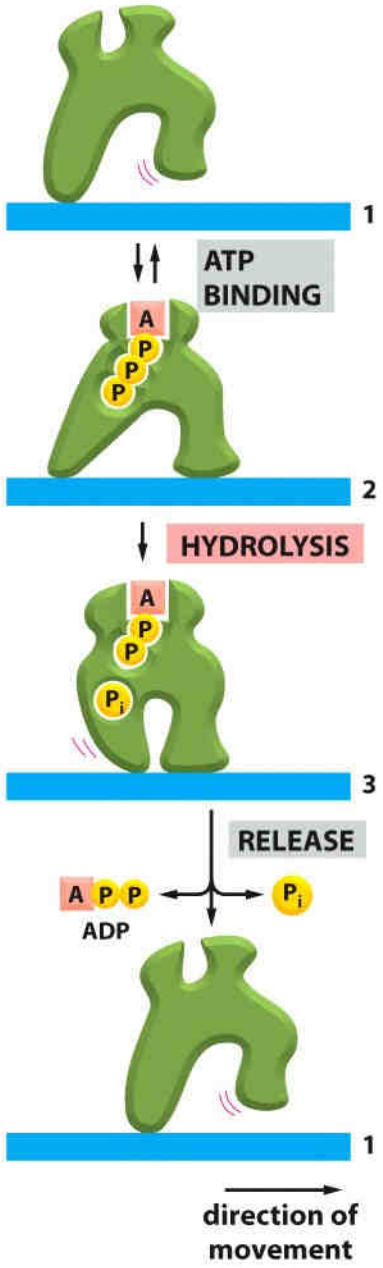


Figure 4-42 *Essential Cell Biology* (© Garland Science 2010)