Computational Biophysics: Algorithms to Applications (CS61060)

Instructor: Pralay Mitra
Email: pralay@cse.iitkgp.ac.in

Course Details

- TA
  - Ashish Malgawa
  - Suyog Shamkant Chadawar
- Lecture Hours
  - Mon (15:00 -16:55); Tue (14:00-15:55)
- Evaluation
  - TA Evaluation 30
  - Mid Semester 30
  - End Semester 40

Needless to say attendance is must.
Fall short of attendance may invoke your de-registration.

Lecture notes and materials

- Will be uploaded at

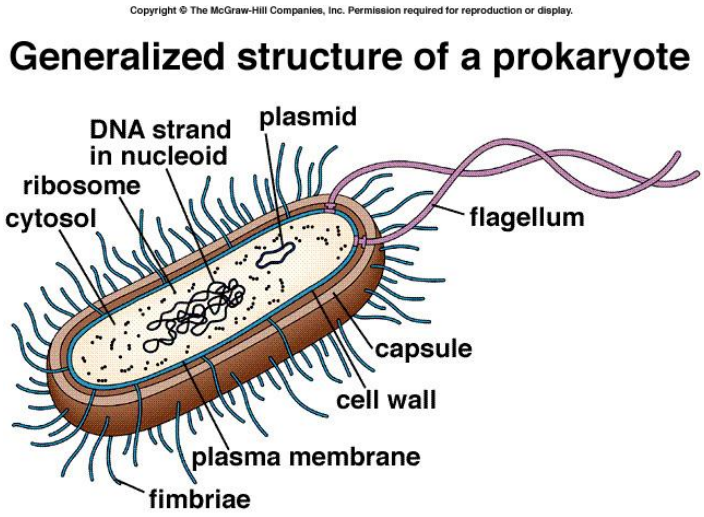
http://cse.iitkgp.ac.in/~pralay/teaching/2019S/CompBio/

References

- **Text Book:**
  1. Neil C. Jones and Pavel A. Pevzner. An Introduction to Bioinformatics Algorithms.
  2. Gary D. Stormo. Introduction to Protein-DNA Interactions: Structure, Thermodynamics, and Bioinformatics.
  3. Bruce R. Donald. Algorithms in Structural Molecular Biology (Computational Molecular Biology).
  4. Dan Gusfield. Algorithms on Strings, Trees and Sequences

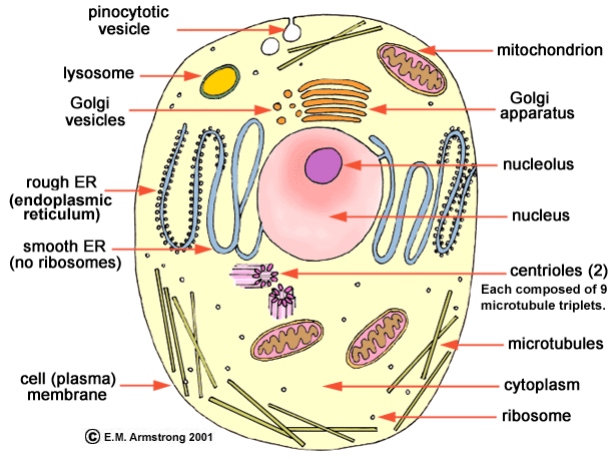
- **Literature:**
  1. Christopher M. Dobson, Andrej Sali, Martin Karplus. (1998) Protein Folding: A Perspective from Theory and Experiment. *Angewandte Chemie International Edition* 37(7):868-893.
  2. Inbal Halperin, Buyong Ma, Haim Wolfson, Ruth Nussinov. (2002) Principles of docking: An overview of search algorithms and a guide to scoring functions. *Proteins: Structure, Function, and Bioinformatics* 47(4):409-443.
  3. Joan-Emma Shea and Charles L Brooks III. (2001). From Folding Theories To Folding Proteins: A Review and Assessment of Simulation Studies of Protein Folding and Unfolding. *Annual Review of Physical Chemistry* **52**:499-535.
  4. Literature will be provided from time to time.

Prokaryotic Cell



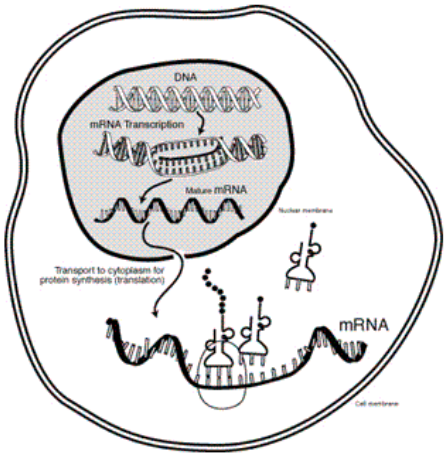
Source: http://classes.midlandstech.edu/carterp/Courses/bio101/labquiz2/prokaryote.jpg

Eukaryotic Cell



Source: http://waynesword.palomar.edu/images/animal4.gif

Central Dogma of Molecular Biology



Source: http://www.ncbi.nlm.nih.gov/Class/MLACourse/Modules/MolBioReview/central_dogma.html

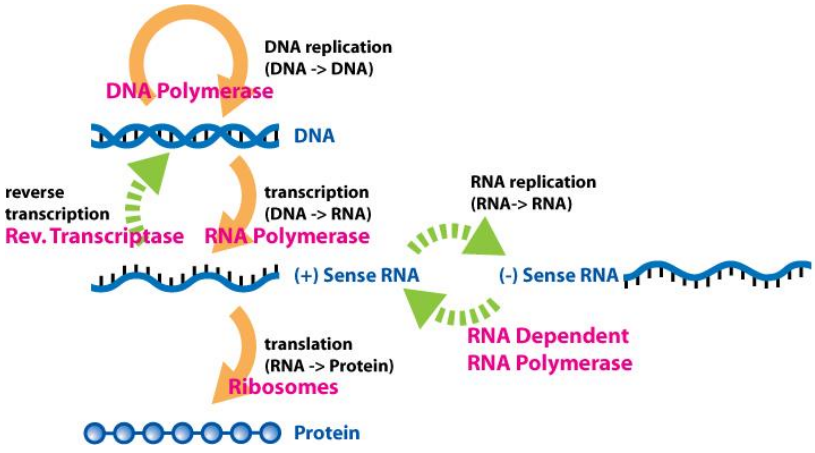
General transfers of biological sequential information

General	Special	Unknown
DNA → DNA	RNA → DNA	protein → DNA
DNA → RNA	RNA → RNA	protein → RNA
RNA → protein	DNA → protein	protein → protein

General transfers of biological sequential information

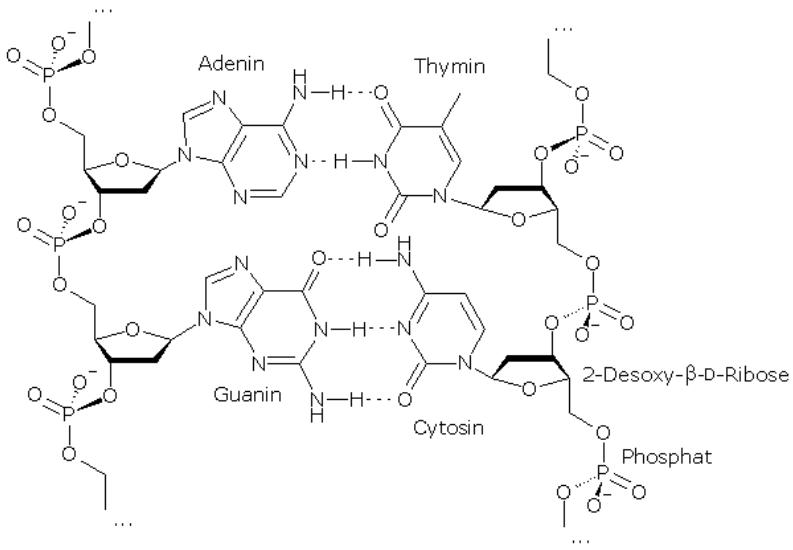
General	Special	Unknown
DNA → DNA (DNA replication)	RNA → DNA (reverse transcription)	protein → DNA
DNA → RNA (transcription)	RNA → RNA (RNA replication)	protein → RNA
RNA → protein (translation)	DNA → protein (direct translation)	protein → protein

Central Dogma with Enzymes

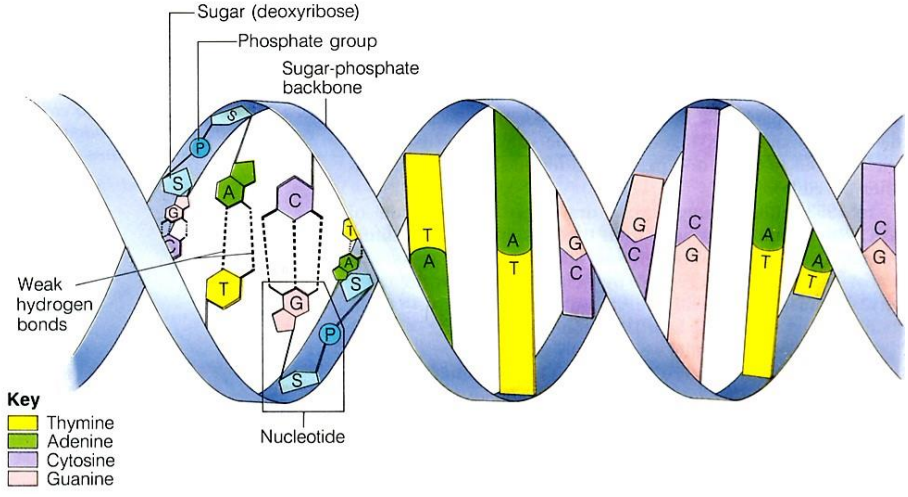


Source: http://en.wikipedia.org/wiki/File:Extended_Central_Dogma_with_Enzymes.jpg

DNA Structure

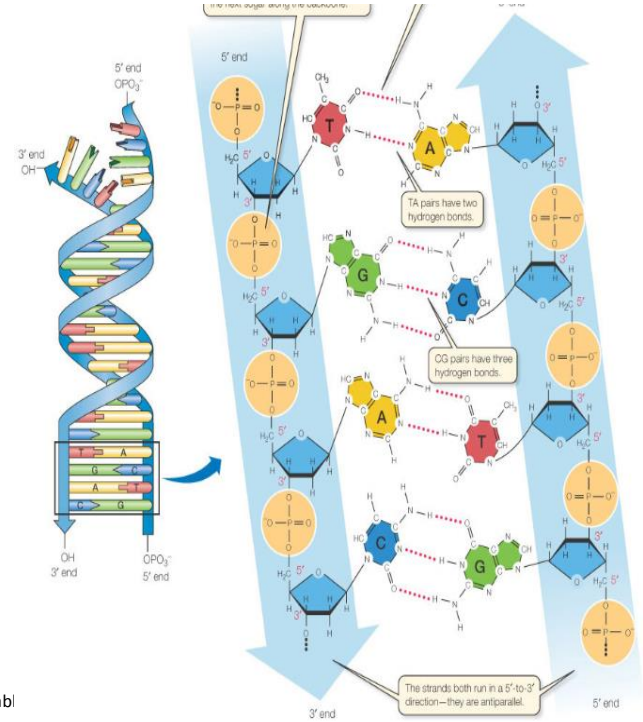


DNA Structure



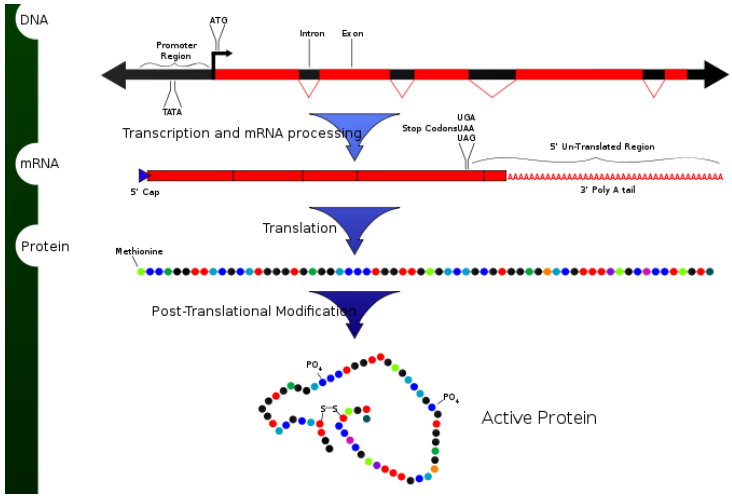
Source: http://karimedalla.files.wordpress.com/2012/11/dna-structure.jpg

DNA Structure



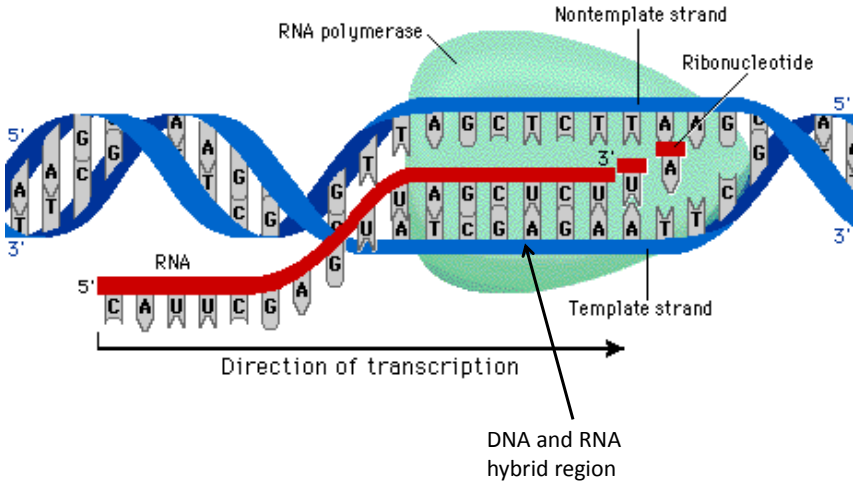
Source: http://www.nature.com/scitabl

Central Dogma of Molecular Biology: Eukaryotic Model



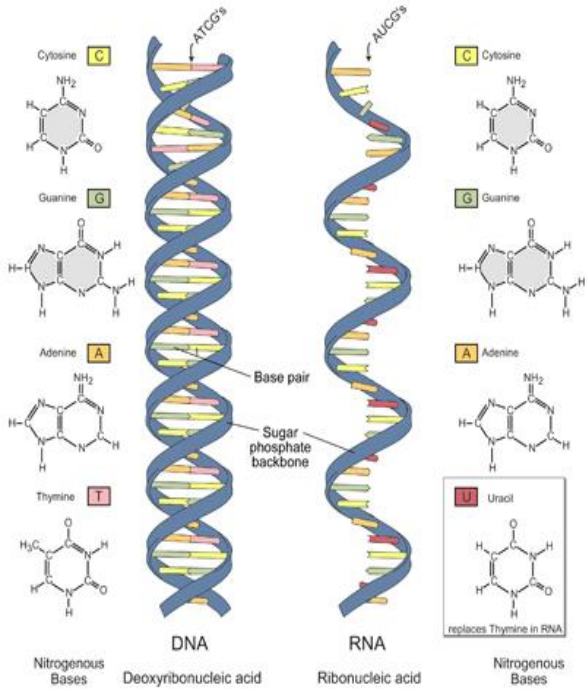
Source: http://en.wikipedia.org/wiki/File:Cdmb.svg

Transcription

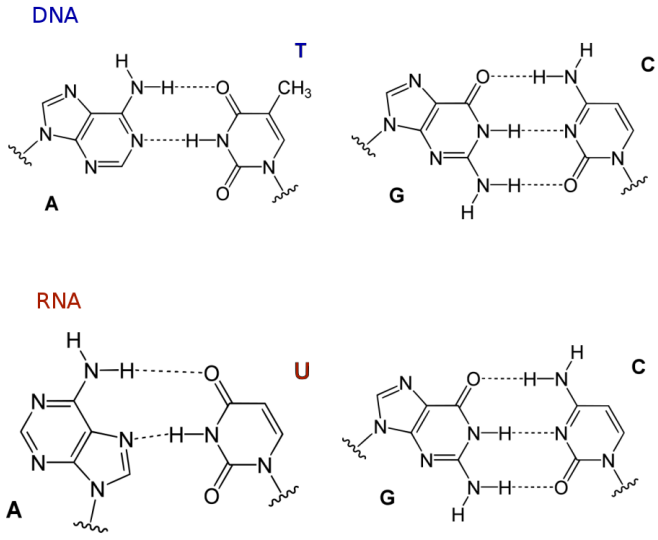


Source: http://www.phschool.com/science/biology_place/biocoach/images/transcription/startrans.gif

DNA vs RNA

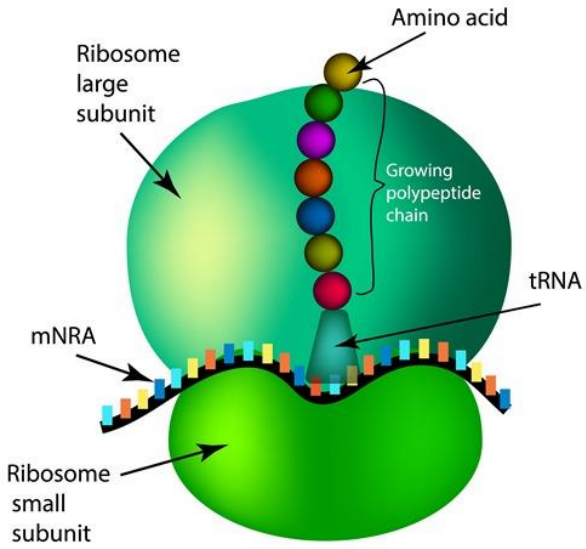


Base Pairs

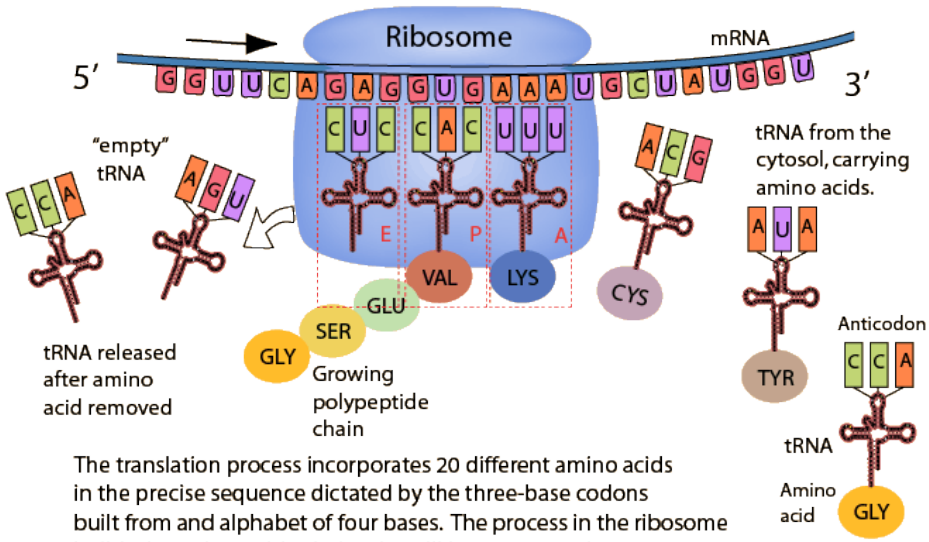


Source: http://andromeda.rut

Ribosome



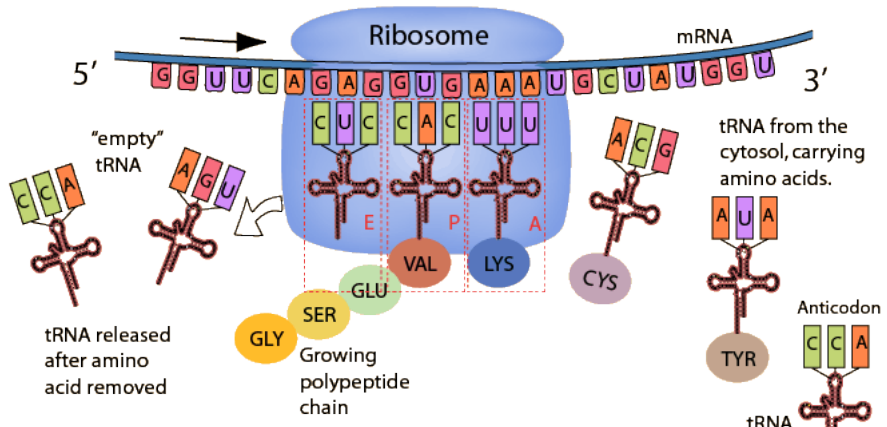
Translation



The translation process incorporates 20 different amino acids in the precise sequence dictated by the three-base codons built from and alphabet of four bases. The process in the ribosome builds the polypeptide chains tha will become proteins.

Source: http://hyperphysics.phy-astr.gsu.edu/hbase/organic/imgorg/translation2.gif

Translation



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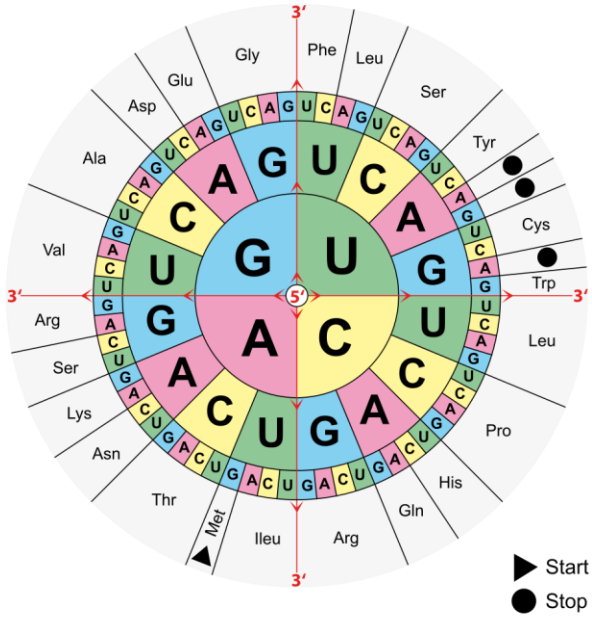
Source: http://hyperphysics.phy-astr.gsu.edu/hbase/organic/imgorg/translation2.gif

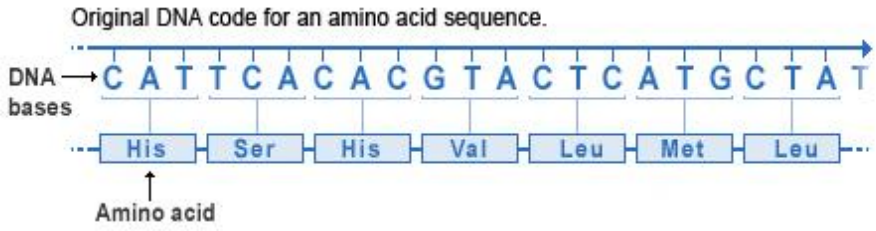
CODON WHEEL



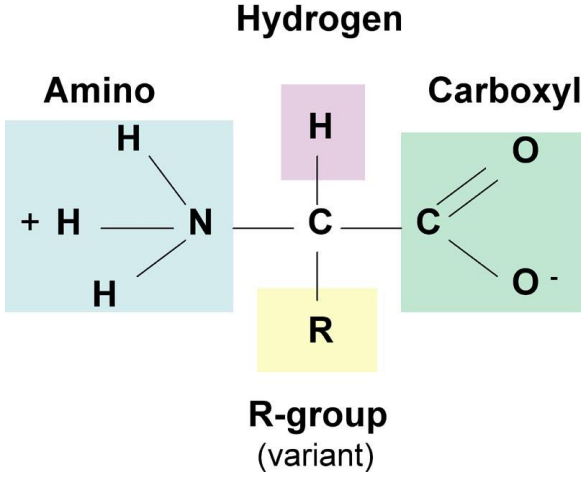
Essential Amino Acids

Amino Acid	3-Letter Code	1-Letter Code
Alanine	Ala	A
Cysteine	Cys	C
Aspartic acid or aspartate	Asp	D
Glutamic acid or glutamate	Glu	E
Phenylalanine	Phe	F
Glycine	Gly	G
Histidine	His	H
Isoleucine	Ile	I
Lysine	Lys	K
Leucine	Leu	L
Methionine	Met	M
Asparagine	Asn	N
Proline	Pro	P
Glutamine	Gln	Q
Arginine	Arg	R
Serine	Ser	S
Threonine	Thr	T
Valine	Val	V
Tryptophan	Trp	W
Tyrosine	Tyr	Y

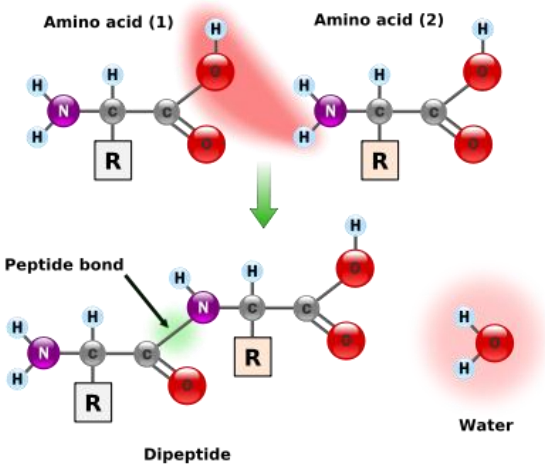
Protein Sequence



Amino Acid Structure

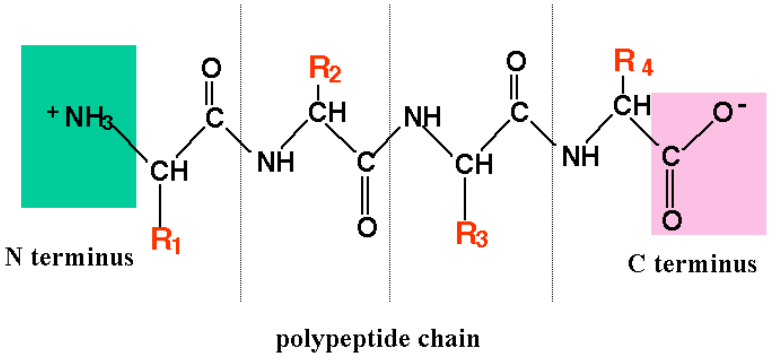


Peptide Bond Formation



Peptide

Peptide = chain of amino acids



Essential Amino Acids

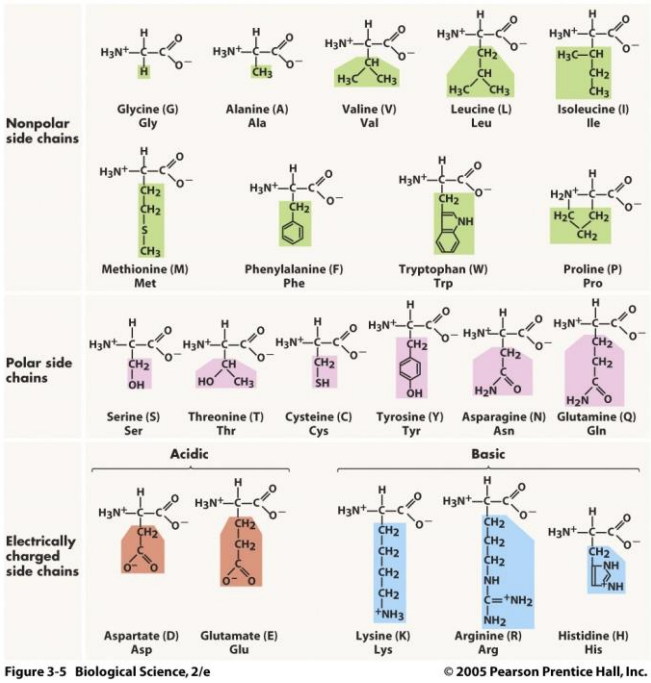
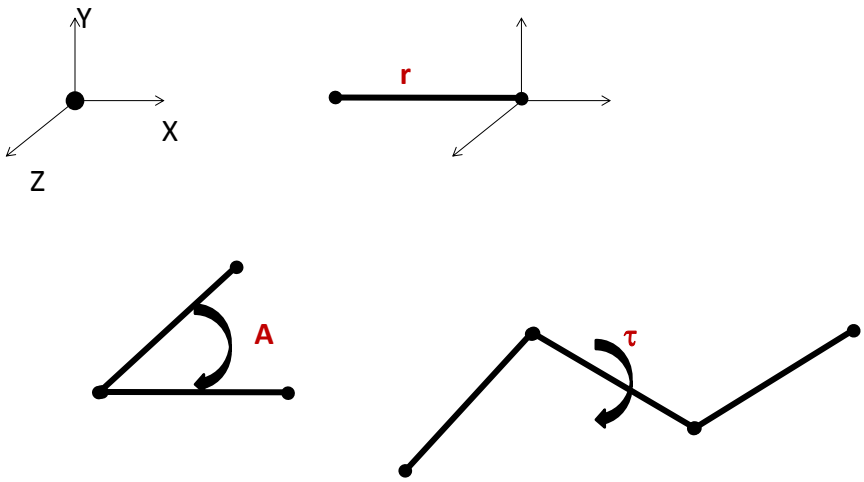


Figure 3-5 Biological Science, 2/e

Point, Line, Angle, Torsional Angle



Peptide

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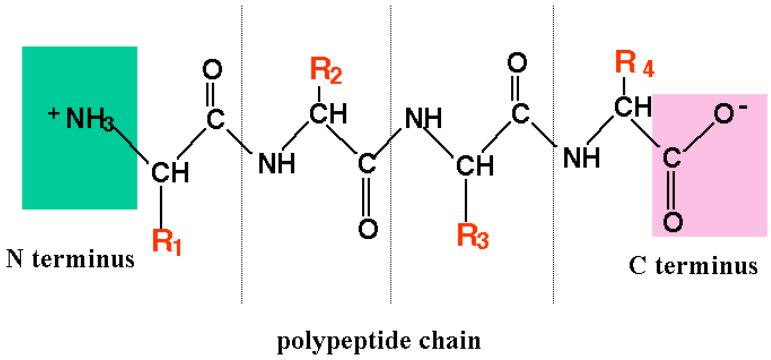
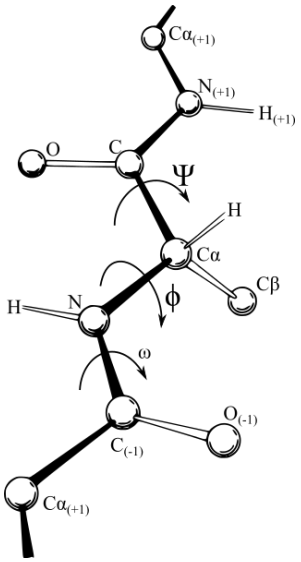
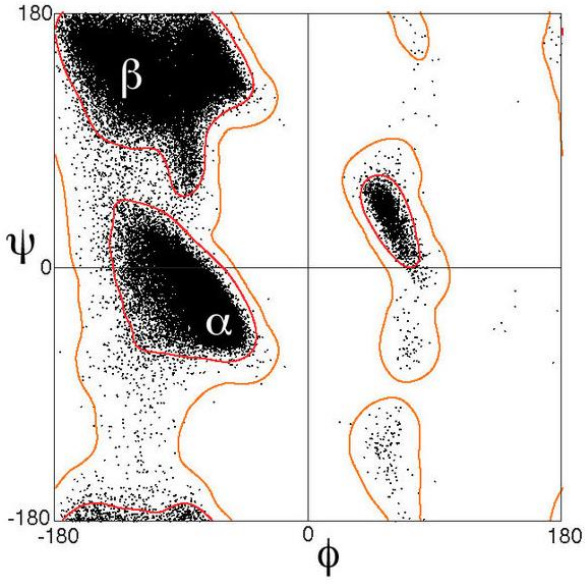


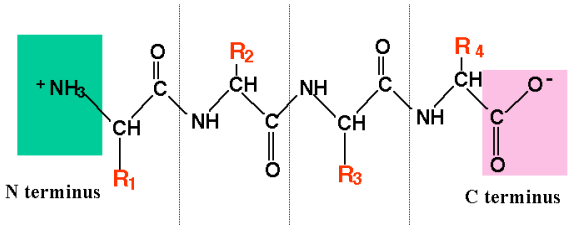
Protein Backbone



Ramachandran Plot



Bonds, Angles and Dihedral Angles



N	11.751	37.846	29.016
CA	**12.501**	**39.048**	**28.539**
C	13.740	38.628	27.754
N	14.235	39.531	26.906
CA	**15.552**	**39.410**	**26.282**
C	16.616	38.913	27.263
N	16.789	39.630	28.369
CA	**17.791**	**39.281**	**29.375**
C	17.598	37.844	29.863
N	16.368	37.519	30.261
CA	**16.004**	**36.186**	**30.742**
C	16.371	35.097	29.741

Homework

Write down a pseudo-code to parse the coordinate file and output the torsional angles.