Computational Biophysics: Algorithms to Applications (CS61060)

Instructor: Pralay Mitra

Email: pralay@cse.iitkgp.ac.in

Course Details

- TA
  - Purnima Gautam (purnimagautam94[at]gmail[dot]com)
  - Shruti Agrawal (shrutiag23@kgpian.iitkgp.ac.in)
  - Suman Kumar Bera (skbera4@kgpian.iitkgp.ac.in)
- Lecture Hours
  - Mon (12:00 -12:55); Tue (10:00-11:55); Thu (08:00-08:55)
- Evaluation
  - TA Evaluation 30
  - Mid Semester 30
  - End Semester 40

Lecture notes and materials

- Will be uploaded at

https://moodlecse.iitkgp.ac.in/moodle/

Login to CSE Moodle. Join to the course

CBP_2024S as Student with enrolment key CBP2024S

Course Coverage

Bioinformatics Topics:

1. Sequence alignment and comparison
2. Secondary structure prediction
3. Structure alignment
4. Protein folding
5. Protein docking
6. Protein Design

PCB Topics:

1. Protein and DNA structure

CS Topics:

1. Dynamic programming
2. Sequencing and Strings
3. Molecular surface
4. Simulation techniques
5. Relevant topics from ML and DL

Tutorials:

1. Databases and their usages
2. PDB file format
3. Rasmol, Pymol;
4. NW, SW, BLAST
5. PSIPred/PSSPred, DSSP, STRIDE
6. NACCESS
7. TM-align, TM-Score
8. Folding and Docking software

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:**

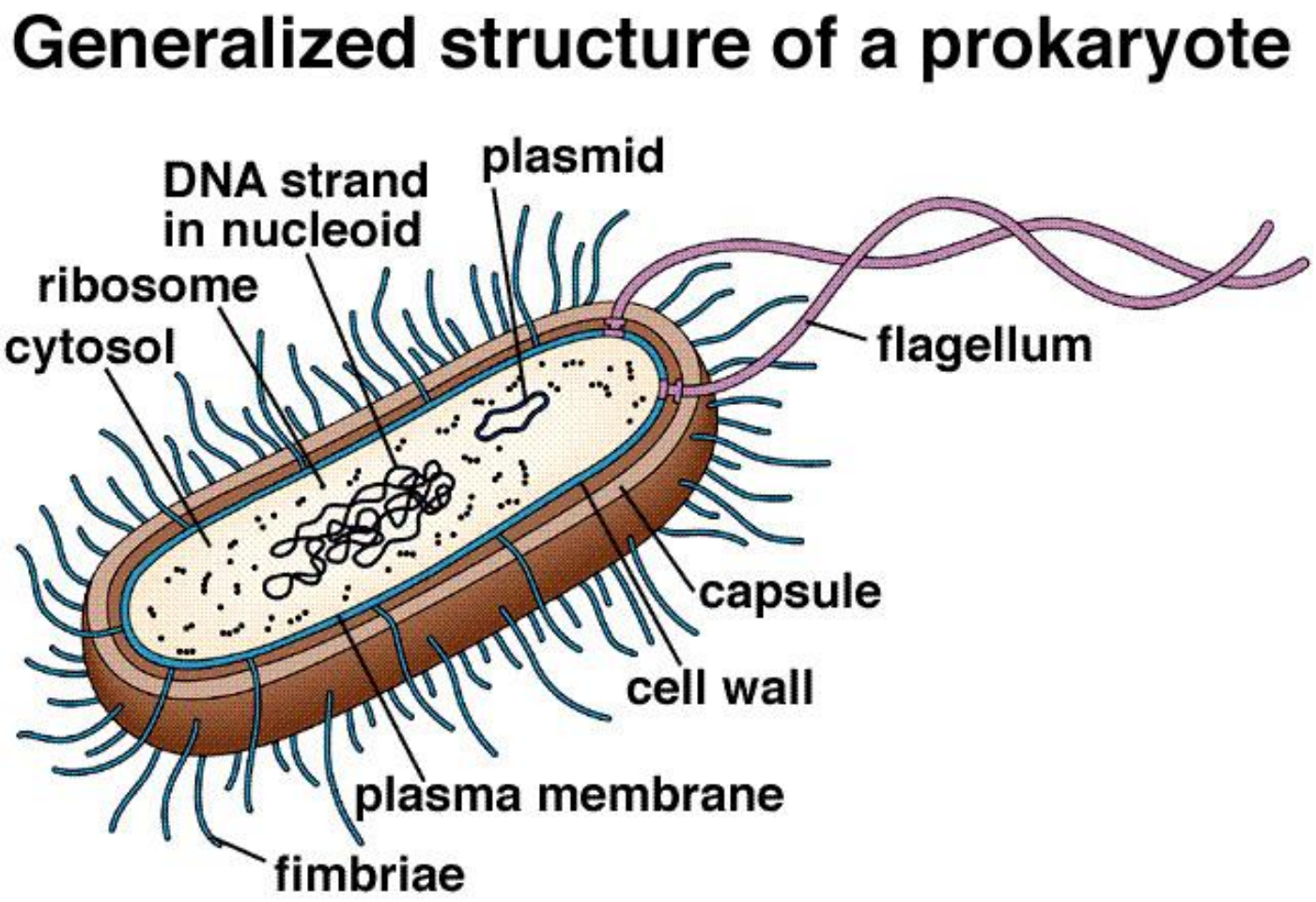
1. Christopher M. Dobson, Andrej Sali, Martin Karplus. (1998) Protein Folding: A Perspective from Theory and Experiment. *Angewandte Chemie International Edition* 37(7):868-893.

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.

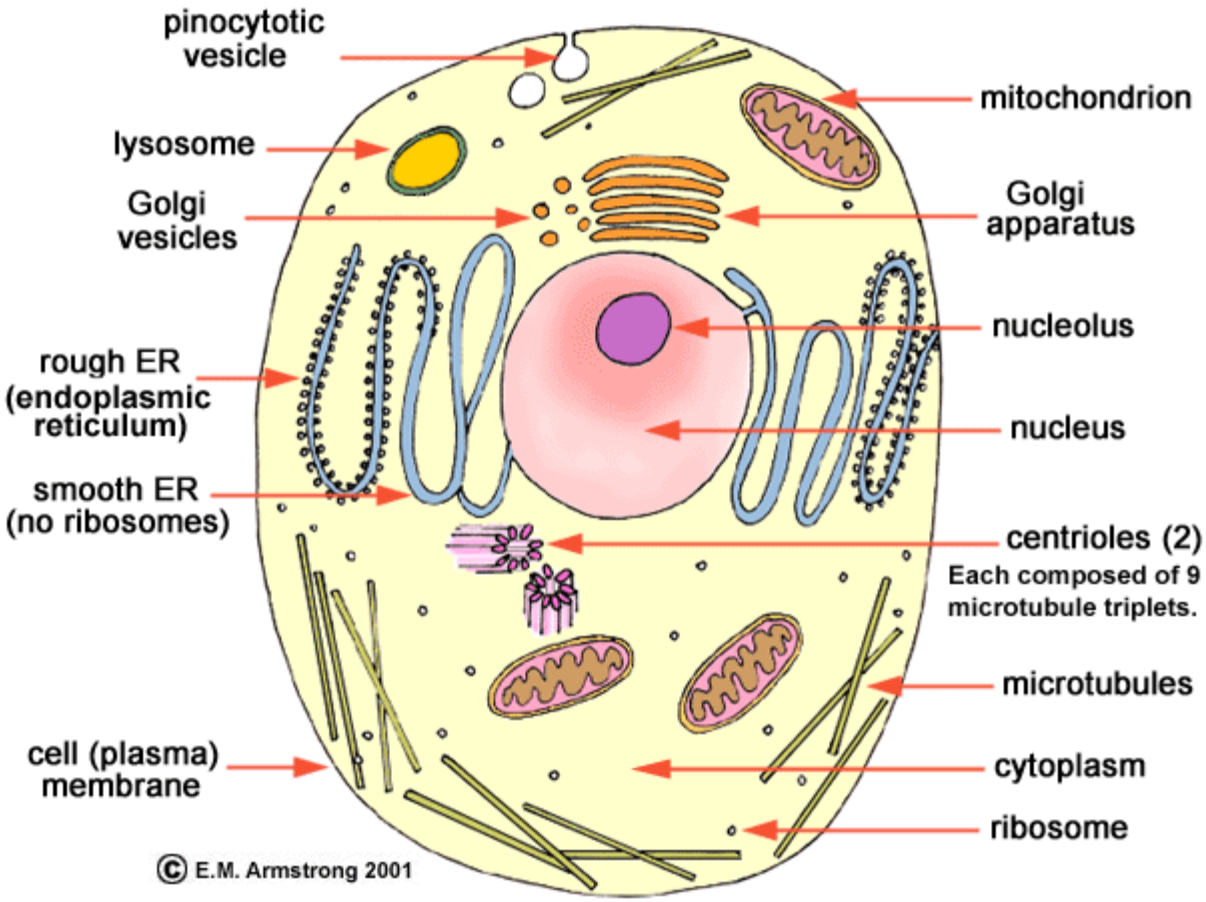
4. Literature will be provided from time to time.

Prokaryotic Cell



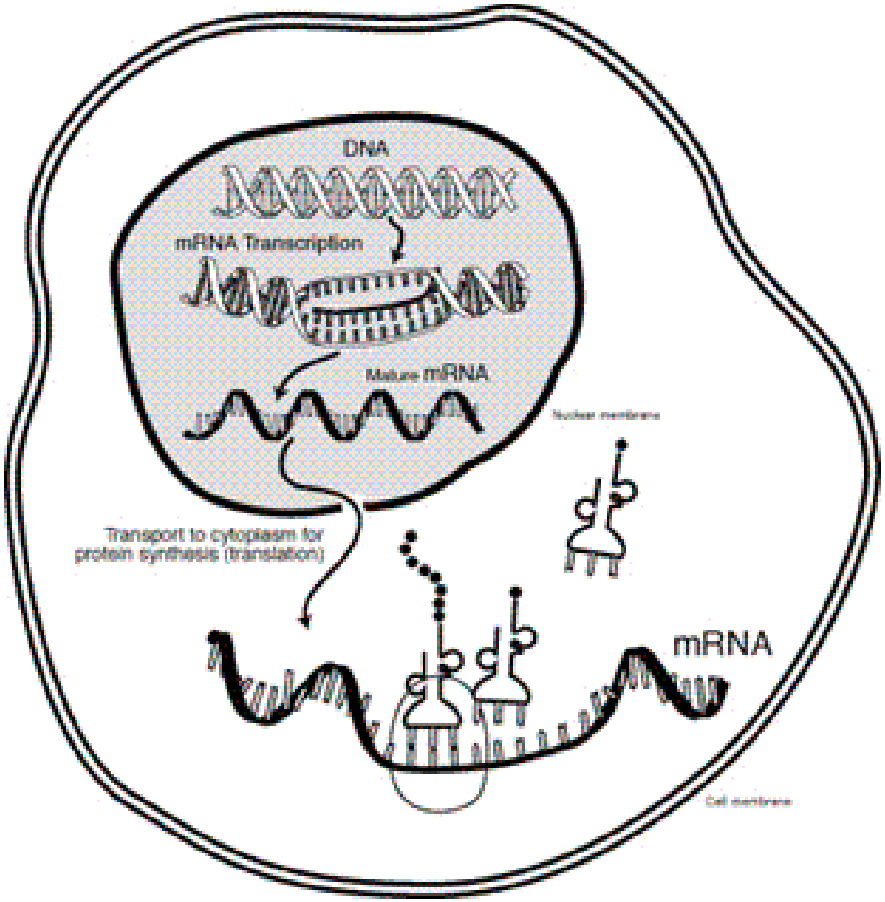
Source: http://classes.midlandstech.edu/carterp/Courses/bio101/labquiz2/prokaryote.jpg

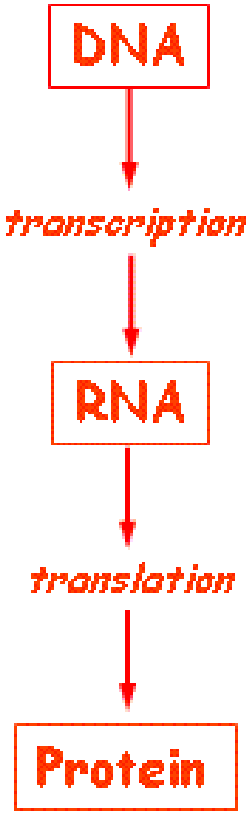
Eukaryotic Cell



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

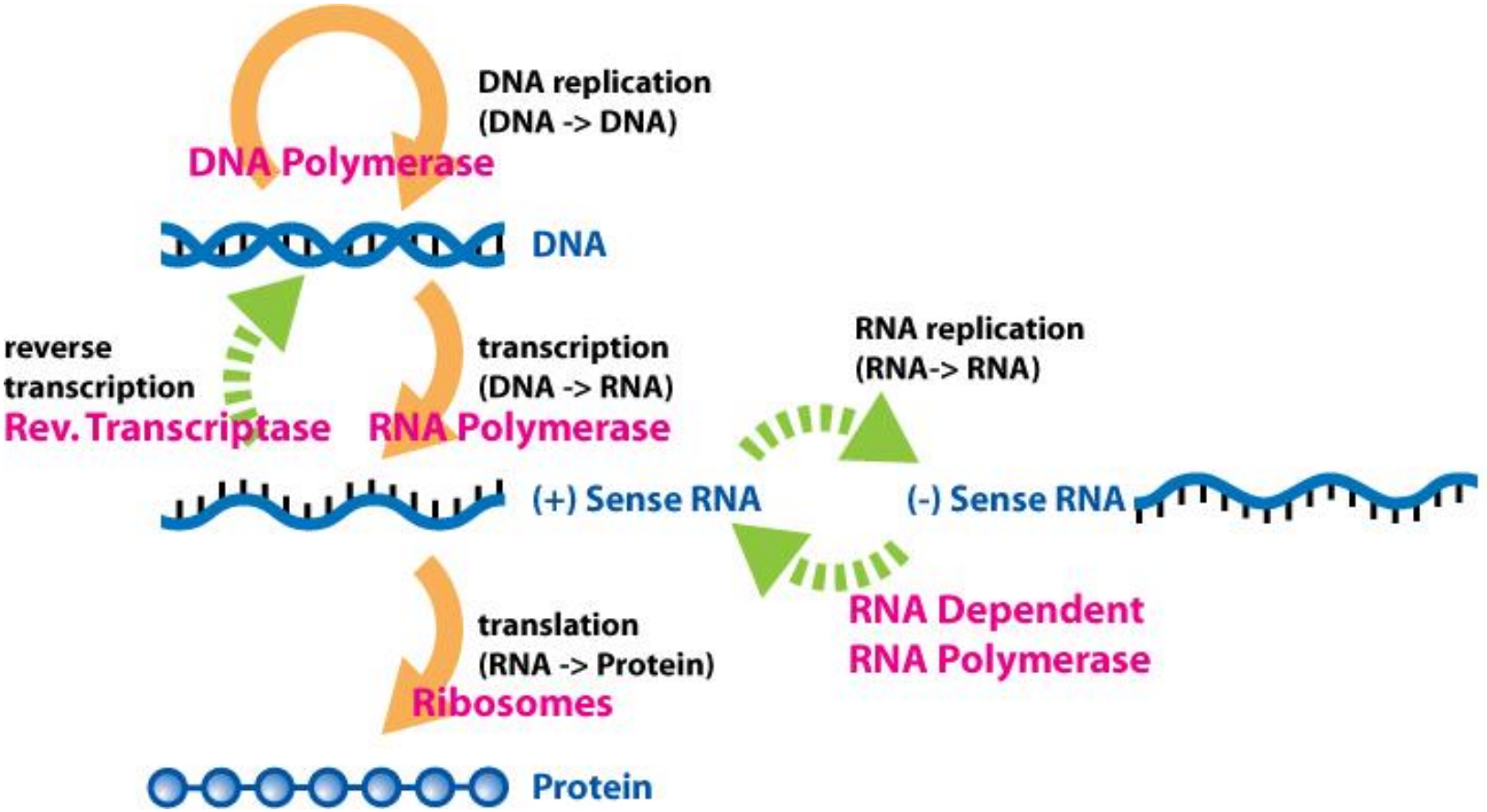
General transfers of biological sequential information

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

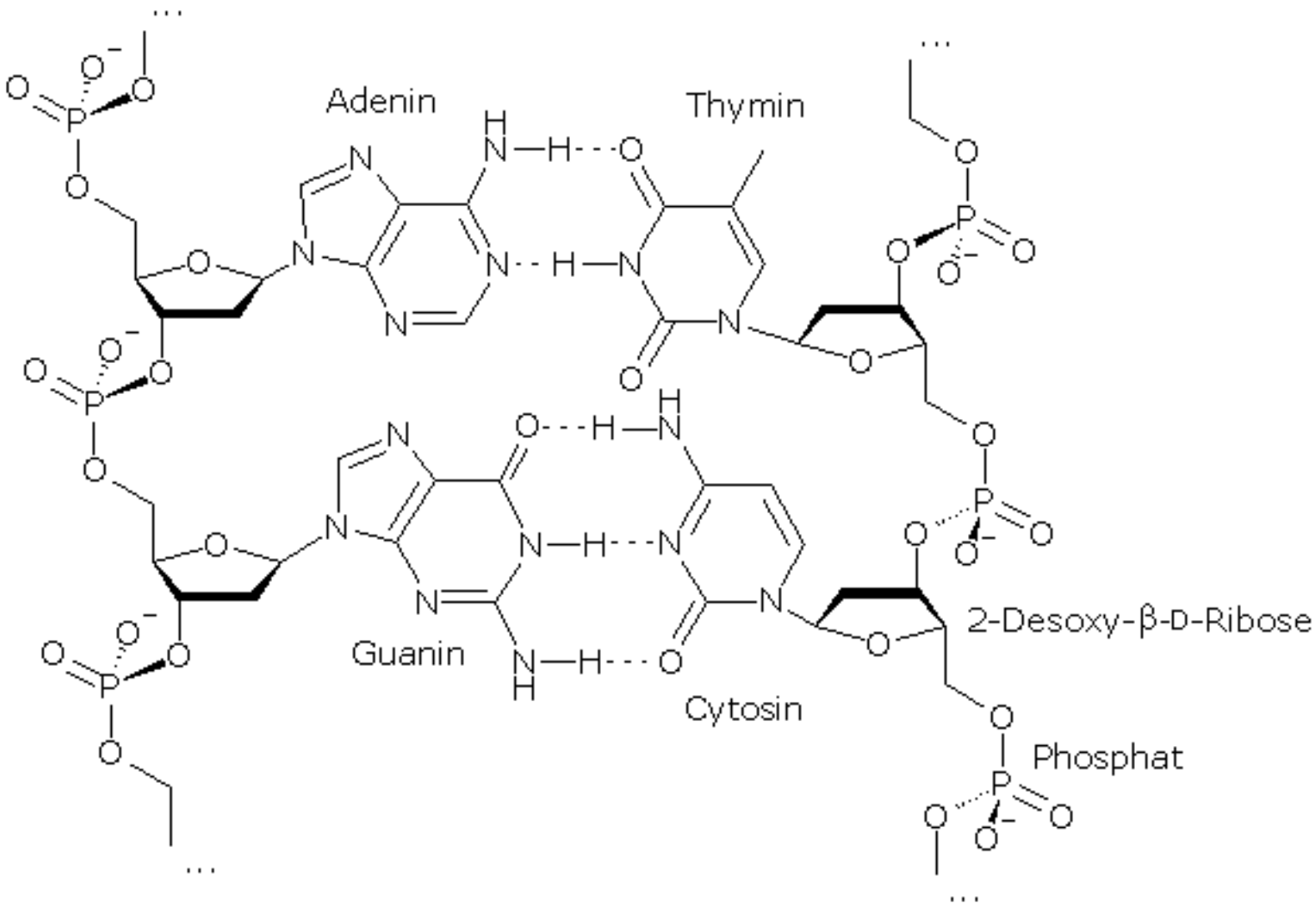
General	Special	Unknown
DNA → DNA (DNA replication)	RNA → DNA (reverse transcription)	protein → DNA
DNA → RNA (transcription)	RNA → RNA (RNA replication)	protein → RNA
RNA → protein (translation)	DNA → protein (direct translation)	protein → protein

Central Dogma with Enzymes

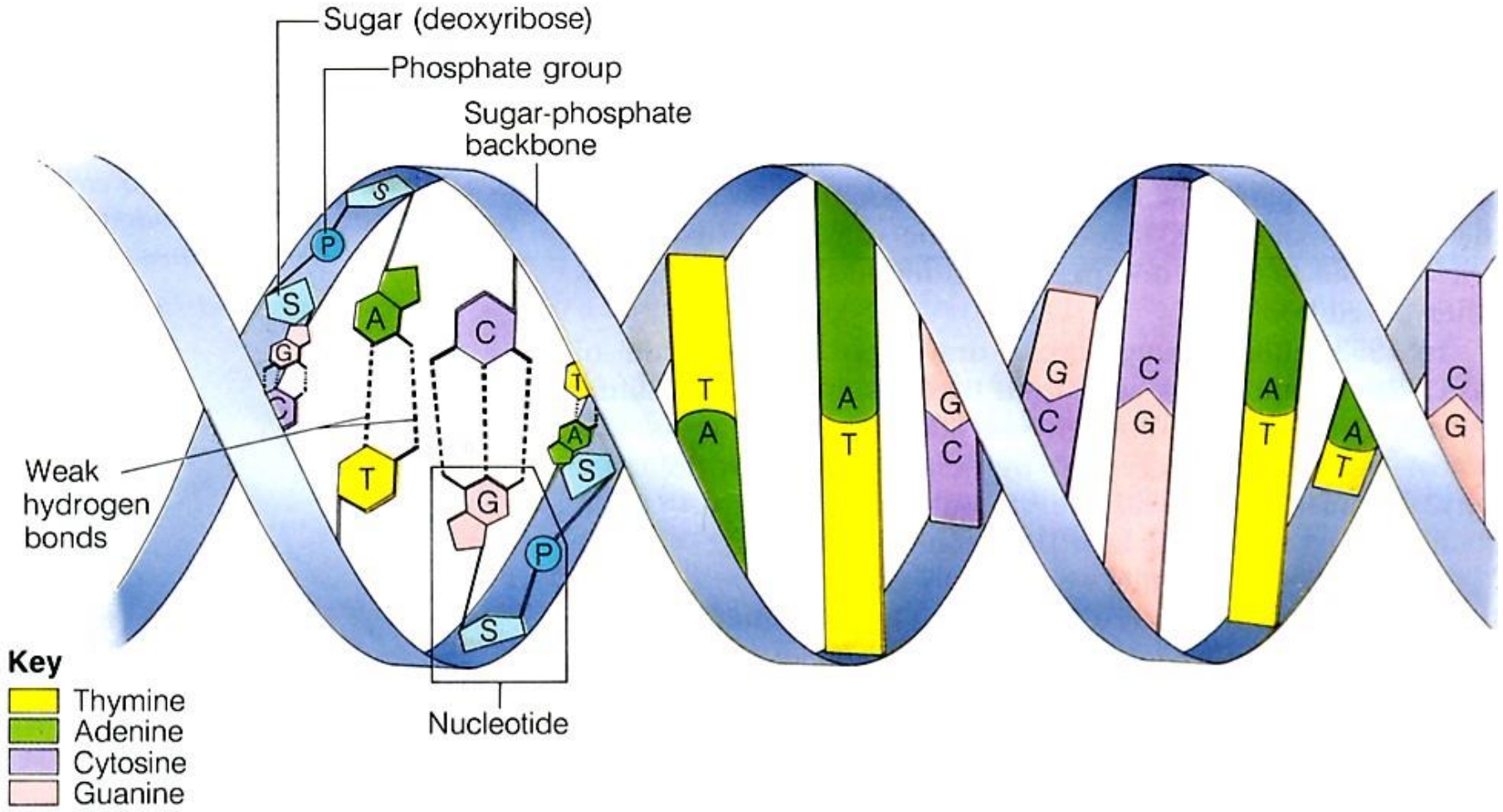


Source: http://en.wikipedia.org/wiki/File:Extended_Central_Dogma_with_Enzymes.jpg

DNA Structure

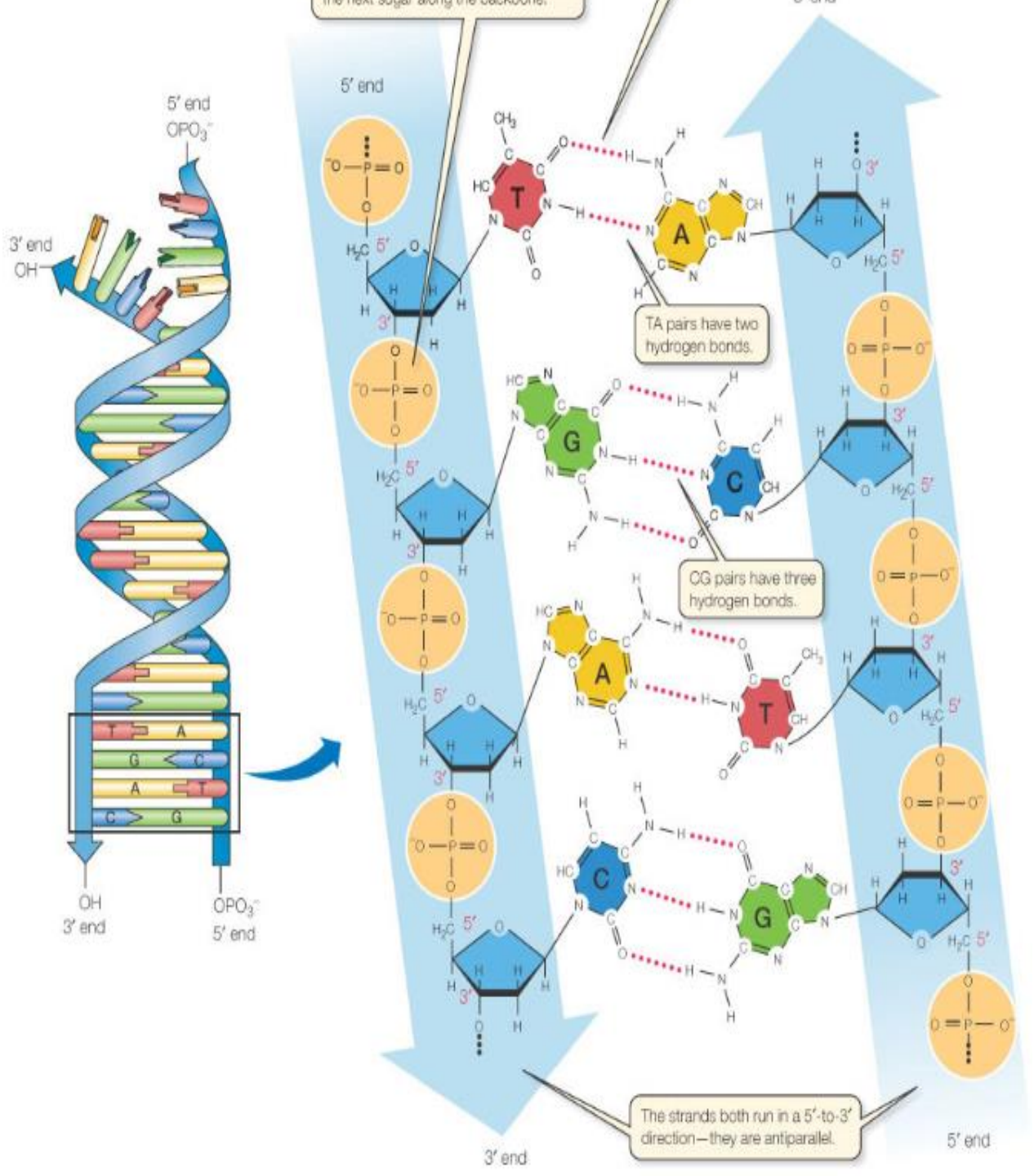


DNA Structure



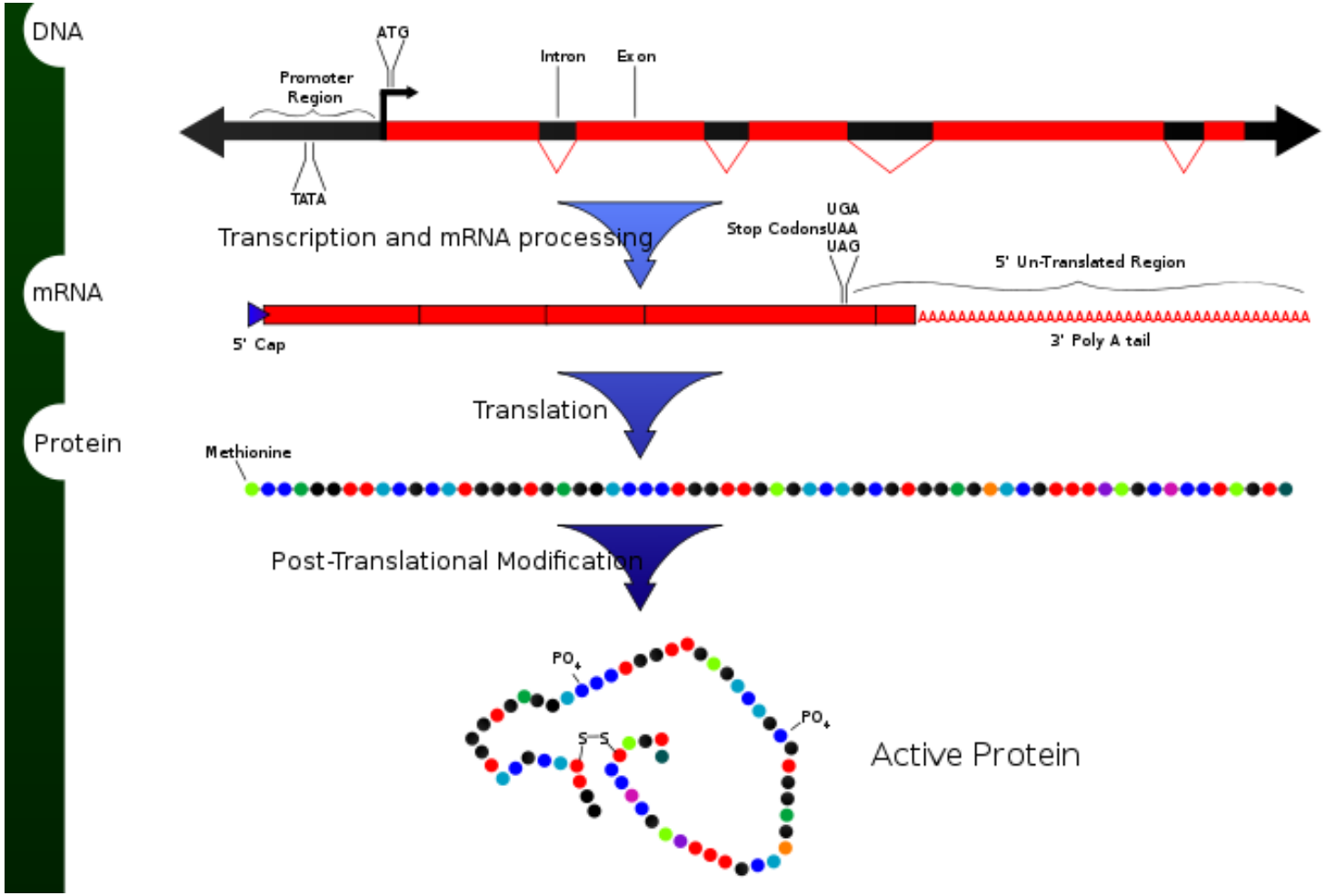
Source: http://karimedalla.files.wordpress.com/2012/11/dna-structure.jpg

DNA Structure



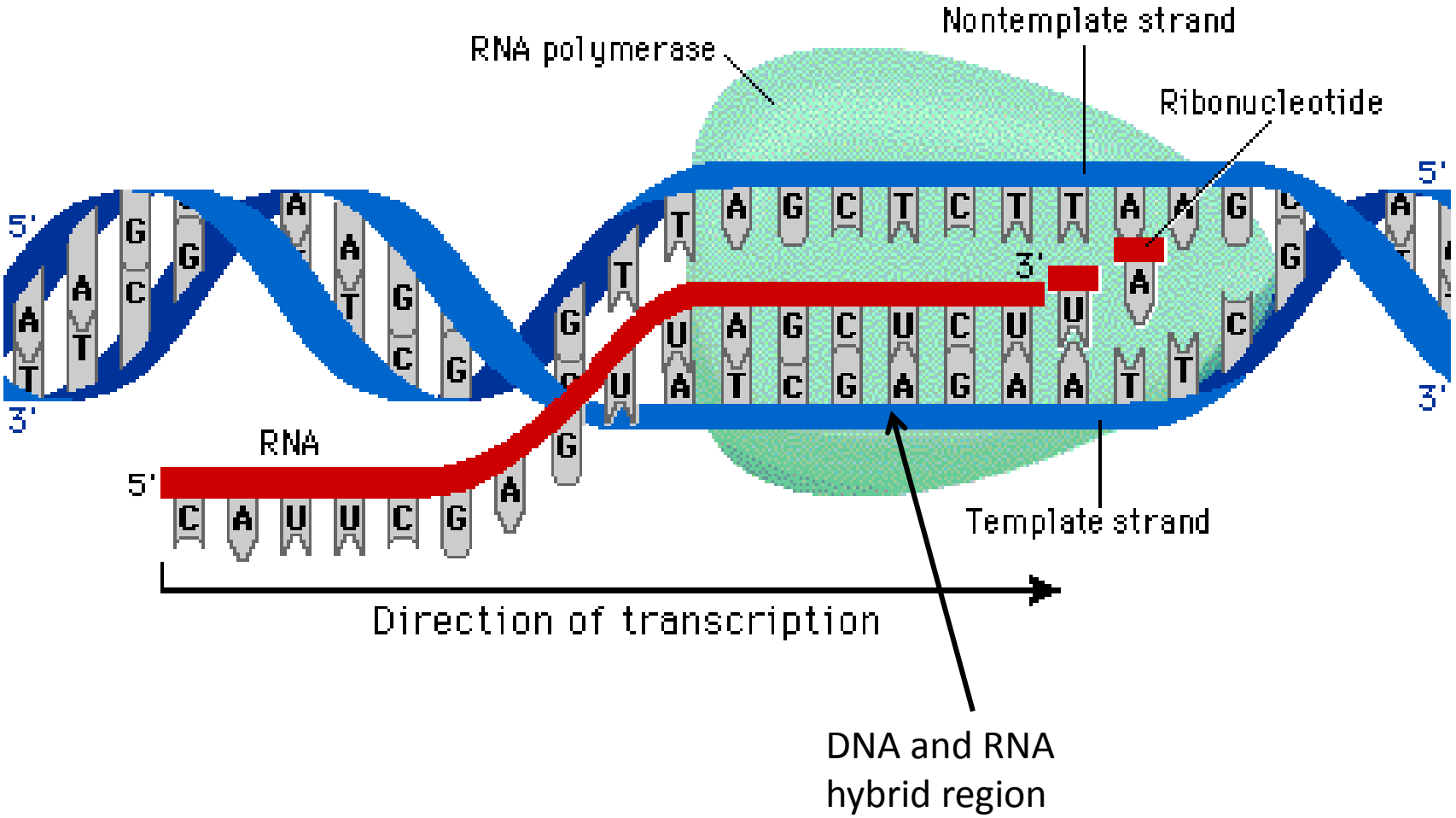
Source: http://www.nature.com/scitab

Central Dogma of Molecular Biology: Eukaryotic Model



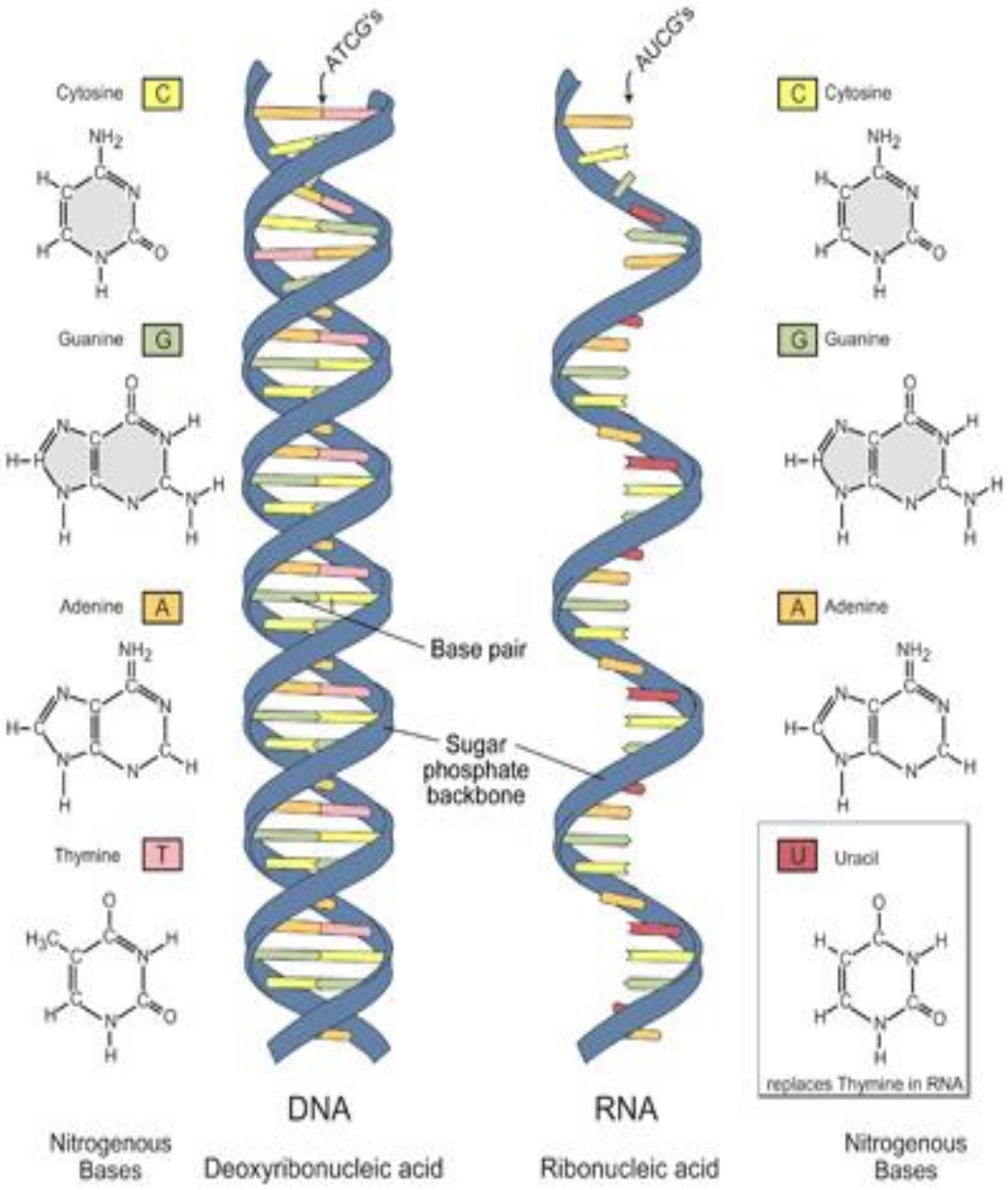
Source: http://en.wikipedia.org/wiki/File:Cdmb.svg

Transcription

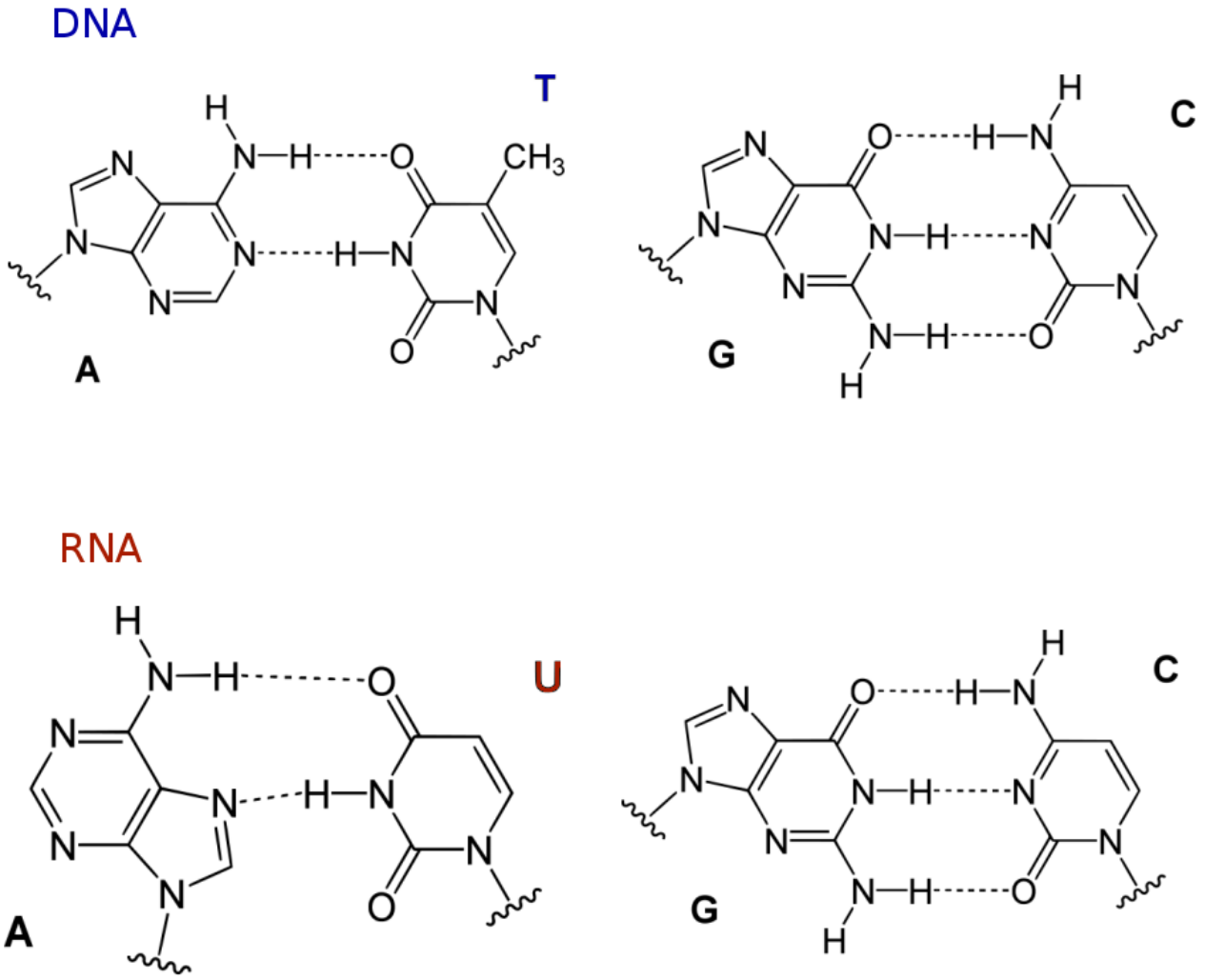


Source: http://www.phschool.com/science/biology_place/biocoach/images/transcription/startrans.gif

DNA vs RNA

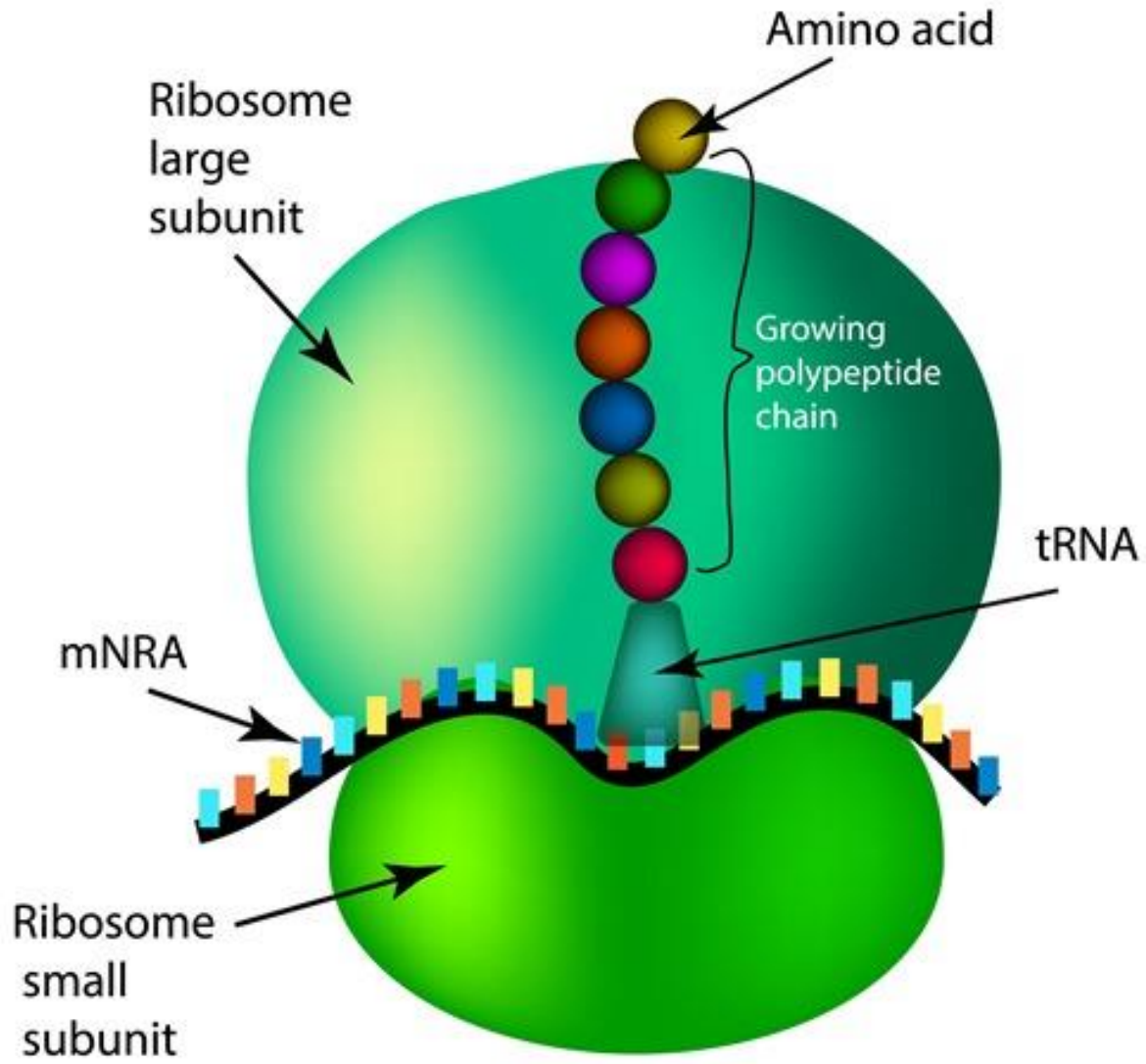

ATCG's
AUCG's
Cytosine
C
Guanine
G
Adenine
A
Thymine
T
Base pair
Sugar phosphate backbone
DNA
Deoxyribonucleic acid
RNA
Ribonucleic acid
Nitrogenous Bases
Uracil
U
replaces Thymine in RNA
Nitrogenous Bases

Base Pairs

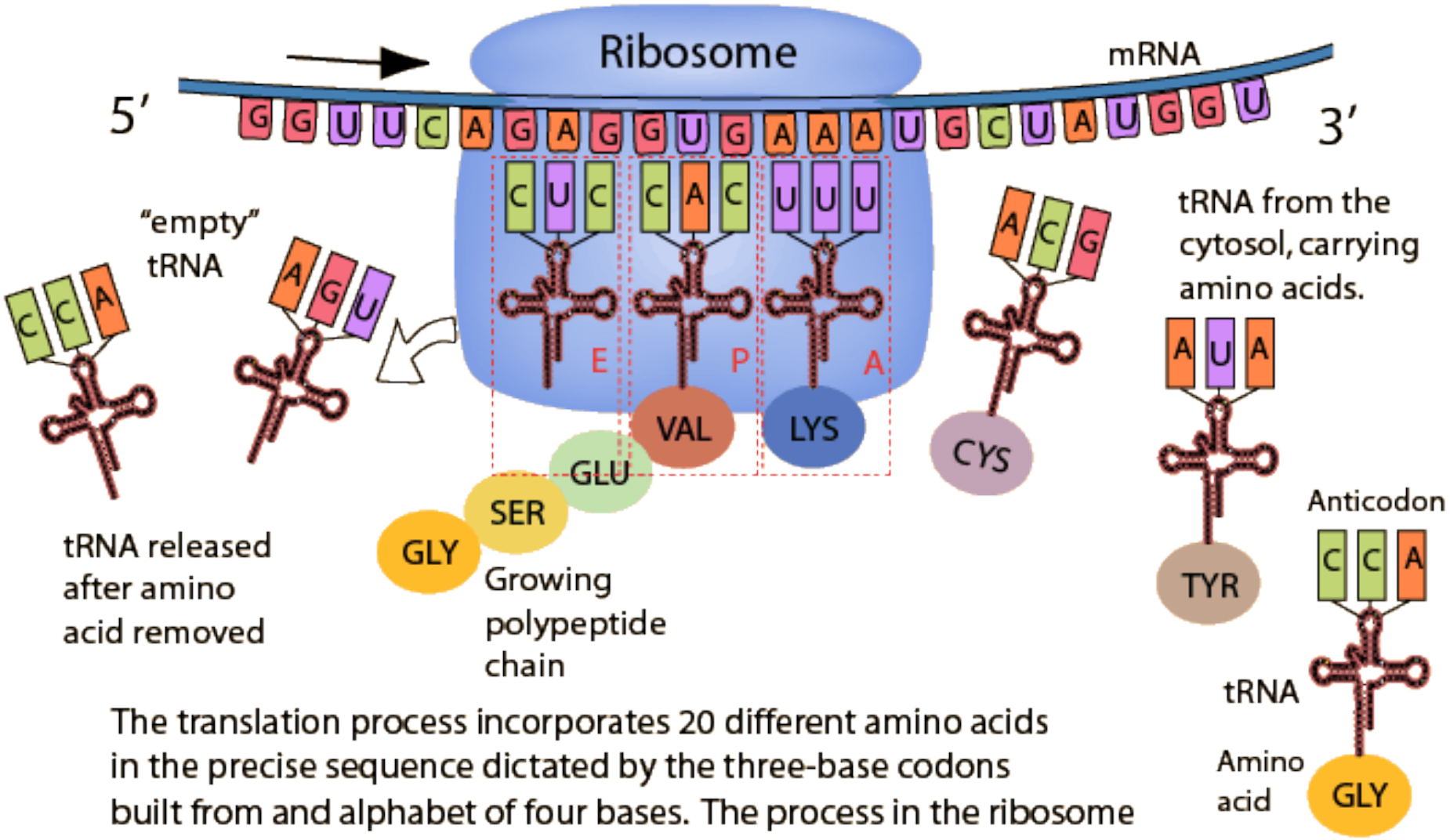


Source: http://andromeda.rutgers.edu/~huskey/images/base_pairs1_w.png

Ribosome


Amino acid
Ribosome large subunit
Growing polypeptide chain
tRNA
mNRA
Ribosome small subunit

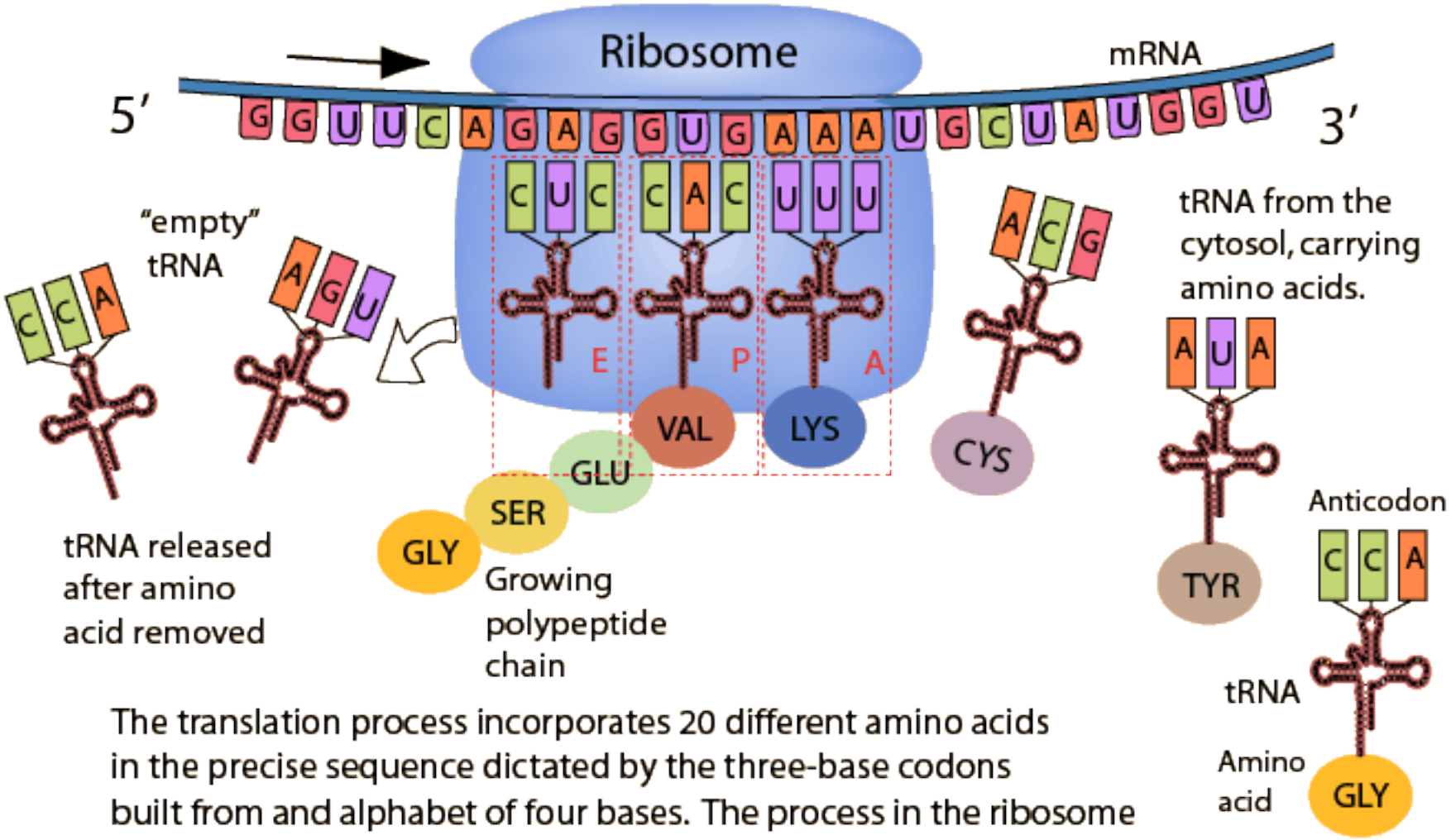
Translation



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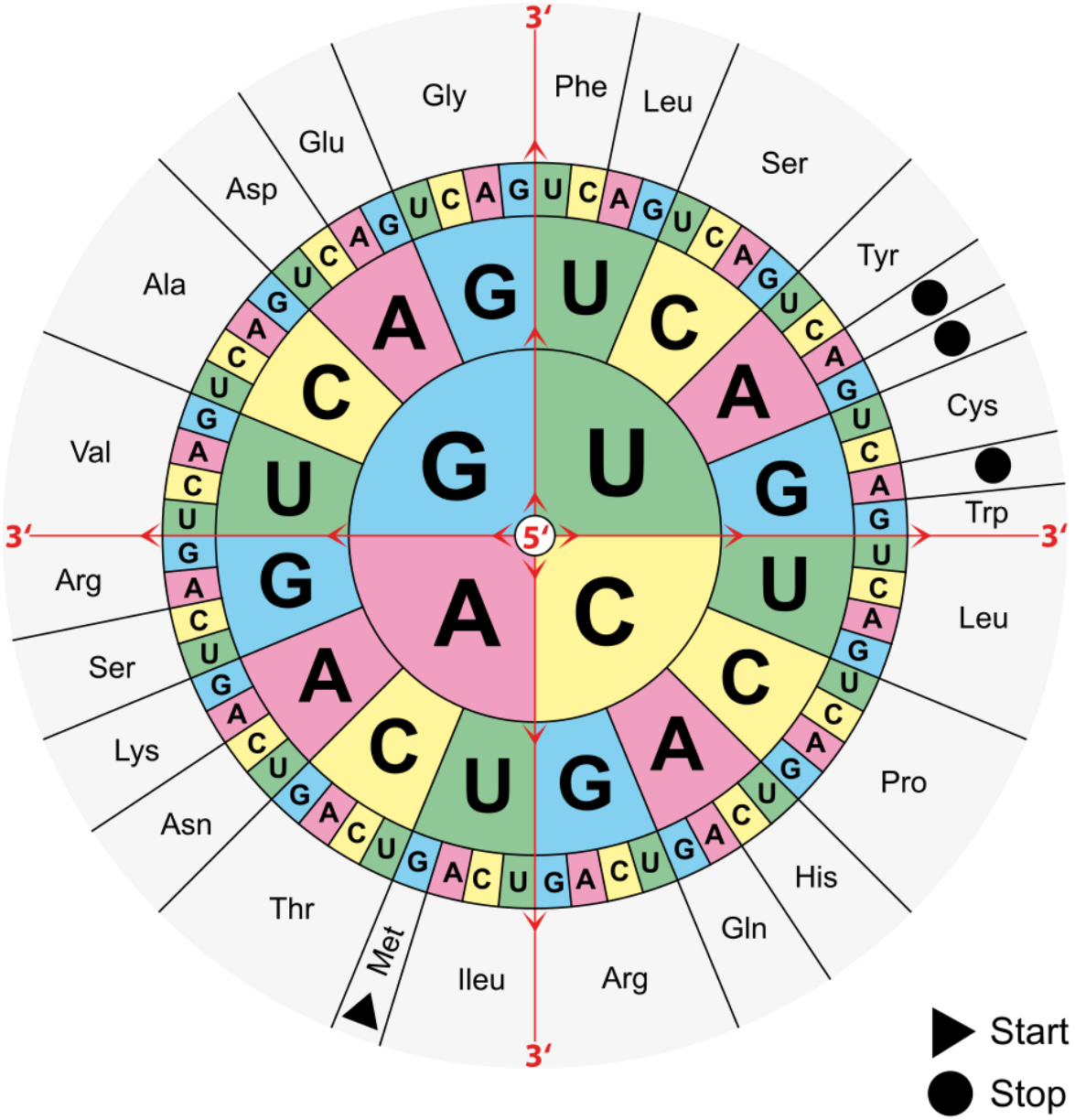
Source: http://hyperphysics.phy-astr.gsu.edu/hbase/organic/imgorg/translation2.gif

CODON WHEEL


3′
5′
Gly
Phe
Leu
Ser
Tyr
Cys
Trp
Leu
Pro
His
Gln
Arg
Ileu
Met
Thr
Asn
Lys
Ser
Arg
Val
Ala
Asp
Glu
Start
Stop

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