

# IBT 432 Aplikasi Bioinformatika

## Protein modelling II: Surfing Protein Data Bank

**Riza Arief Putranto**

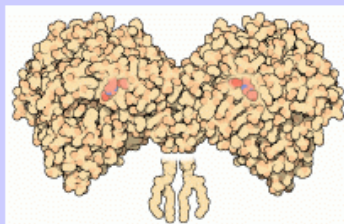
# Rencana Perkuliahan

- ~~1. Kontrak belajar dan pengenalan bioinformatika aplikatif~~
- ~~2. Database sekuen dan analisis genomika~~
- ~~3. Anotasi sekuen ke genom - Praktik~~
- ~~4. Analisis komparasi genomika I~~
- ~~5. Analisis komparasi genomika II~~
- ~~6. Analisis komparasi genomika III~~
- ~~7. Analisis komparasi genomika - Praktik~~
- ~~8. Protein modelling I~~
9. Protein modelling II
10. Protein modelling III
11. Protein modelling - Praktik
12. Visualisasi protein modelling
13. Visualisasi protein modelling - Praktik
14. Presentasi mahasiswa

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25760 Structures  
Last Update: 01-Jun-2004  
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[Molecule of the Month:](#)  
[Acetylcholinesterase](#)

The Protein Data Bank (PDB) is operated by Rutgers, The State University of New Jersey; the San Diego Supercomputer Center at the University of California, San Diego; and the Center for Advanced Research in Biotechnology/UMBI/NIST -- three members of the [Research Collaboratory for Structural Bioinformatics \(RCSB\)](#).

The RCSB PDB is supported by funds from the [National Science Foundation \(NSF\)](#), the [National Institute of General Medical Sciences \(NIH\)](#), the [Office of](#)

# RCSB PDB

PROTEIN DATA BANK

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1-June-2004

### [TargetDB and Ligand Depot papers published in Bioinformatics](#)

Two papers have been published online that describe the TargetDB and Ligand Depot resources. [\[MORE...\]](#)

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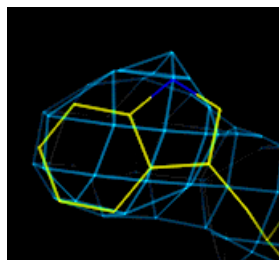
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*\*RCSB partner*

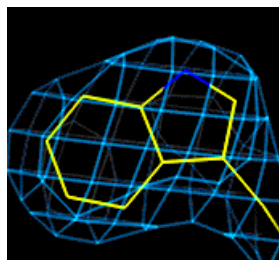
In citing the PDB please refer to:

H.M. Berman, J. Westbrook, Z. Feng, G. Gilliland, T.N. Bhat, H. Weissig, I.N. Shindyalov, P.E. Bourne: [The Protein Data Bank](#). *Nucleic Acids Research*, **28** pp. 235-242 (2000)

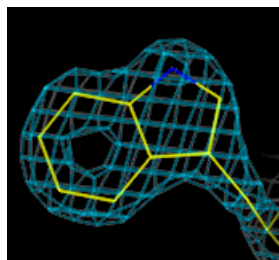
# Remember the resolution importance



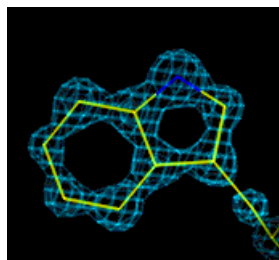
4 Å



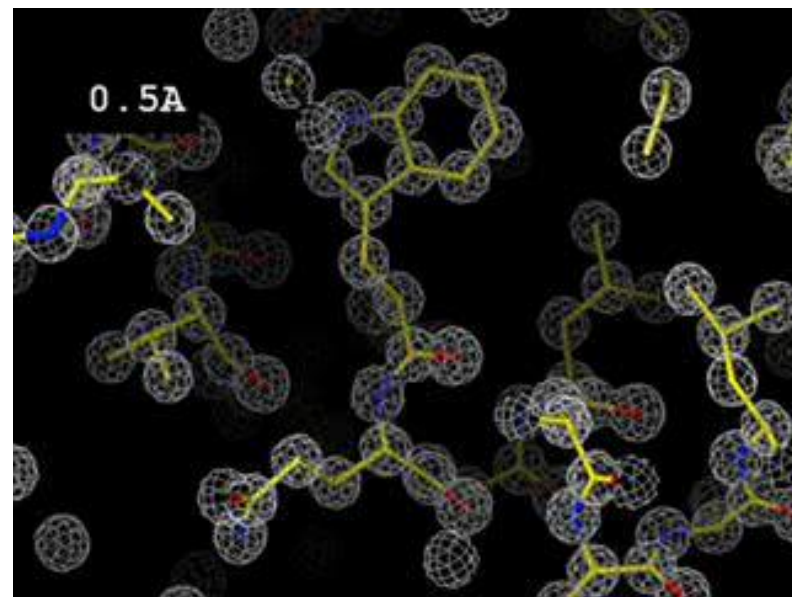
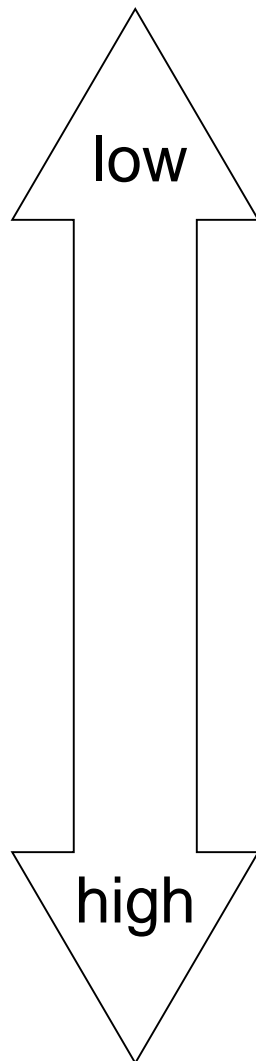
3 Å



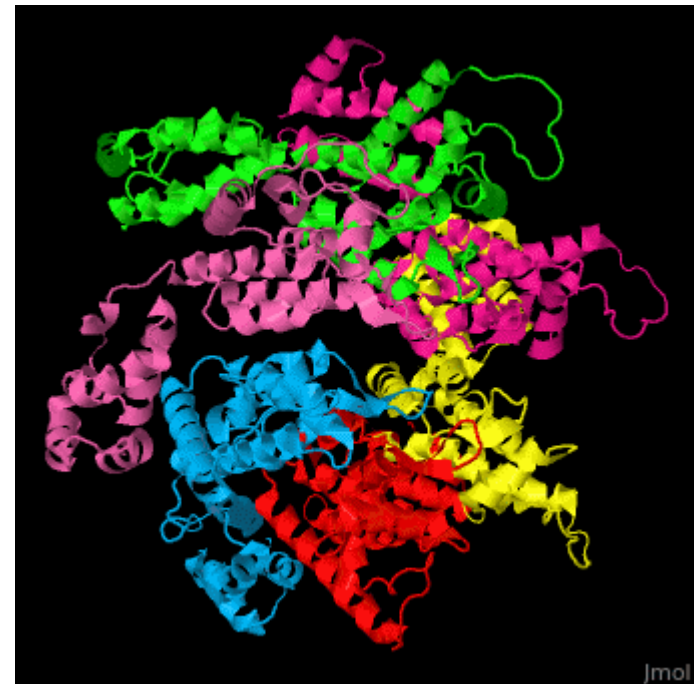
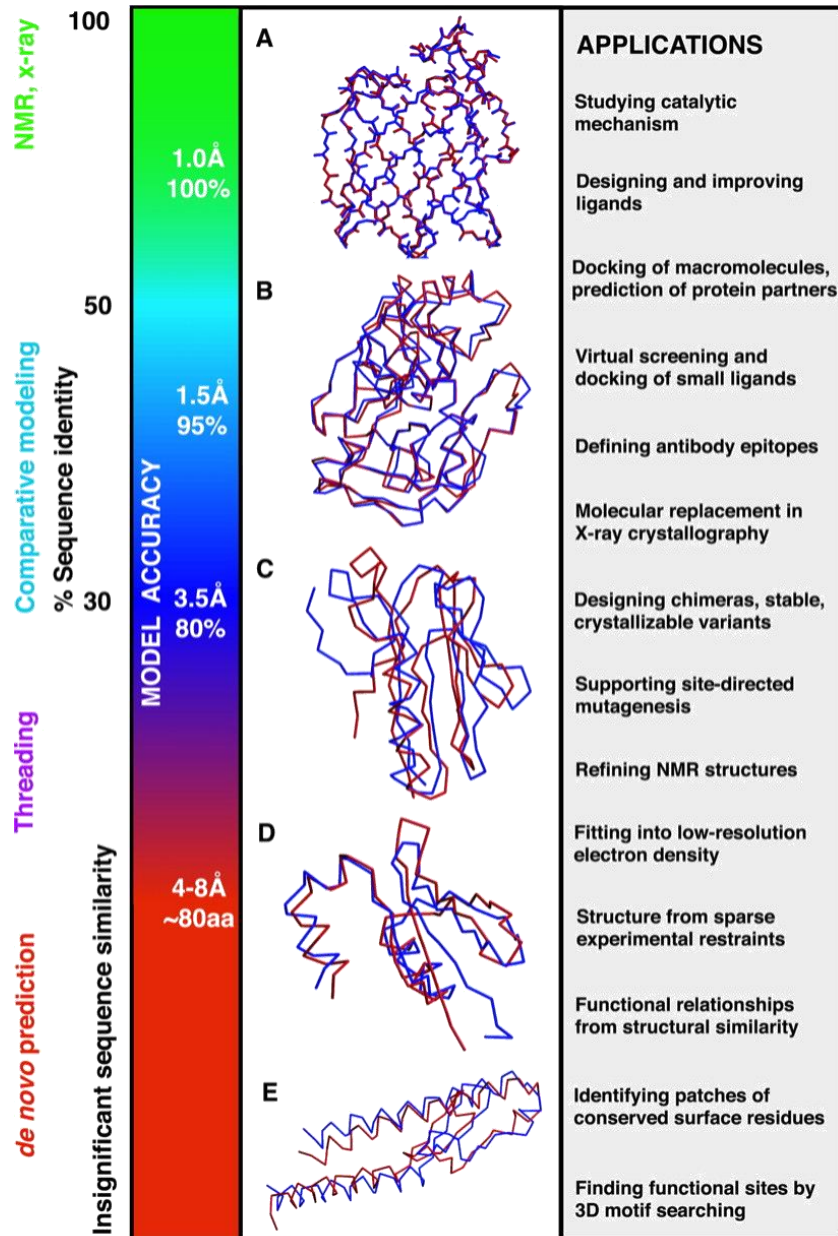
2 Å



1 Å



# Remember the resolution importance

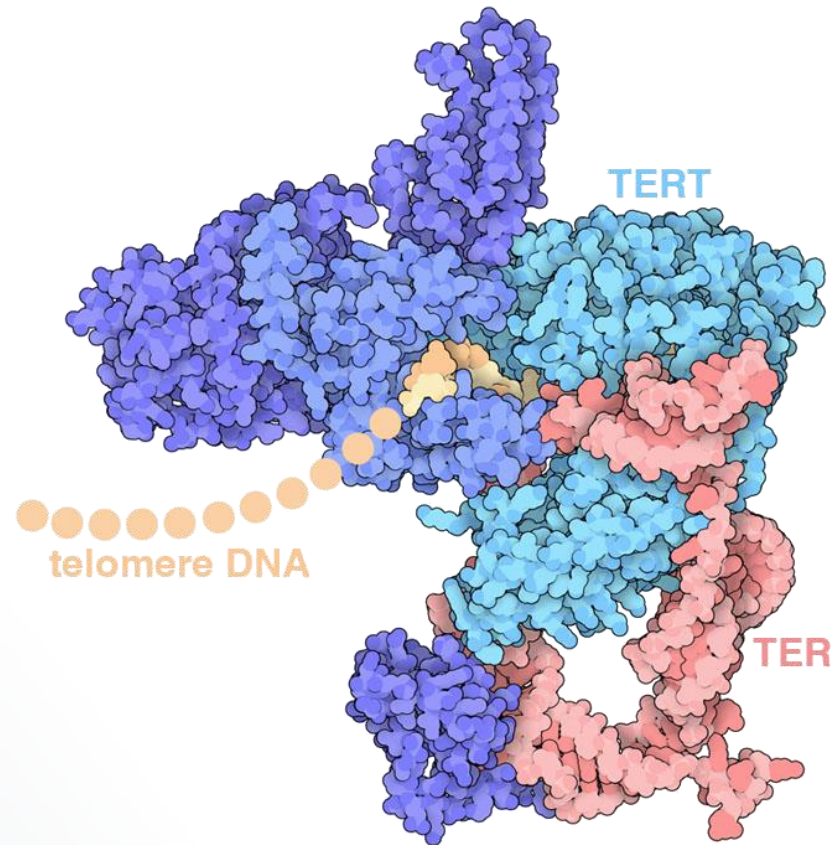




# The PDB's Molecule of The Month

<http://pdb101.rcsb.org/motm/227>

**Telomerase** is most active during development of embryos, when cells divide many times to create our entire body. Later in life, it is far less active in most cells, and telomeres gradually shorten as we age. Improper regulation of telomerase, however, can cause serious problems. For example, cancer cells very often have mutations that lead to production of higher levels of telomerase. This allows them to maintain their telomeres as they rapidly divide and form a tumor.



# Structural view of a Myoglobin

Ribbon cartoon

5OJA

Structure of MbQ

DOI: [10.2210/pdb5OJA/pdb](https://doi.org/10.2210/pdb5OJA/pdb)

Classification: [OXIDOREDUCTASE](#)

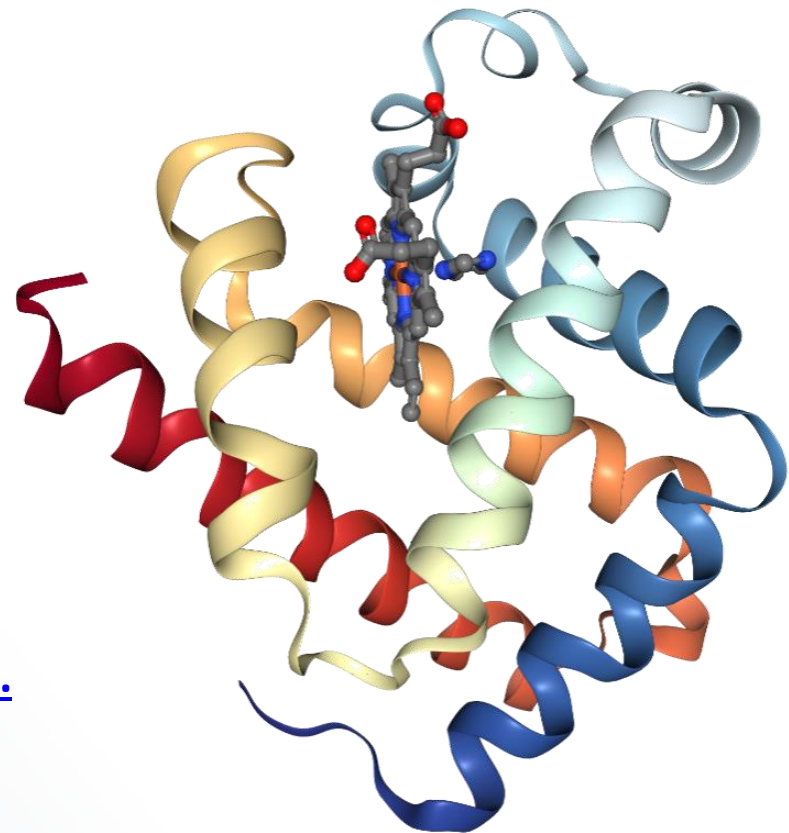
Organism(s): [Physeter catodon](#)

Expression System: [Escherichia coli](#)

Deposited: 2017-07-21

Released: 2018-01-24

Deposition Author(s): [Hayashi, T.](#), [Pott, M.](#), [Mori, T.](#), [Mittl, P.](#), [Green, A.](#), [Hivert, D.](#)



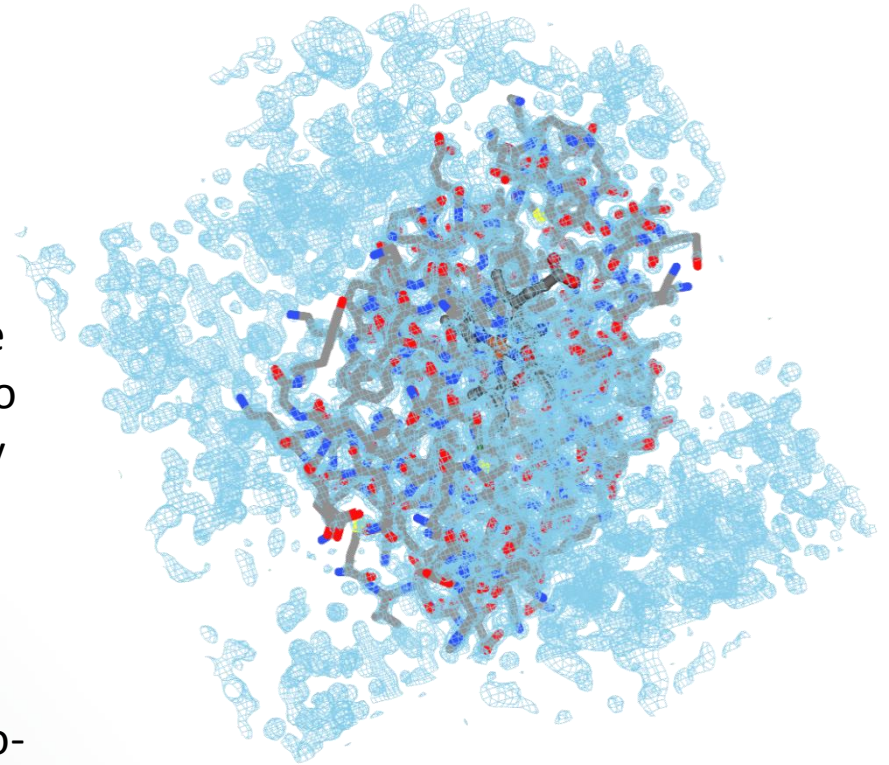
3D View: [Structure](#)

# Structural view of a Myoglobin

## Electron Density Maps: 2fo-fc map

### Electron density maps

combine the **structural model (coordinates)** and the **experimentally-collected data from an X-ray structure determination** and serve to represent the fit of the model to the data. There are two types of electron density maps commonly used by researchers: the 2fo-fc map and the fo-fc map. The fo-fc (also called a difference or omit map) map shows what has been overrepresented or not accounted for by the model, while the 2fo-fc map includes the fo-fc map and electron density around the model.



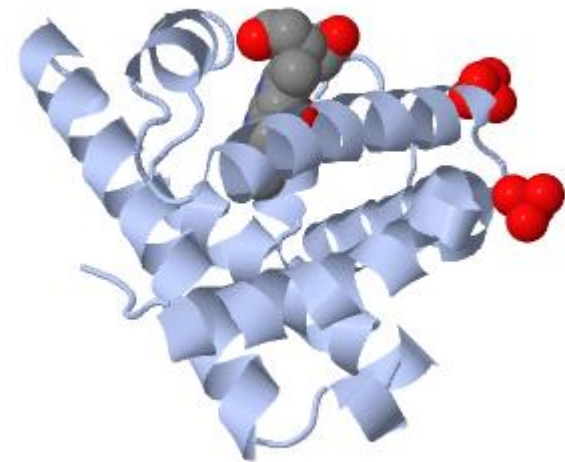
3D View: [Structure](#)



# Task II

## Hemoglobin

1. Find **10 hemoglobins** of any species in RCSB PDB
2. **Screenshot** each of them and save it in a ppt file, one for each image
3. 1 hemoglobin **should have** X-RAY RESOLUTION less than 1.5 Å
4. Send your task to [rizaputranto@gmail.com](mailto:rizaputranto@gmail.com) before 24 Nov 2018



It was still the ninth course, don't  
get dizzy yet

