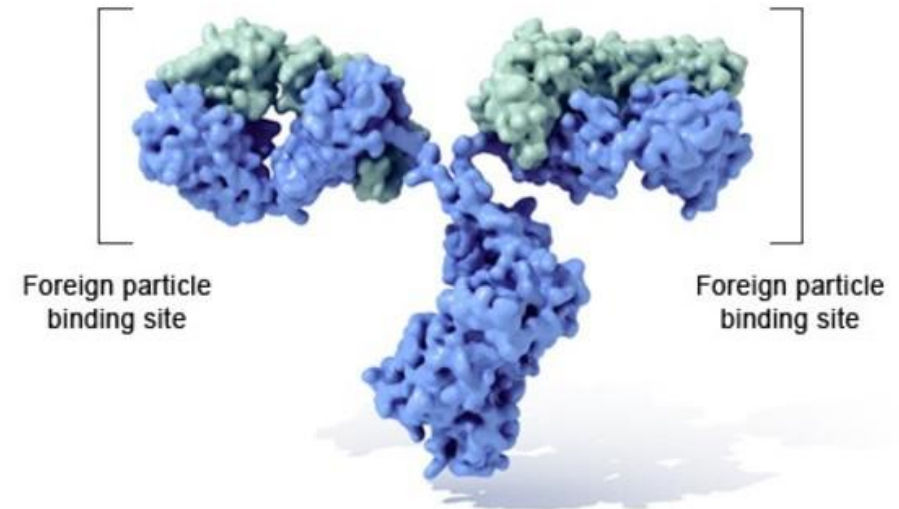


# Antibody

- Antibodies bind to specific foreign particles, such as viruses and bacteria, to help protect the body.

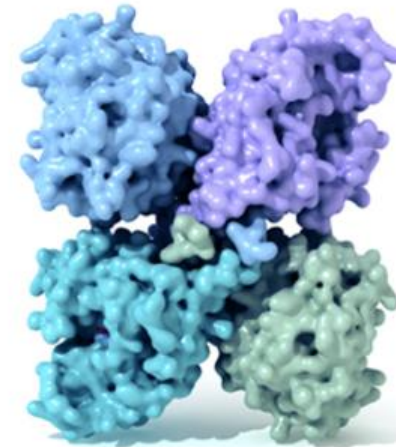
Immunoglobulin G (IgG)



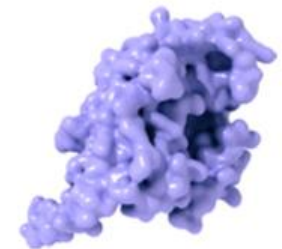
# Enzymes

- Enzymes carry out almost all of the thousands of chemical reactions that take place in cells. They also assist with the formation of new molecules by reading the genetic information stored in DNA.

Phenylalanine hydroxylase



Phenylalanine hydroxylase  
protein consisting of 4 subunits



Single phenylalanine  
hydroxylase subunit

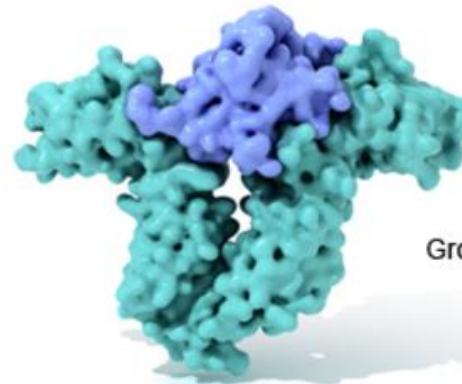
# Messenger

- Messenger proteins, such as some types of hormones, transmit signals to coordinate biological processes between different cells, tissues, and organs.

Growth hormone



Growth hormone

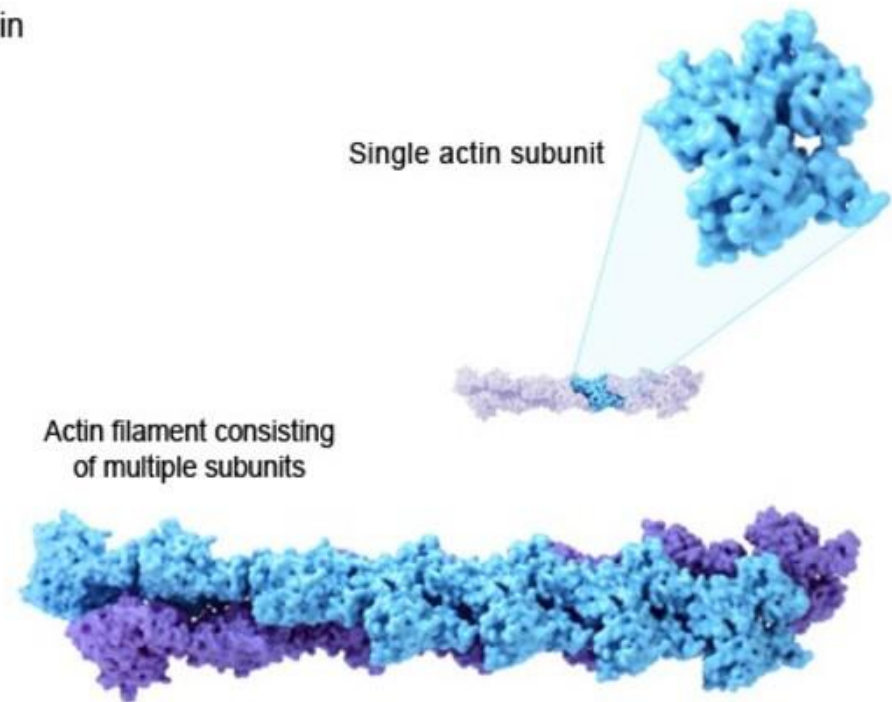


Growth hormone bound  
to receptor

# Structural component

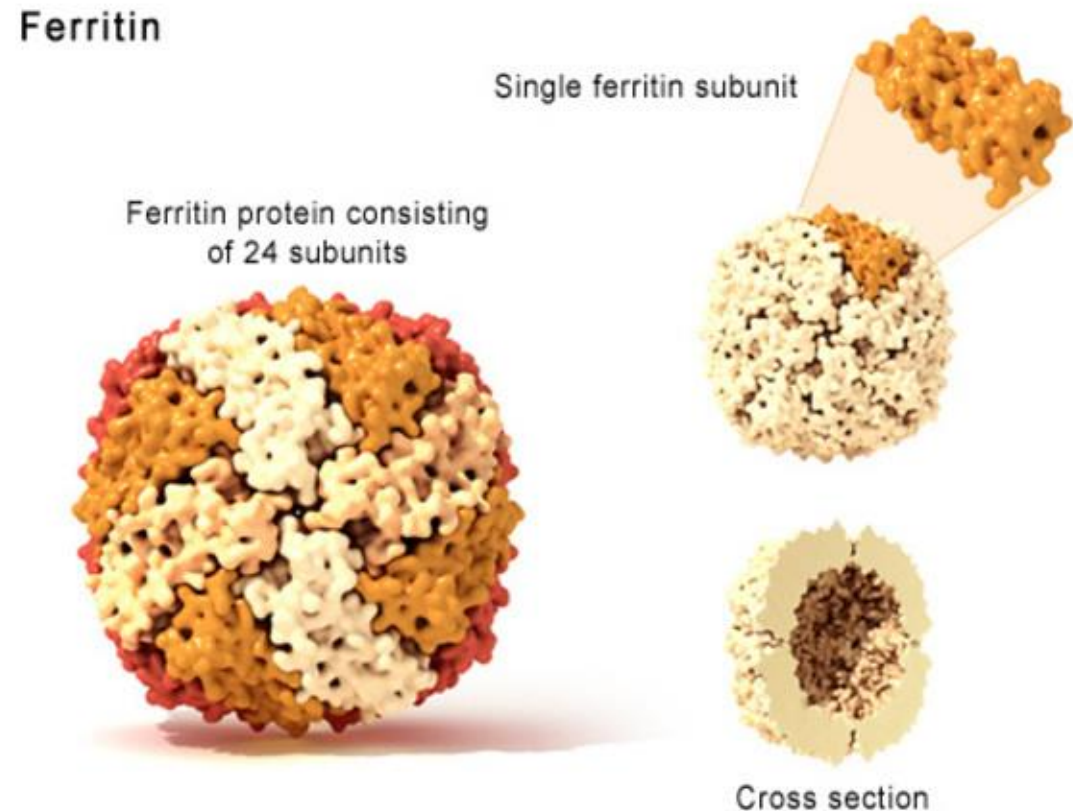
- These proteins provide structure and support for cells. On a larger scale, they also allow the body to move.

Actin



# Transport/storage

- These proteins bind and carry atoms and small molecules within cells and throughout the body.



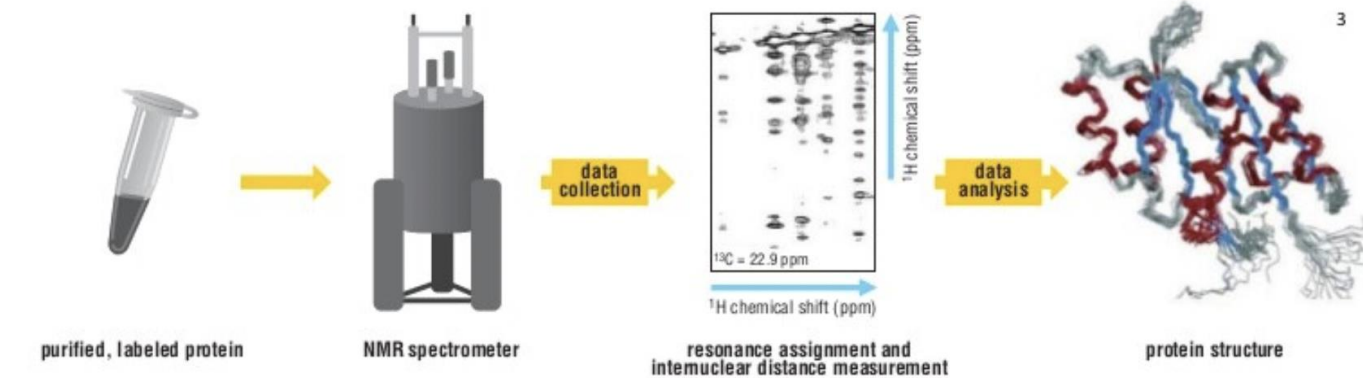
# problems

- Mutation
- Chimera protein
- Domain grafting
- De-novo design
- Vaccine design
- Interface design
- Antibody redesign
- PPI or multimer protein design
- Starting and final structures

# Protein structure

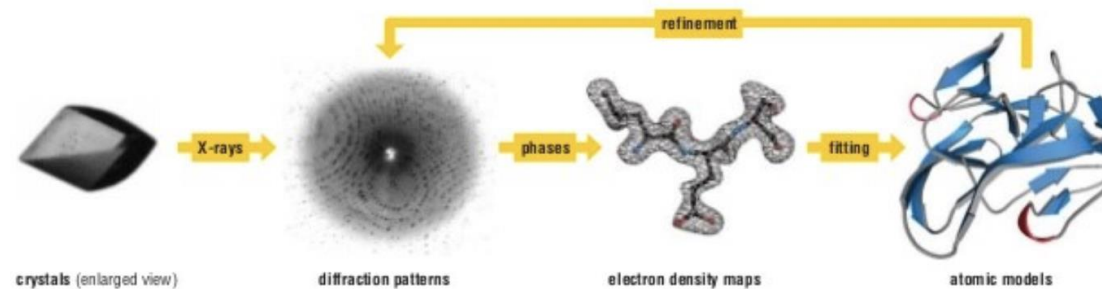
## NMR & X-ray crystallography

### NMR:



<sup>3</sup> Gregory, A.; Dagmar, R.; Protein Structure and Function: Chapter 5, Structure determination; New Science Press Ltd, 2004; pp 168-173 For X-ray description

### X-ray Crystallography:



<sup>4</sup> Gregory, A.; Dagmar, R.; Protein Structure and Function: Chapter 5, Structure determination; New Science Press Ltd, 2004; pp 168-173 For X-ray description

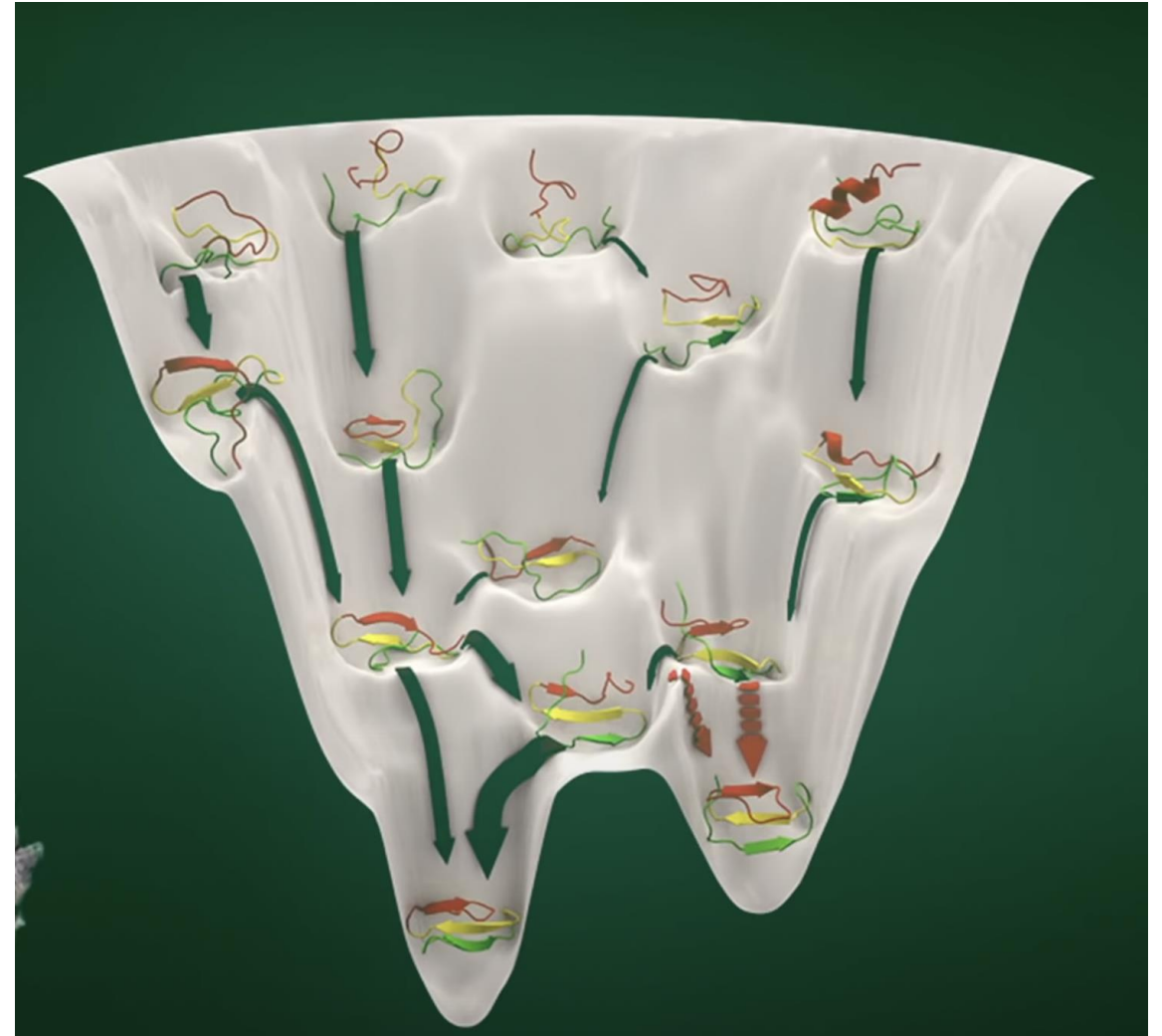
# Anfinsen's dogma





# Searching space prablem

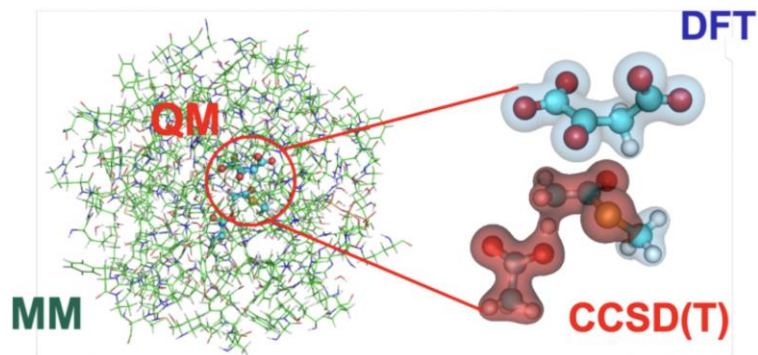
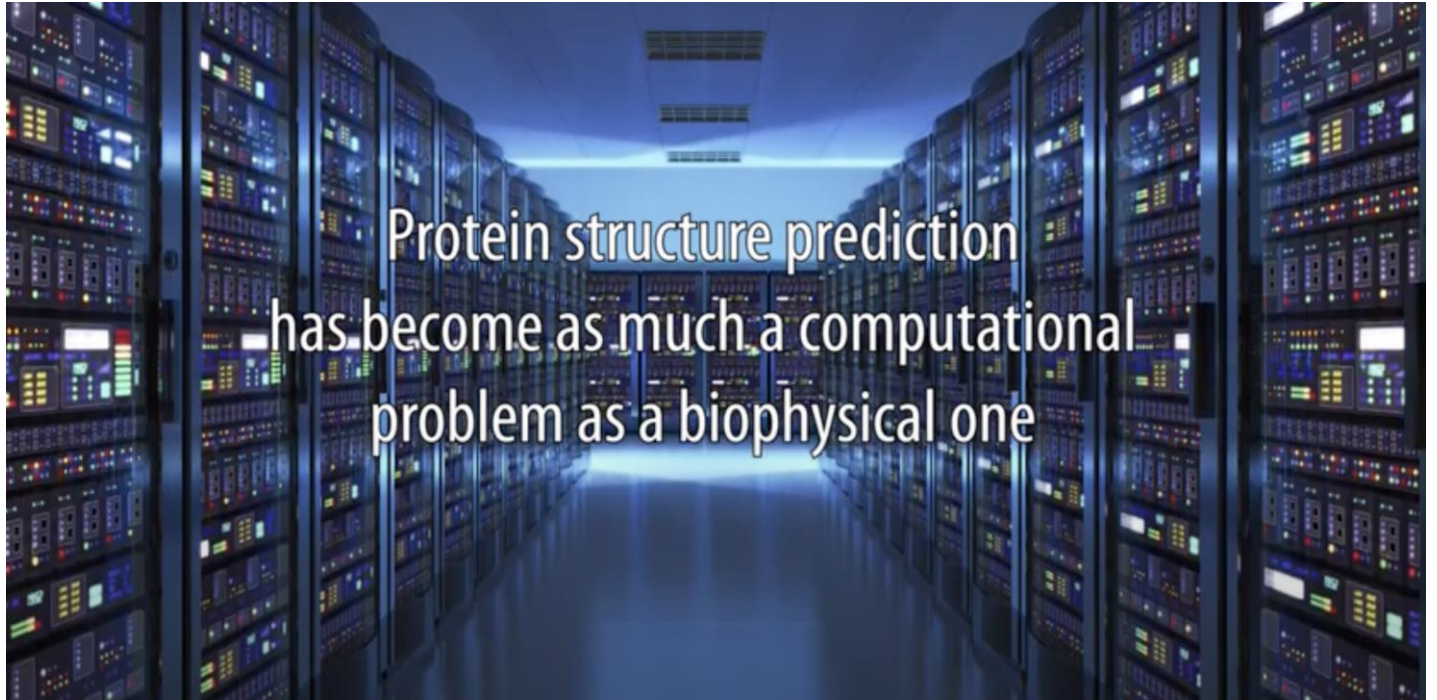
- Levintal paradox
- $2^{100} = 10^{30}$
- 1ps for each conformation = 30
- billion years



# Cpu problems

Homology modeling  
 Denovo modeling

MM and QM  
 schrodinger equation



# Homology Modeling

- %70 similarity
- Swiss model
- Modeller
- Shcrodinger
- Itasser
- **alphafold**

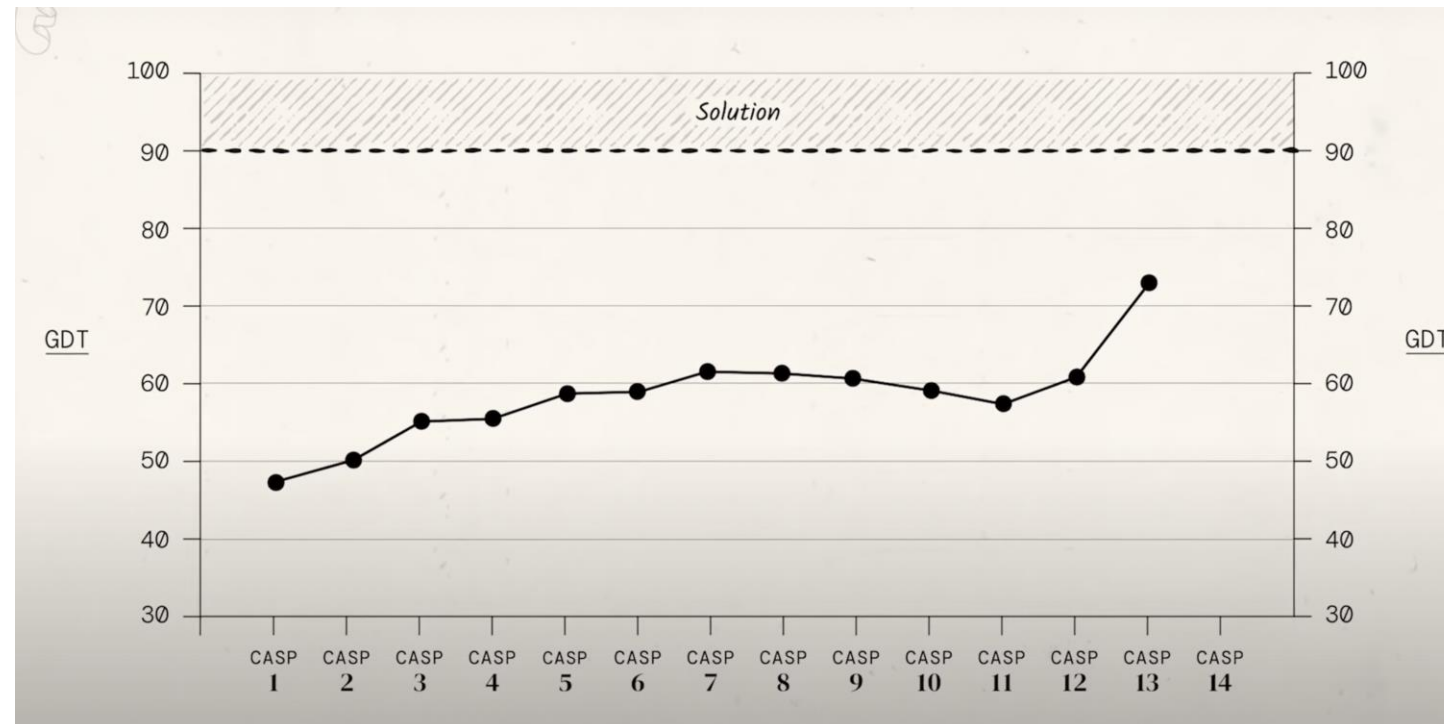
Pymol

chimera

Vmd

# casp

- **Critical Assessment of protein Structure Prediction (CASP)** is a community-wide, worldwide experiment for [protein structure prediction](#) taking place every two years since 1994.

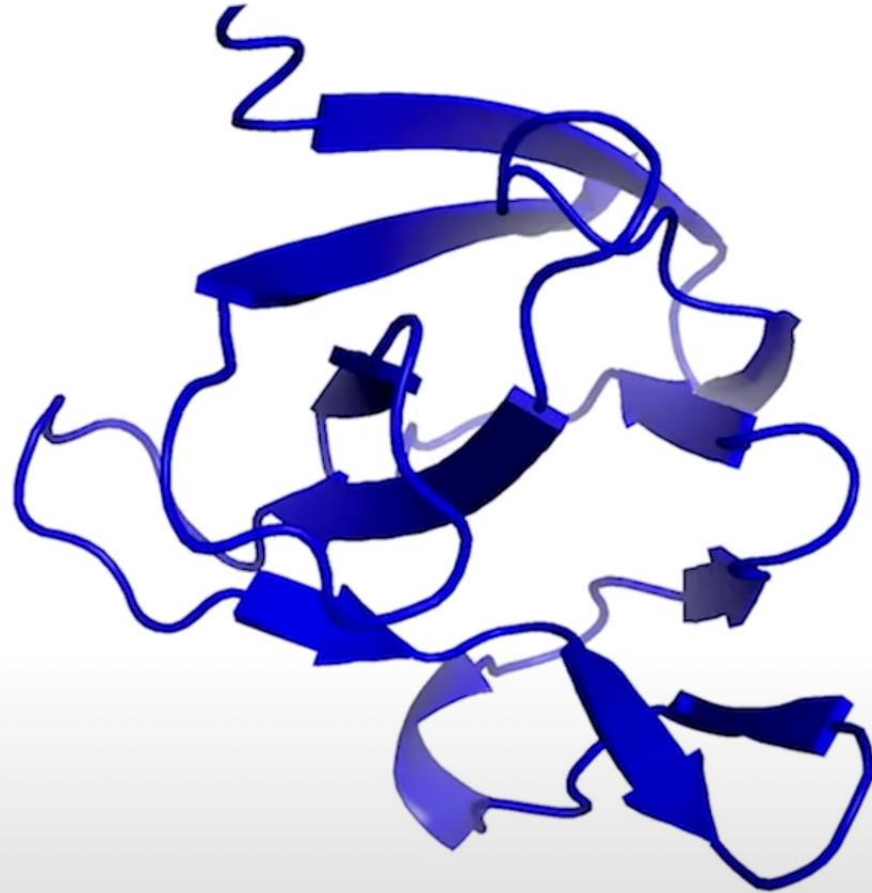


# CASP 14 Prediction

## Target T1064

**Description:**  
Orf8 Protein

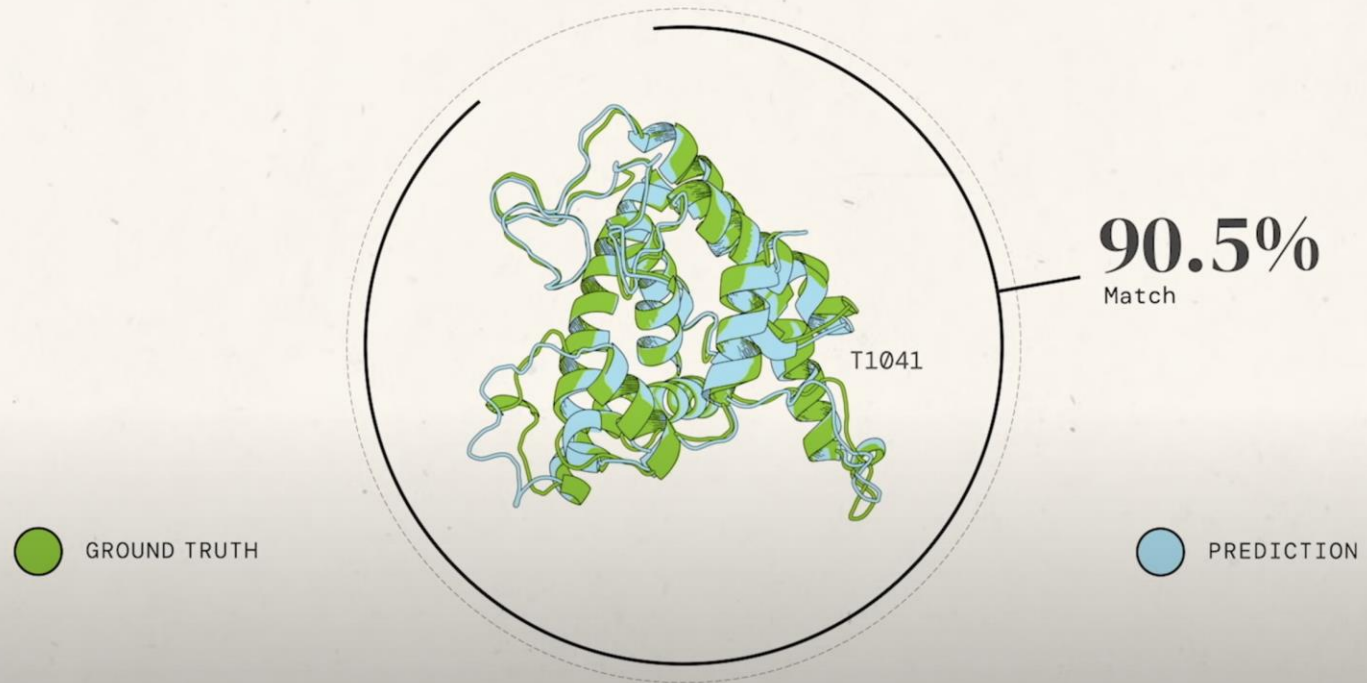
**Organism:**  
SARS-CoV-2





Google AI

Global Distance Test



Global Distance Test





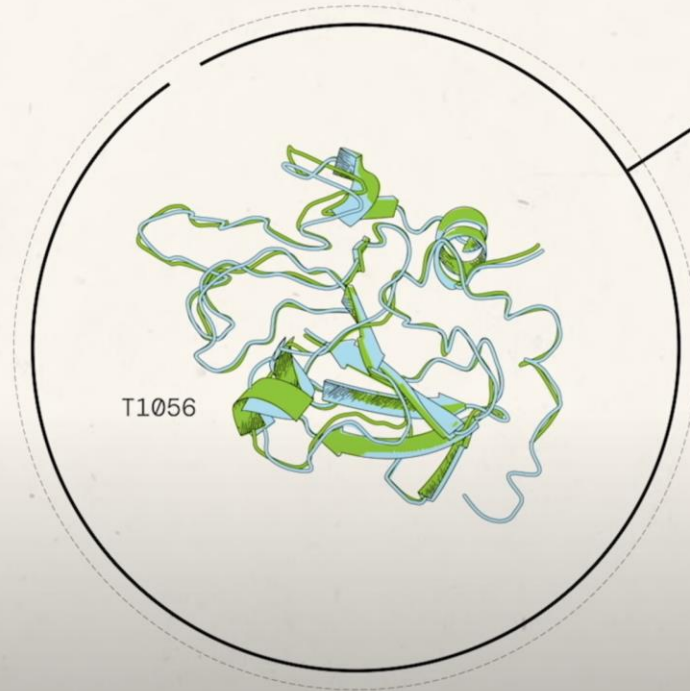
Global Distance Test

**98.22%**  
Match

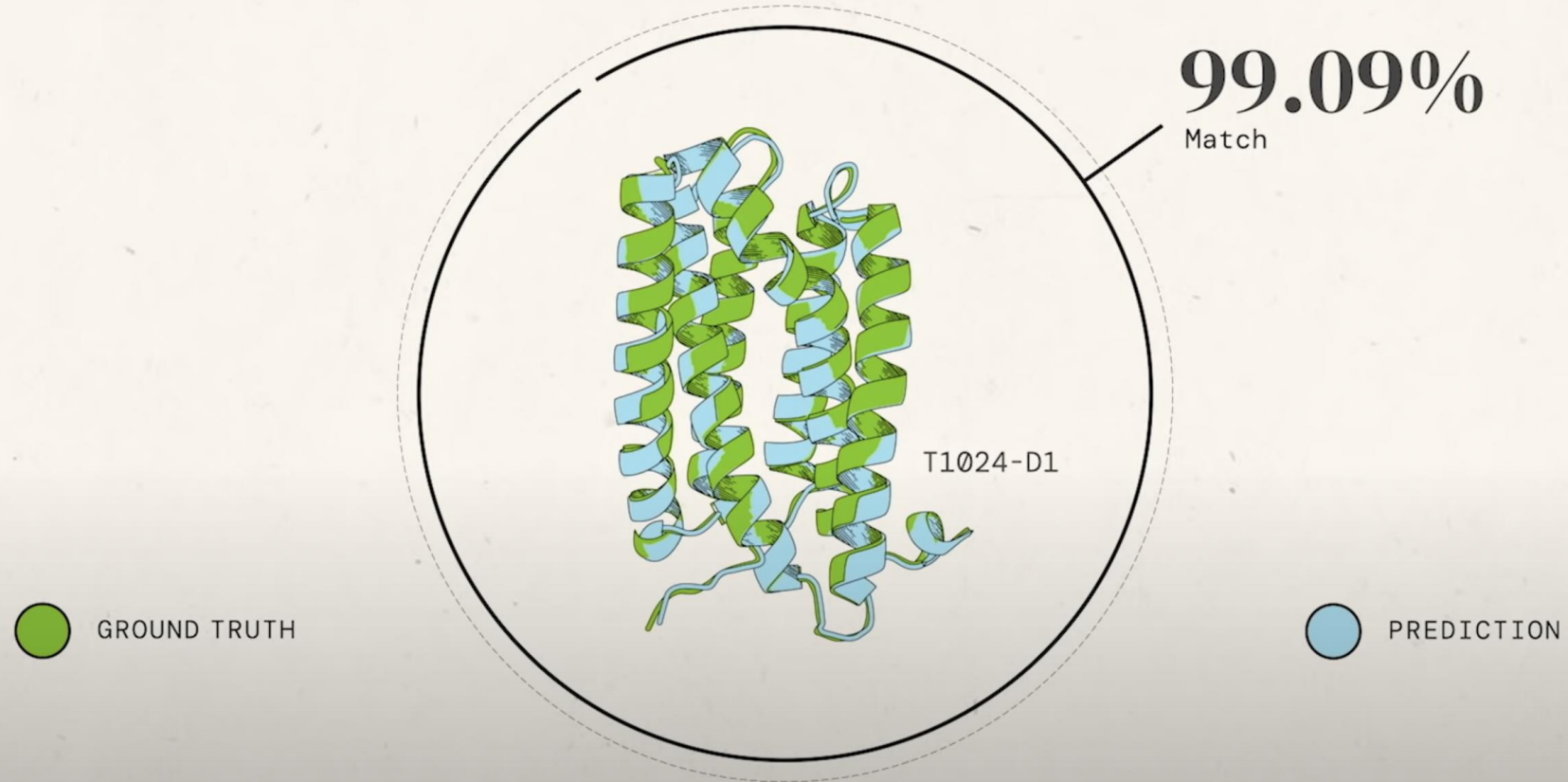
T1056

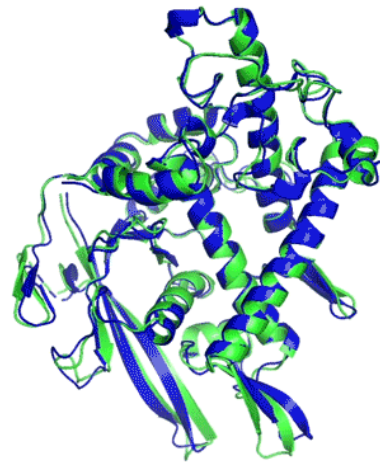
● GROUND TRUTH

● PREDICTION

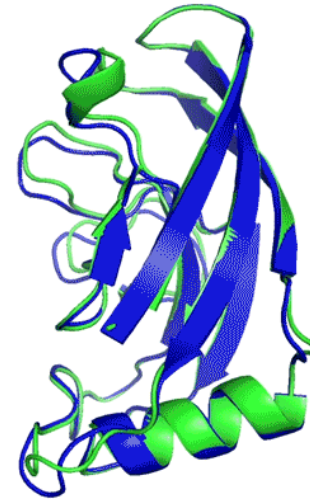


Global Distance Test





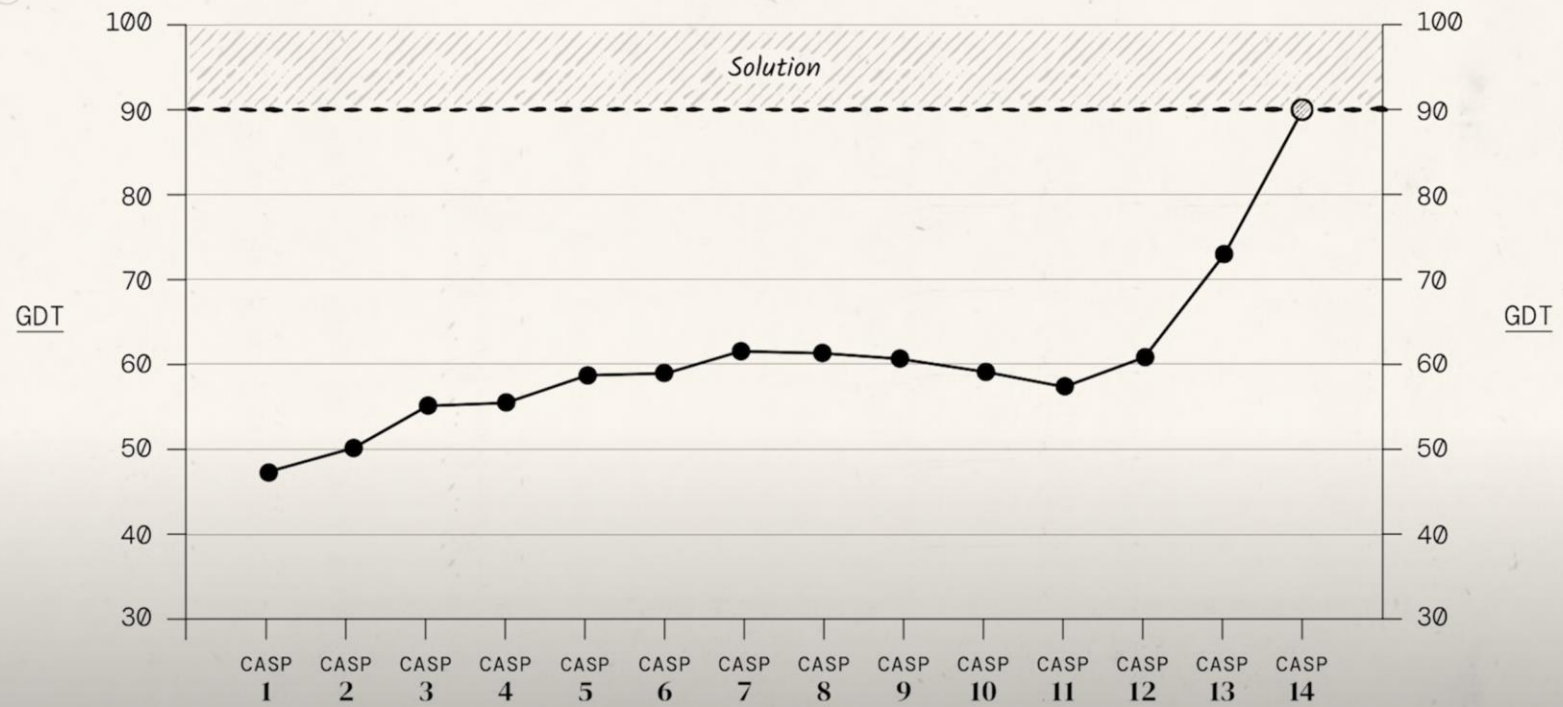
**T1037 / 6vr4**  
90.7 GDT  
(RNA polymerase domain)

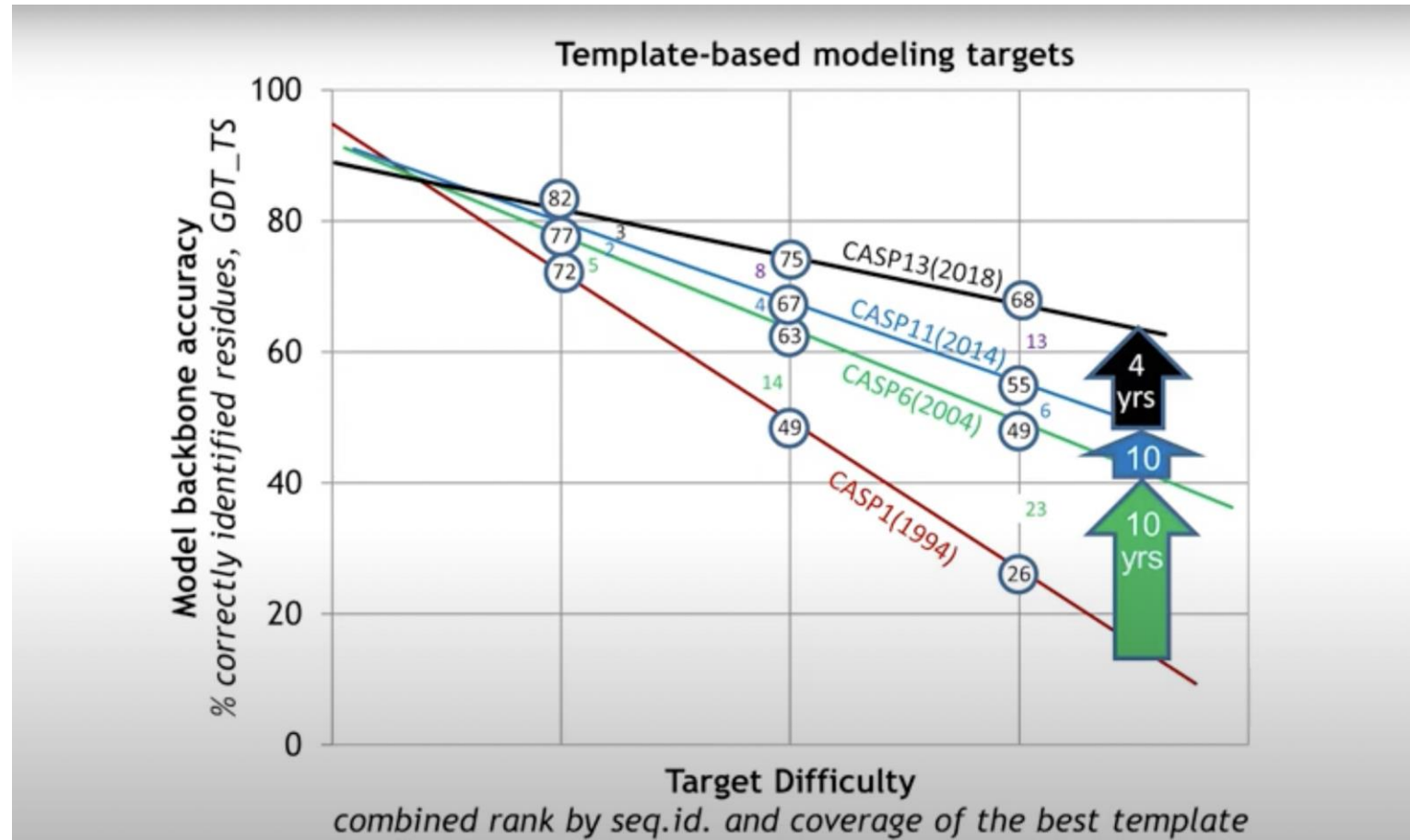


**T1049 / 6y4f**  
93.3 GDT  
(adhesin tip)

- Experimental result
- Computational prediction

### Critical Assessment of Structure Prediction





# AlphaFold Protein Structure Database

Developed by DeepMind and EMBL-EBI

Search for protein, gene, UniProt accession or organism

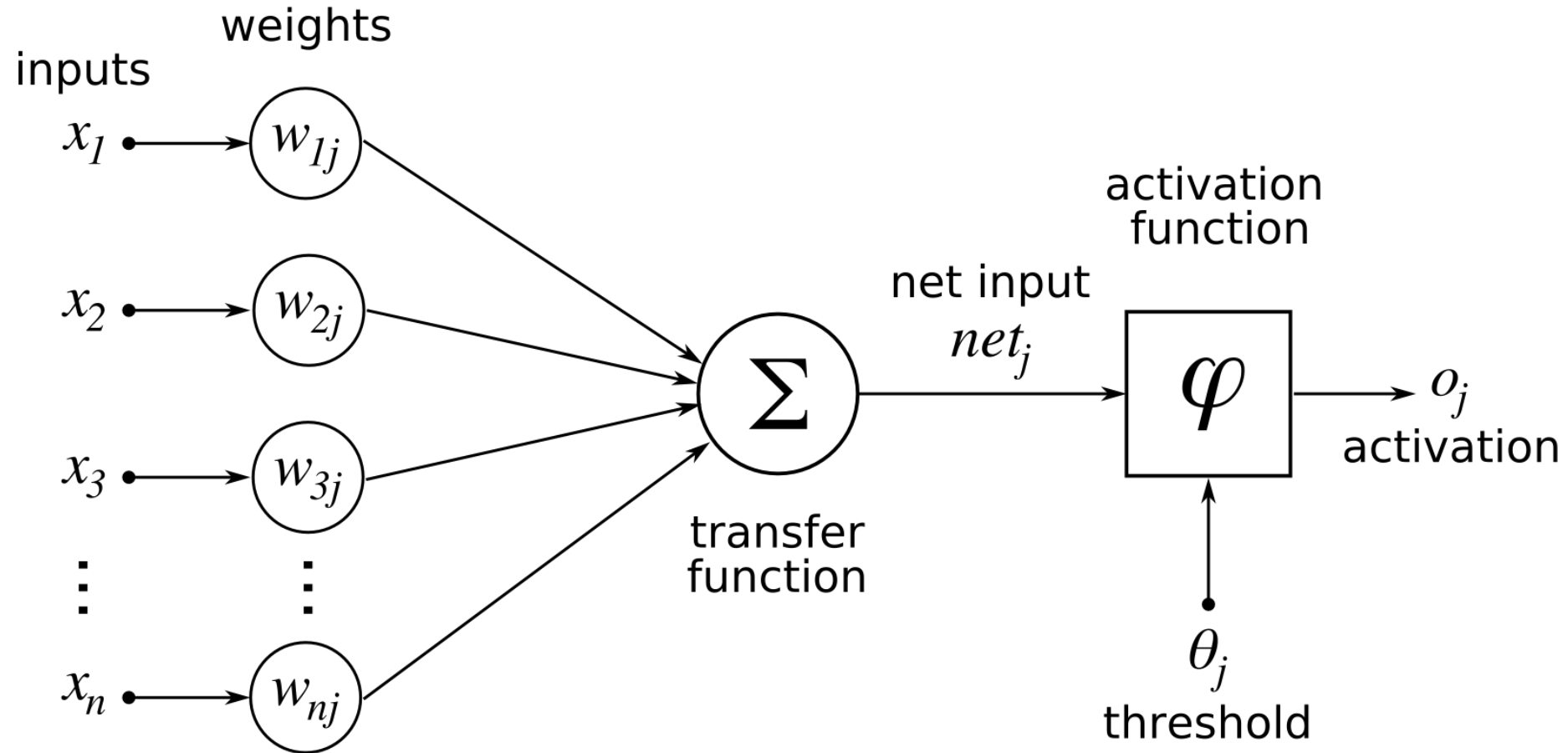
BETA

Search

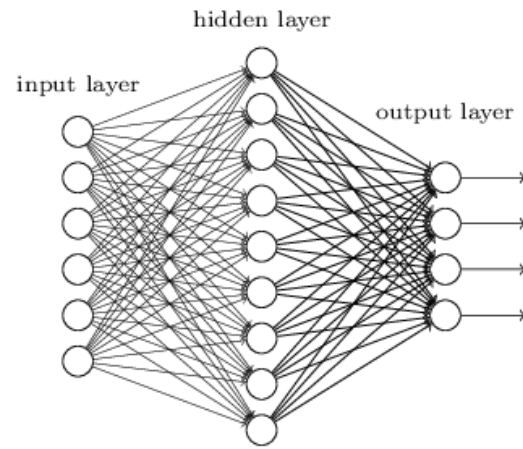
Examples: [Free fatty acid receptor 2](#) [At1g58602](#) [Q5VSL9](#) [E. coli](#) Help: [AlphaFold DB search help](#)

AlphaFold DB provides open access to protein structure predictions for the human proteome and 20 other key organisms to accelerate scientific research.

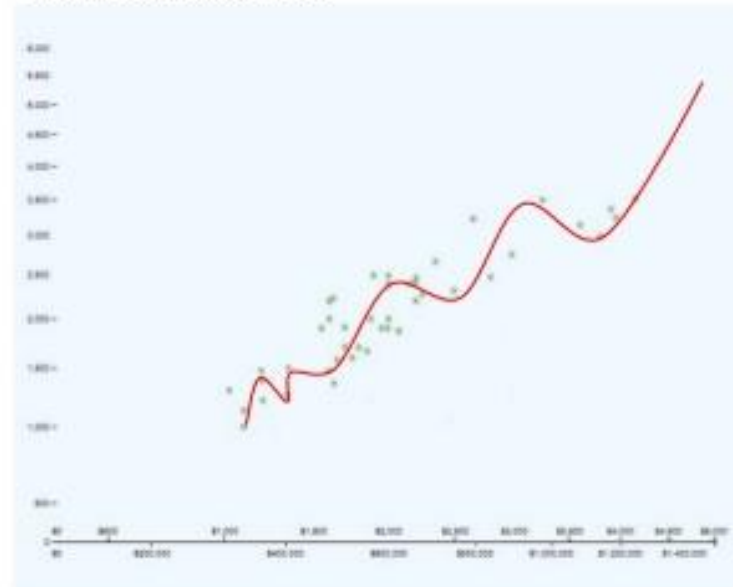
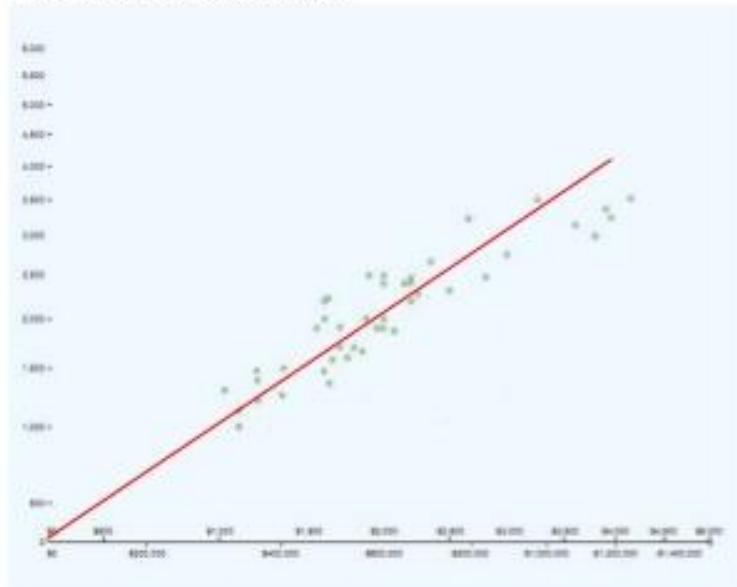
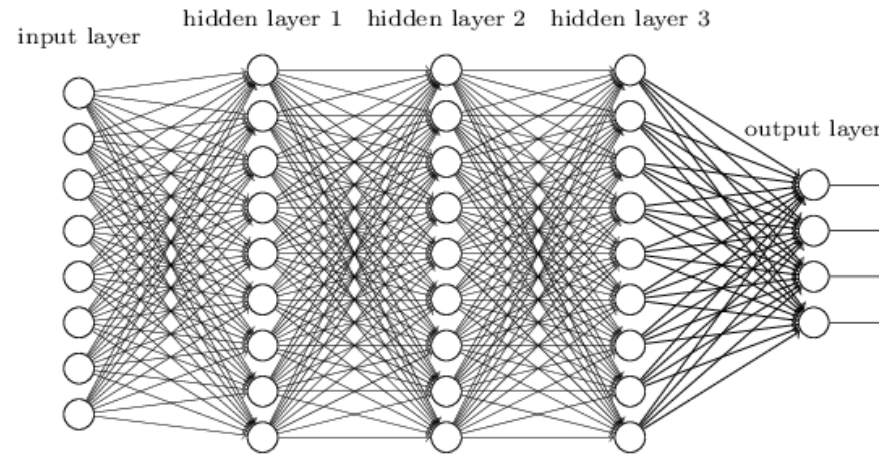
## ANN



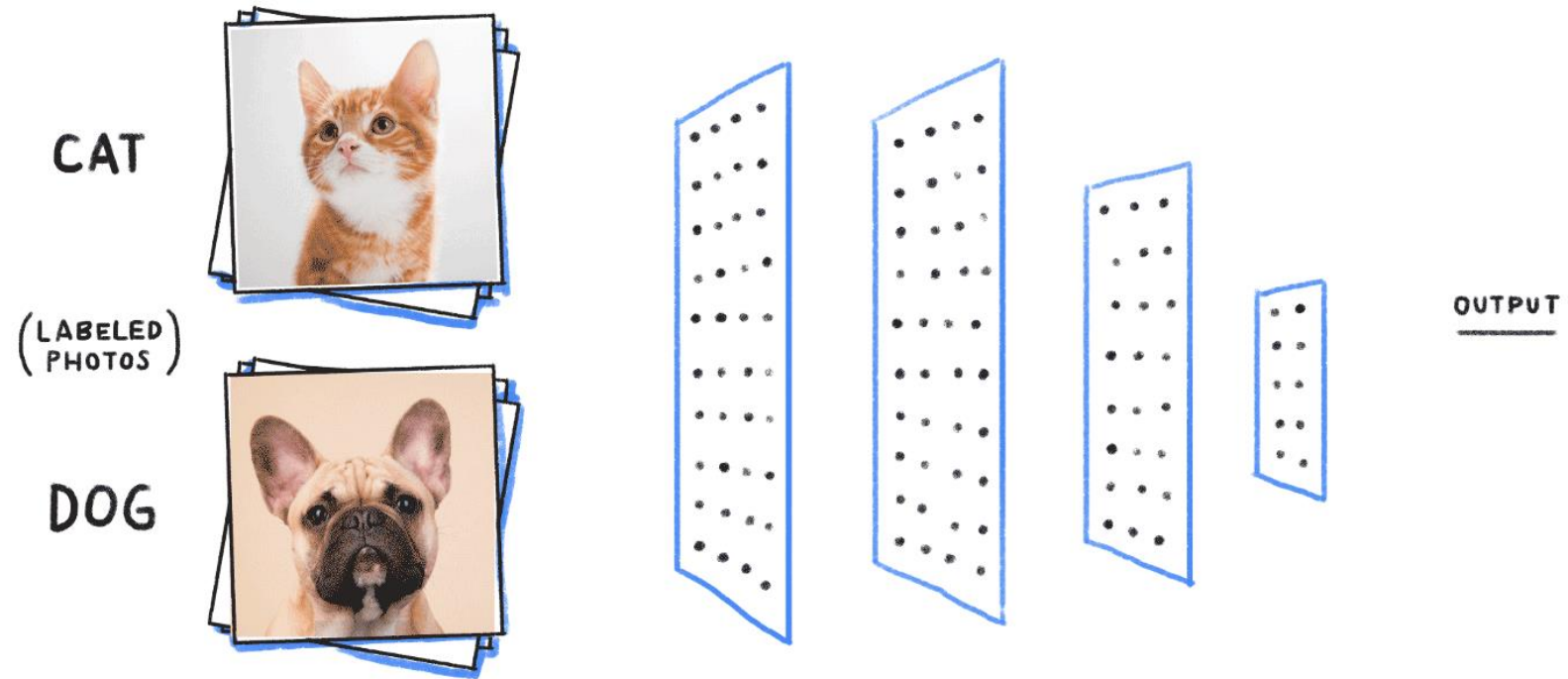
"Non-deep" feedforward neural network



Deep neural network

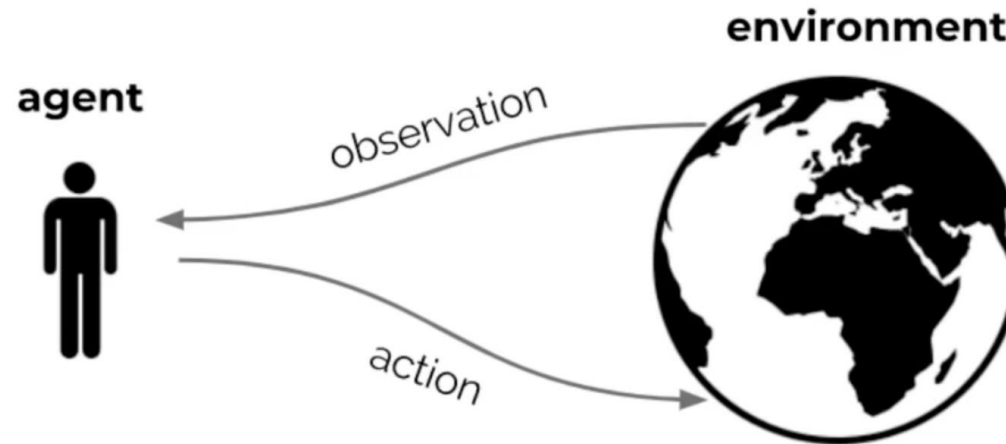




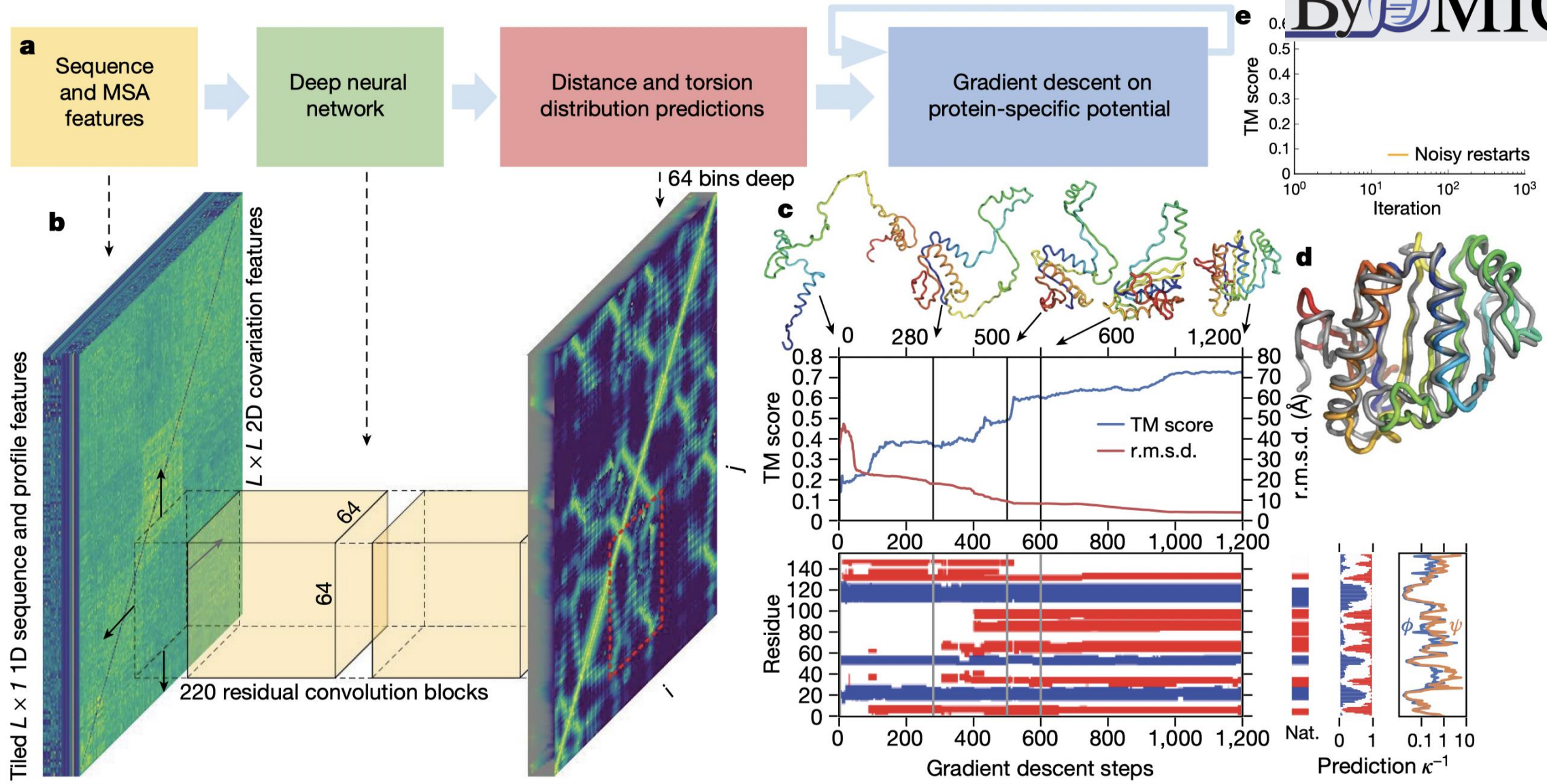


# Reinforcement learning

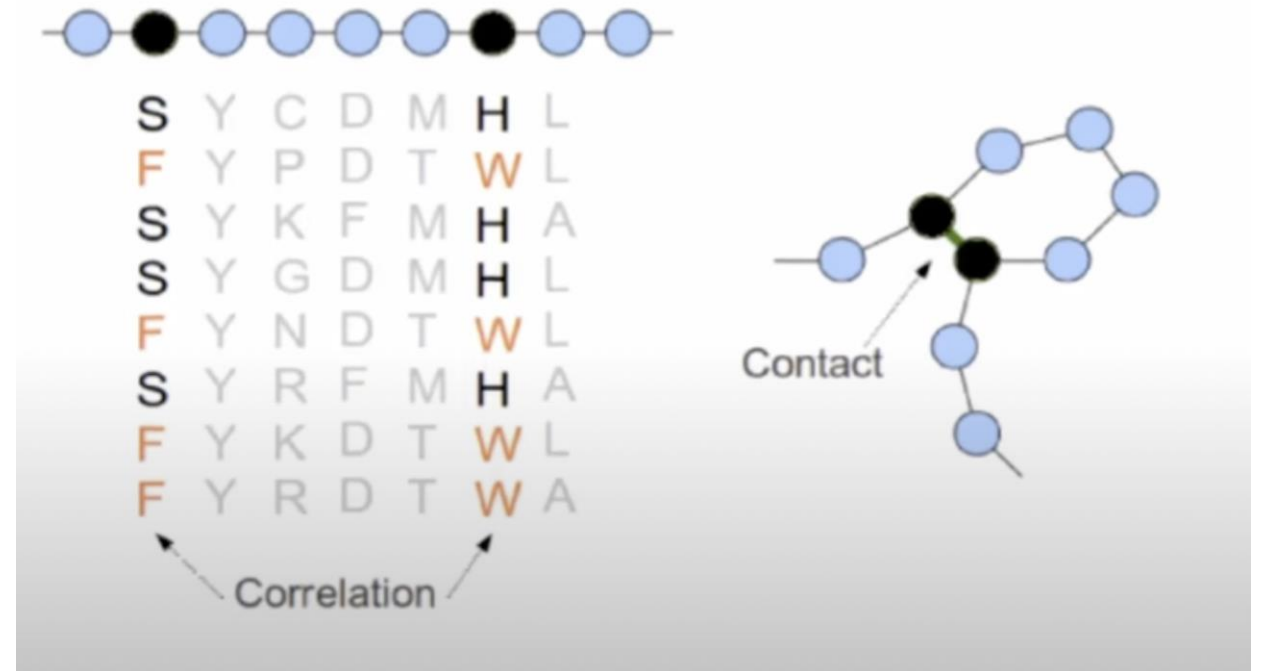
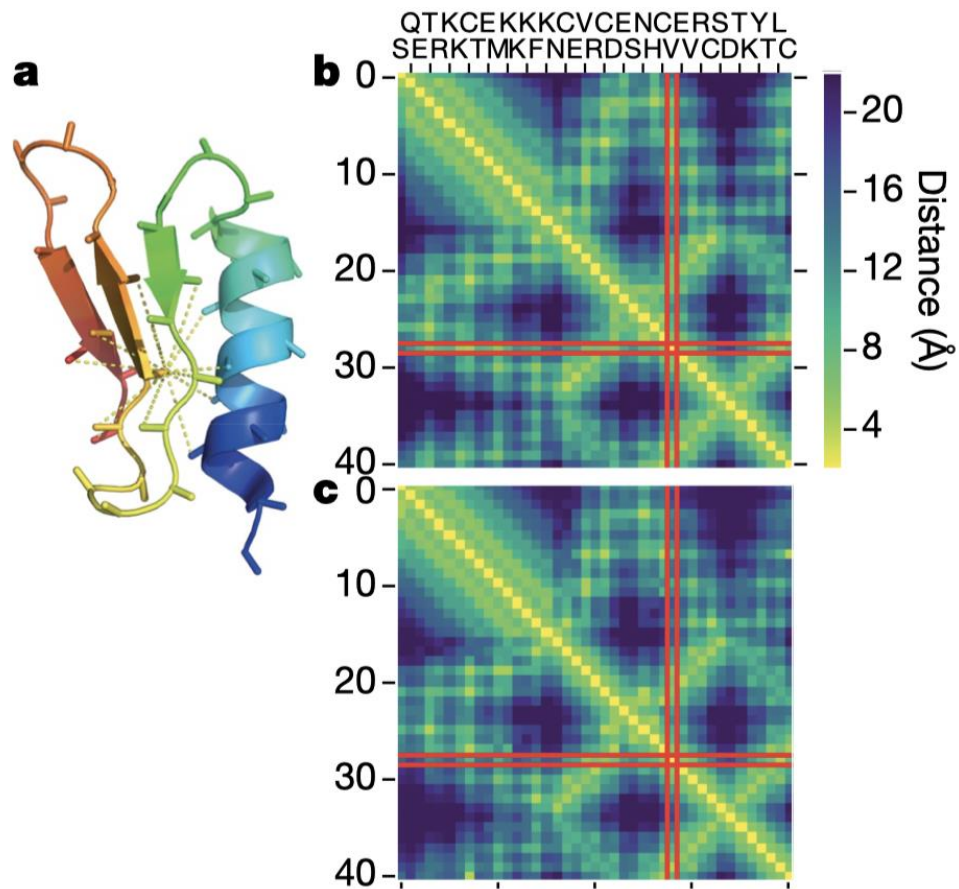
## Agent and Environment



- ▶ At each step  $t$  the agent:
  - ▶ Receives observation  $O_t$  (and reward  $R_t$ )
  - ▶ Executes action  $A_t$



(helix in blue, strand in red)



# AlphaFold Protein Structure Database

Developed by DeepMind and EMBL-EBI

Search for protein, gene, UniProt accession or organism

BETA

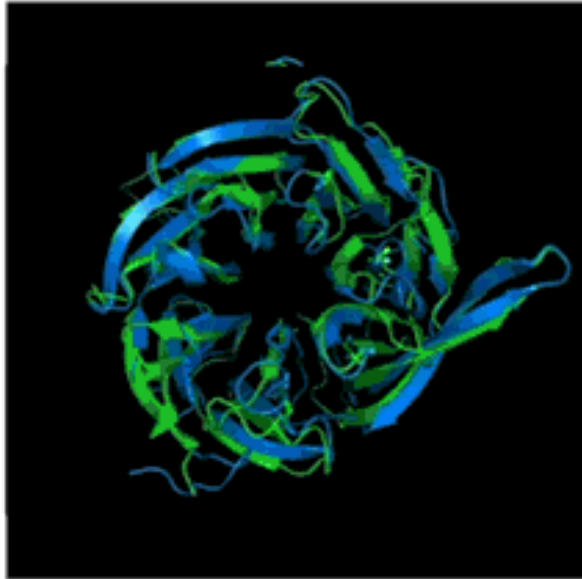
Search

Examples: [Free fatty acid receptor 2](#) [At1g58602](#) [Q5VSL9](#) [E. coli](#) Help: [AlphaFold DB search help](#)

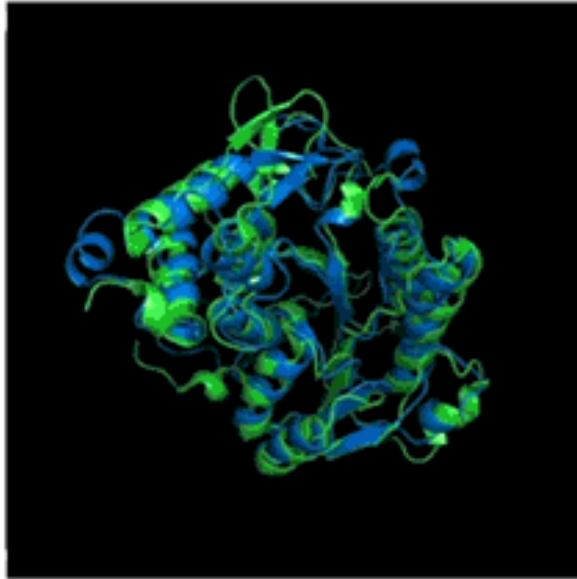
AlphaFold DB provides open access to protein structure predictions for the human proteome and 20 other key organisms to accelerate scientific research.

Structures:  
Ground truth (green)  
Predicted (blue)

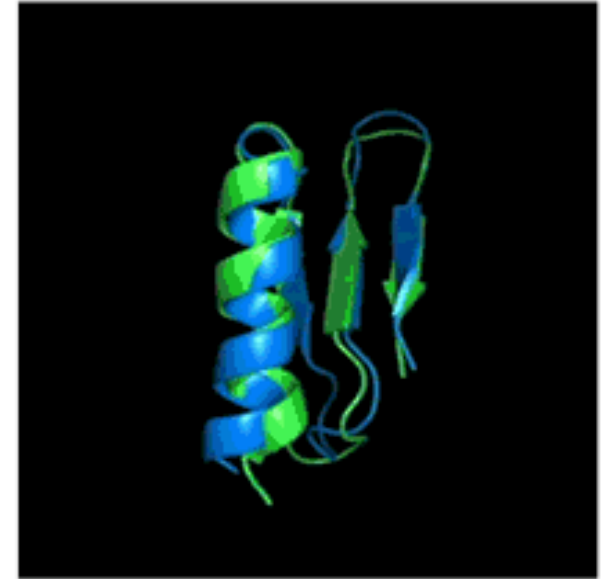
T0954 / 6CVZ



T0965 / 6D2V



T0955 / 5W9F













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 <b>Augustin-Zidek and Copybara-Service</b> Accept any ordering given by ListDir in t... 1d43aaaf 15 days ago 25 commits
 <b>alphafold</b> Skip obsolete PDB templates that don't have a replacement. 15 days ago
 <b>docker</b> Fix a few typos. 2 months ago
 <b>imgs</b> Initial release of AlphaFold. 2 months ago
 <b>notebooks</b> Fix TensorFlow versions in AlphaFold Colab notebook. last month
 <b>scripts</b> Remove a redundant space. last month
 <b>.dockerignore</b> Collapse hh-suite install steps into single layer. 2 months ago
 <b>CONTRIBUTING.md</b> Initial release of AlphaFold. 2 months ago
 <b>LICENSE</b> Initial release of AlphaFold. 2 months ago
 <b>README.md</b> Update the bibtex citation with the issue number and pages 25 days ago




**About**  
Open source code for AlphaFold.  
Readme  
Apache-2.0 License

**Releases 1**  
 **Initial release** Latest  
on Jul 16

**Packages**  
No packages published

main ▾ alphafold / notebooks / AlphaFold.ipynb Go to file ...

 a-googler Fix TensorFlow versions in AlphaFold Colab notebook. Latest commit b1d772d on Aug 25 History

   3 contributors

694 lines (694 sloc) | 33 KB <> Raw Blame Copy Edit Delete

## AlphaFold Colab

This Colab notebook allows you to easily predict the structure of a protein using a slightly simplified version of [AlphaFold v2.0](#).

### Differences to AlphaFold v2.0

In comparison to AlphaFold v2.0, this Colab notebook uses **no templates (homologous structures)** and a selected portion of the [BFD database](#). We have validated these changes on several thousand recent PDB structures. While accuracy will be near-identical to the full AlphaFold system on many targets, a small fraction have a large drop in accuracy due to the smaller MSA and lack of templates. For best reliability, we recommend instead using the [full open source AlphaFold](#), or the [AlphaFold Protein Structure Database](#).

Please note that this Colab notebook is provided as an early-access prototype and is not a finished product. It is provided for theoretical modelling only and caution should be exercised in its use.

### Citing this work

Any publication that discloses findings arising from using this notebook should [cite](#) the [AlphaFold paper](#).

### Licenses

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