

ESM vs Alphafold - ELOV7_HUMAN

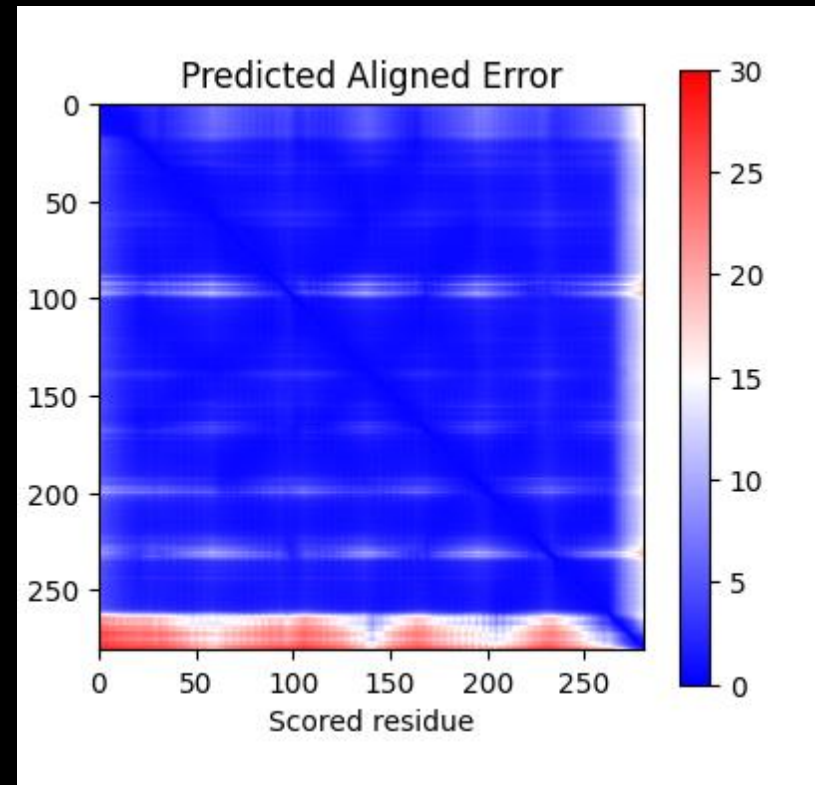
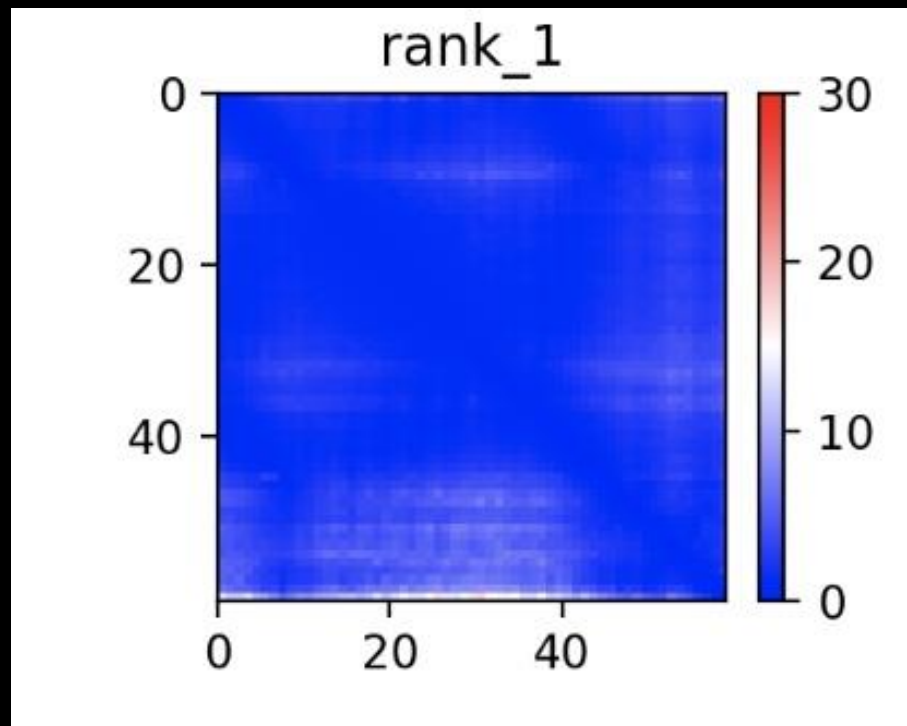
By Daniel Boudagian

ELOV7_HUMAN

- 280 Amino Acids
- Full name = Elongation of very long-chain fatty acids protein 7, human
- It is present within human cells, where it functions in the endoplasmic reticulum
- This protein is particularly important for the elongation of fatty acids, contributing to the synthesis of very long-chain fatty acids (VLCFAs)
- It plays a crucial component for various cellular structures and plays important roles in biological processes such as lipid metabolism and membrane function.

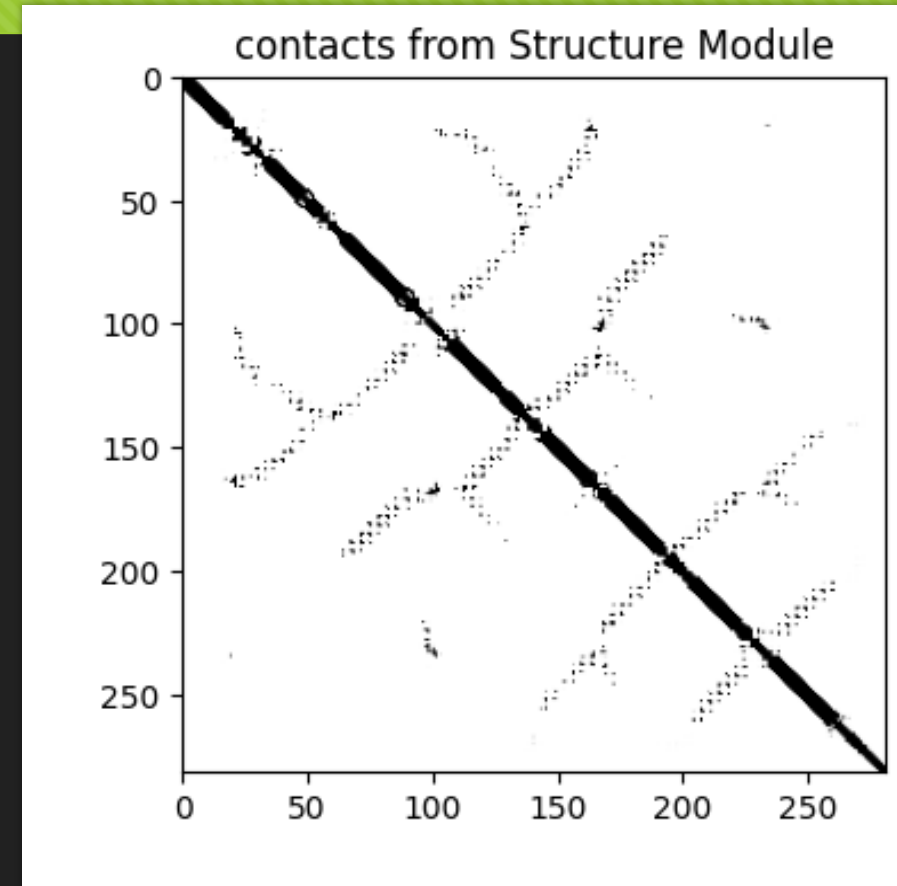
Predicted Aligned Error

- PAE is pairwise, i.e. it has a value for every residue pair
- It measures the **confidence in the relative position of two amino acids**



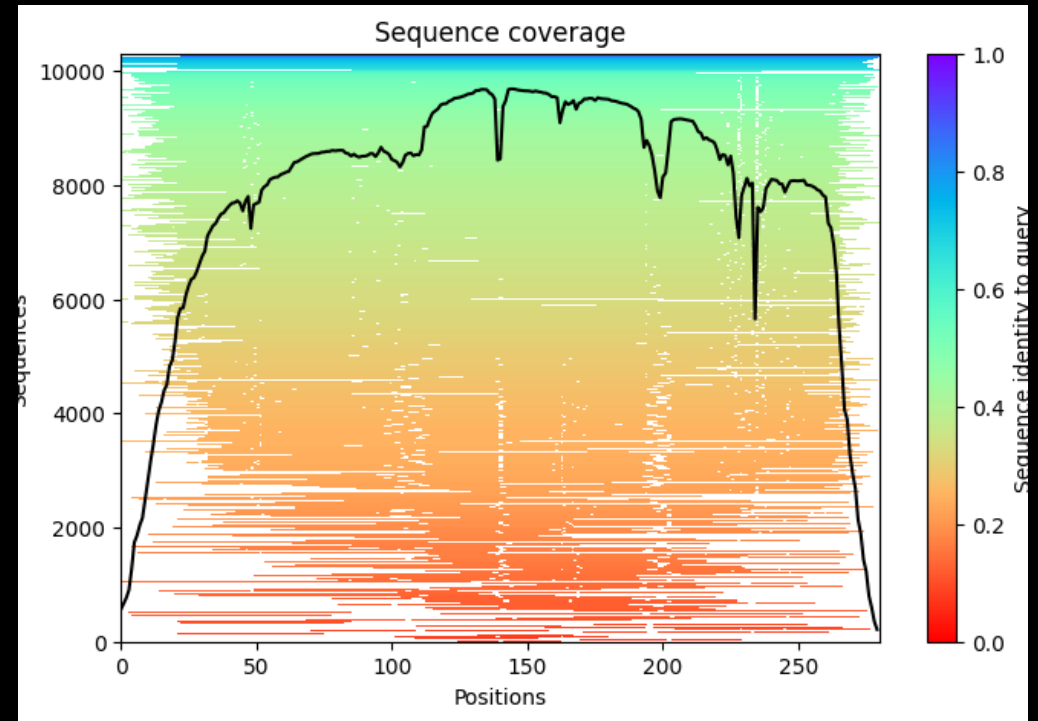
Contacts from Structure Model

- shows the predicted interactions between amino acids within a protein that are close enough to affect each other's position in the protein's three-dimensional structure.
- The patterns of contacts can suggest how the protein folds, which regions come together, and which configurations are stable



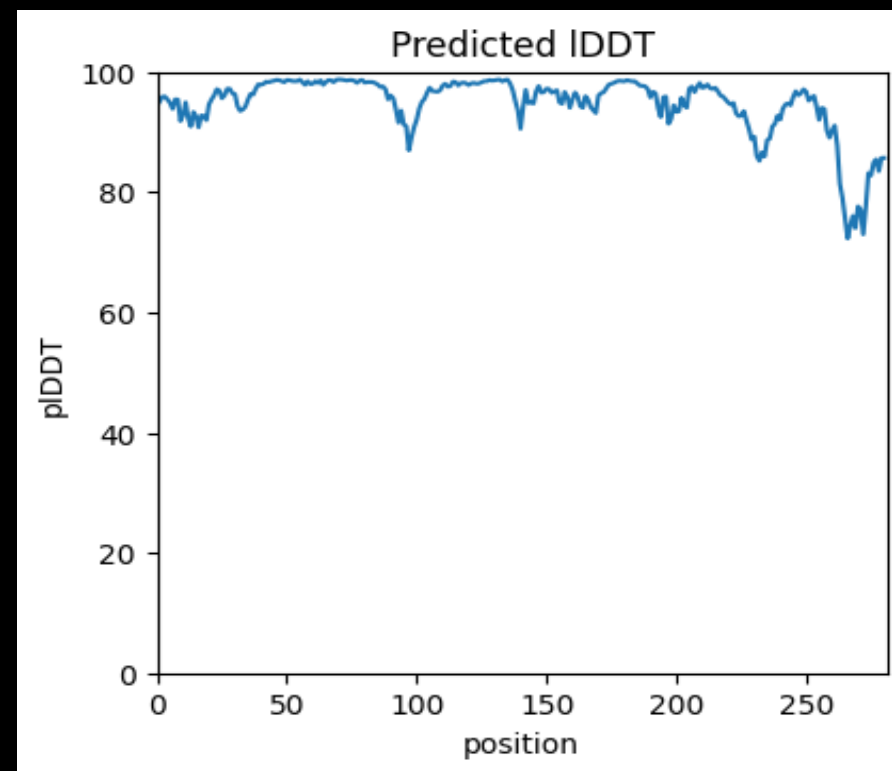
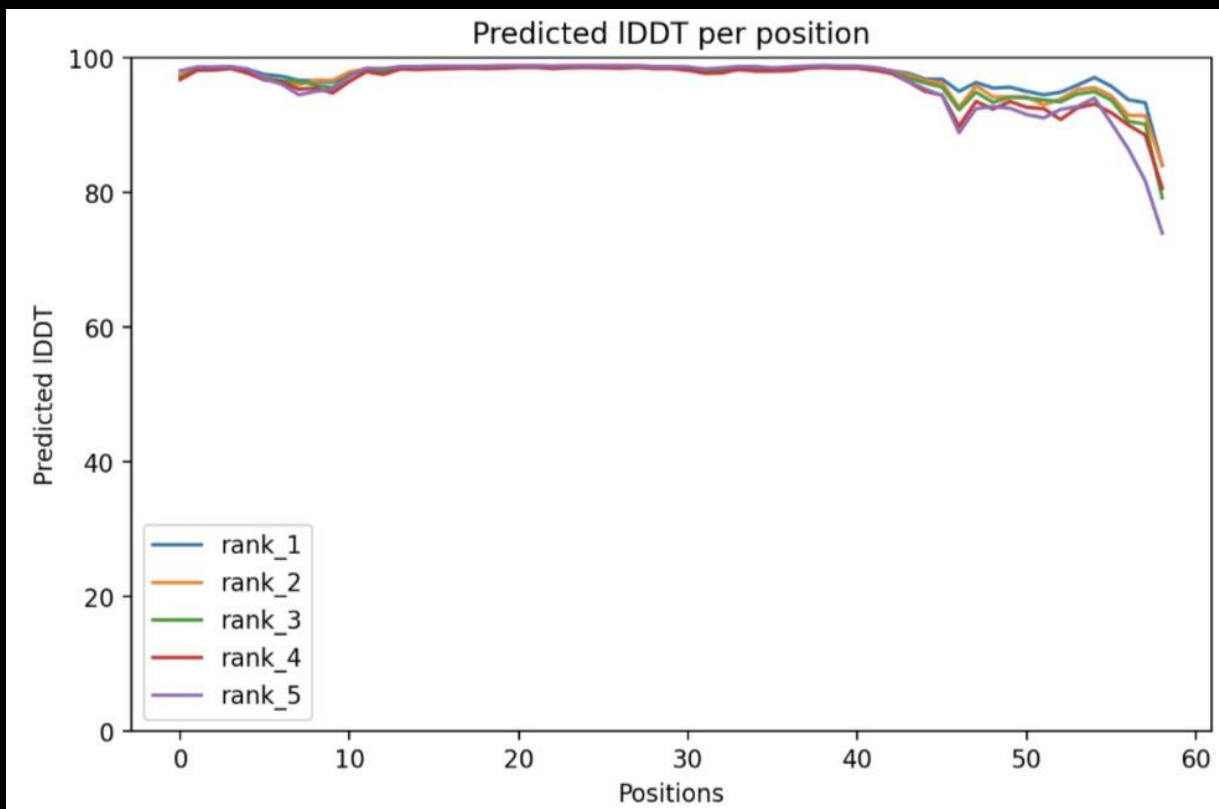
Multiple Sequence Alignment (MSA)

- - Multiple Sequence Alignment (MSA) aligns multiple sequences to the input sequences
- - Larger identities are at the top and lower at the bottom
- - The black line showing relative coverage with all the aligned sequences



PLDDT Plot

- Amino acid-level confidence measure is called PLDDT
- It is a **local accuracy metric**. Rewards **locally correct structures**, and **getting individual domains right**.
- The range of PLDDT scores is between 0 and 100

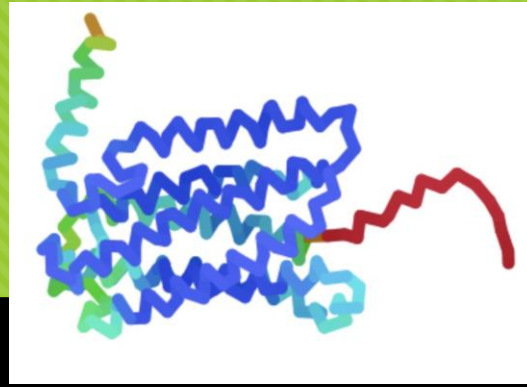


Scores

Rank 1- Model 1

pLDDT = 83.4

PTM = 0.811



Max_msa = 16:32

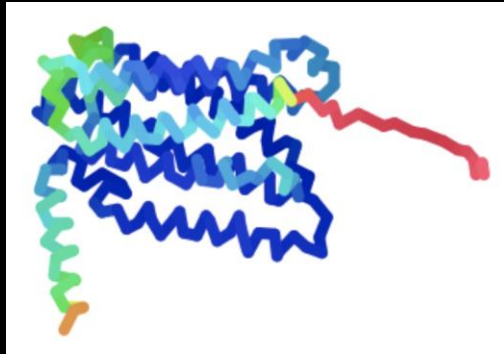
Dropout = True

Model_type = alphafold2_ptm

Num_recycles = 3

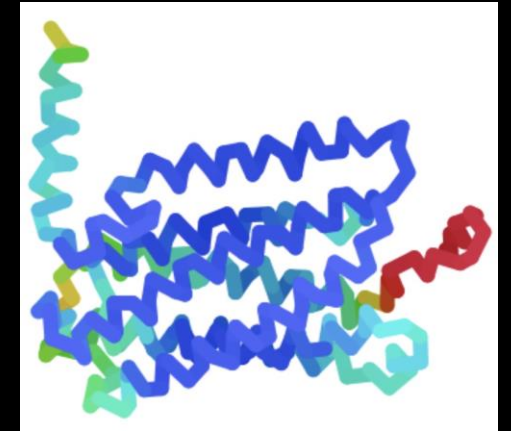
Rank 2 – Model 4

pLDDT = 83.2



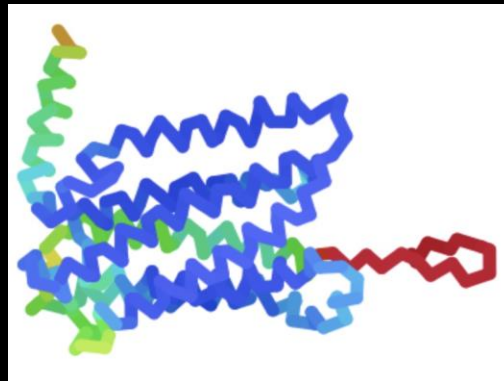
Rank 3 – Model 3

pLDDT = 83.2



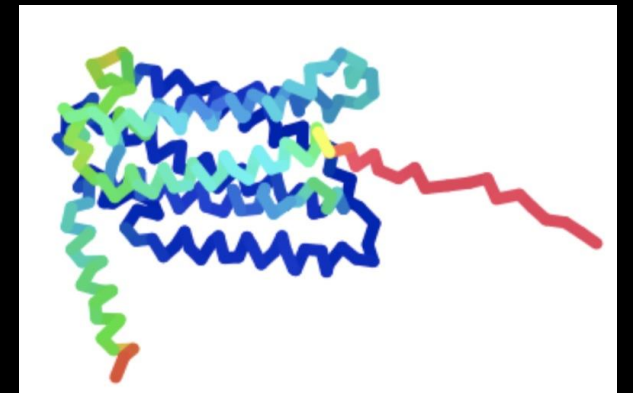
Rank 4 – Model 5

pLDDT = 83.1



Rank 5 – Model 2

pLDDT = 82.1



Scores

ESM Fold

pLDDT = 94.703

PTM = 0.925

Dpi = 100

Num_recycles = 3

