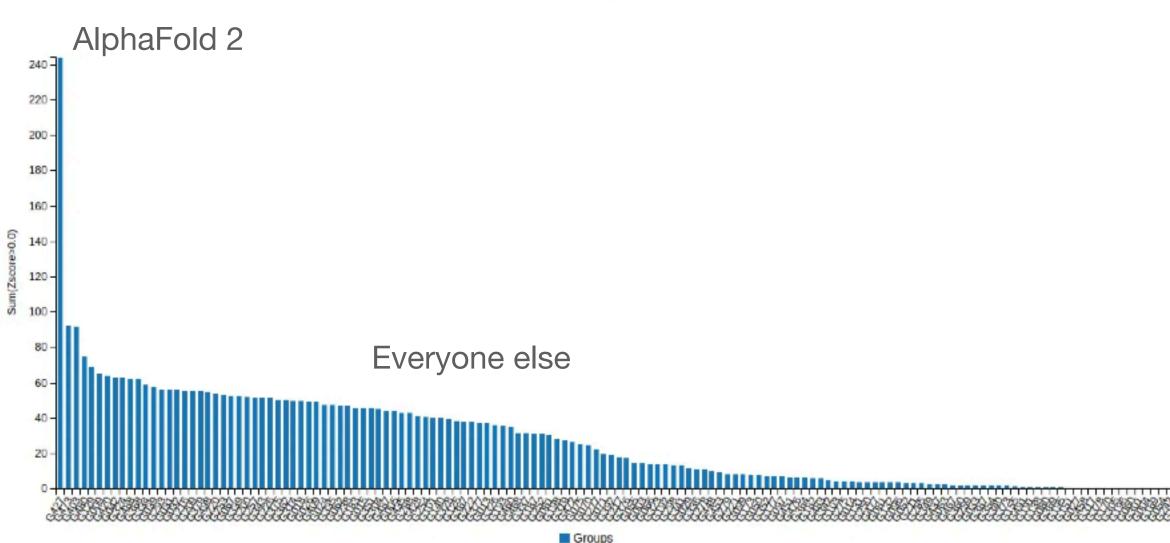
ML for protein folding

- Critical Assessment of protein Structure Prediction (CASP) biannual competition
- Predicting protein structures from amino acid sequences
- In the past two competitions, Google DeepMind used machine learning in their AlphaFold system to great success

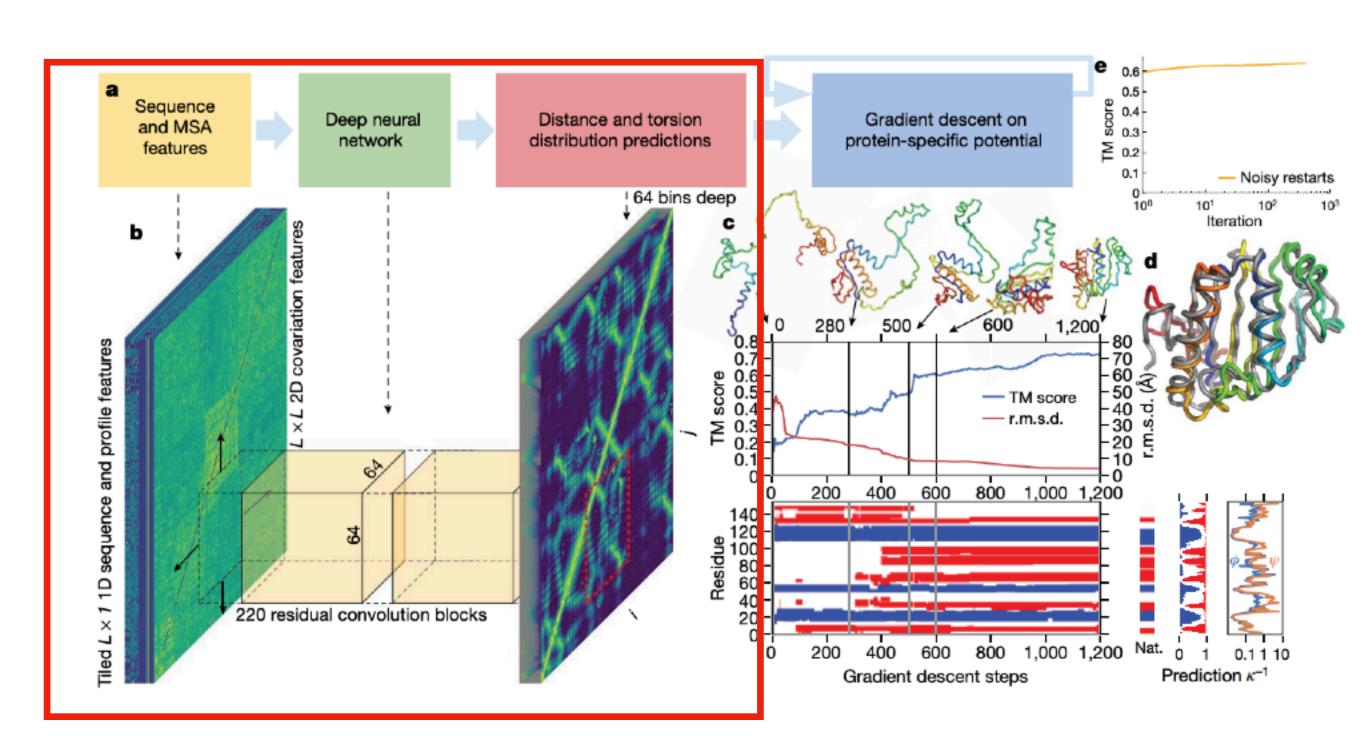
Median Free-Modelling Accuracy





AlphaFold 1 System

- The AlphaFold 1 System [2] consists of multiple components
- Specifically, the ML subcomponent contains a supervised learning task
 - Input: amino acid sequence
 - Output: a matrix of interresidue distances and torsion angles



Machine learning portion of the AlphaFold 1 System

^[2] Improved protein structure prediction using potentials from deep learning