

## Introduction

- Adaptive immune system is a key element for fighting diseases
- T cells are responsible for cell-mediated immune response
- T cell receptors (TCR) bind to pMHC complexes (protein – Major Histocompatibility Complex) to trigger immune response
- Problem:** Predict TCR-pMHC binding
- Input data [1]:**
  - Protein sequence
  - Per-residue energy terms
  - Global energy term
- Input dimensions:**
  - x observations
  - y peptide positions
  - z channels, including sequence embedding and energy terms

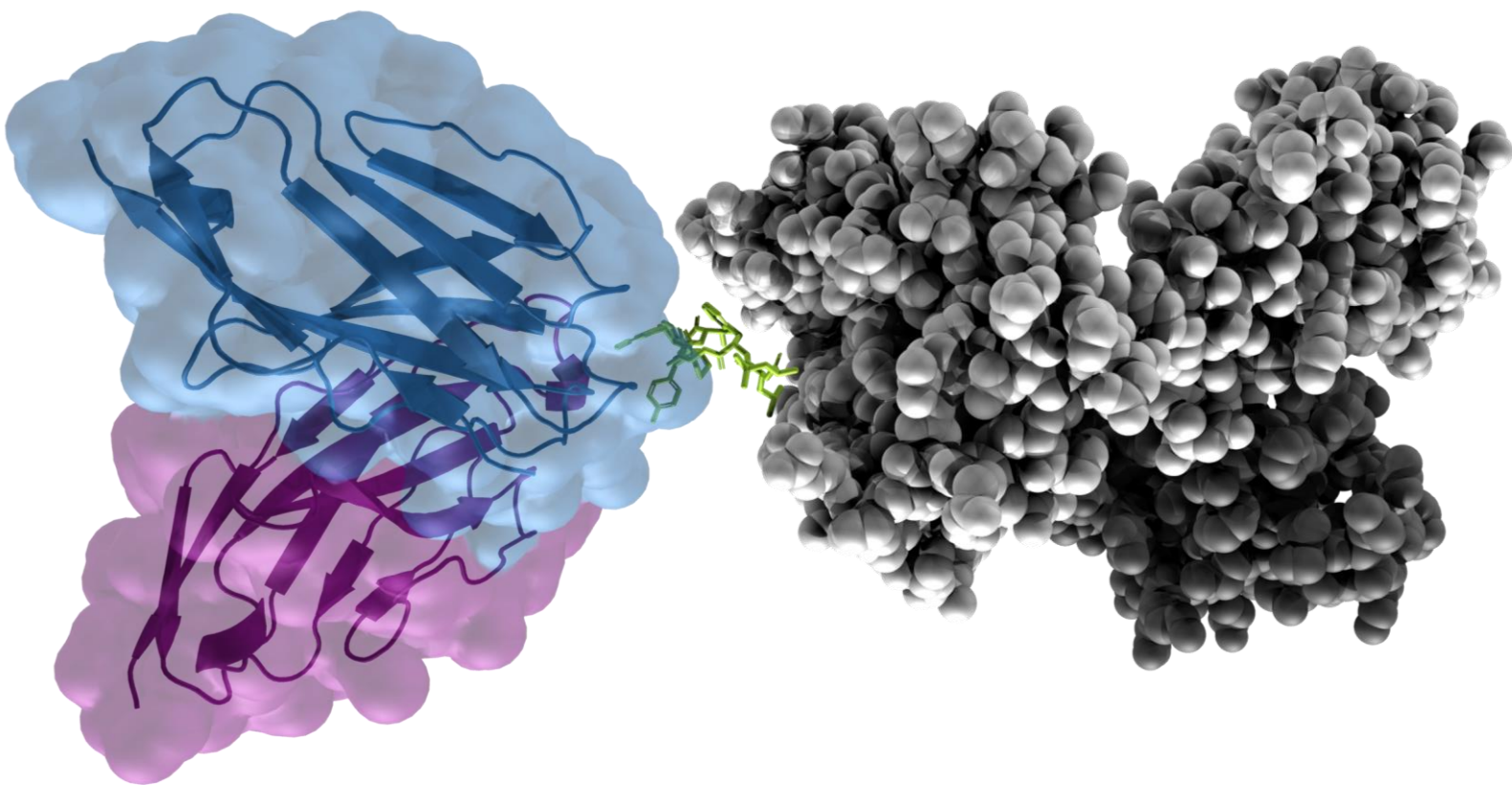


Figure 1. Three dimension visualization of the TCR-pMHC complex. Blue: TCR-α, Purple: TCR-β, Green: Peptide, Grey: MHC.

## Methods

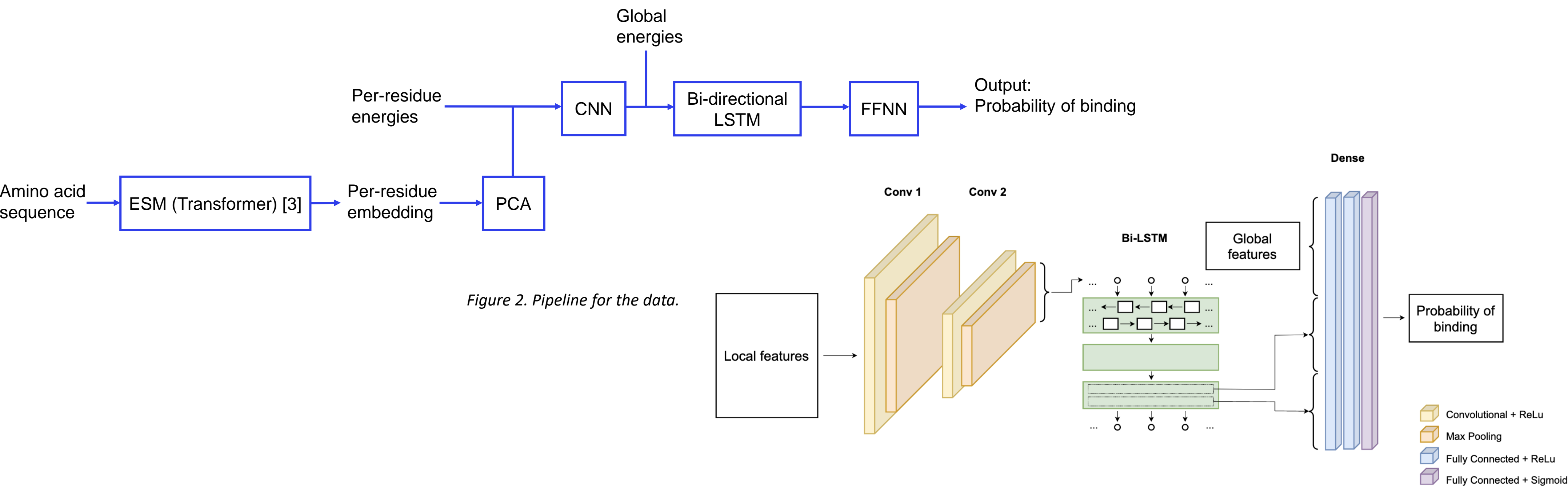


Figure 3. Architecture of the neural network.

## Results

Table 1. Comparison between our results and the result from the Master Thesis authored by Ida Meitil [2].

	AUC	MCC	Accuracy	Precision	Recall	F1
Our results						
Ida Meitil's results	0.84	0.63	0.88	0.79	0.61	0.69

Comparison with Ida [2]

MCC on test  
Confusion matrix  
AUC plot

## Discussion

High number of negative  
BERT  
Graph based approach

## References

[1] Magnus H. Høie. (2021). T-cell binding prediction challenge (TCR-pMHC). Github repository, Link: <https://github.com/CBH2021/tcr-pmhc>  
 [2] Ida Kristine Sandford Meitil. (2021). Using deep learning for improving TCR homology modeling and its application to immunogenicity prediction [Master's Thesis, DTU]  
 [3] Rives, A. et al. (2021). Biological structure and function emerge from scaling unsupervised learning to 250 million protein sequences. *Proceedings of the National Academy of Sciences*, 118(15).