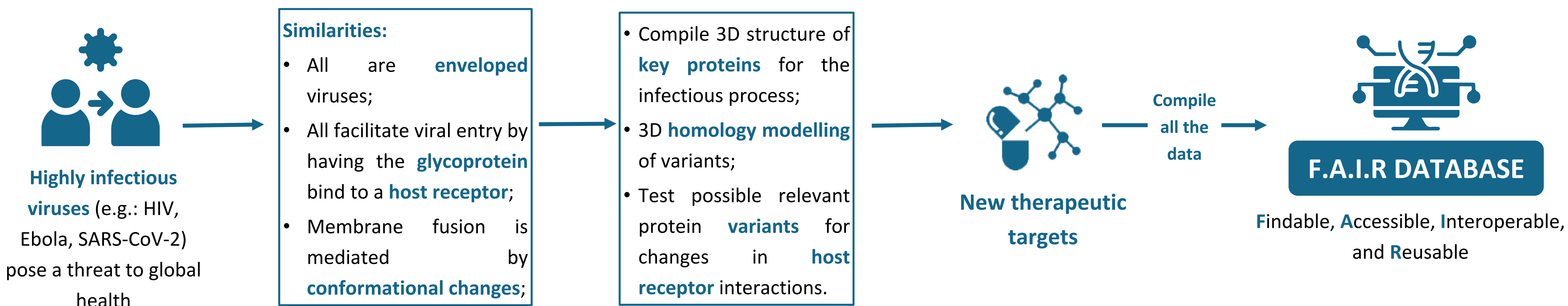


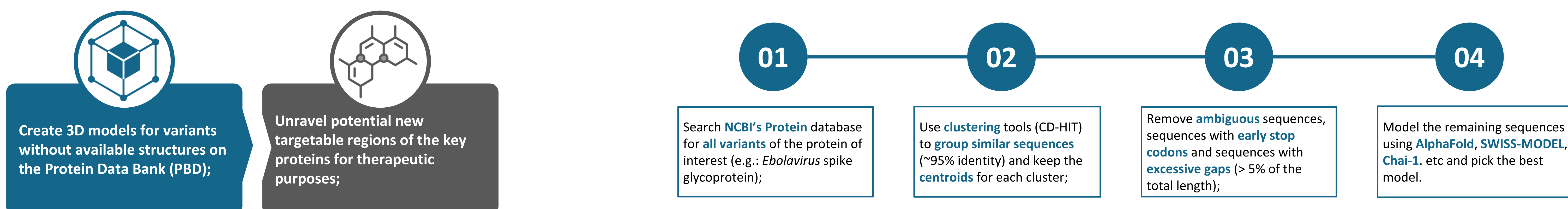
## INTRODUCTION

## AIM



## OBJECTIVES

## WORKFLOW EXAMPLE



## PRELIMINARY RESULTS

**Retrieved:**

- 2578 sequences for Ebola spike glycoprotein
- 7 sequences after filtering

- NP\_066246.1 [Zaire ebolavirus]
- AAB37093.1 [Tai Forest ebolavirus]
- AAB37096.1 [Sudan ebolavirus]
- AAC24346.1 [Reston ebolavirus]
- AAR11463.1 [Sudan ebolavirus]
- ACI28624.1 [Bundibugyo virus]
- ASJ82195.1 [Bombali virus]

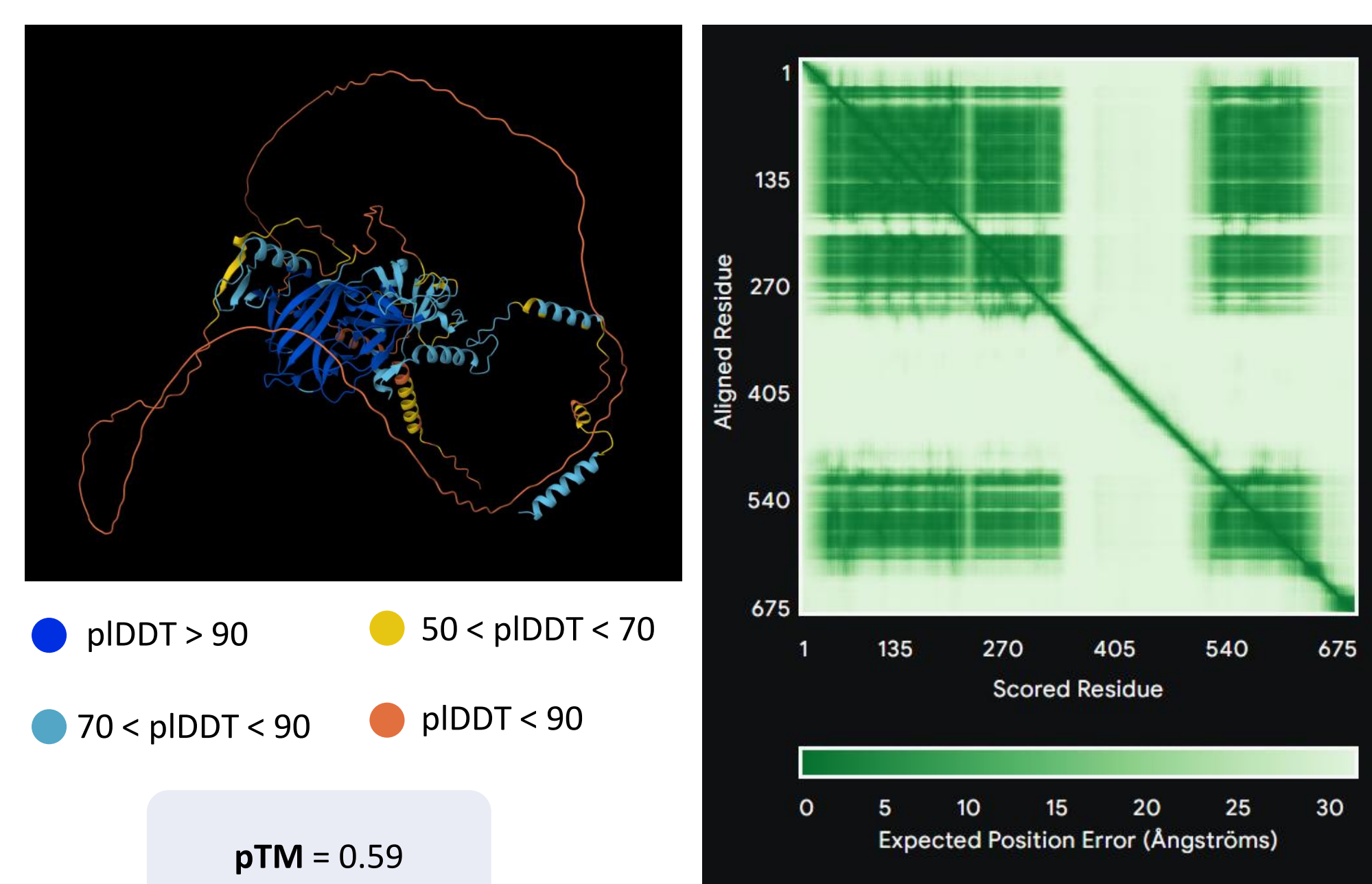


Figure 1. AlphaFold3's prediction for the structure of AAB37093.1 and the respective predicted template modelling (pTM) and per-atom confidence estimate (pLDDT) scores (left). The graph for the predicted aligned error (PAE) (right) shows low expected position errors in the receptor binding (residues 54-201) and coiled coils (residues 524-595, associated with oligomerization and fusion activity) regions.

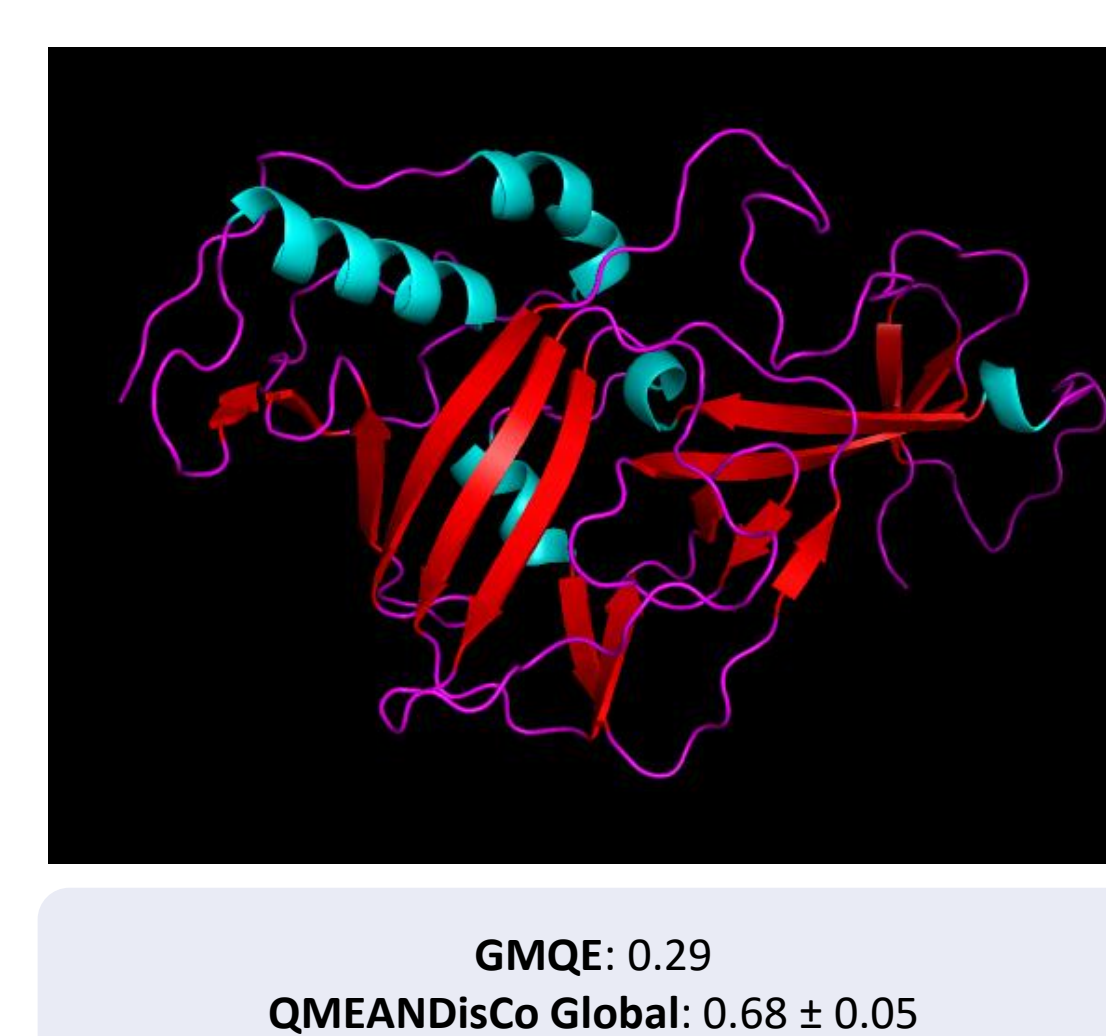
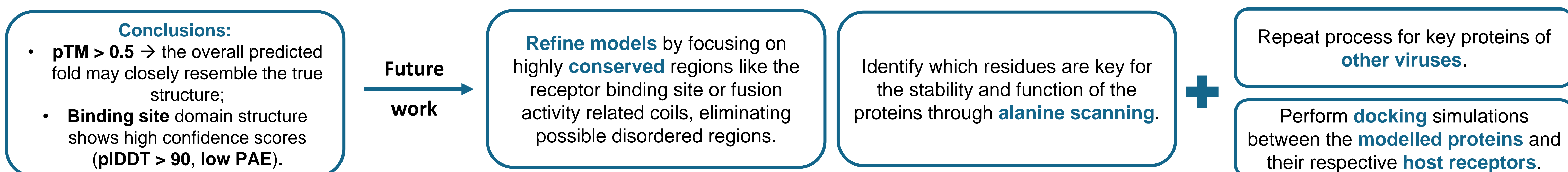


Figure 2. SWISS-MODEL's prediction for the partial structure (residues 32-311) of AAB37093.1. Global Model Quality Estimate (GMQE) evaluates the model based on template-alignment and template structure properties; thus it is coverage-dependent, which might explain the low score. QMEANDisCo Global evaluates the model "as-is", with scores closer to 1 meaning higher quality.

Table 1. MolProbity reference values and respective model scores.

Score	Goal	Model score
MolProbity Score	As low as possible	1.25
Clash Score	As low as possible	0.91
Ramachandran Favoured	≥ 98%	92.45%
Ramachandran Outliers	≤ 0.05%	1.80%
Rotamer Outliers	≤ 0.3%	0.41%
C-Beta Deviations	Zero	0
Bad Bonds	< 0.01%	0%
Bad Angles	< 0.1%	0.4%

## FINAL CONSIDERATIONS AND FUTURE WORK



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