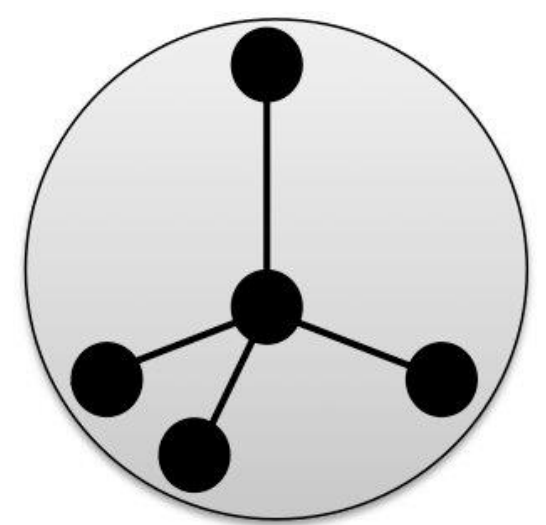




Does inclusion of residue-residue contact information boost protein threading?



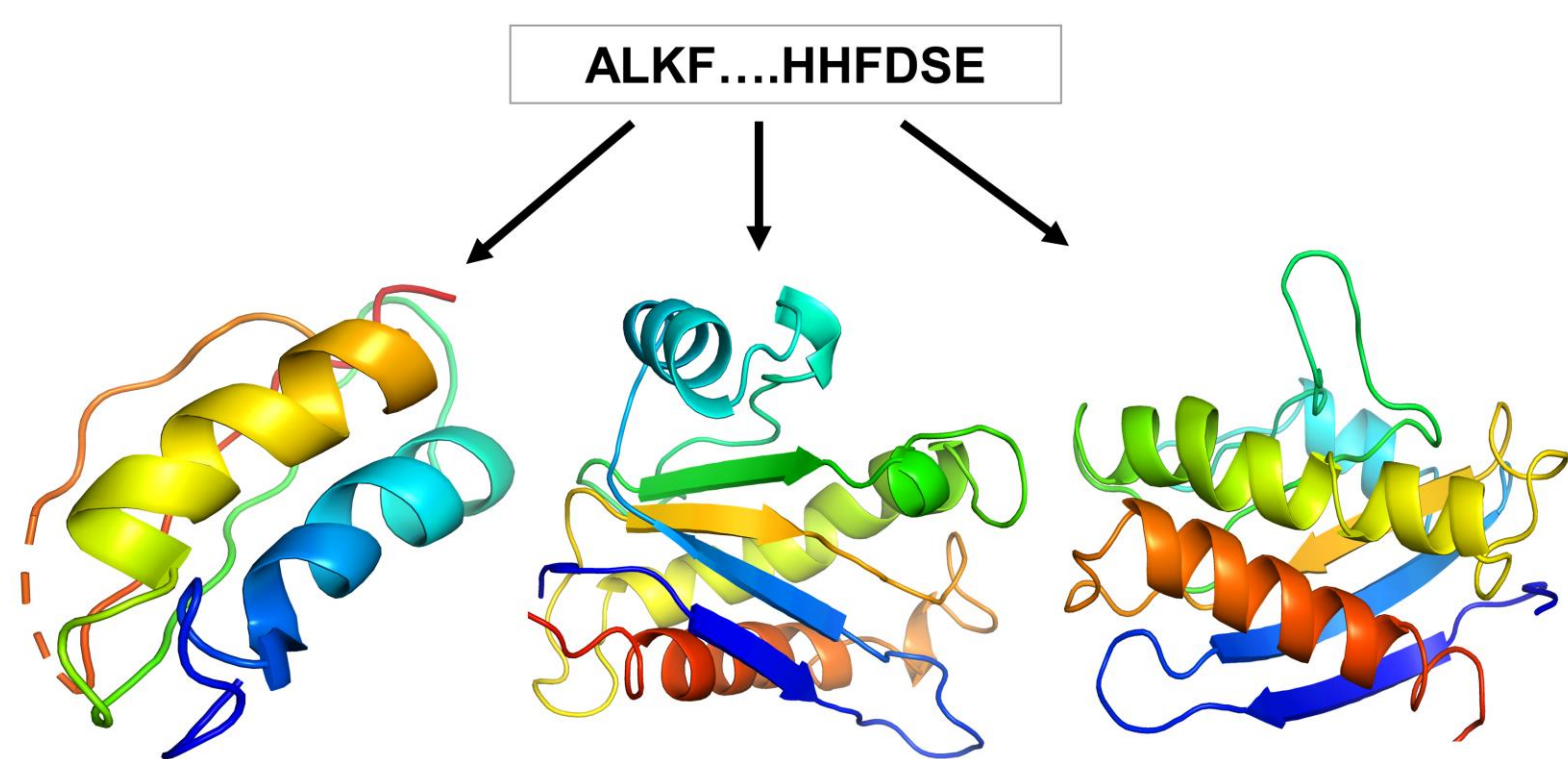
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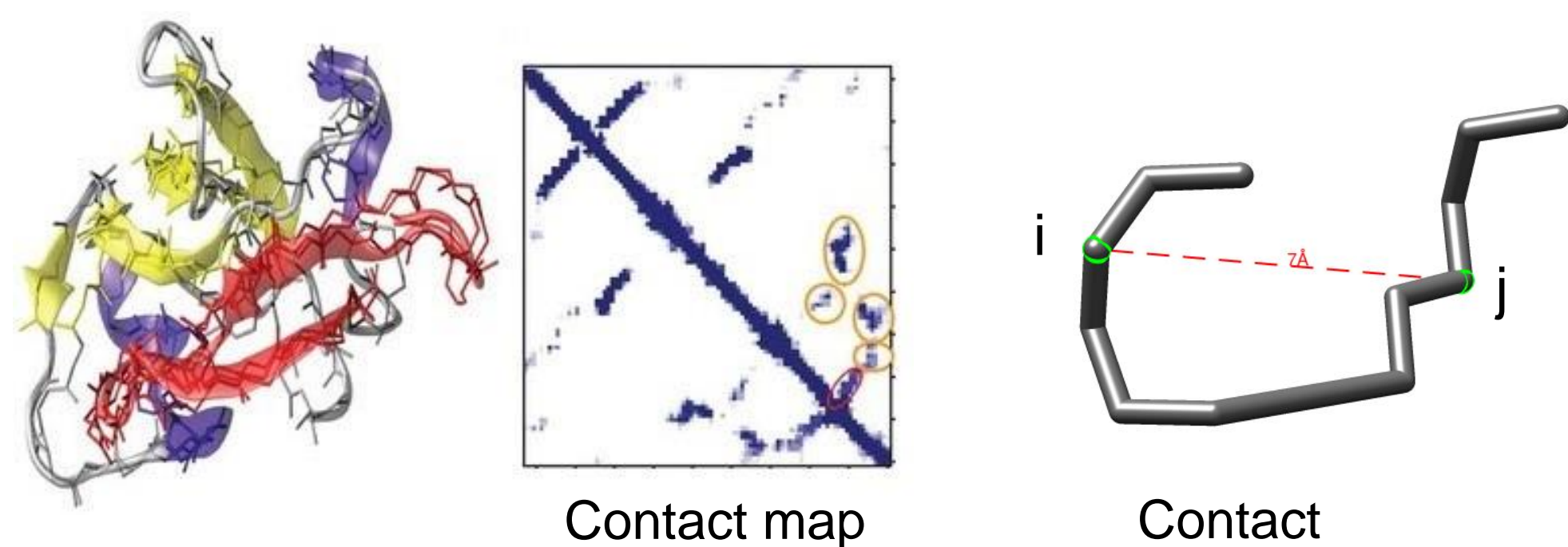
Introduction

“Given an amino acid sequence, what is the protein three-dimensional structure?”

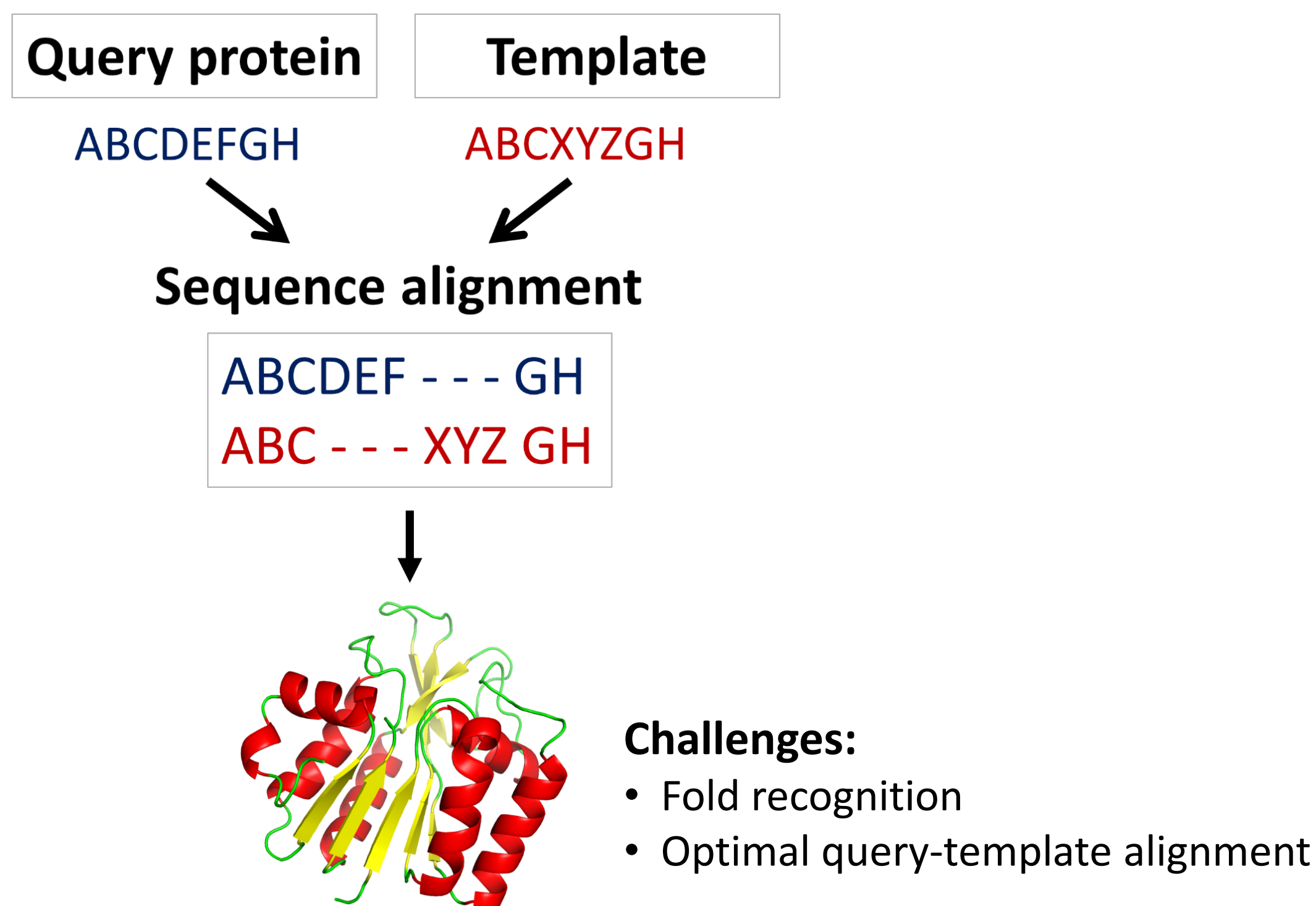


Background

Residue-residue contact map



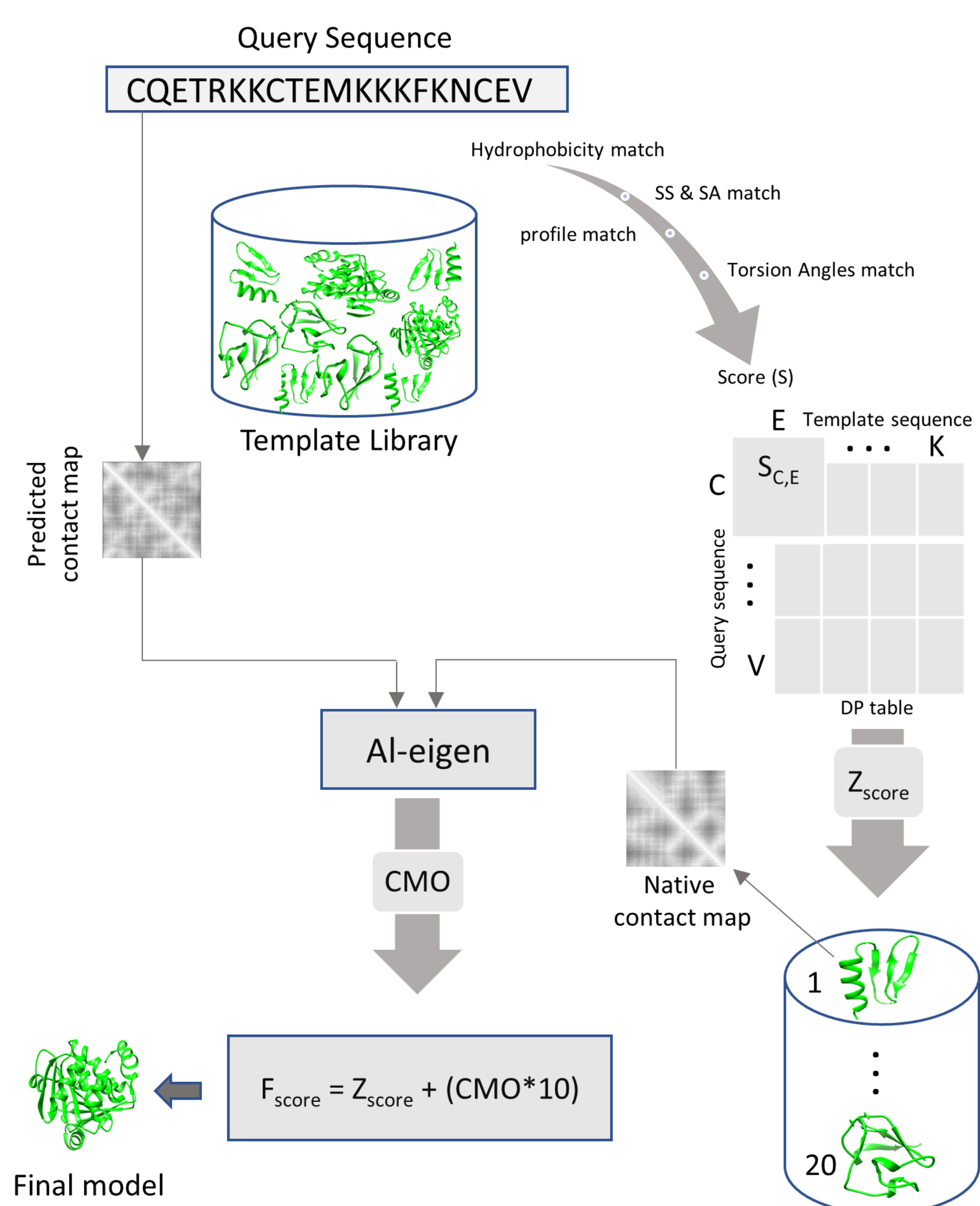
Protein threading



Research question ?

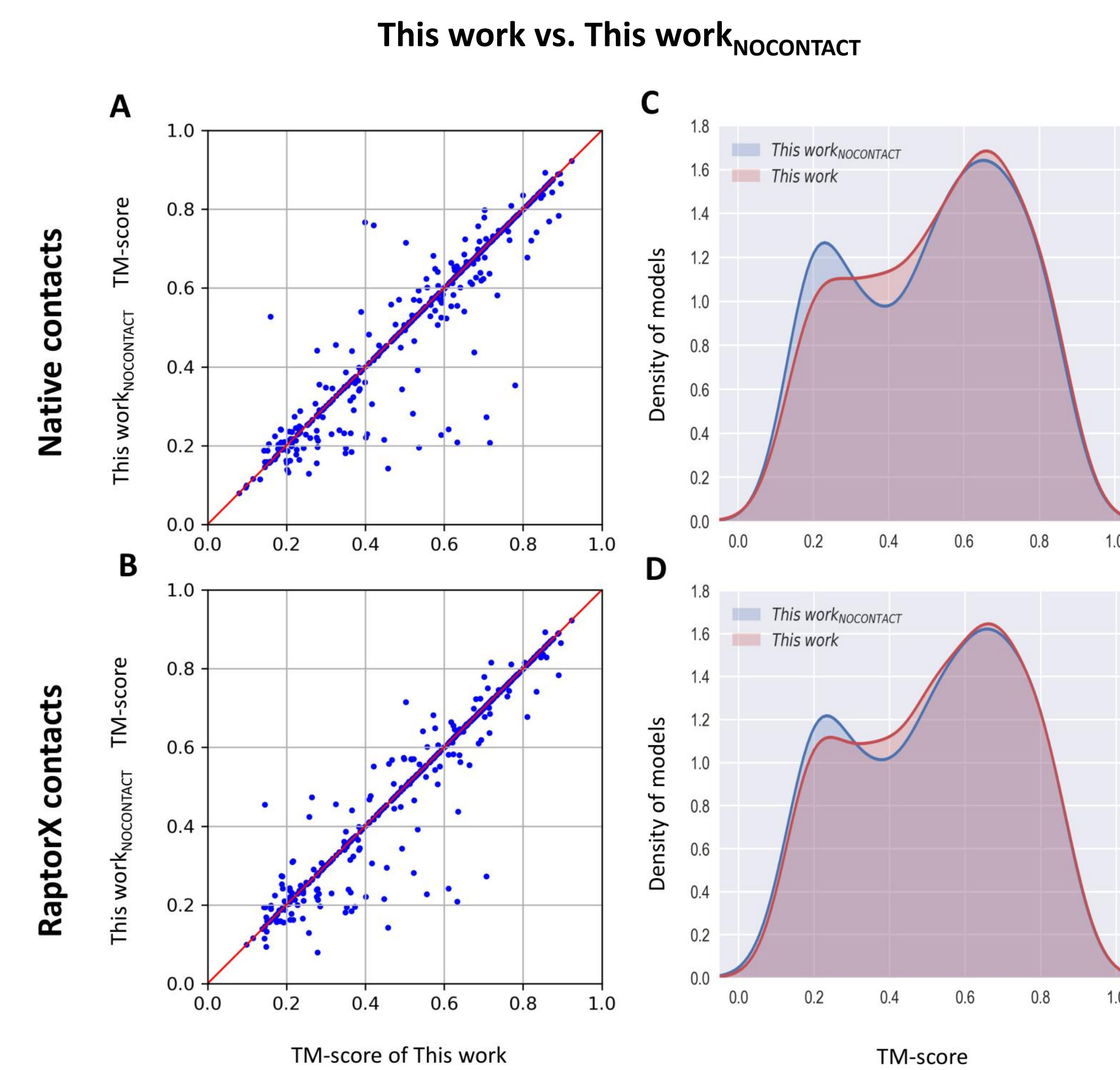
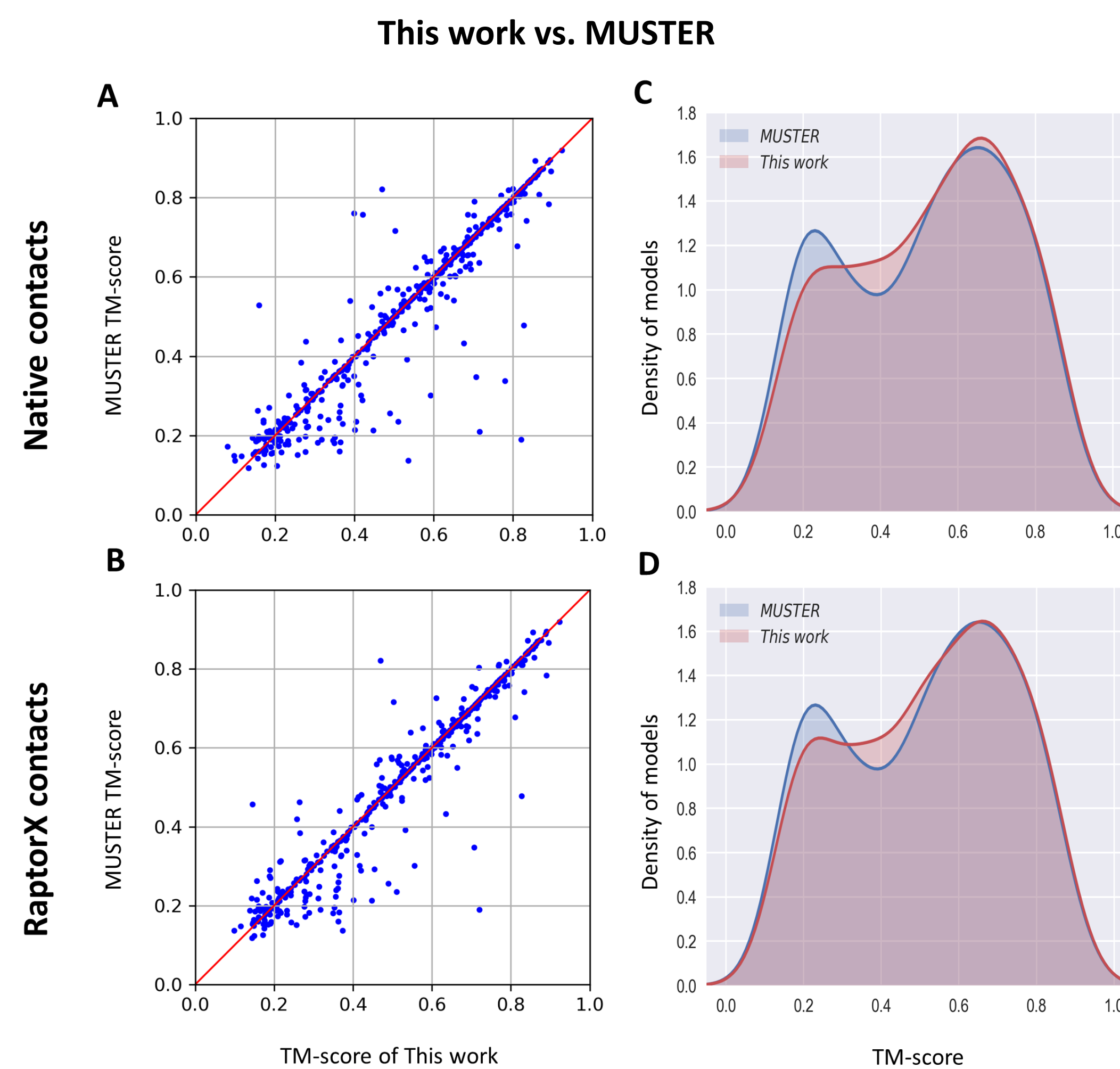
Does contact map boost protein threading?

Methods

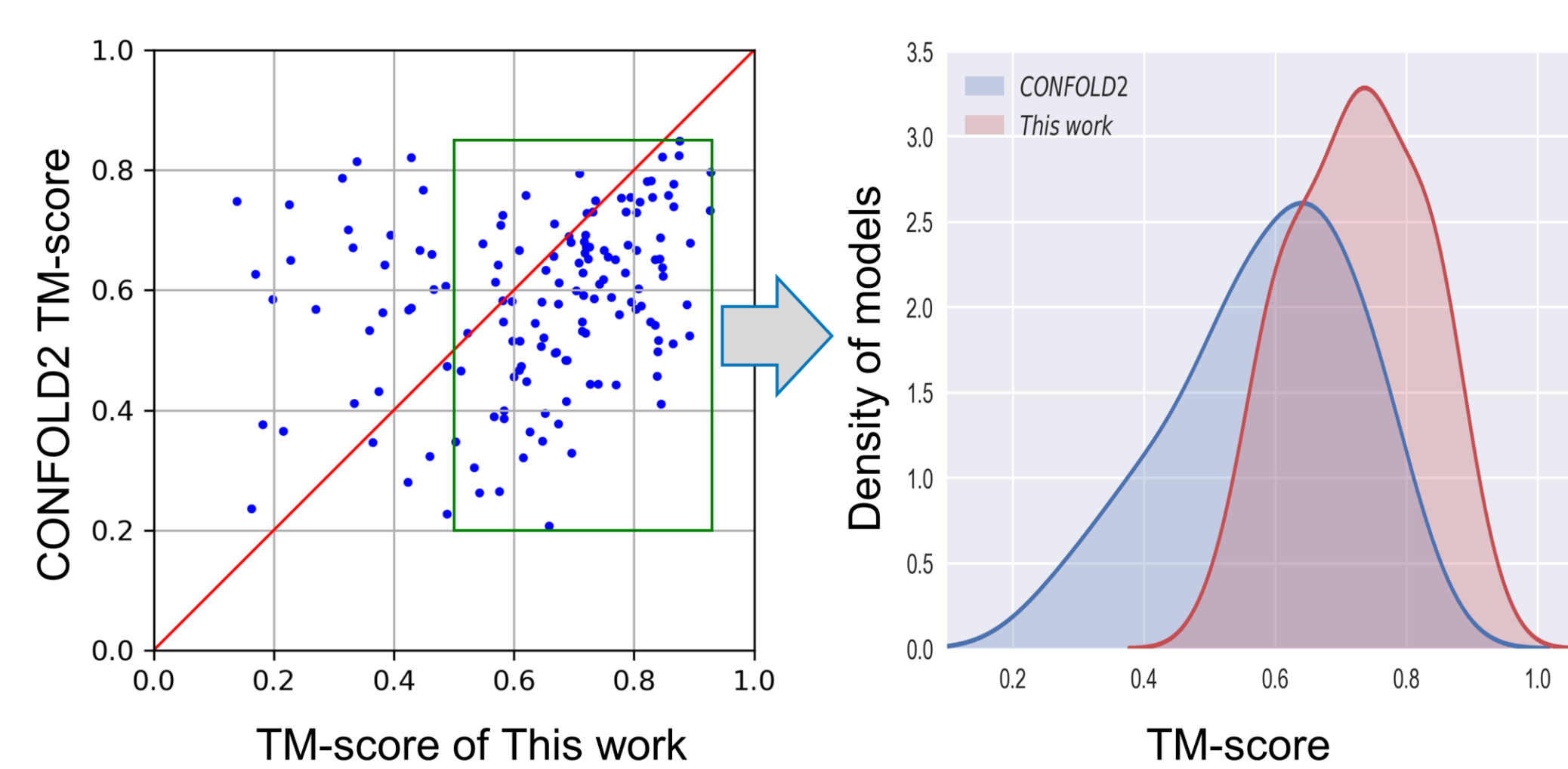


Results

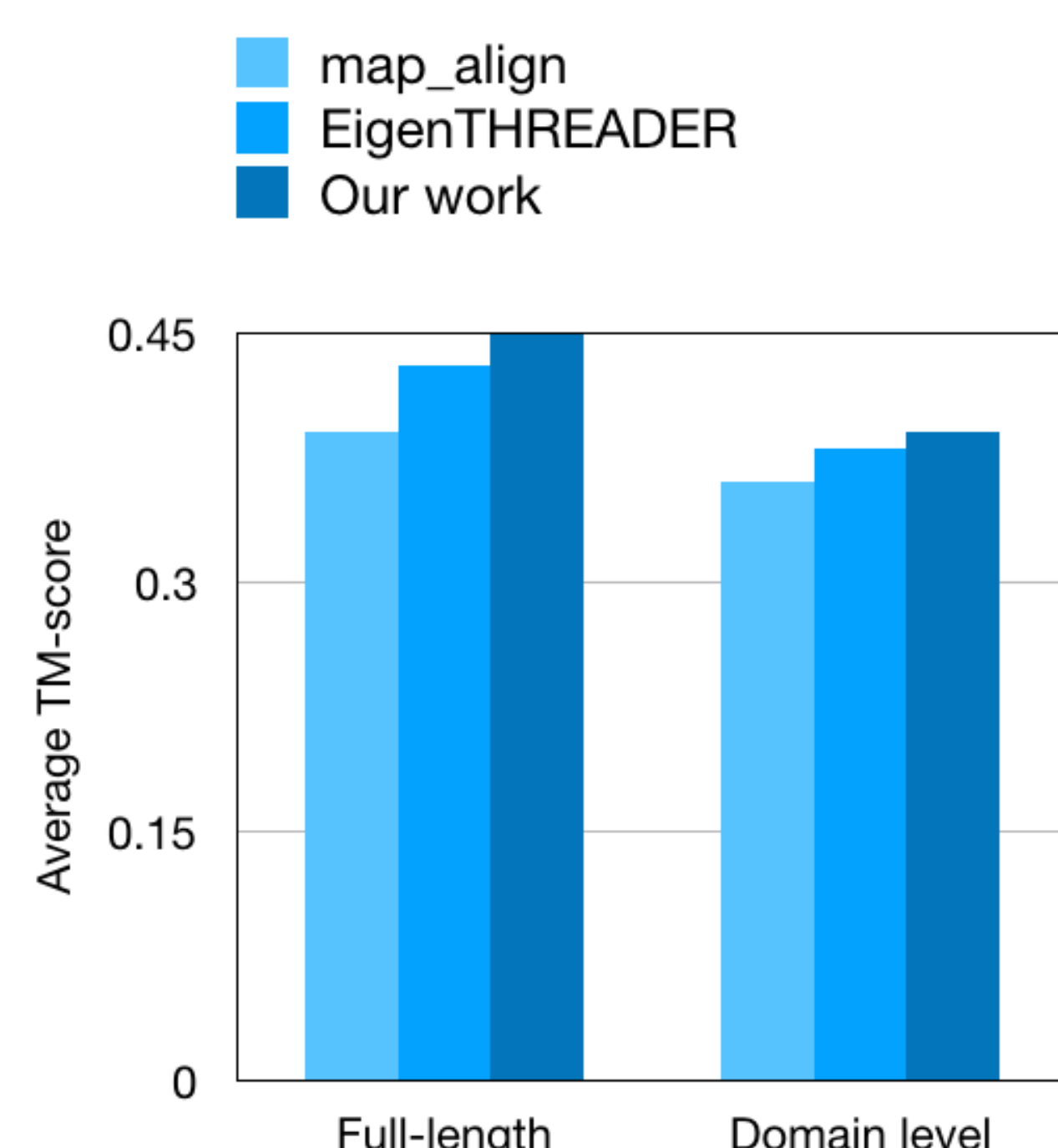
(1) Performance on Test500 dataset



(2) Performance on PSICOV150 dataset



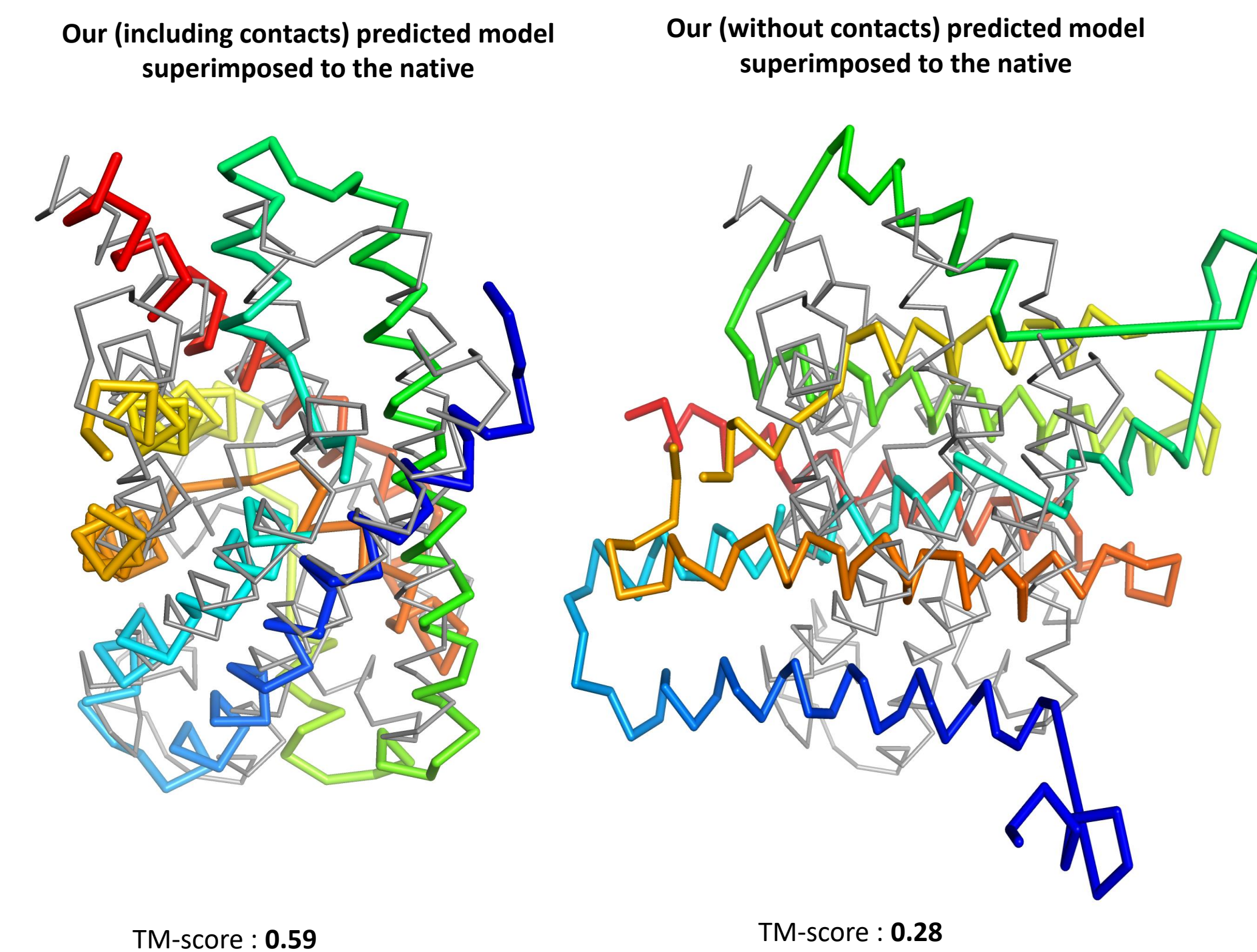
(3) Performance on CASP13 dataset



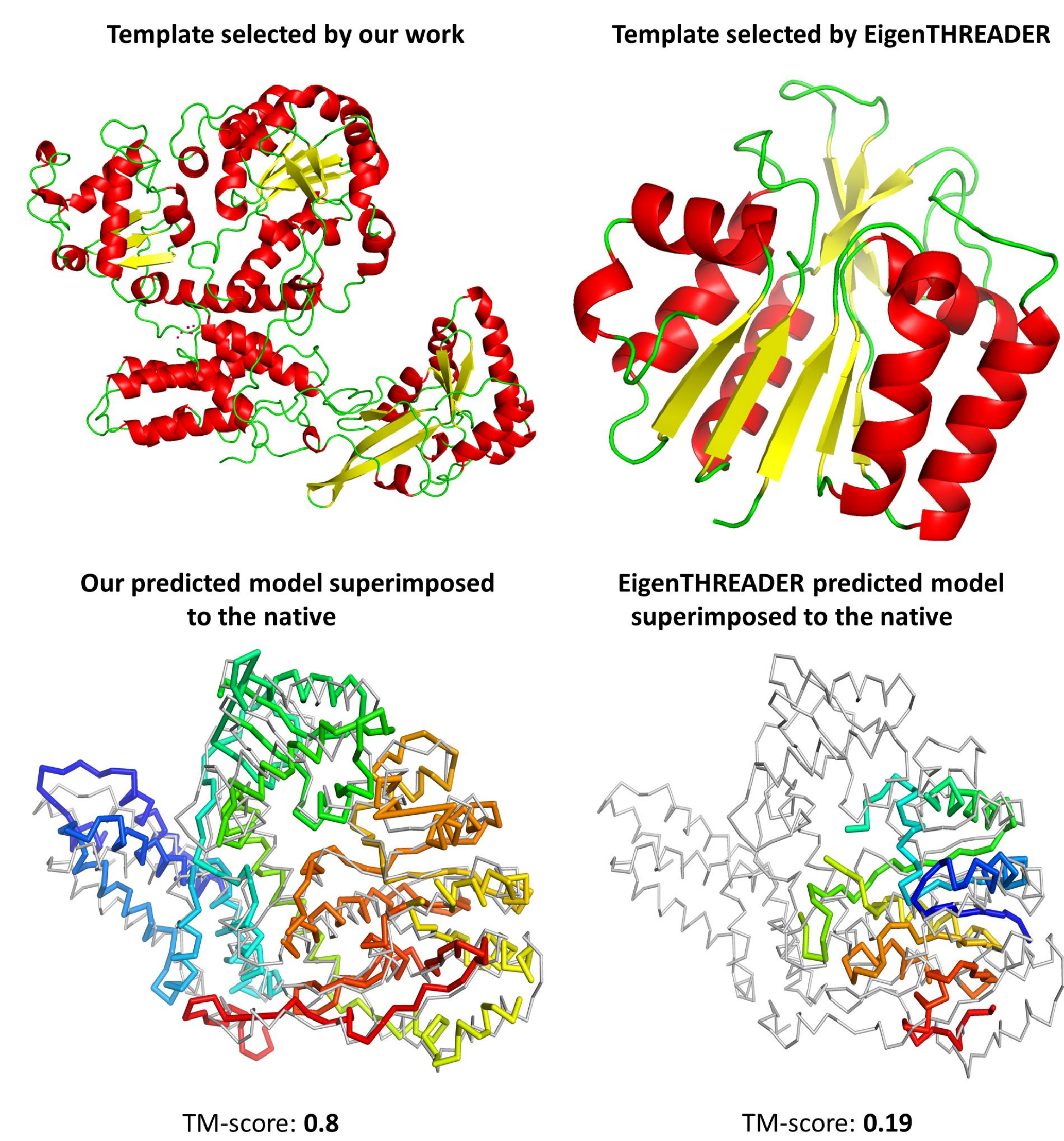
Results – con't

Case study:

Target: 2f2ba (245 residues)



Target: T0966 (494 residues)



Conclusions

- Test500: contact + threading better than pure threading
- PSICOV150: contact + threading better than contact-assisted ab initio folding method
- **Contact boosts threading.**

Future works

- Does contact improve query-template **alignment**?
- Is **distance** more informative than **contact** in improving protein threading?

Reference

- Bhattacharya, S. and Bhattacharya, D. (2019), Does Inclusion of Residue-Residue Contact Information Boost Protein Threading?. Proteins. Accepted Author Manuscript. doi:10.1002/prot.25684