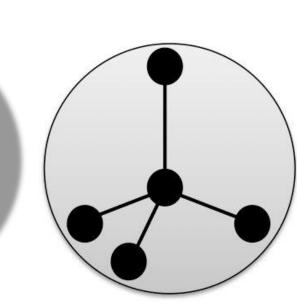


Does inclusion of residue-residue contact information boost protein threading?

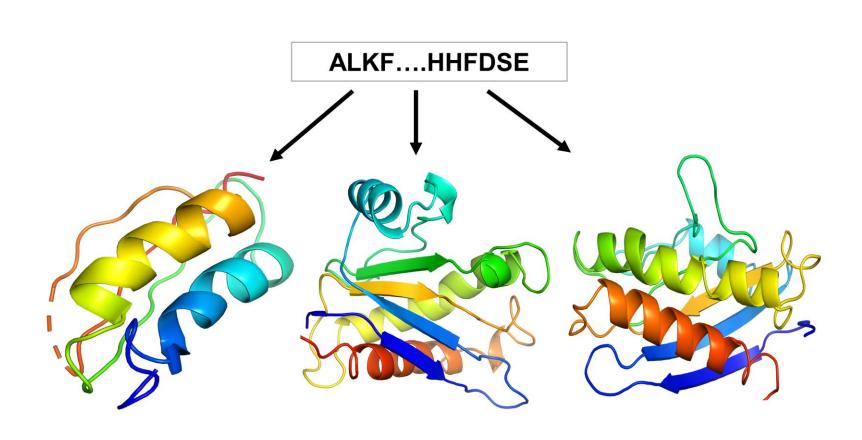


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*Corresponding Author: bhattacharyad@auburn.edu

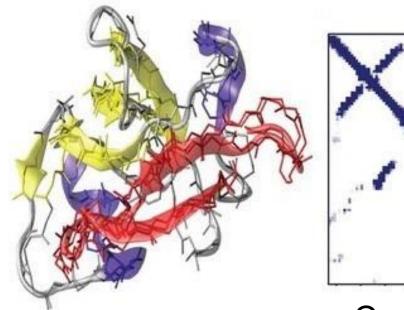
Introduction

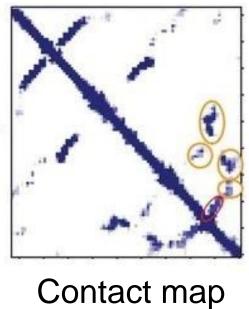
"Given an amino acid sequence, what is the protein threedimensional structure?"

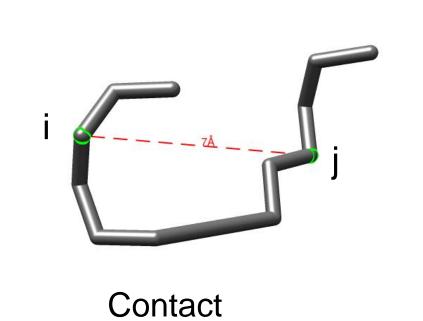


Background

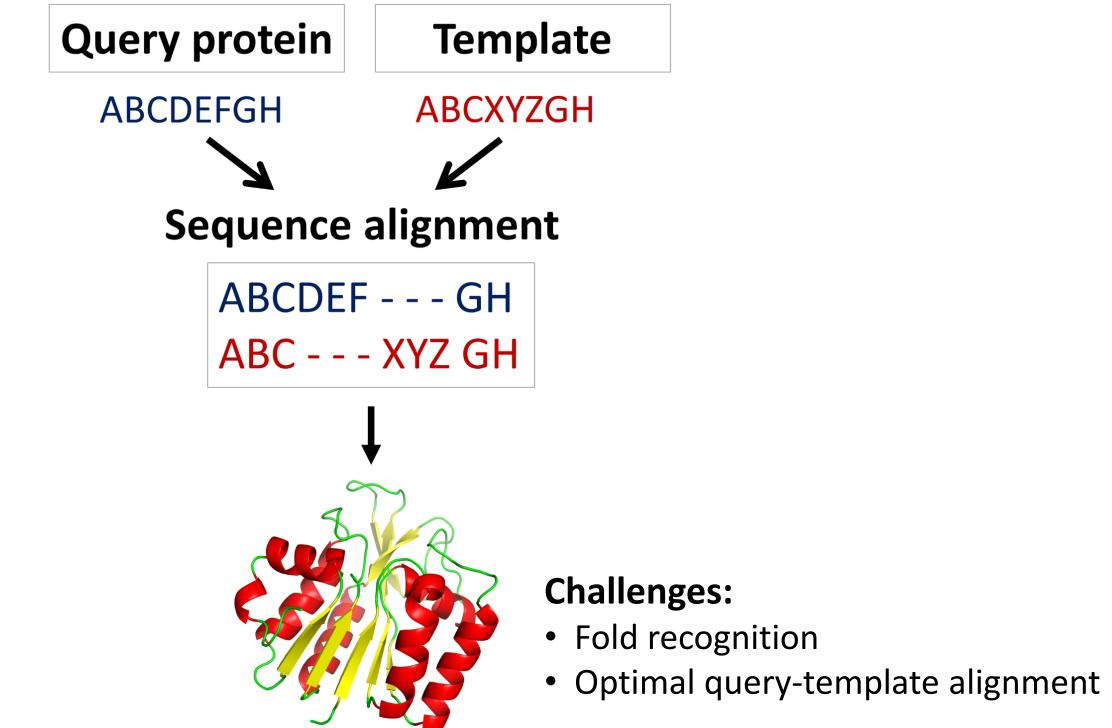
Residue-residue contact map







Protein threading



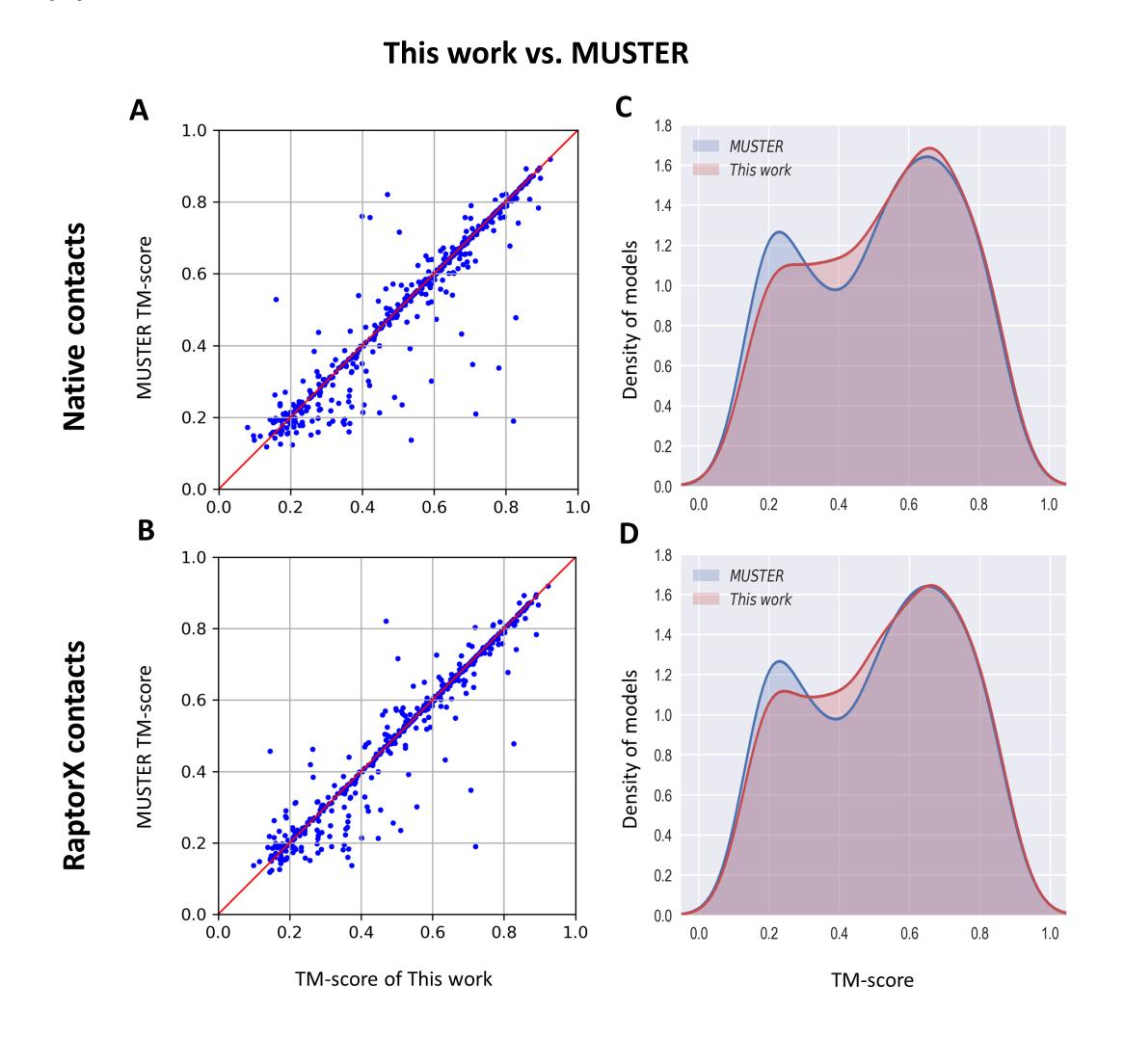
Research question?

Does contact map boost protein threading?

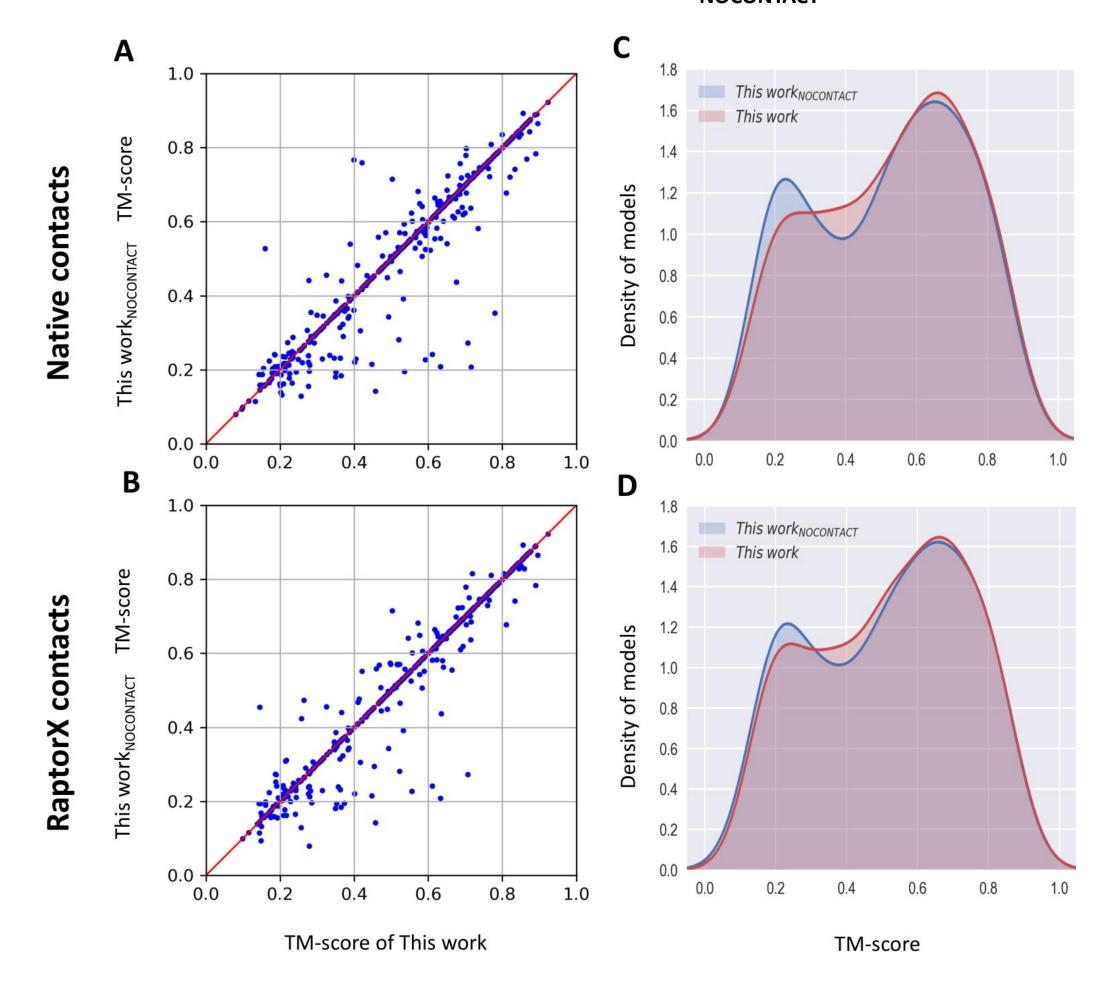
Methods **Query Sequence** CQETRKKCTEMKKKFKNCEV Hydrophobicity match SS & SA match profile match Torsion Angles match Score (S) F Template sequence **Template Library** DP table Al-eigen CMO Native contact map $F_{\text{score}} = Z_{\text{score}} + (CMO*10)$ Final model

Results

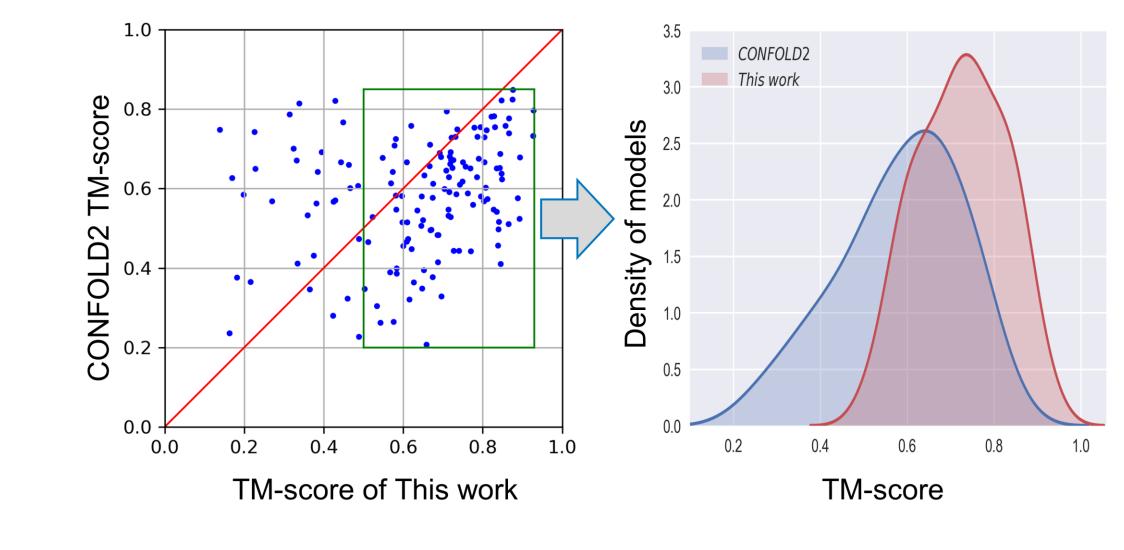
(1) Performance on Test500 dataset



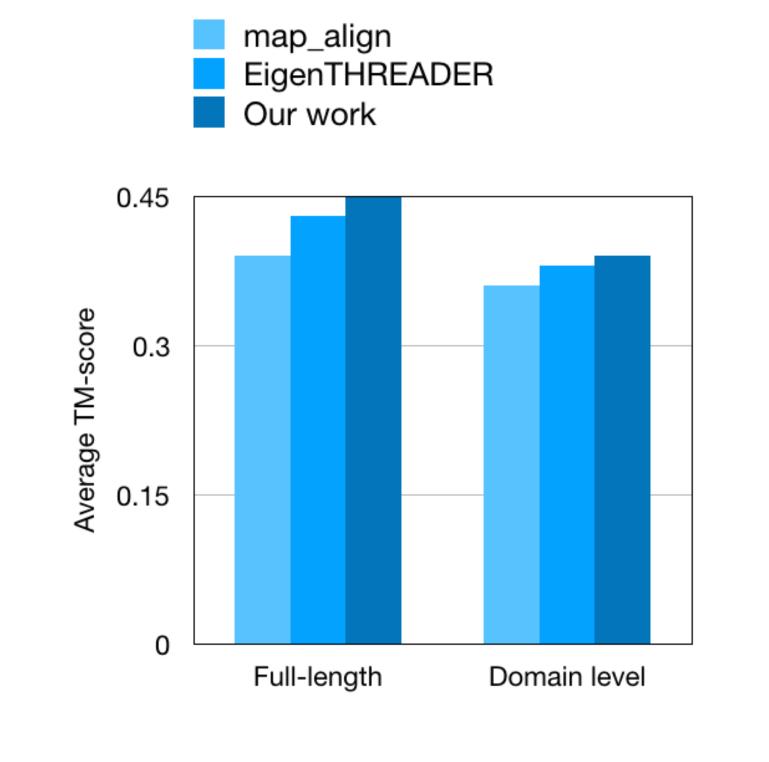
This work vs. This work_{NOCONTACT}



(2) Performance on PSICOV150 dataset



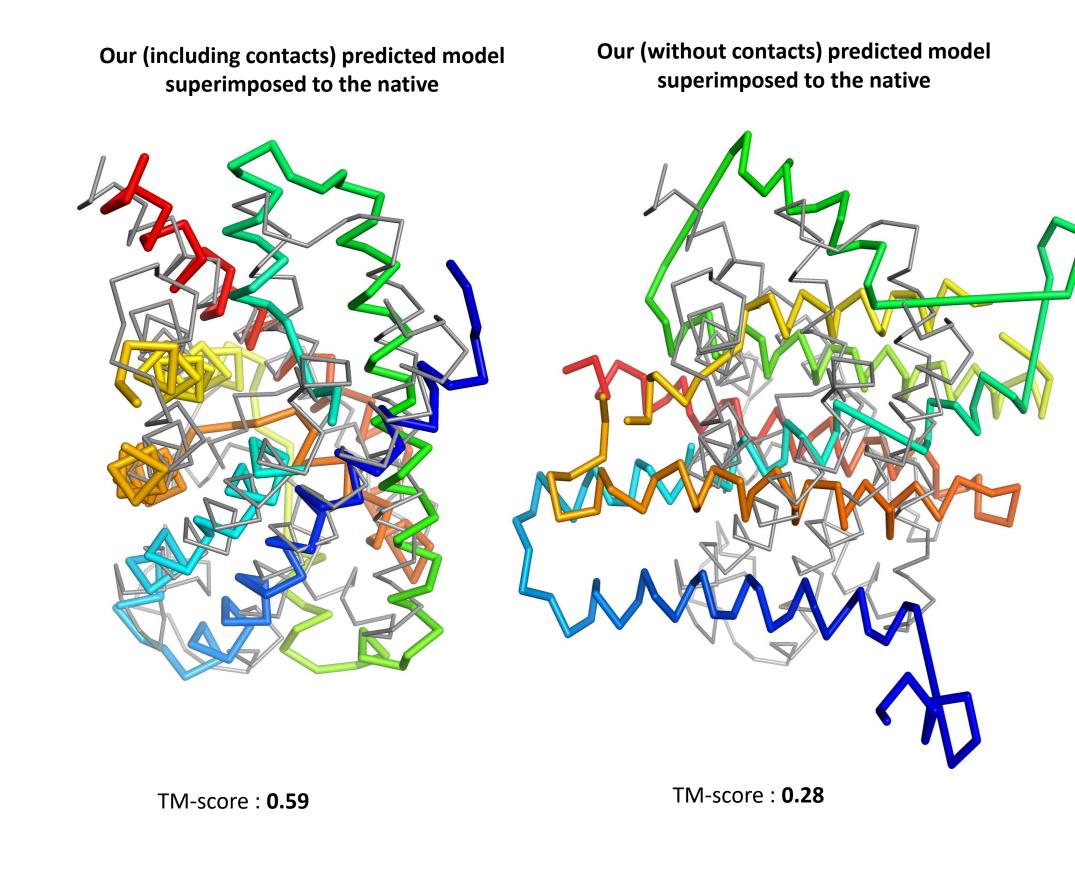
(3) Performance on CASP13 dataset



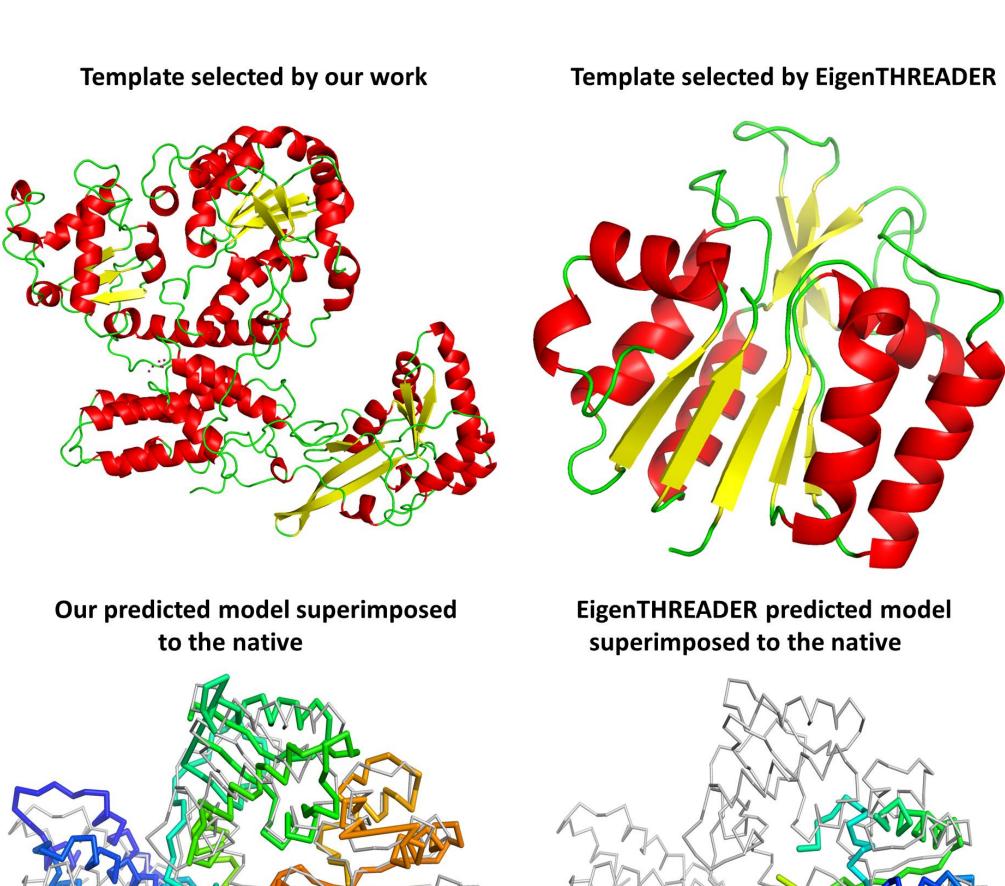
Results – con't

Case study:

Target: **2f2ba** (245 residues)



Target: **T0966** (494 residues)



TM-score: 0.8

TM-score: **0.19**

Conclusions

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

Future works

- query-template contact improve Does 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