

First multi-template model

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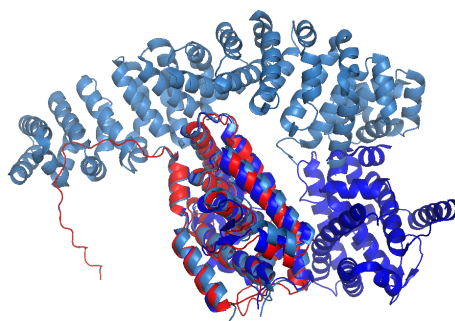


Fig. 1: Example of a multiple model, our unknown sequence threaded onto 3XT7 and 3PLZ. Colors: red = our model, blue = templates.

I have written a script that uses more than one model into a sequence/structure MSA and then threads our unknown sequence onto the alignment of all structures (somehow). An example using only two templates is shown in Fig. 1.

I have also written a small pymol script that outputs figures of a) the original structure with the predicted one and b) all templates with the predicted one. The results are presented in Fig. 2.

We still need to “present results in a convenient way”. According to Sven’s hint, this should amount to calculate overlap between our predicted sites and the true structure, or the templates...? The latter seems to be a silly way of evaluating a prediction, but – oh, well.

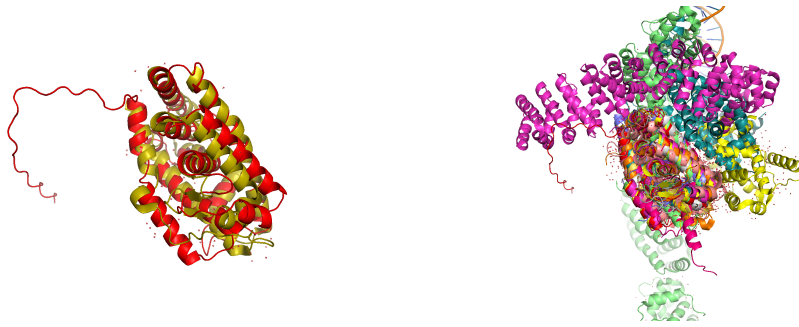


Fig. 2: Example of a multiple model, our unknown sequence threaded onto ten similar PDB entries. Left hand side: the predicted structure against the true one; right hand side: the same against all ten models. Colors: red = our model, gold = true structure, other = templates.