Interpreting the Output of the Undertaker Protein-Folding Algorithm

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- SAM-T06, T04, and T2K Hidden Markov Models iterate through databases for similar alignments and helix and sheet patterns
- Undertaker algorithm produces probable structure based on:
  - Alignment with fragments
  - Probabilistic burial, calculated from other sequences
- Extra parameters are introduced to improve accuracy

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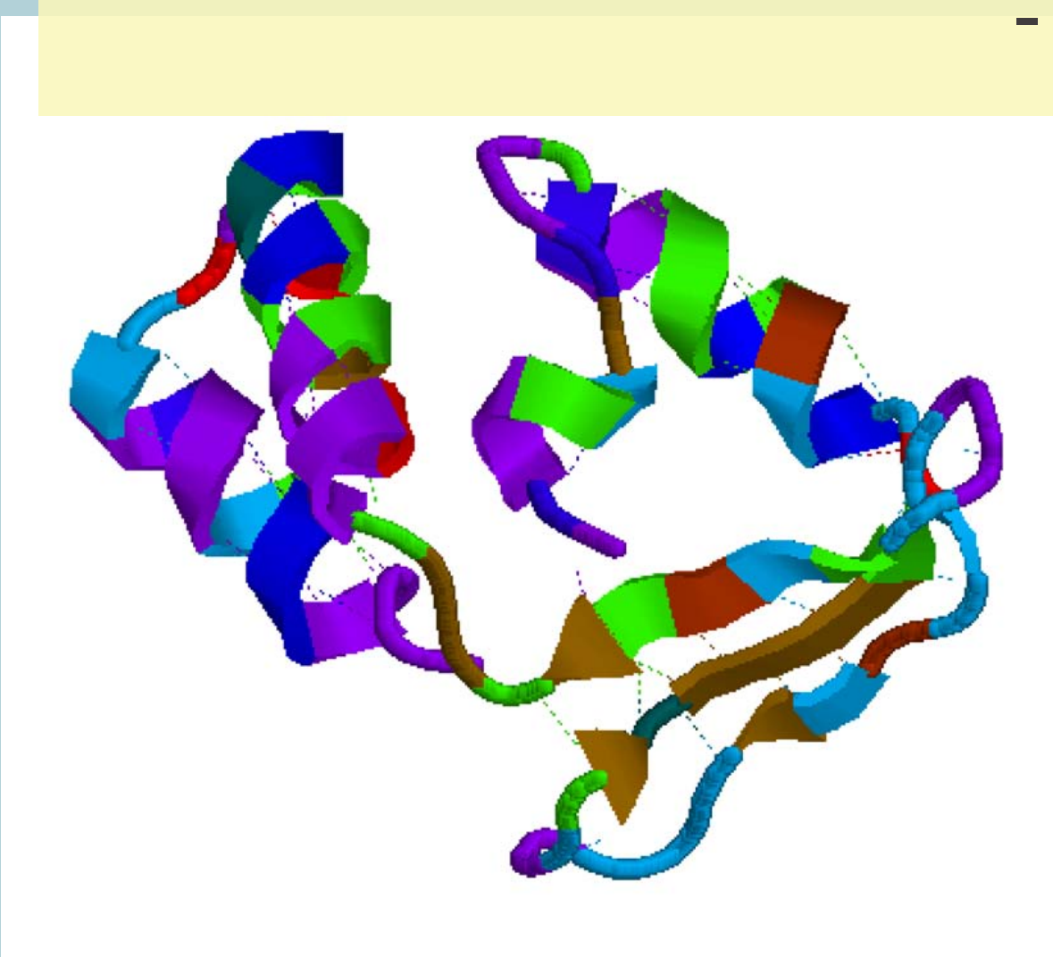
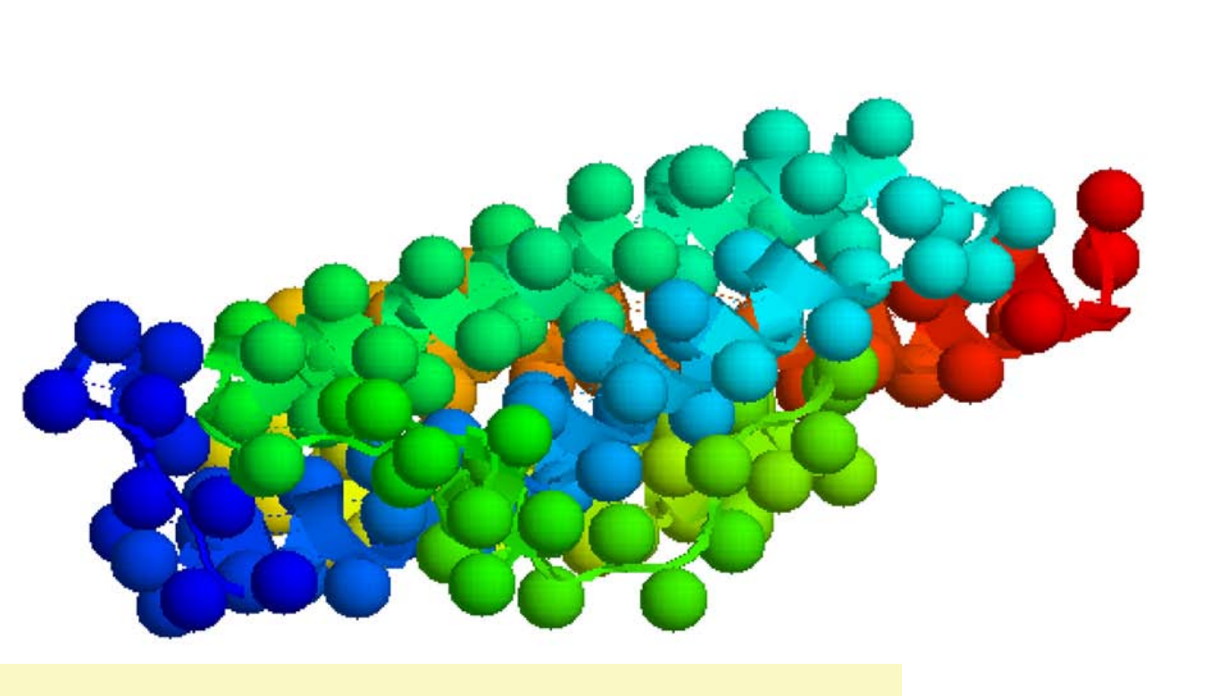
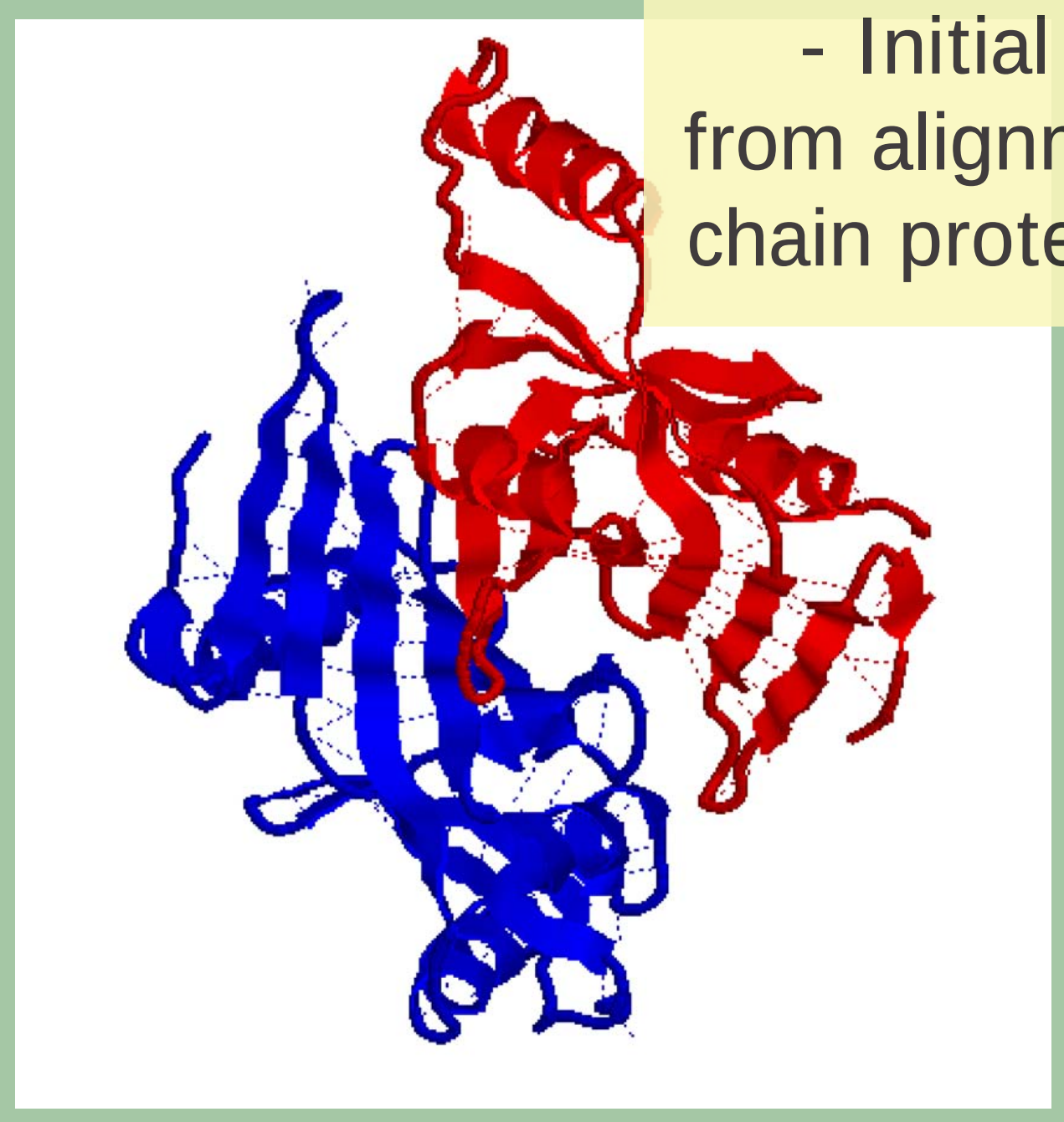
CRITICAL ASSESSMENT FOR PROTEIN STRUCTURE PREDICTION

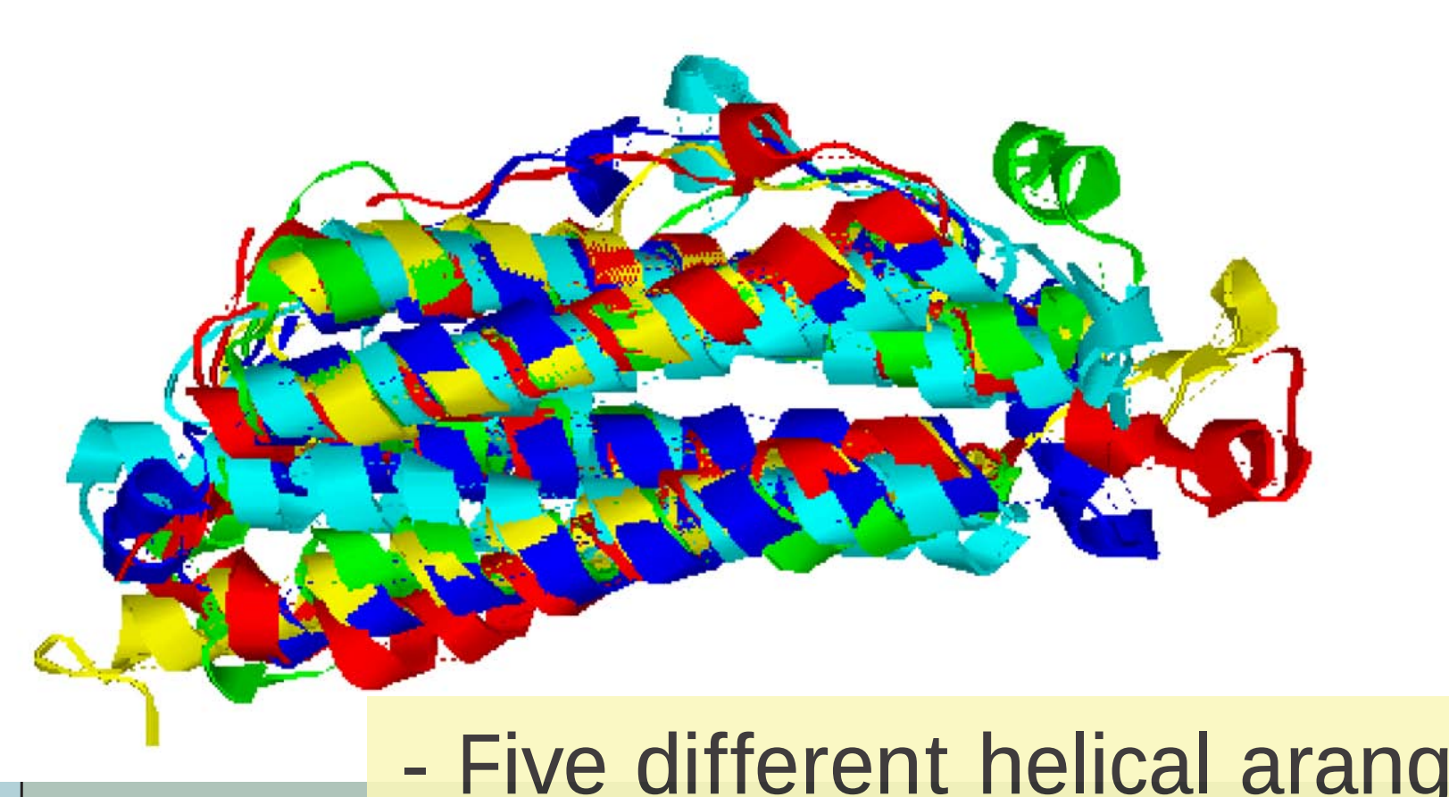
INITIAL ALIGNMENT


- Purple residues - calculated to be exposed
- Brown residues - calculated to be buried
- Model violates this

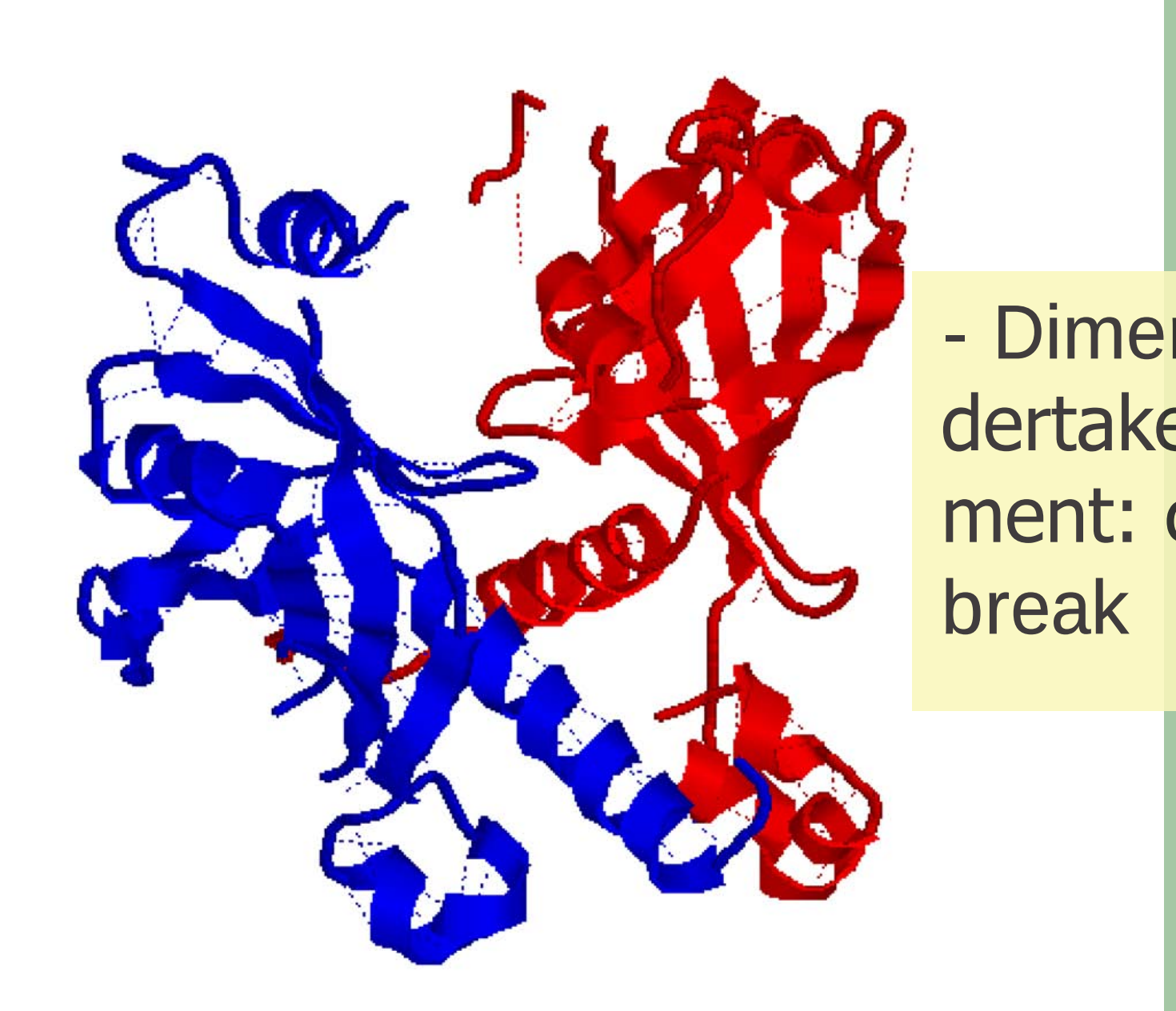

- Single alignment hand specified
- Every third atom of the backbone shown in spacefill


- Initial dimer, created from alignment with two-chain protein from server

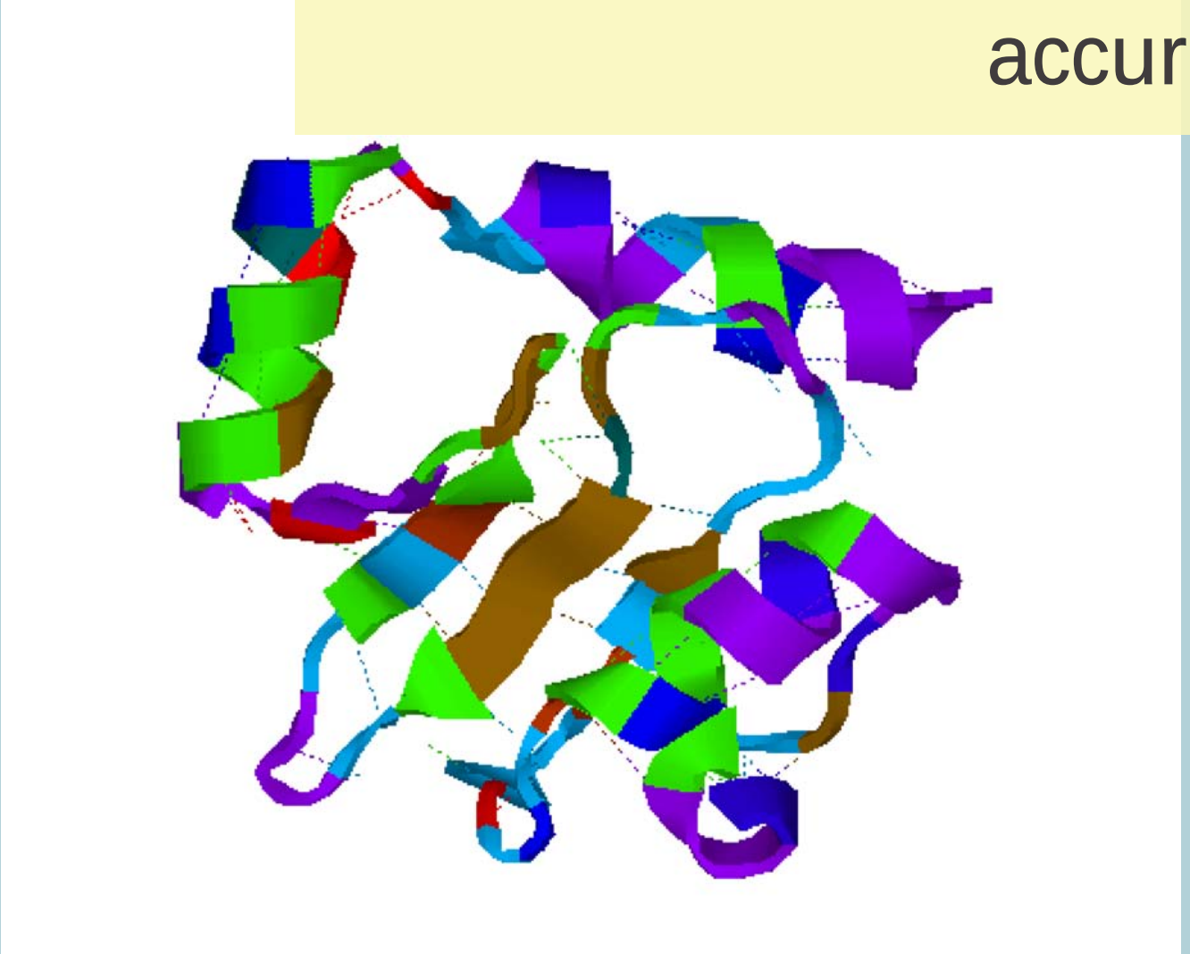

- Better alignment proudced by using a shorter segment of the chain


- Five different helical arangements produced by manipulating molecules in the backbone

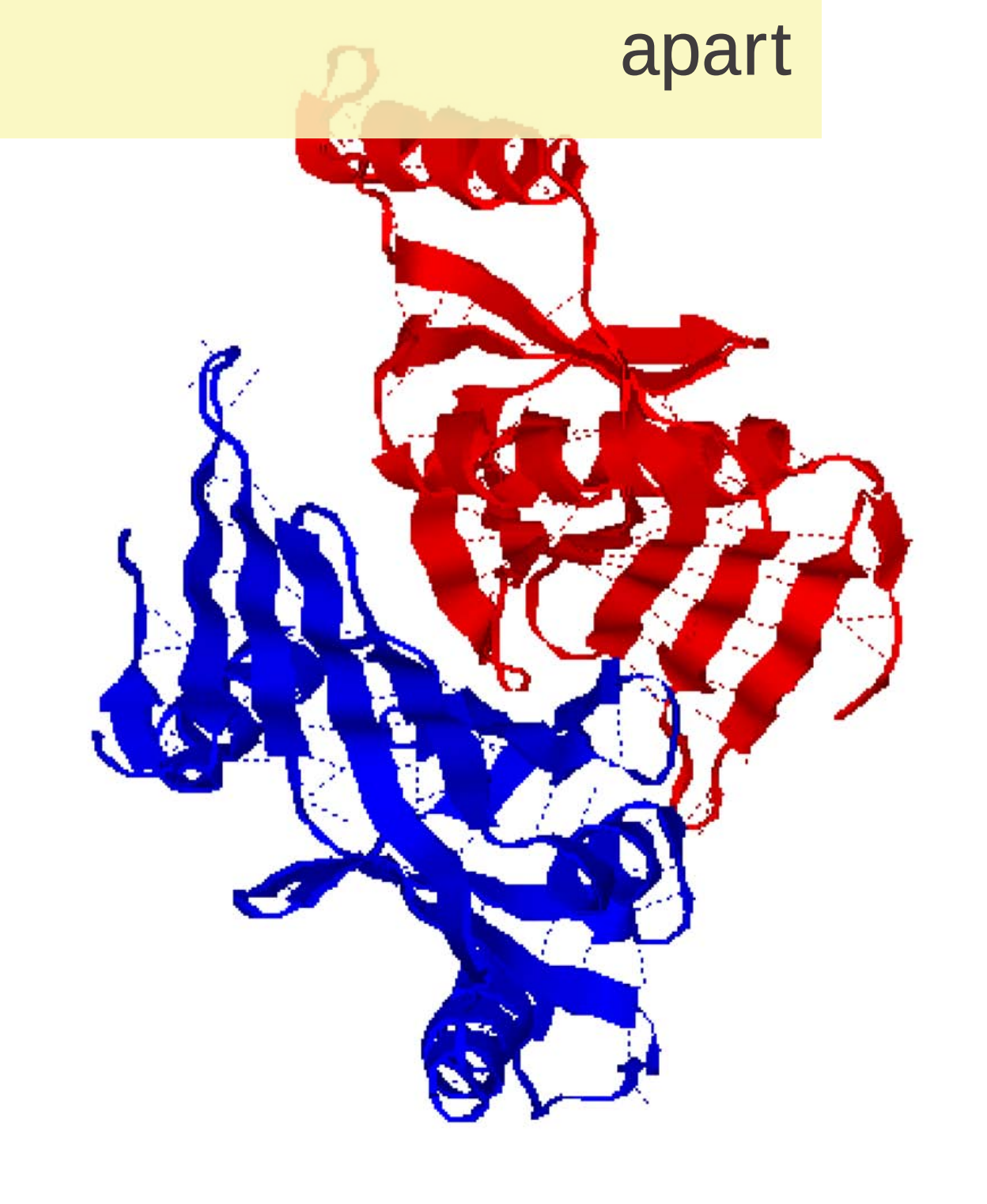
T0385


- Dimer, optimized by Undertaker to fix flaws in alignment: chains drift apart and break

SUBMISSIONS


- Combining models made of smaller chains produces greater accuracy overall

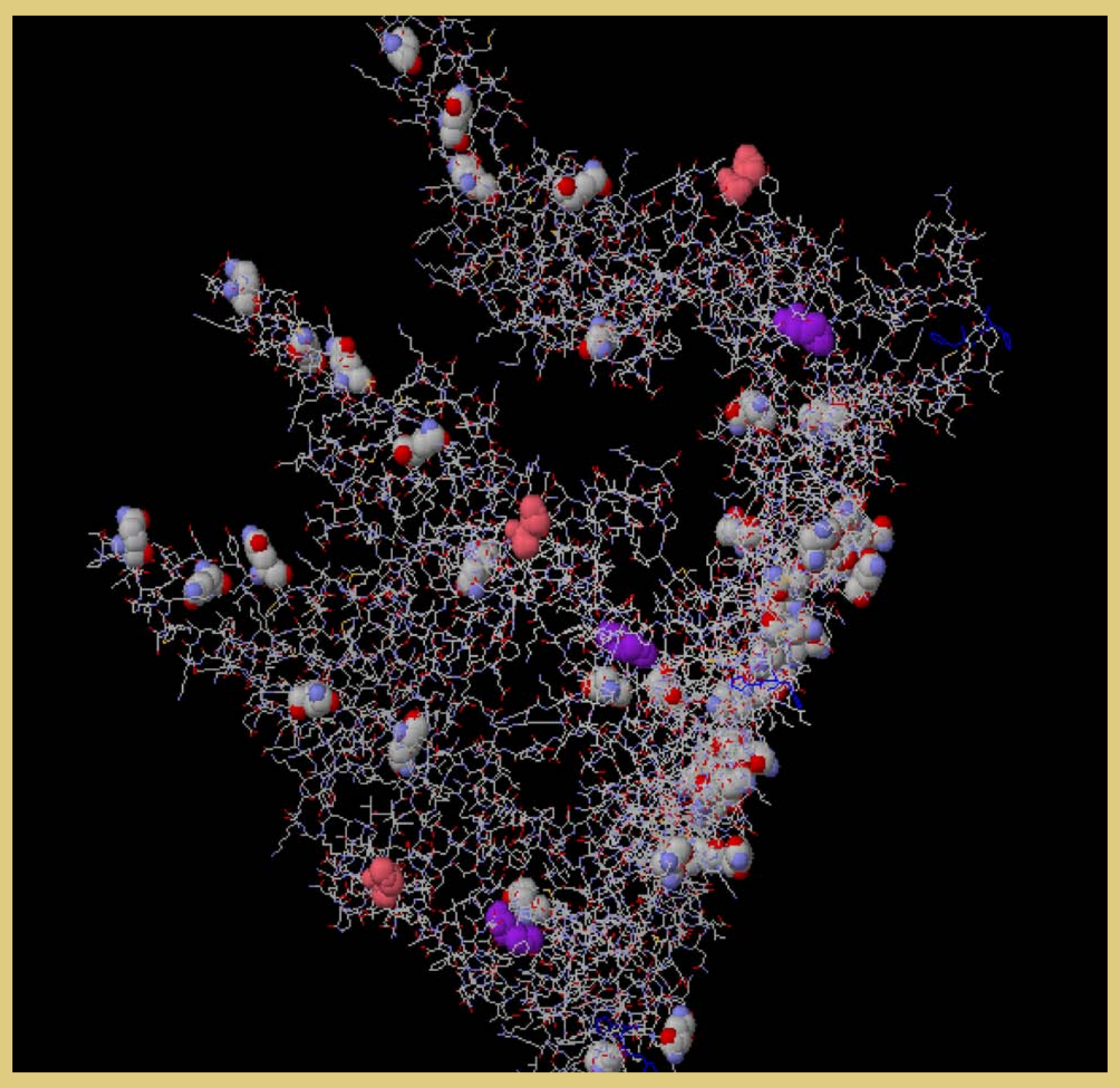
T0358

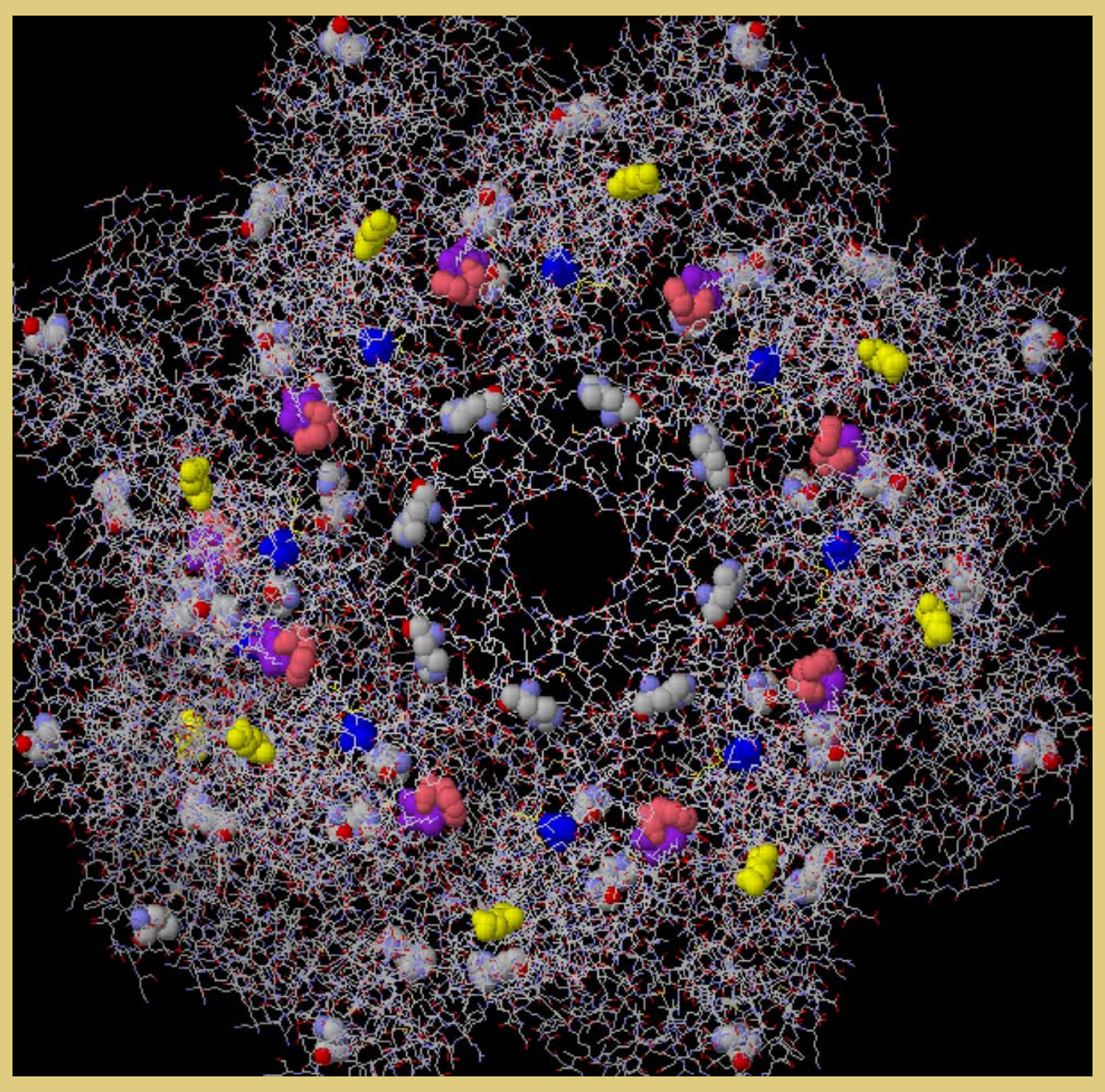

- Distance constraints prevent dimers from drifting too far apart

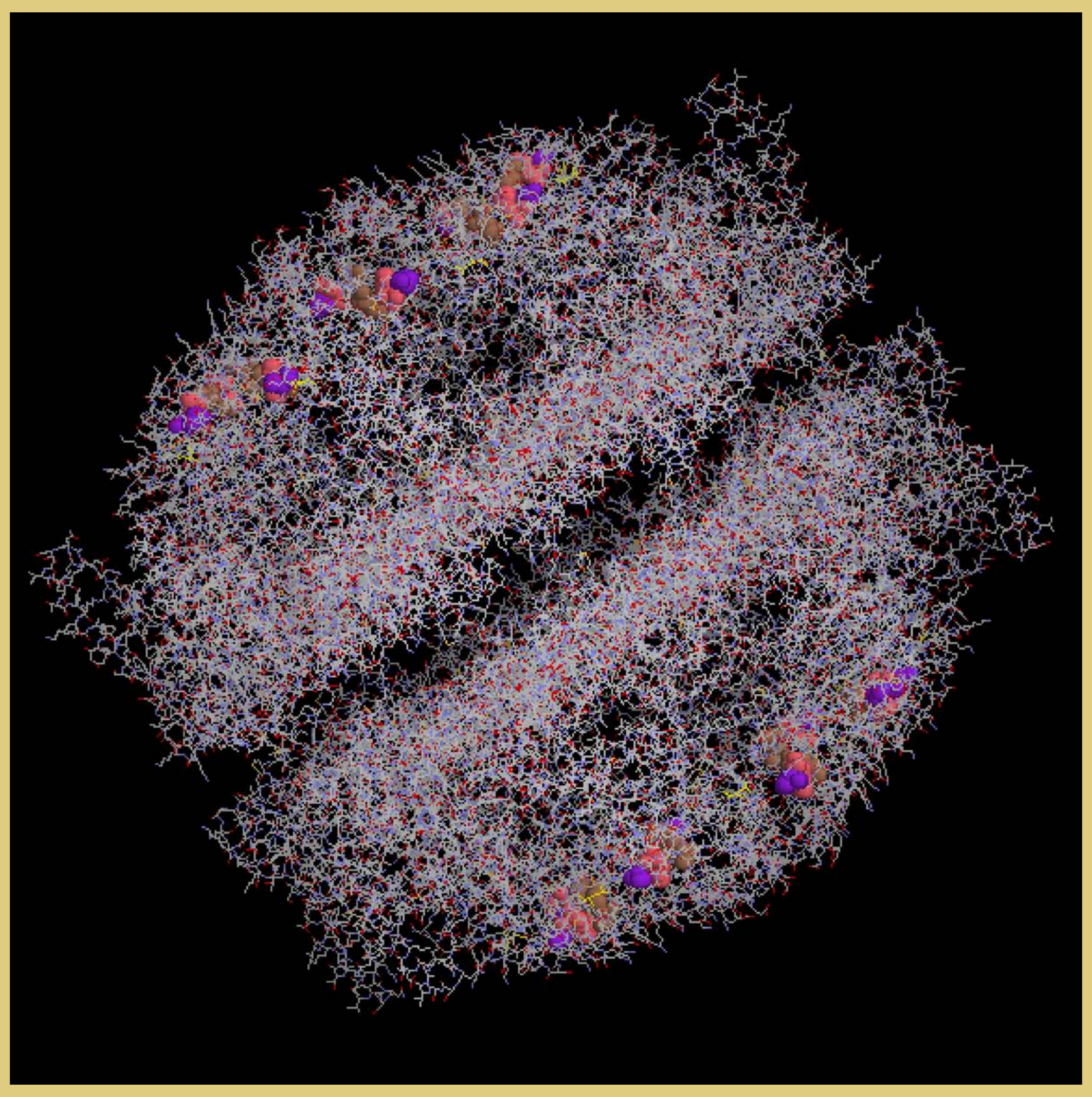
T0370

Heat Shock Proteins

- HSPs from *S. Shibatae* archaebacteria form **rosettasomes** - two rings of nine subunits each
- Higher percentage of alpha and beta types in high temperatures (92° C)
- Higher percentage of gamma in cooler temperatures (60° C)
- Alpha and beta (but **not gamma**) are both able to form **filaments** in presence of metals


Three gamma subunits


Beta subunits


Rosettasome of alpha subunits, from alignments

- **<u>RESULTS:</u> Metal binding** amino acids shown in color and spacefill