

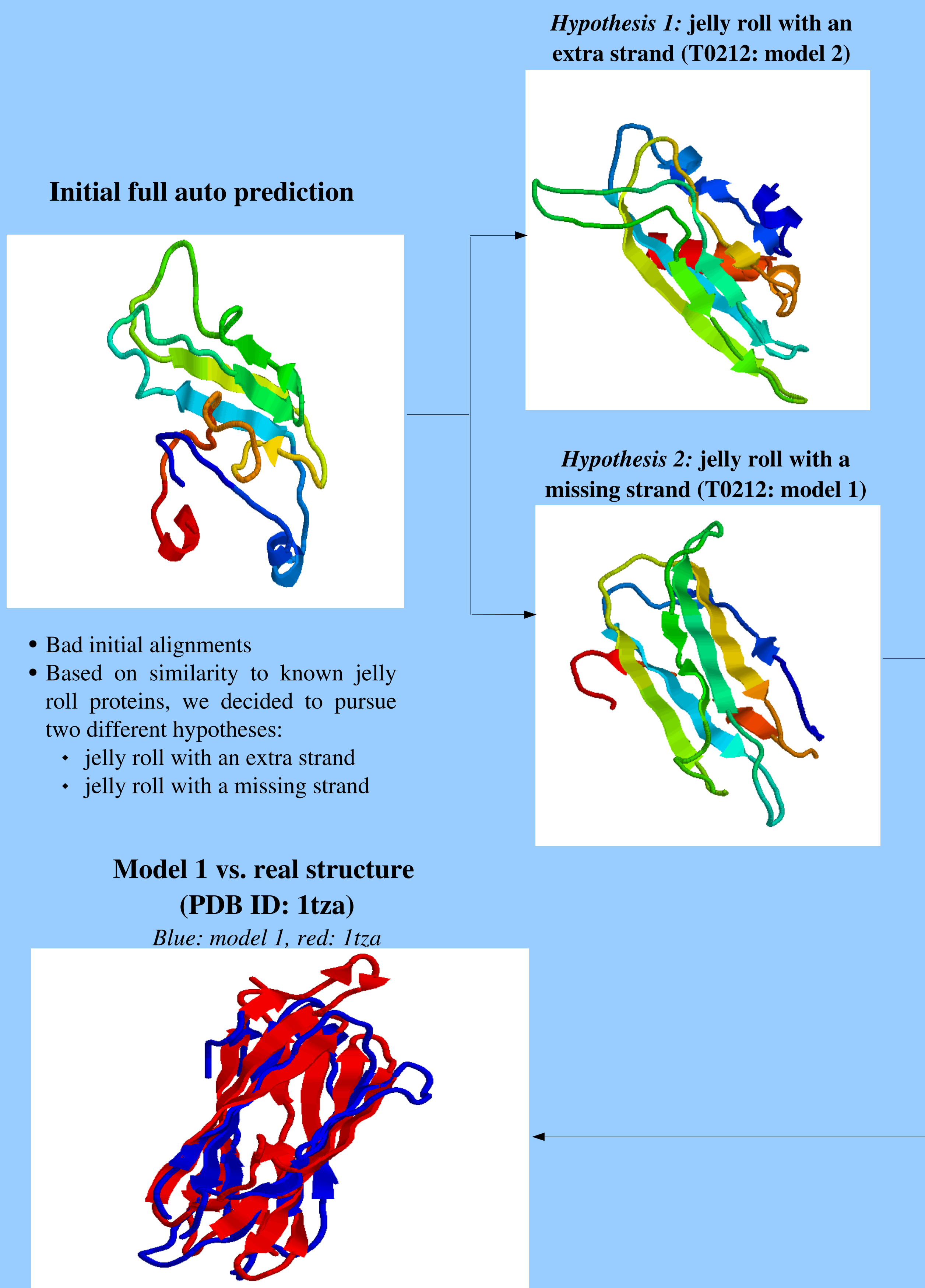
Human Interaction with Undertaker for the Structure Prediction of Targets T0212 and T0198

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Undertaker is UCSC's fragment-packing program. It was used during CASP6 for the generation of 3D models that were consistent with alignments and constraints. After the generation of an initial model, produced by an automatic run, subsequent models for a given target were produced after a hand examination of the result and a modification of the Undertaker cost function aimed at improving the models.

We present two examples (T0212 and T0198) of our interaction with Undertaker during the structure prediction process. The results allow us to gain some understanding of the abilities and limitations of the program, as well as to assess the human-added value to the quality of the predictions.

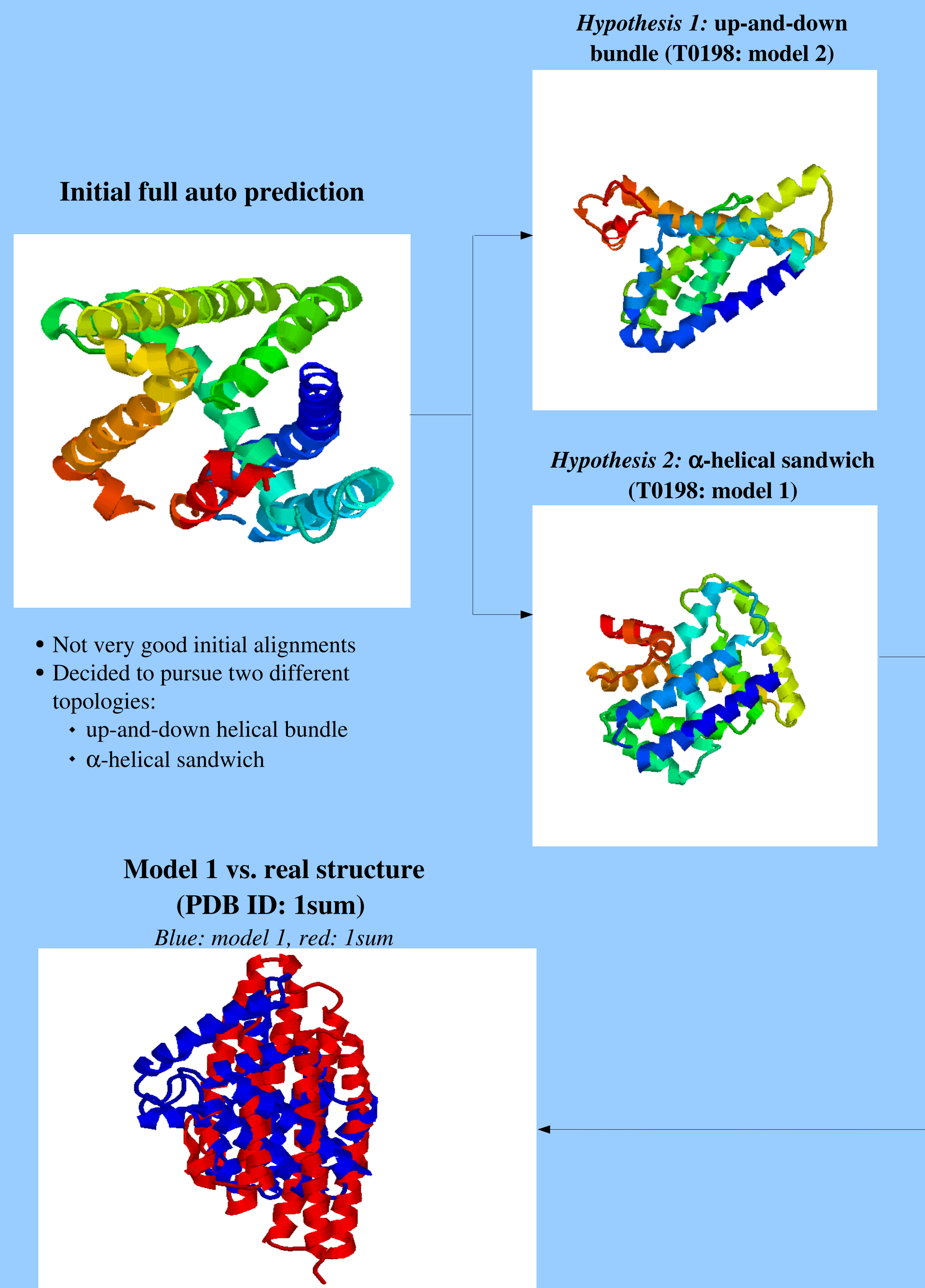
Target T0212 (FR/A)



Results for T0212 (FR/A)

- **Real PDB:** 1tza
- **Length:** 124 aa
- **Protein (organism) name:** SOR45 (*S. oneidensis*)
- **Smooth GDT score for model 1:** 28.0245%
- **RMSD C α for model 1:** 9.7256 Å
- Model 1, which predicted a jelly-roll-like structure with a missing N-terminal strand, was our best submitted model. Swapping the N- and C-terminal strands of the model would have made it relatively close to the real structure. Strand T60-A66 was off by one residue.

Target T0198 (FR/A)



Results for T0198 (FR/A)

- **Real PDB:** 1sum
- **Length:** 225 aa
- **Protein (organism) name:** 1170B (*T. maritima*)
- **Smooth GDT score for model 1:** 12.44%
- **RMSD C α for model 1:** 20.1124 Å
- Model 1 was not a successful choice in terms of both smooth GDT and RMSD C α scores. We predicted models that were closer to the real structure, but did not choose them for submission. The best smooth GDT score among our models was 19.2123%, while the best RMSD C α was 10.0664 Å.

Conclusions

- **T0212:** Undertaker was successful in assembling the sheets into a jelly-roll-like structure. The poor initial full auto model was improved after the careful selection of better alignments and the incorporation of appropriate strand and sheet constraints into the subsequent models. The human involvement led to an overall improvement of the initial models.
- **T0198:** Undertaker did not manage to successfully pack the helices of T0198 into a helical bundle, despite our efforts in that direction. The human involvement did not add value to the prediction, since the final models were not better than the initial full auto model. Any attempts to include constraints that would force a model into a bundle led to the assembly of the helices into either an α -helical sandwich, or a loosely packed structure that only somewhat resembled a helical bundle.

Acknowledgments: Kevin Karplus and the SAM-T04-hand team (Jenny Draper, Sol Katzmann, George Shackelford, Marcia Soriano, Bret Barnes and Richard Hughey)