

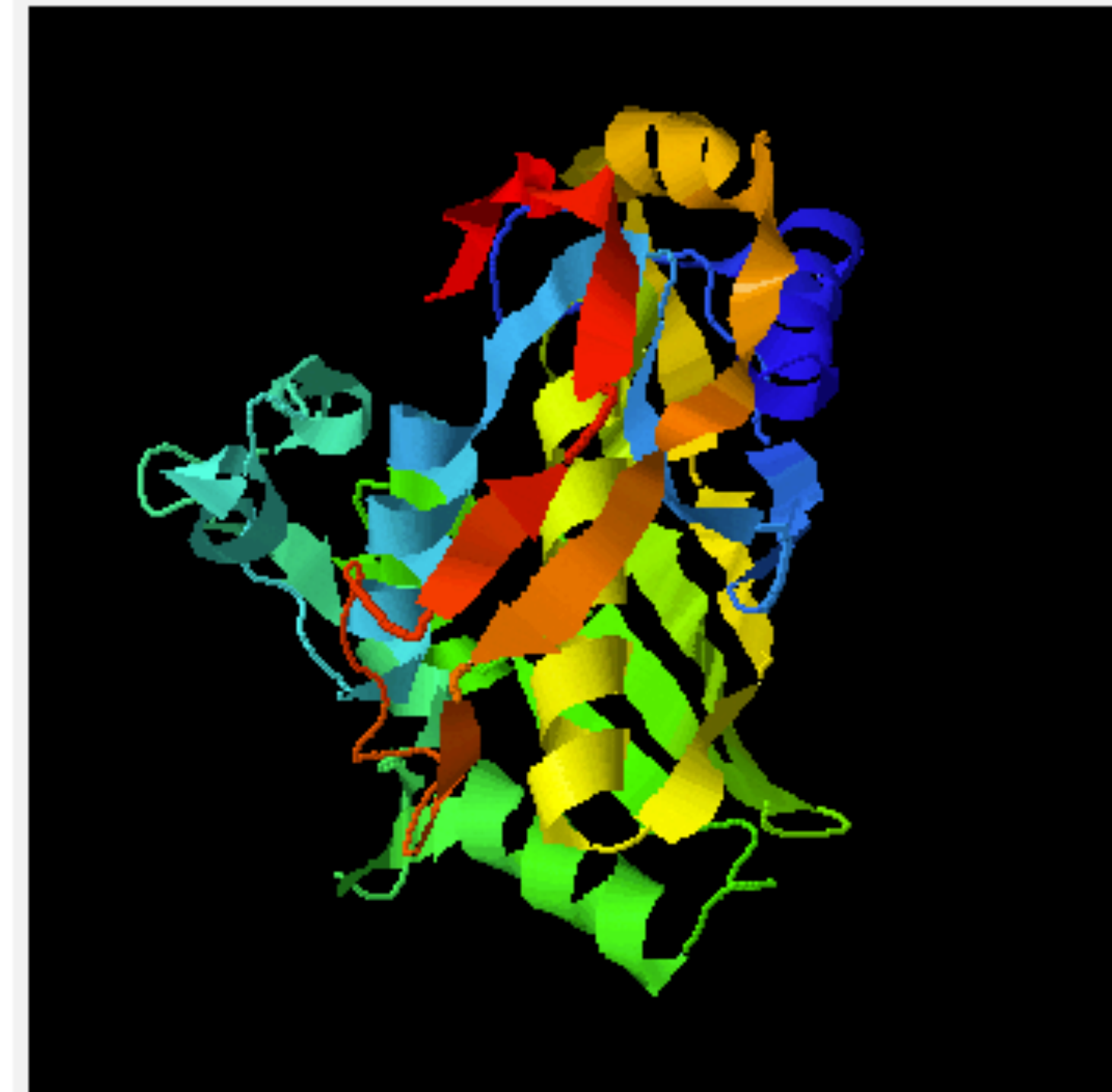
- The confidence of each model is quantitatively measured by C-score that is calculated based on the significance of threading template alignments and the convergence parameters of the structure assembly simulations. C-score is typically in the range of $[-5, 2]$, where a C-score of a higher value signifies a model with a higher confidence and vice-versa. TM-score and RMSD are estimated based on C-score and protein length...
- Is I-TASSER confident about its final model? Yes.

Top 5 final models predicted by I-TASSER

(For each target, I-TASSER simulations generate a large ensemble of structural models quantitatively measured by C-score that is calculated based on the significance of threading template alignments and the convergence parameters of the structure assembly simulations. C-score is typically in the range of $[-5, 2]$, where a C-score of a higher value signifies a model with a higher confidence and vice-versa. TM-score and RMSD are estimated based on C-score and protein length following the correlation observed between these rank models as seen in our benchmark tests. If the I-TASSER simulations converge, the top 5 models are shown below.)

- [More about C-score](#)
- [Local structure accuracy profile of the top five models](#)

(By right-click on the images, you can export image file or change the orientation.)



☐ Spin On/Off

- [Download Model 1](#)
- C-score=1.91 ([Read more about C-score](#))
- Estimated TM-score = 0.99 ± 0.04
- Estimated RMSD = $2.2 \pm 1.7 \text{ \AA}$

Structure Preparation

- None of the structures were ready for electrostatic potential calculation
- The human structure, 1HVY
 - has 4 chains, but we are only interested in 2
 - I used MultiSeq to write separate files for each chain, merged the files for chains A and B, and then modified “END” after chain A into “TER”
- The E. coli structure, 6NNR
 - is not aligned with the human structure
 - I used MultiSeq to write separate files for each chain, used MultiSeq STAMP structural alignment to superpose E. coli chains A and B on top of the respective human chains, wrote the aligned files, and merged and modified them as with 1HVY
- The W.g.b. homology model
 - is not aligned with the human structure
 - I used MultiSeq STAMP structural alignment to superpose W.g.b. chains A and B on top of the respective human chains, wrote the aligned files, and merged and modified them as with 1HVY