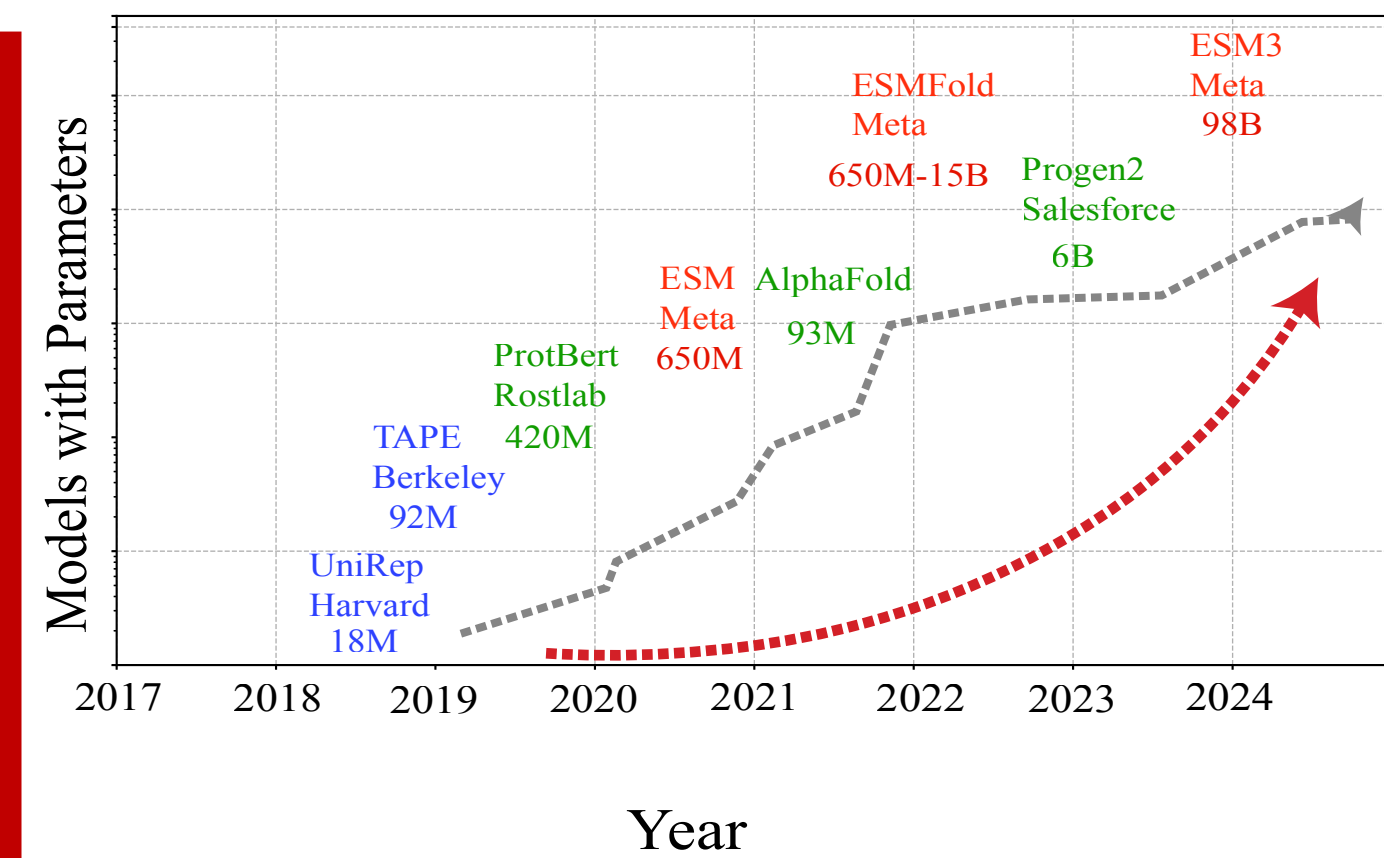
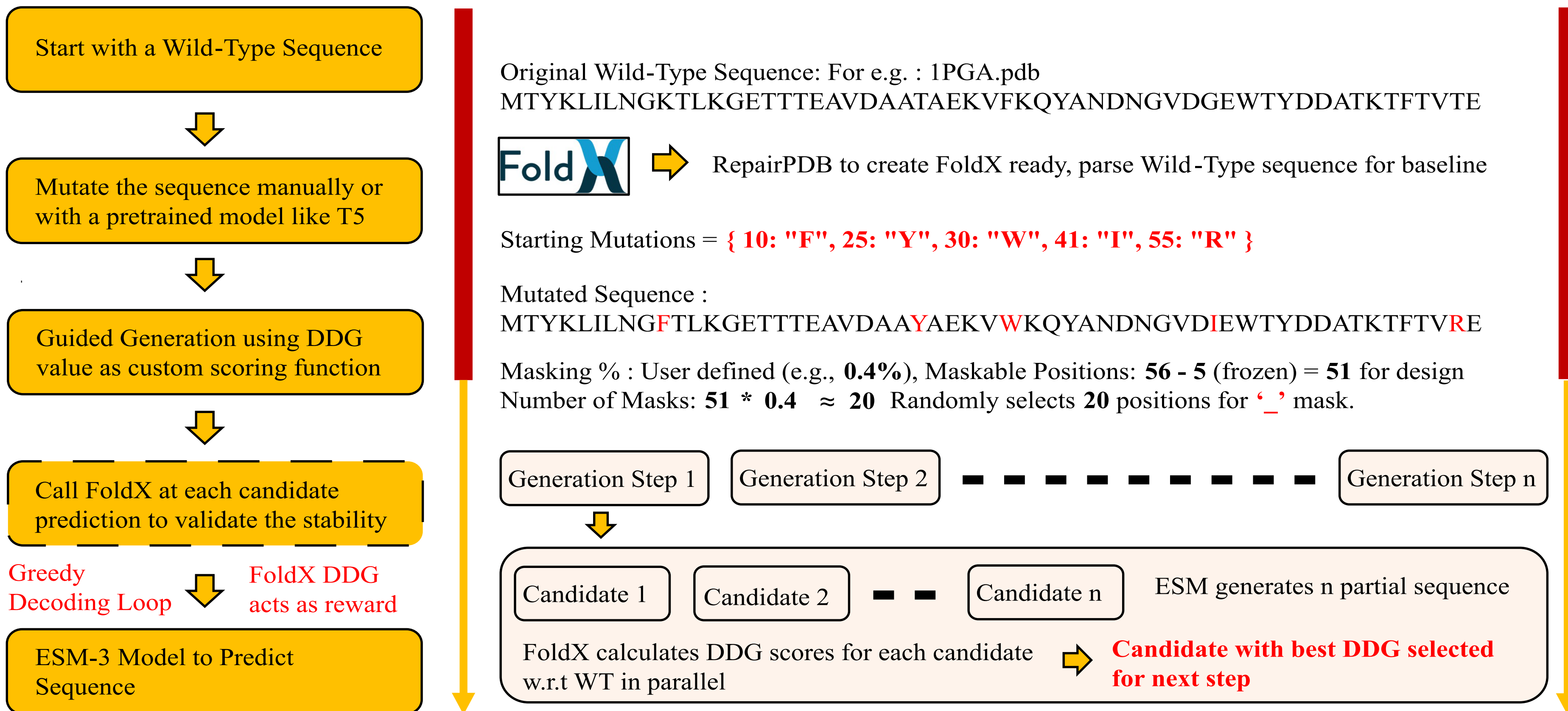
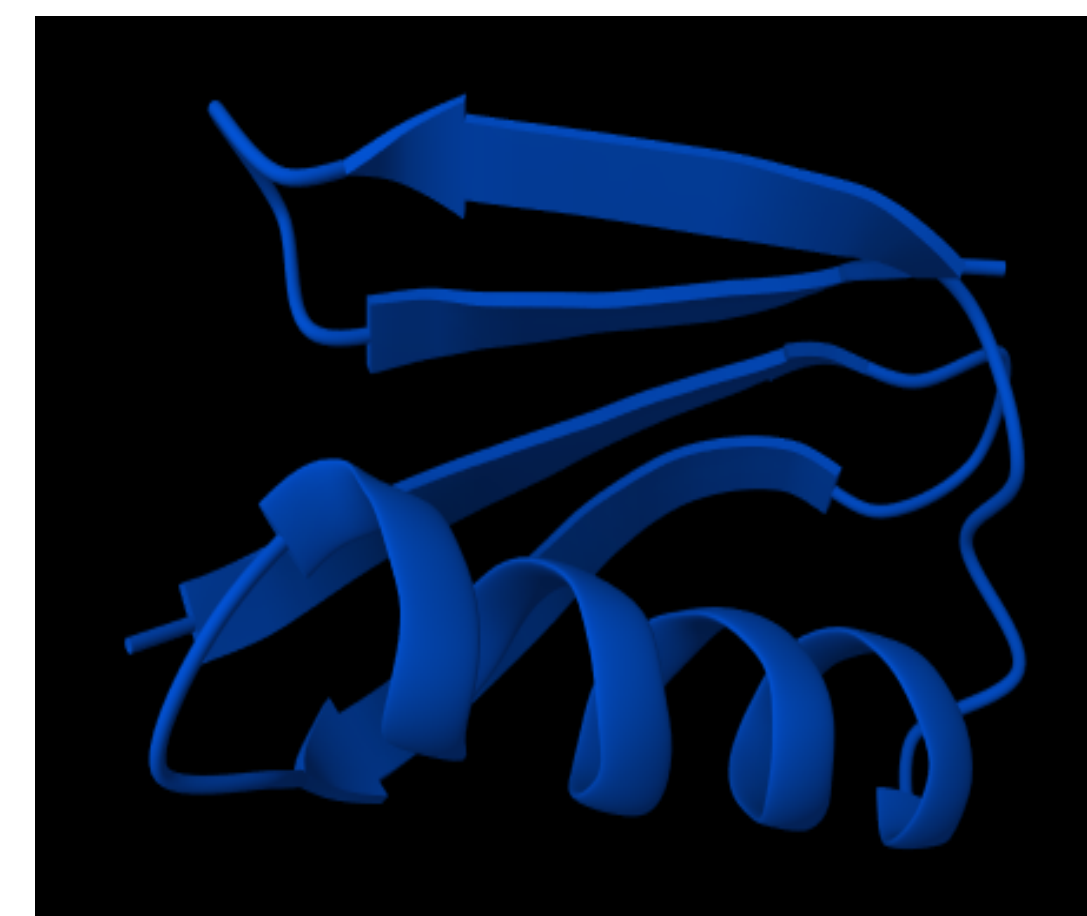
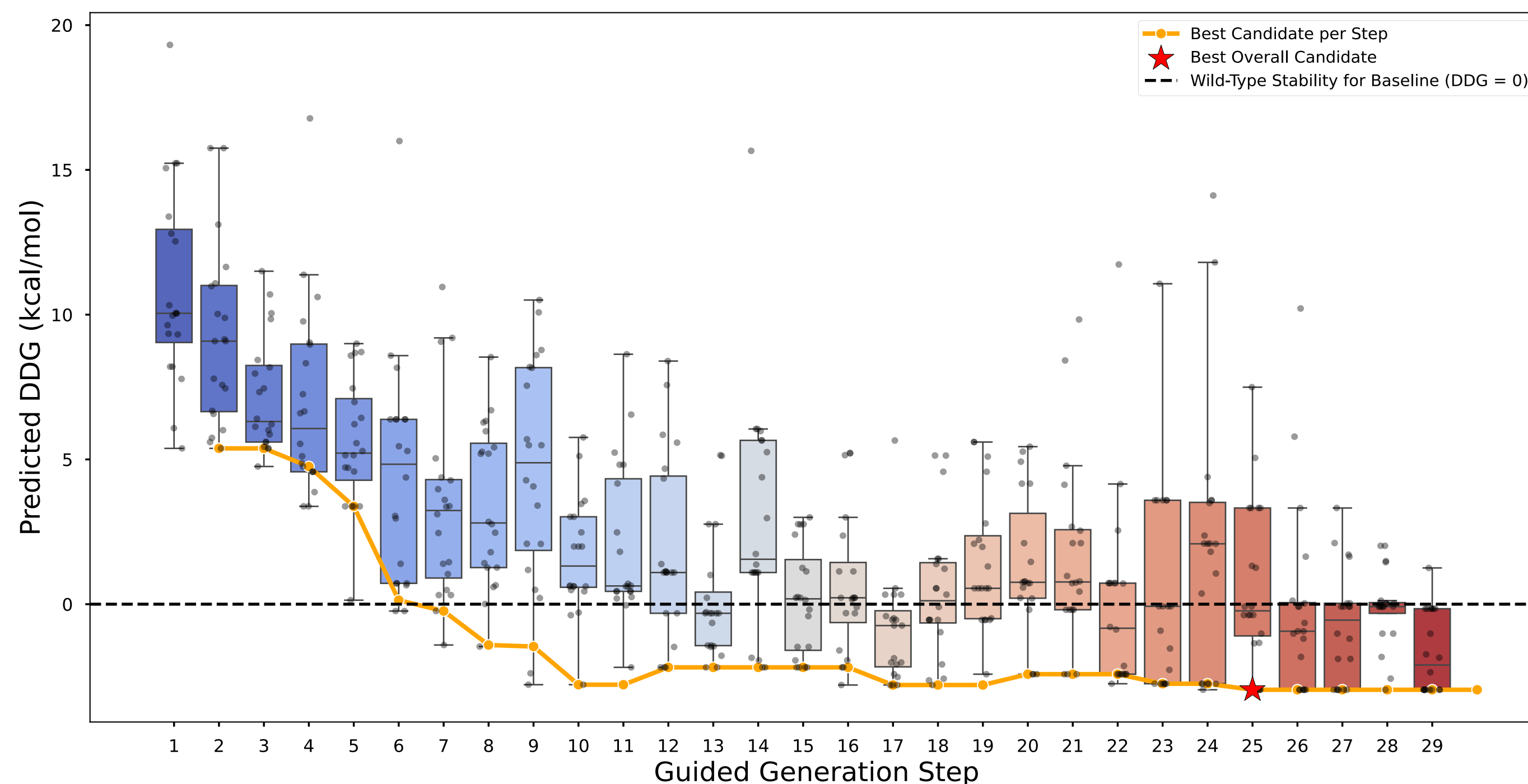


Guided - Generation Framework Overview

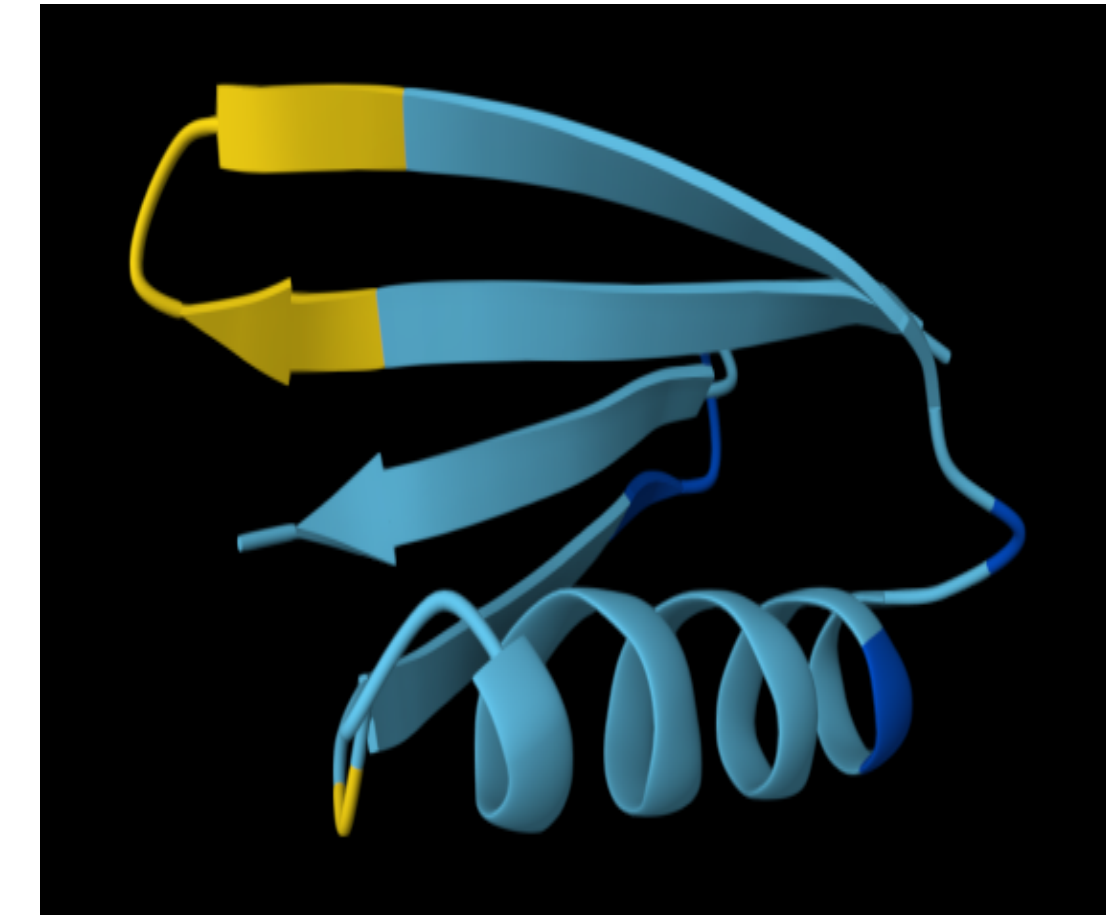


- The optimization algorithm uses proportional schedule. It is adaptive, efficient, and robust.
- Guided Generation Step - Total run step
- Number of Candidate - Denoised Prediction in each step.
- Number of Position to Unmask = $\max(1, \text{masked_position} // \text{remaining_steps})$
- The proportional schedule is designed to finish unmasking right at last step.

ESM3-FoldX Guided Generation using DDG scores



Original structure of 1PGA



Best Optimized structure using Guided-Generation Framework