Improved cryoEM-Guided Iterative Molecular Dynamics−Rosetta Protein Structure Refinement Protocol for High Precision Protein Structure Prediction

Supplemental Figures

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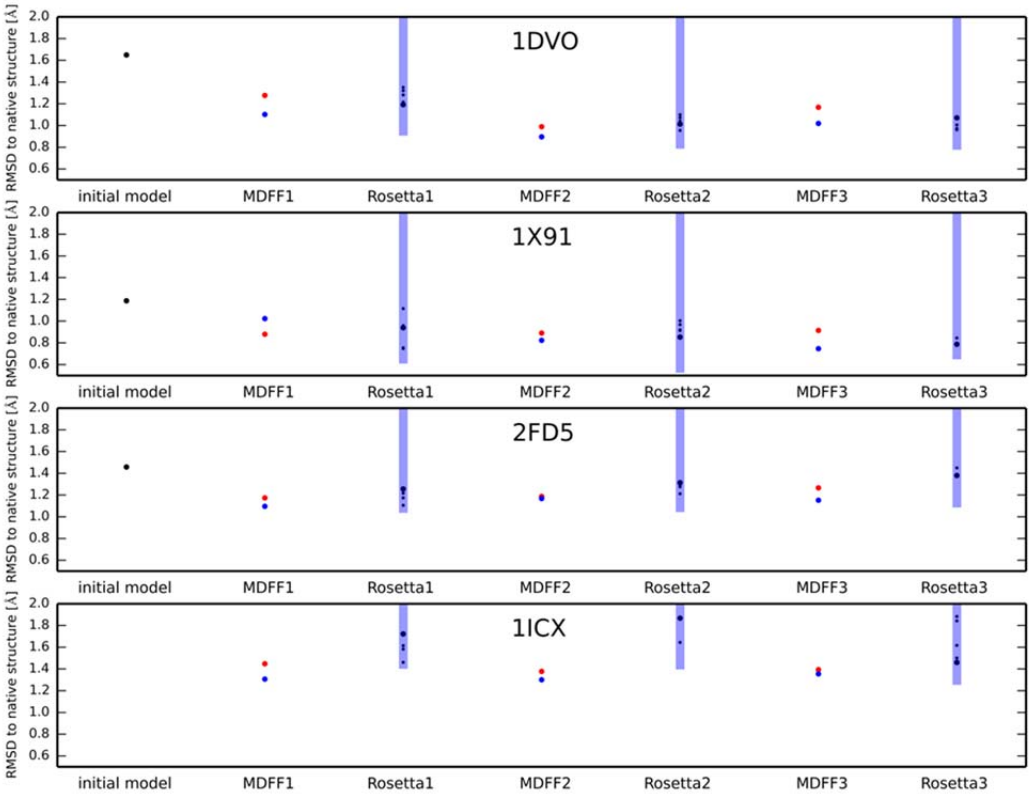
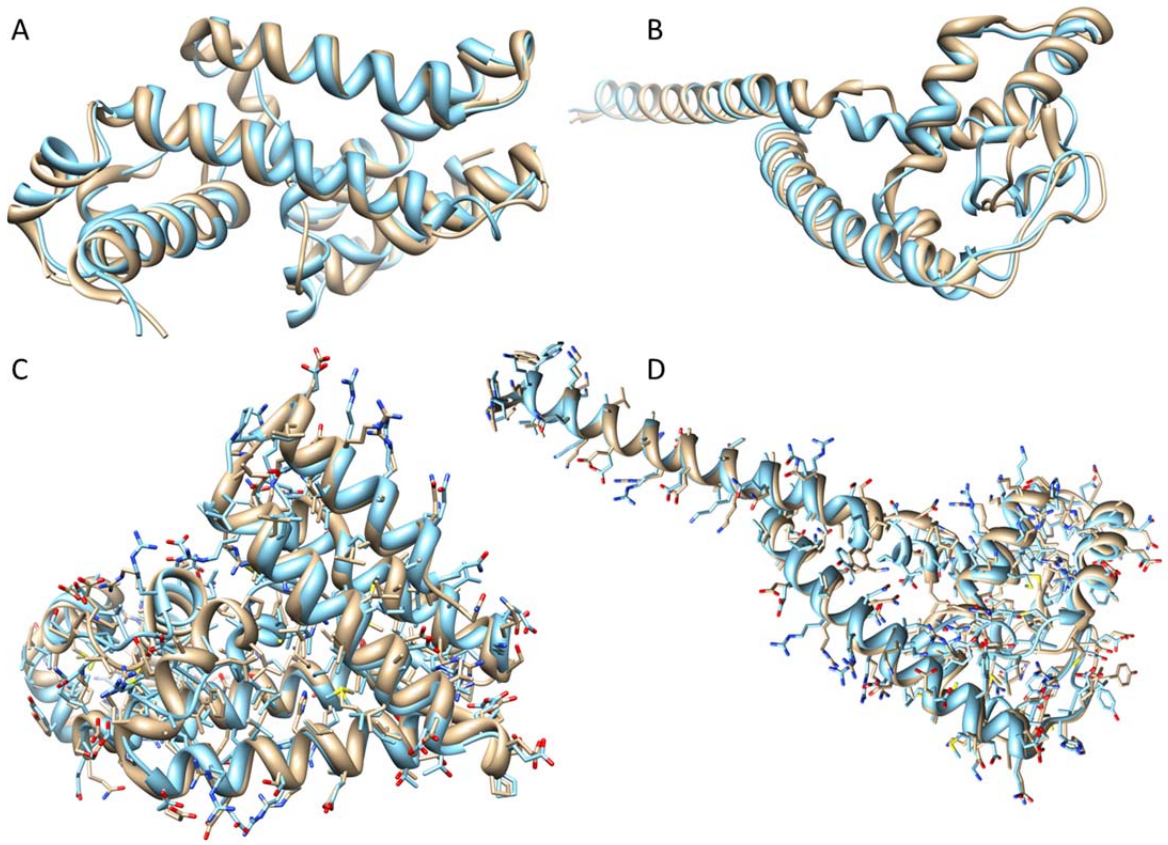


Supplemental Figure 1. Summary of the results of all rounds of the iterative MDFF – Rosetta refinement. The RMSD values over protein residues in secondary structure elements with respect to the native structure SSEs in all three rounds of iterative cryoEM-guided protein structure refinement are shown. The first panel (black dot, labeled initial model) shows the top-scoring model of the last round of Rosetta-only refinement in (1). For the MDFF simulations, final models after each of the two separate steps (MD simulation with low density forces (red) and subsequent minimization with high forces (blue)) are shown. For each of the three rounds of Rosetta refinement, the RMSD values of the top scoring model (thick black dot) and the subsequent four best-scoring models (four thin black dots) are shown. A blue bar indicates the range of the RMSDs of all models built during that round of Rosetta refinement (irrespective of their individual scores), with the low-RMSD end of the bar corresponding to the lowest-RMSD model built. The high-RMSD end of the bar is beyond the plotting limit of 3 Å for all proteins and rounds.



Supplemental Figure 2. Lowest RMSD models after three rounds of iterative MD / Rosetta refinement for 2FD5 (panel A and C) and 1DVO (panel B and D). The native structure is shown in gold while the model is shown in turquois. A, B) Ribbon backbone representation of the proteins. The overall structure within secondary structure elements has been recovered in the models. C, D) Side chain non-hydrogen coordinates are shown in addition to Ribbon backbone representation. Most side chain conformations within the interface of secondary structure elements have been built correctly.

1. Lindert, S., N. Alexander, N. Wotzel, M. Karakas, P. L. Stewart, and J. Meiler. 2012. EM-fold: de novo atomic-detail protein structure determination from medium-resolution density maps. Structure 20:464-478.