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De novo main-chain modeling for EM maps using MAINMAST

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An increasing number of protein structures are determined by cryo-electron microscopy (cryo-EM) at near atomic resolution. However, tracing the main-chains and building full-atom models from EM maps of ~4–5 Å is still not trivial and remains a time-consuming task. Here, we introduce a fully automated de novo structure modeling method, MAINMAST, which builds three-dimensional models of a protein from a near-atomic resolution EM map. The method directly traces the protein's main-chain and identifies Cα positions as tree-graph structures in the EM map. MAINMAST performs significantly better than existing software in building global protein structure models on data sets of 40 simulated density maps at 5 Å resolution and 30 experimentally determined maps at 2.6–4.8 Å resolution. In another benchmark of building missing fragments in protein models for EM maps, MAINMAST builds fragments of 11–161 residues long with an average RMSD of 2.68 Å.