Supplementary Material

Supplementary Figure 1. Narrowly defined dihedral angle restraints improve the accuracy of individual helices within the calculated structures. Average rmsds broken down to the TM helix level for ensembles calculated in Figure 5, with loose (black) or narrow (white) definitions for dihedral angle boundaries. (The indicated helix from each ensemble was superimposed onto the corresponding helix from the target structure for each calculation.) The rmsd between the target helix structure superimposed into a canonical helix of the same length is also shown (gray bars) as a measure of the maximum theoretical accuracy that can be obtained using these dihedral angle definitions. Except for the single GpA TM helix, all other TM helices are indicated with the first initial of the protein name and the helix number as it occurs in the protein sequence. Even when the target helix structure deviated significantly from canonical values (*e.g.* AMC helices 1 and 3), no adverse affect on single helix accuracy resulted from the imposition of these restraints. Otherwise, the accuracy of helices that were not yet at the theoretical maximum with the conventional dihedral angle restraints closely approached this maximum when narrow boundaries were imposed.