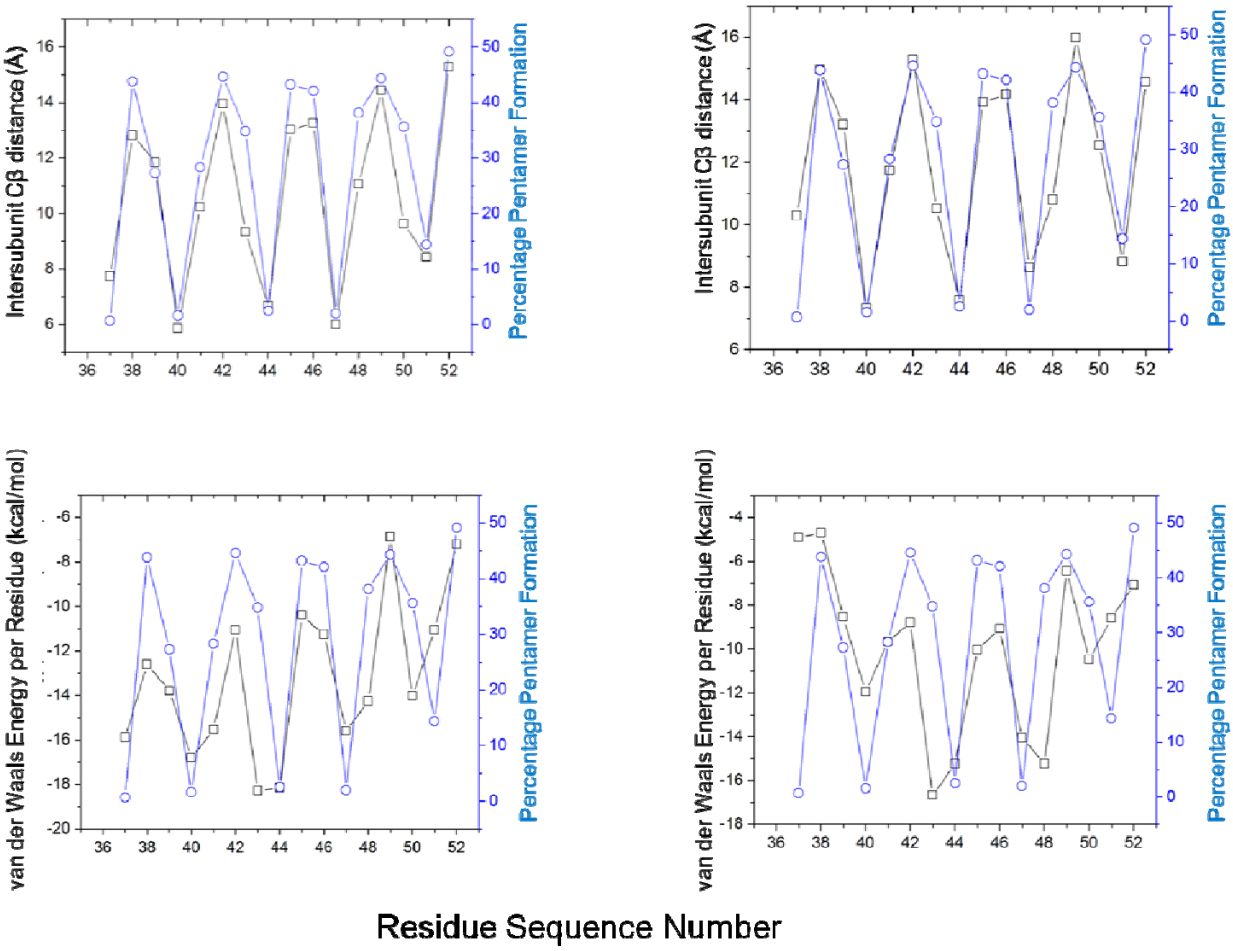
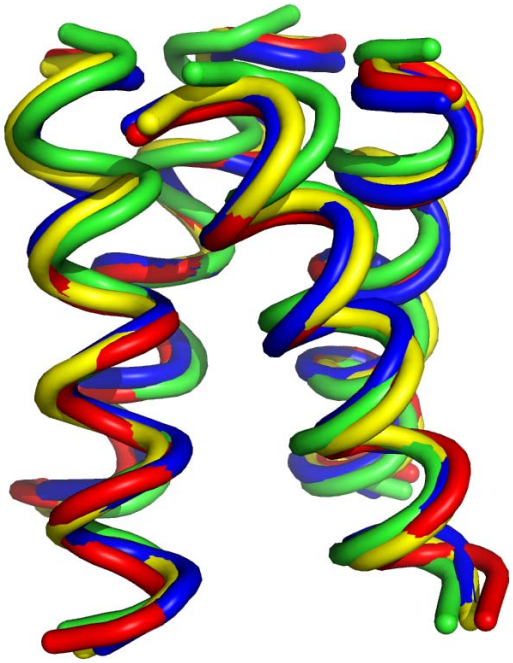
Supplementary Figure 1— Inter-subunit Cβ distance versus percentage pentamer formation for native phospholamban (upper left pannel) and the best scoring model (upper right panel). A similar profile is shown using van der Waals interaction energy per residue versus percentage pentamer formation for native phospholamban (lower left panel) and the best scoring model (lower right panel). The van der Waals interaction energy per residue was obtained using the CHARMM22 force field implementation in XPLOR-NIH.



Supplementary Figure 2— Structural heterogeneity between different structures of M2 that include the solution NMR structure (green, PDB ID 2RLF), a high-resoltion X-ray structure (blue, PDB ID 3LBW), a solid-state NMR structure from Mei Hong's group (yellow, PDB ID 2KQT) and a solid-state NMR structure from Tim Cross' group (red,  PDB 2LOJ)



Only the TM portion of the structures are shown.