

**Figure 4S. Optimized model of the MRR from CagY.** This structure corresponds to the central chain of the trimmer optimized by a 10 ns Equilibrium Molecular Dynamics.As it is described in the document, only this central chain reached the conformational equilibrium (RMSD approximately constant). The structure shown here corresponds to frame 95 of 100 (time 9.5 ns), which was estimated as the average representative conformation for the stable trajectory. All three chains in the trimer had the same orientation. N and C terms are highlighted.