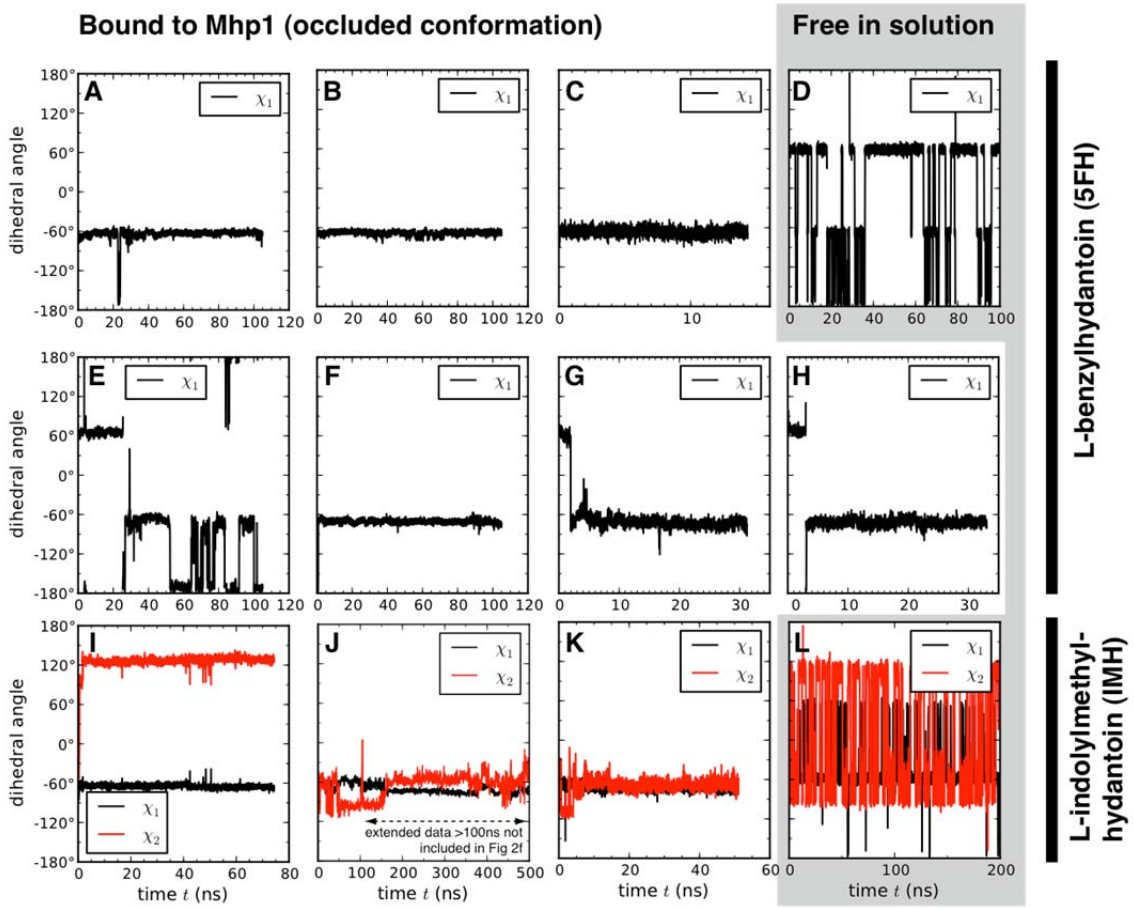

Figure S3. Time evolution of dihedral angles in L-BH (ligand code 5FH) and L-IMH from MD simulations. (**A-C**) Simulations 5FH(g^-) MD_001–MD_003 (L-BH bound to Mhp1, started from the extended conformation as seen for the IMH-bound structure). (**D**) L-BH in solution. (**E-H**) Simulations 5FH(g^+) MD_001–MD_004 (L-BH bound to Mhp1, started from the U-shaped folded over conformation as modeled in 2JLO). (**I-K**) Simulations IMH(g^-) MD_001–MD_003 (L-IMH bound to Mhp1 as seen in the crystal structure). (**I**) L-IMH in solution. (**J**) Extended to 500 ns. (**L**) L-NMH in solution.