**Fig. S4.** Interface residue selections *in magenta* highlighted over a protein target (Receptor, *in green* and ligand, *in blue*). The four residues selections are as follows: (1) 5.5 Å interface patch, (2) 8 Å interface patch (3) 5.5 Å interface patch + loops, (4) 8 Å interface patch + loops. Note that, we also performed a test set by including all the residues of the protein for backbone sampling, however, with T-REMC, such simulations resulted in distortion of the protein quaternary structure (i.e. resulted in protein unfolding). Therefore, we chose to exclude that test.