

Figure S5. Prediction of FlgM in complex with Sigma 28 improves accuracy

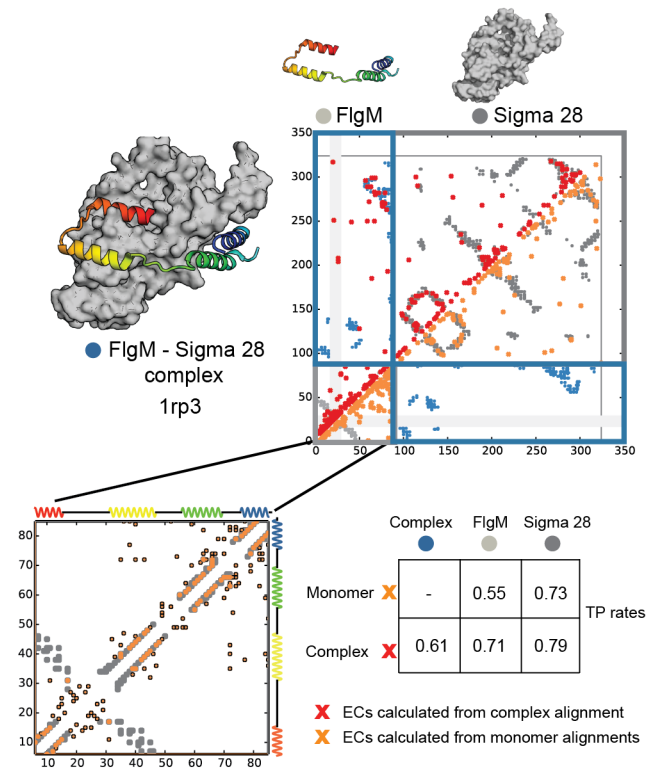


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Anti- σ factor, FlgM is disordered in solution and forms an extended α -helical structure upon binding σ factor 28 (PDB id 1rp3) (Sorenson et al., 2004). In order to capture intermolecular constraints between FlgM and sigma 28, ECs were calculated from a concatenated alignment of the two proteins (O66683_AQUAE and O67268_AQUAE) (Hopf et al., 2014). High-ranking ECs correspond to intermolecular contacts (left panel – significant ECs for monomer FlgM; right panel – significant ECs for complex alignments), and predict the binding interface of helix 3 and 4. Notably, complex based intra-molecular ECs for both FlgM and sigma 28 more accurately capture the internal contacts, suggesting that the information for the fold of the one protein is encoded also in the protein partner (TP ECs are 0.55 vs. 0.71 and 0.73 vs. 0.79).