Figure 3. Evolutionary couplings predict close residues in known ordered states of disordered proteins.

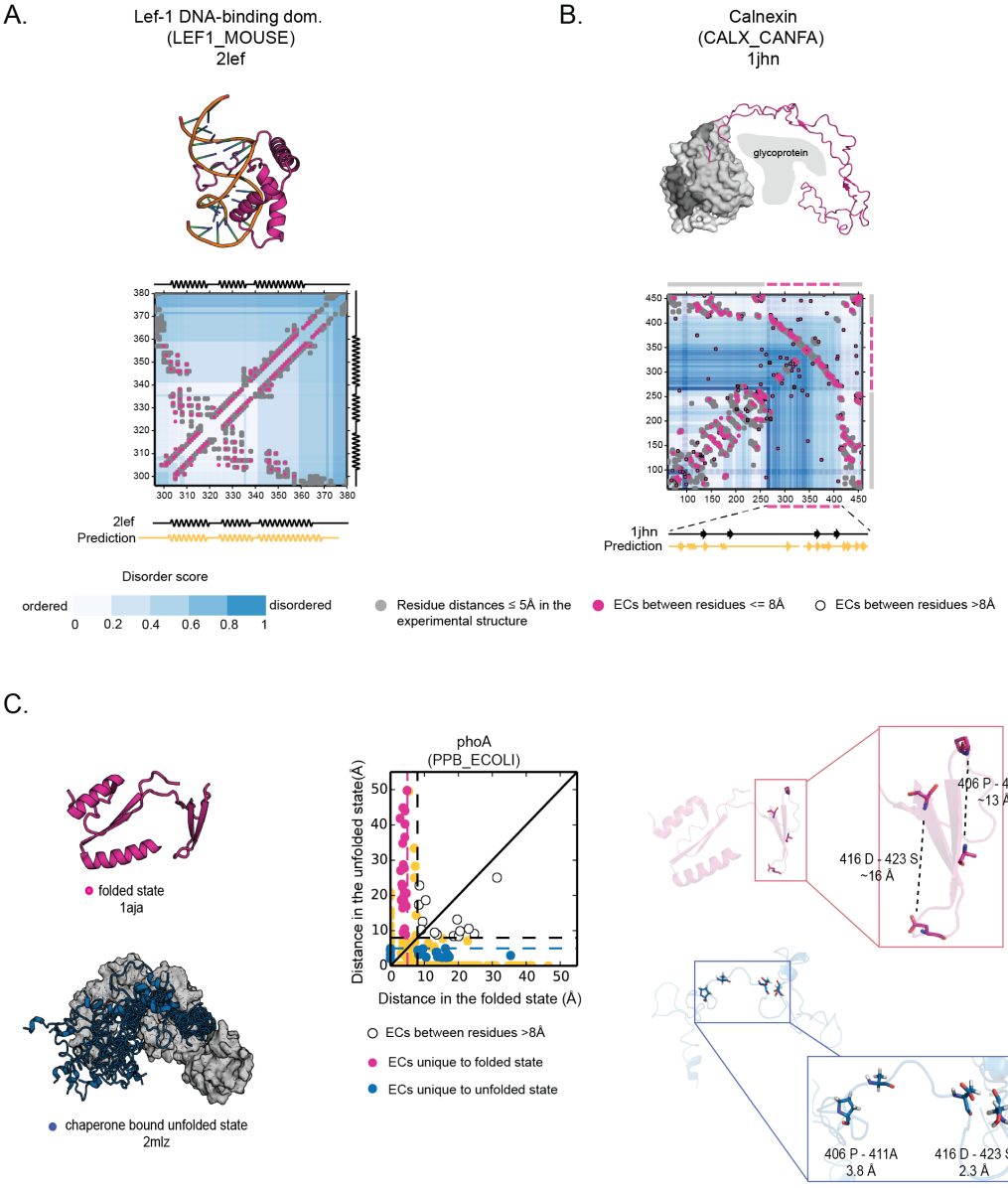

Figure 3. Evolutionary couplings predict close residues in known ordered states of disordered proteins. **(A)** ECs (pink circles) perfectly recapitulate the experimental contacts (grey circles- residue-residue distance <5 Å) of the folded, DNA-bound state of Lef-1 that is partially unstructured in the absence of DNA (2lef, Precision=1.00). **(B)** ECs predict the overall contact map of Calnexin chaperone, including the disordered luminal domain, which only folds when binding unfolded glycoprotein (1jhn, Precision=0.58). **(C)** phoA has been captured experimentally in the folded state (1aja) and unfolded state when bound to a chaperone (2mlz) (left panel). ECs capture contacts that are unique to the folded state (pink circles) and some unique to the unfolded state (blue circles) (middle panel). Specifically two pairs of ECs predict residue pairs that are only close in the "unfolded" state (between 416D-423S, and 406P-411A, ~16 and ~13 Å apart in the folded state and 3.8 and 2 Å apart in the unfolded state) (right panel).