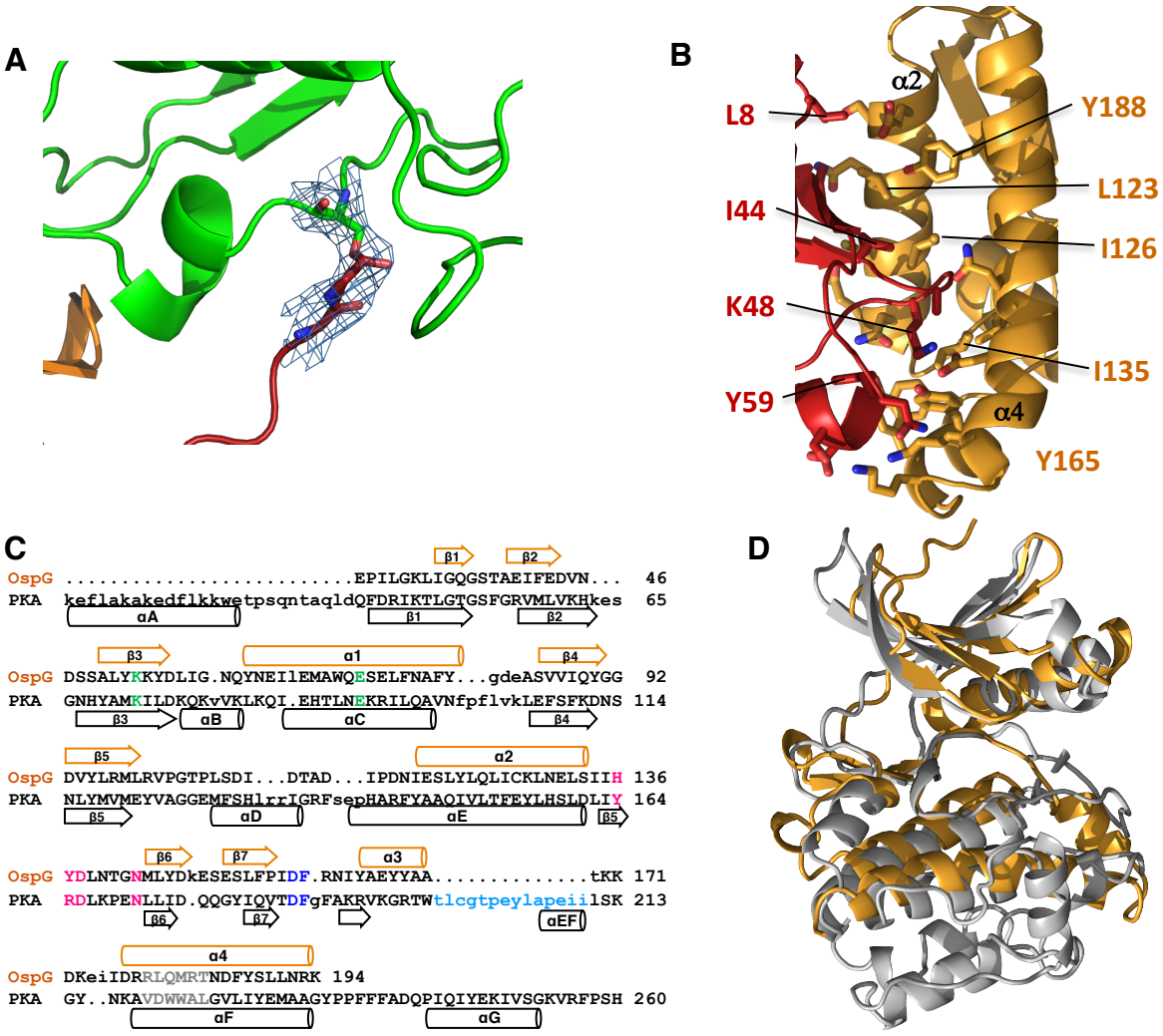
Supplemental Figure 1: OspG/UbcH5c~Ub crystal structure and comparison to PKA and structurally similar kinase domains



Supplemental Figure 1: OspG/UbcH5c~Ub crystal structure

a) 2Fo-Fc composite map plotted at 1.5σ defining the conformation of the UbcH5c~Ub oxyester linkage. **b)** Interacting residues in the OspG (orange)/Ub (red) interface. Backbone atoms are depicted as ribbon representations and side chains involved in the interface are shown as stick representations. Specific residues from OspG and Ub are labeled, as are OspG helices $\alpha 2$ and $\alpha 4$. **c)** Sequence alignment of OspG and PKA based on the structure alignment. Secondary structural elements are shown in orange for OspG and in black for PKA. Residues that form the structural features described in Fig. 1 are colored. Important highlighted features are the conserved Lys-Glu salt bridge (green), critical active site residues (magenta), the regulatory loop (cyan), and the αF helix (grey) All PKA residue numbering used here and in the text matches PDB entry 1ATP. **d)** Global superposition of the OspG and PKA (PDB ID 1ATP) kinase domains. This superposition was used to generate overlaid structures depicted in the main text. **e)** Representative residue contact maps were generated for the kinase domains of OspG, PKA (PDB ID 1ATP), and RIO1 (PDB ID 1ATH). Contacts highlighted in red represent direct interactions between the N- and C-terminal lobes of the kinase. Residues highlighted in green on the diagonal correspond to residues in the hinge segment that connects the N- and C-lobes. Only the structurally homologous regions of the kinases are plotted. PKA has additional N- and C-terminal lobe interactions that occur from protein segments outside the regions structurally homologous to OspG.