

Supplemental Figure S5

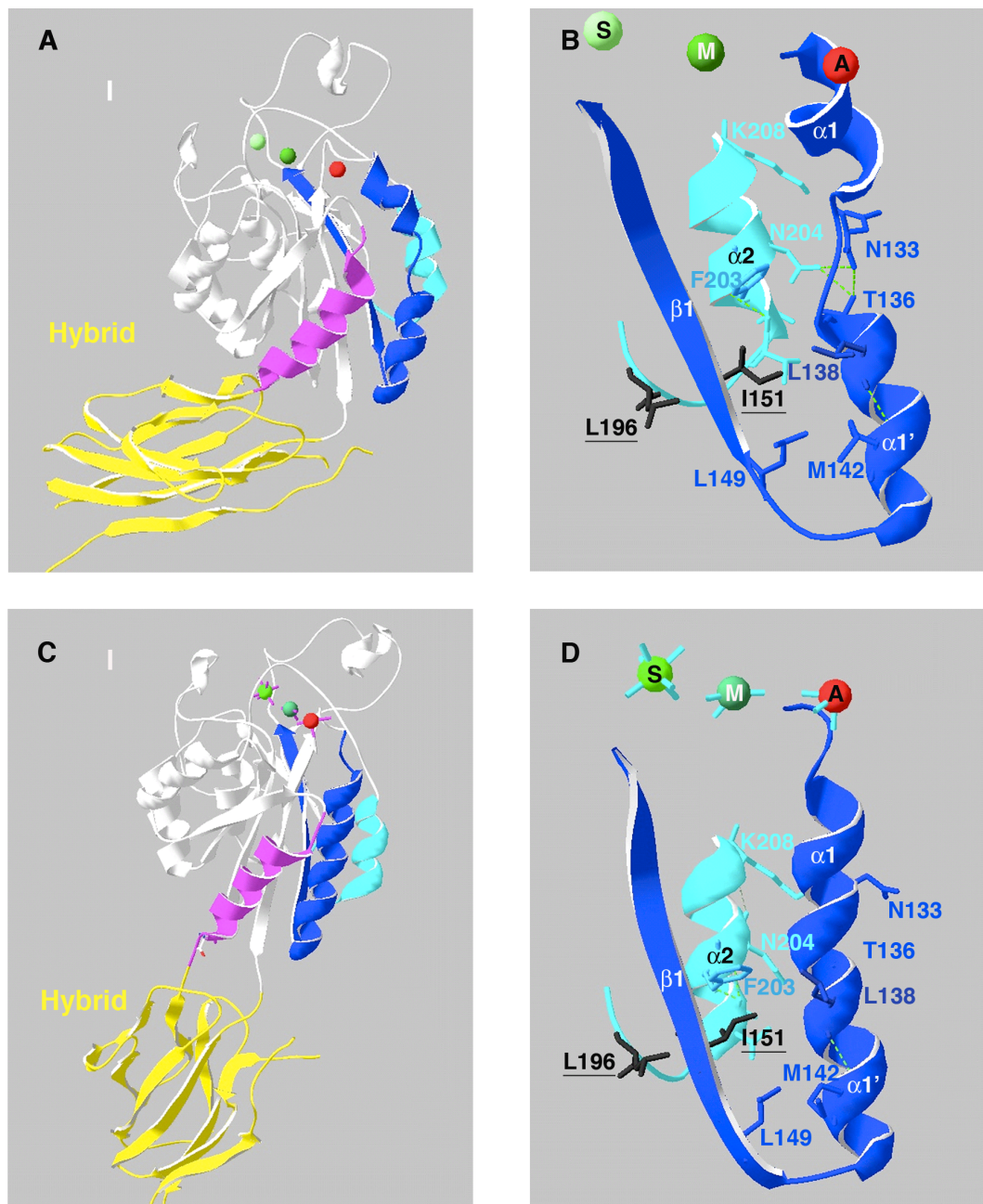


Fig. S5. Mutations that disrupt  $\alpha1,1'$  interactions in the closed conformation increase ligand binding. *A* & *C*. Ribbon structure [from (28,30)] depicting the I and Hybrid (yellow) domains in the closed, (*A*) and open (*C*) conformations.  $\alpha1,1'$ -loop- $\beta1$  (blue),  $\alpha7$  (magenta), and loop- $\alpha2$  (light blue) are highlighted and expanded in *B* (closed) and *C* (open). Amino acids corresponding to those mutated in *Drosophila*  $\beta$ PS and analyzed for ligand binding are labeled (black and underlined). Cations are; SyMBS  $\text{Ca}^{2+}$  (S, light green), MIDAS  $\text{Mg}^{2+}$  (M, green) and ADMIDAS  $\text{Ca}^{2+}$  (A, red). Hydrogen bonds are shown as green dashed lines in *B* and *D*.