Supplemental Figure S7

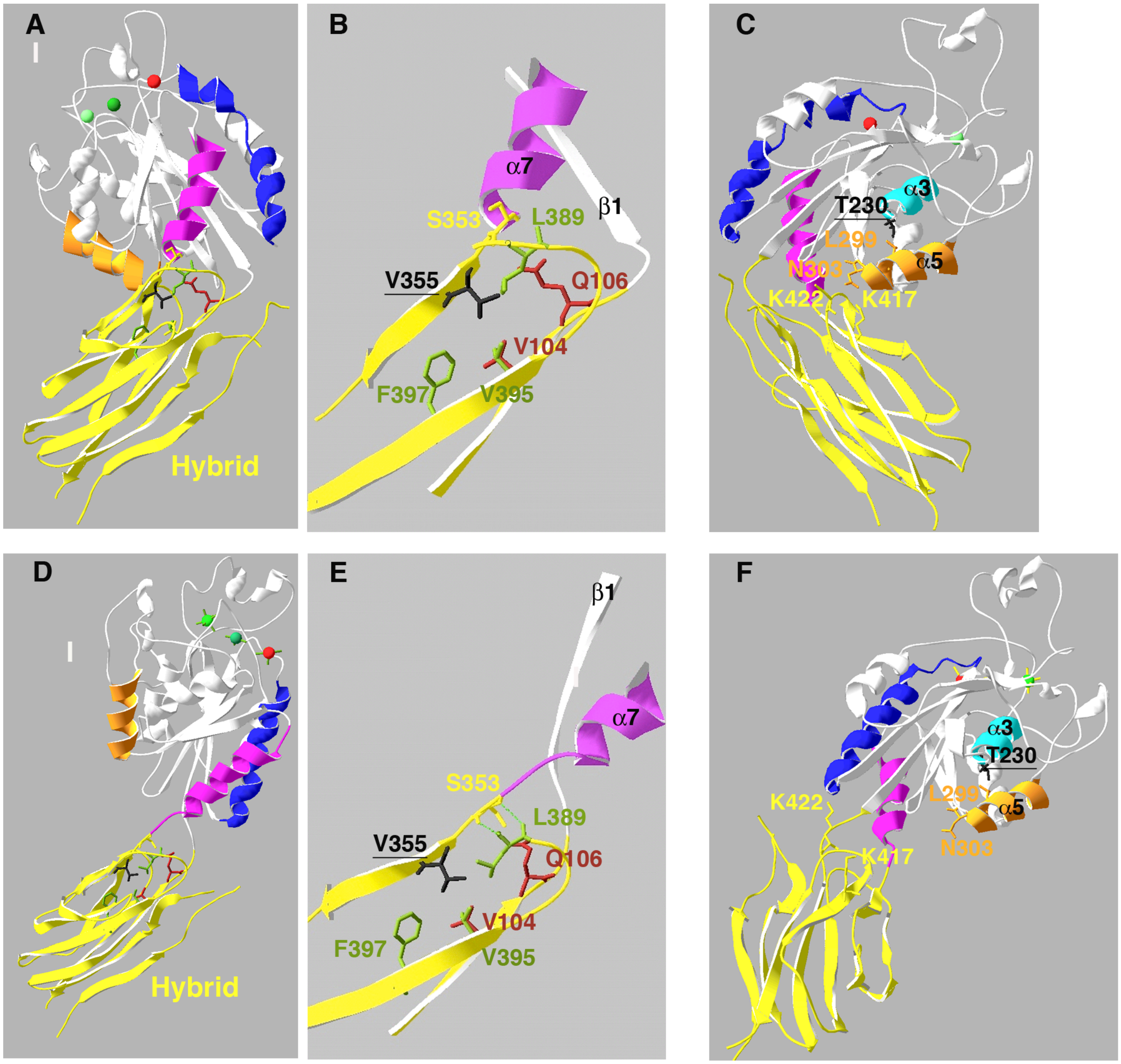

Fig. S7. Hybrid residue **V355** immediately following $\alpha 7$ maintains the closed conformation. *A* and *D*. Ribbon structure [from (28,30)] depicting the $\beta 3$ integrin I (white) and Hybrid (yellow) domains in the closed (A) and open (D) conformations. $\alpha 7$ (magenta), $\alpha 5$ (orange), and $\alpha 1,1'$ (blue) are highlighted. Expanded views of **V355** (mutated in mys^{b27}; black underlined) and residues with altered interactions between the closed (B) and open (E) states. In the closed state **V355** is within 3.4 Å of **V104** (dark red) and **Q106** (dark red) and separated from **L389** (green) by 3.9 Å. **V395** and **F397** (green) are further away at 4.6 and 4.5 Å. In the open state **V355** shifts away from **Q106** (more than 5.9 Å) and closer to **V395** and **F397** (now within 3.9 Å). **L389** hydrogen bonding with **S353** is also altered and this brings it closer to **V355** in the open conformation (3.3 Å versus 3.9 Å). *C* and *F*. Ribbon structures in *A* and *D* rotated approximately 180° with $\alpha 3$ (light blue) additionally highlighted. In the closed conformation (C) **N303**, at the base of $\alpha 5$ (orange), is very near (within 3.0 and 3.8 Å) **K417** and **K422** in the Hybrid domain (yellow). These distances increase to over 20 Å in the open (F) conformation. **T230** (mutated in mys^{b30}; black underlined) at the base of $\alpha 3$ contacts **L299** of $\alpha 5$. $\alpha 5$ is likely to be key to restraining the Hybrid domain in the closed conformation. Cations in *A* and *D* are SyMBS Ca^{2+} (light green), MIDAS Mg^{2+} (green) and ADMIDAS Ca^{2+} (red). Hydrogen bonds are shown as green dashed lines (E).