## **Supplemental Figure 7** Ro 08-2750 RoOH Ro A6 0 0 $\Delta G$ : $-5.5 \pm 0.3$ $\Delta G$ : $-6.2 \pm 0.3$ $\Delta G$ : -5.1 ± 0.2 -1 -1 ΔG<sub>bind</sub> (kcal/mol) **-**2 -2 **-**2 -3 -3 **-**3 -4 -5 -5 -6 -6 -6 -7 -7 10 20 5 15 5 10 15 20 5 10 15 20 Cutoff distance (Å) В Ro 08-2750 **RoOH** Ro A6 **Complex** Apo RoOH Ro 08-2750 С Ro 8-2750 Ro A6 D Cluster 0 ~ 25.7% Cluster 1 Ε ~ 32.2% **RoOH** Cluster 0 Cluster 3 Cluster 7 Cluster 14 ~10.0% ~ 17.7% ~12.8% ~8.6% Cluster 6 ~ 34.8%