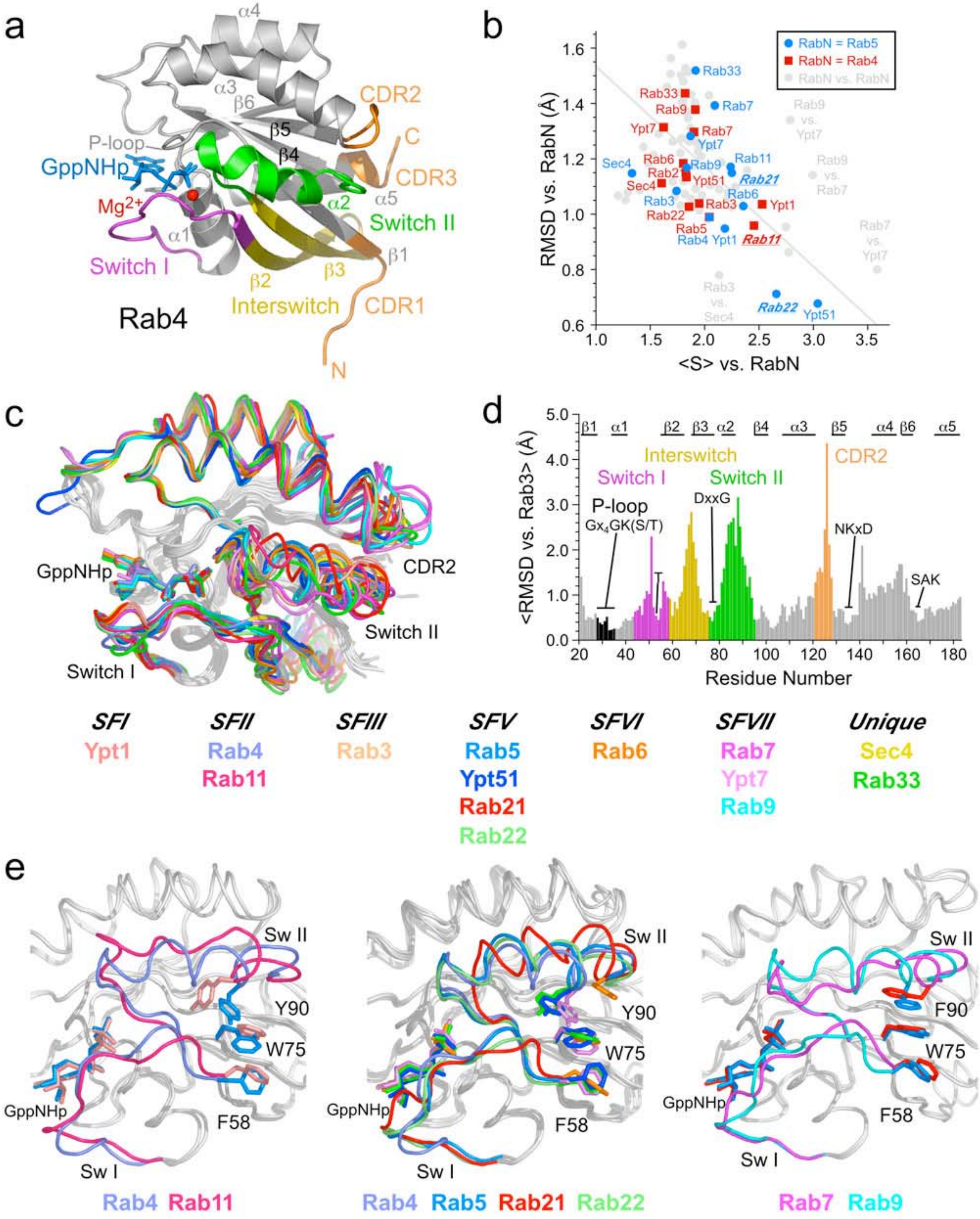

Supplementary Figure 3. Survey of structural similarity, variability, and plasticity in the Rab family

a, Ribbon rendering of the GppNHp-bound structure of Rab4. **b,** Correlation of structural and sequence similarity for the active forms of 14 Rab GTPases. Gray circles represent a pairwise comparisons of all 14 Rab GTPases. Red squares and blue circles denote pairwise comparisons with Rab4 and Rab5, respectively. RMSD denotes the root mean squared deviation of Cα atoms following superposition. <S> denotes the average log odds score for pairwise sequence comparison calculated with the Blosum 62 substitution matrix. **c,** Comparison of the active structures of Rab GTPases determined in this study or available in the protein data bank (see Supplementary Table 3). The figure was rendered following pairwise superposition with the most representative structure (Rab3). Colors and subfamily organization are indicated underneath the superposition. **d,** Average deviation from the most representative structure calculated with respect to the superposition in SF 3C. Residues numbers correspond to Rab5. **e,** Comparison of active structures from subfamily II (left), subfamilies II and V (middle), and subfamily VII (right). Also shown are invariant aromatic residues in the switch and interswitch regions. Residues numbers correspond to Rab5.