

Figure S1. Global dynamical comparisons of Parkin variants. (A) RMSD of the entire Parkin protein over time throughout the course of the simulation. (B) Domain map of the Parkin Wildtype (WT). (C) Overlap of the WT and Y143E. (D) Overlap of the WT and V393D. (E) Overlap of the WT and A401D. (F) Overlap of the WT and W403A.

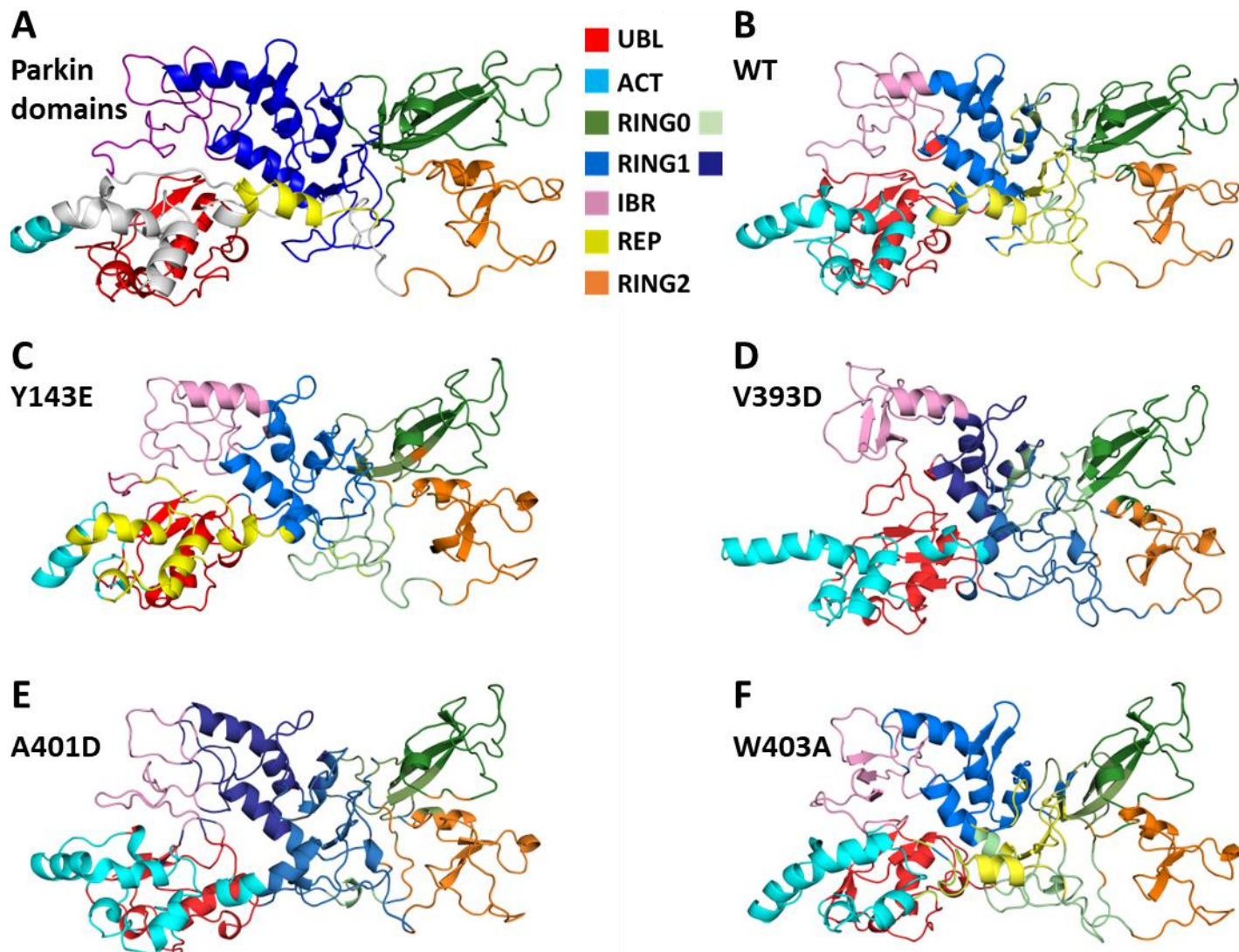


Figure S2. Structural network comparisons of Parkin variants. (A) 3D domain map of Parkin. (B) Dynamical network of WT Parkin, colored to correspond to the domain map. (C) Dynamical network of Y143E. (D) Dynamical network of V393D. (E) Dynamical network of A401D. (F) Dynamical network W403A.

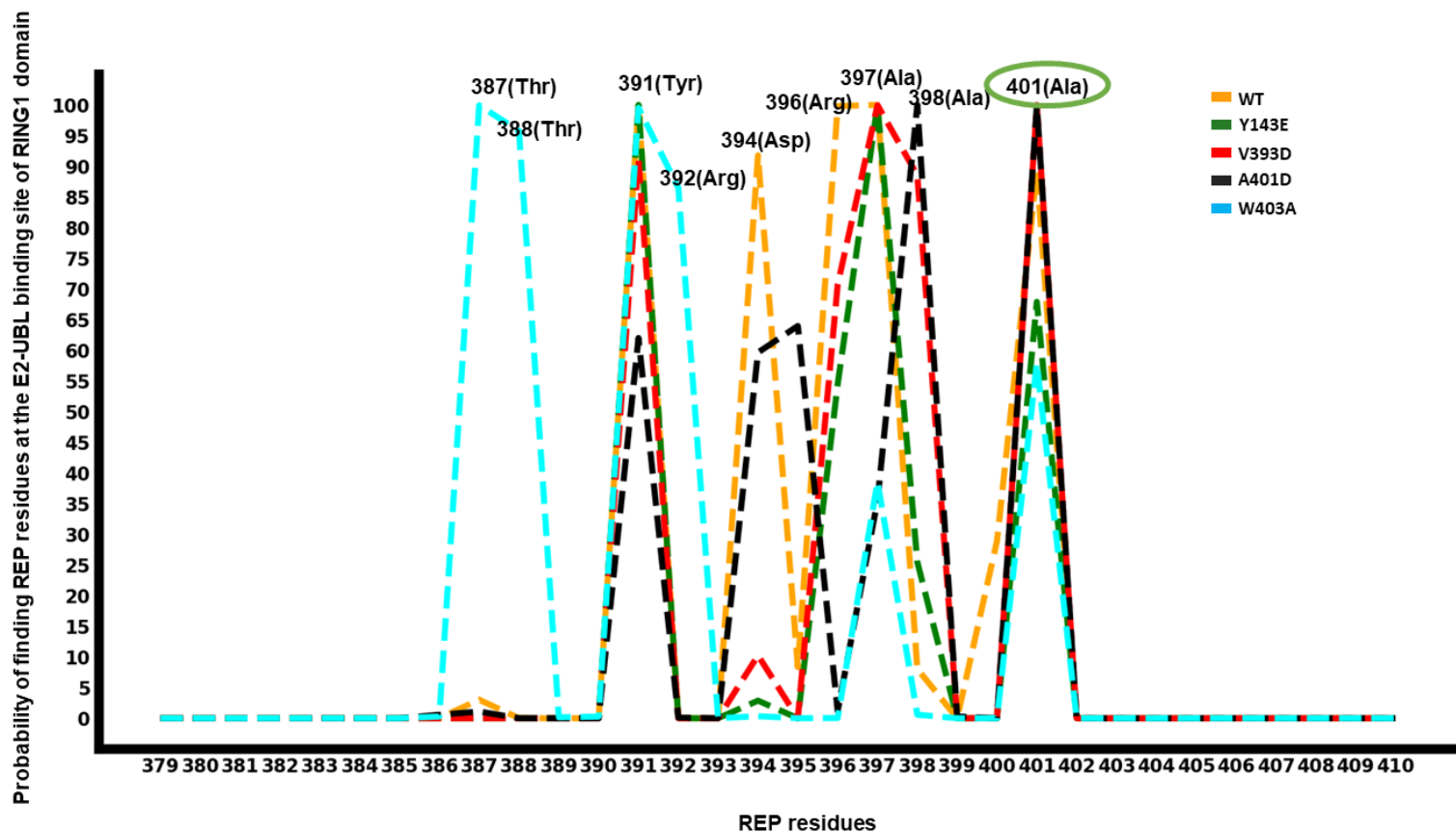


Figure S3. Global dynamical comparisons of Parkin variants. Probability of finding REP residue at the E2-UBL binding site of RING1 domain for different mutations, as well as for WT Parkin.

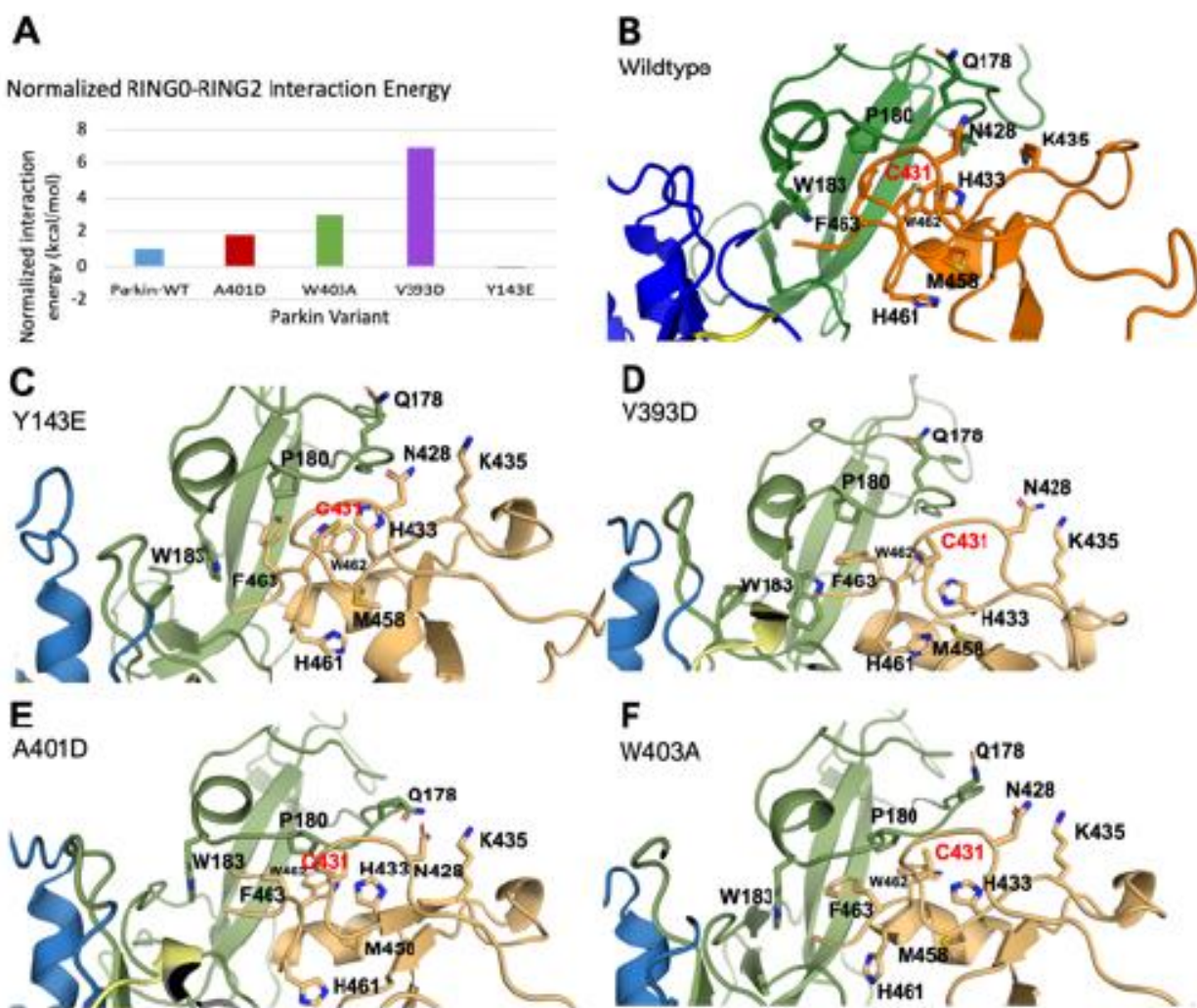


Figure S4. RING0-RING2 regional dynamical comparisons of Parkin variants. Domain-Domain interactions between the (A) RING0 and RING2 domains over time throughout the course of the simulation. Close up of the RING0-RING2 interactions for (B) WT, (C) Y143E, (D) V393D, (E) A401D, and (F) W403A.

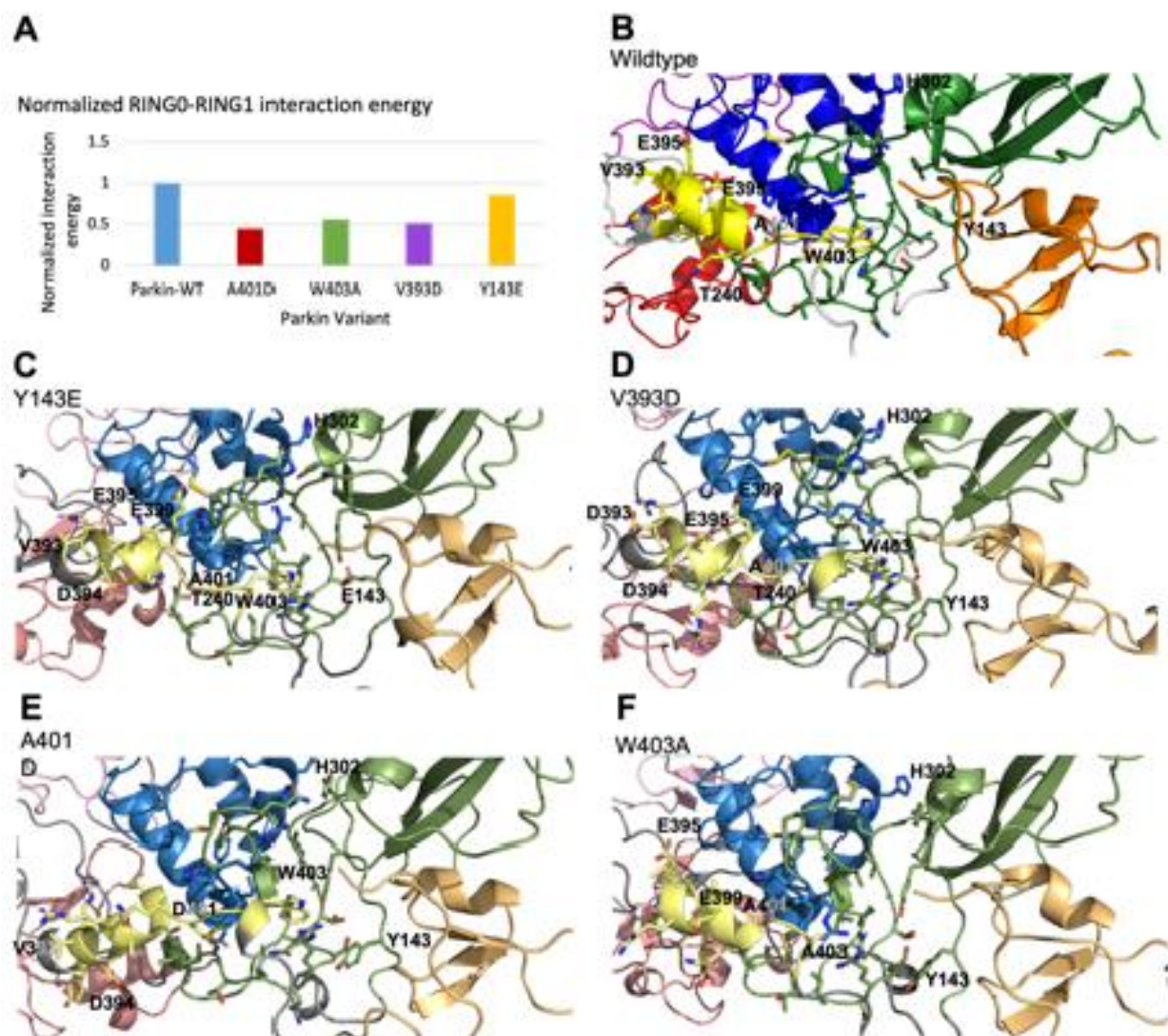


Figure S5. RING0-RING1 regional dynamical comparisons of Parkin variants. Domain-Domain interactions between the (A) RING0 and RING1 domains over time throughout the course of the simulation. Close up of the RING0-RING1 interactions for (B) WT, (C) Y143E, (D) V393D, (E) A401D, and (F) W403A.