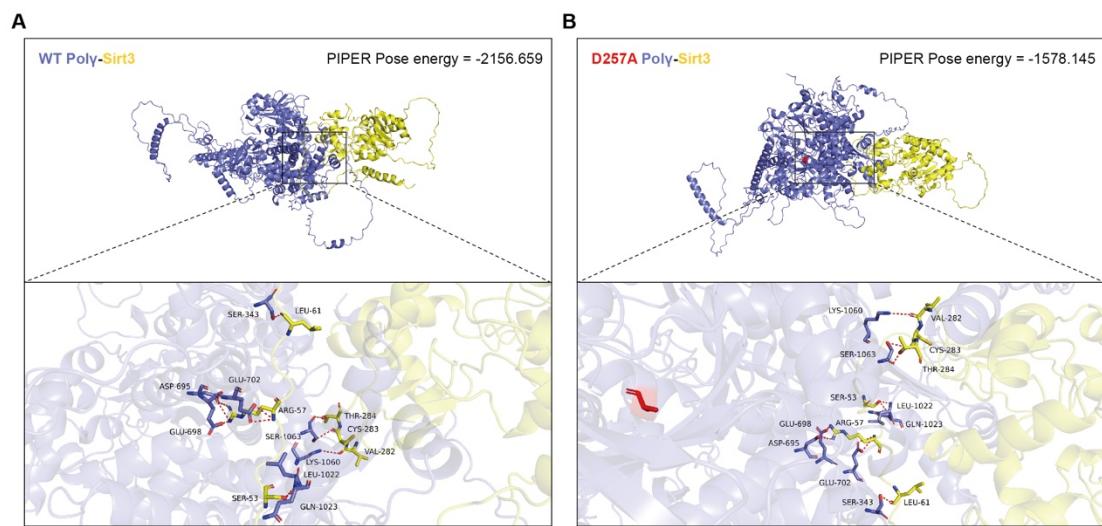
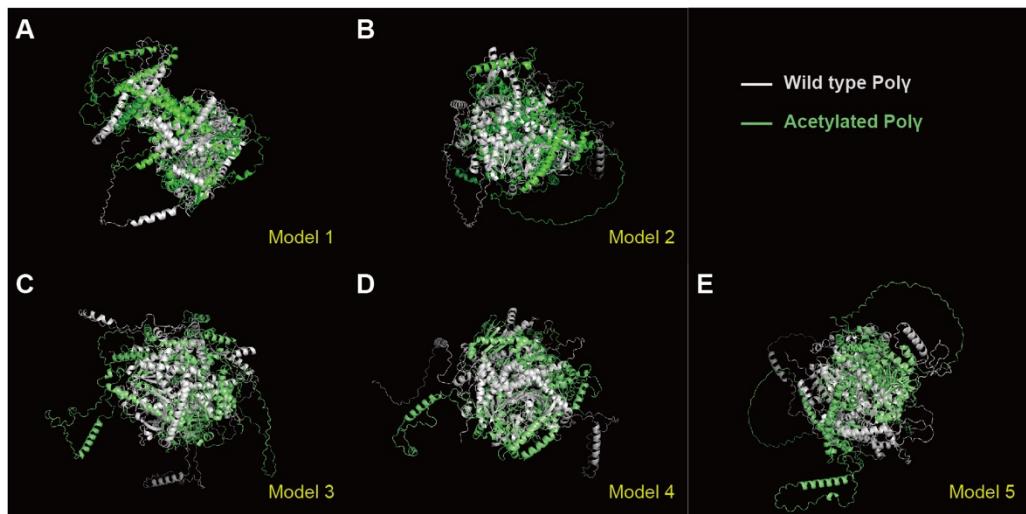


Figure S1. D257A mutation reduced binding between Poly and Sirt3 by molecular docking.



D257A mutation reduced binding between Poly and Sirt3 by molecular docking. (A) The predicted structural model of the wild-type Poly- Sirt3 complex, with Poly depicted in blue and Sirt3 in yellow. The interface analysis predicts potential interfacial residues mediating the interaction between the two proteins. (B) The predicted structural model and potential interfacial residues of the D257A mutated Poly- Sirt3 complex, with Poly depicted in blue (D257 site in red) and Sirt3 in yellow.

Figure S2. K1039 acetylation altered the spatial structure of Poly.



K1039 acetylation altered the spatial structure of Poly. (A-E) AlphaFold3 was employed to predict the structures of both wild-type Poly and K1039-acetylated Poly (acetyl group in K1039 site). Five representative structural models were generated for each form.