

Fig. S1 The β -strands are named from A to H. The F and H strands are located in the other monomer of the same dimer. Arrows point from the hydrogen bond donor to the acceptor. The α -helix is from Asp 74 to Ala 81.

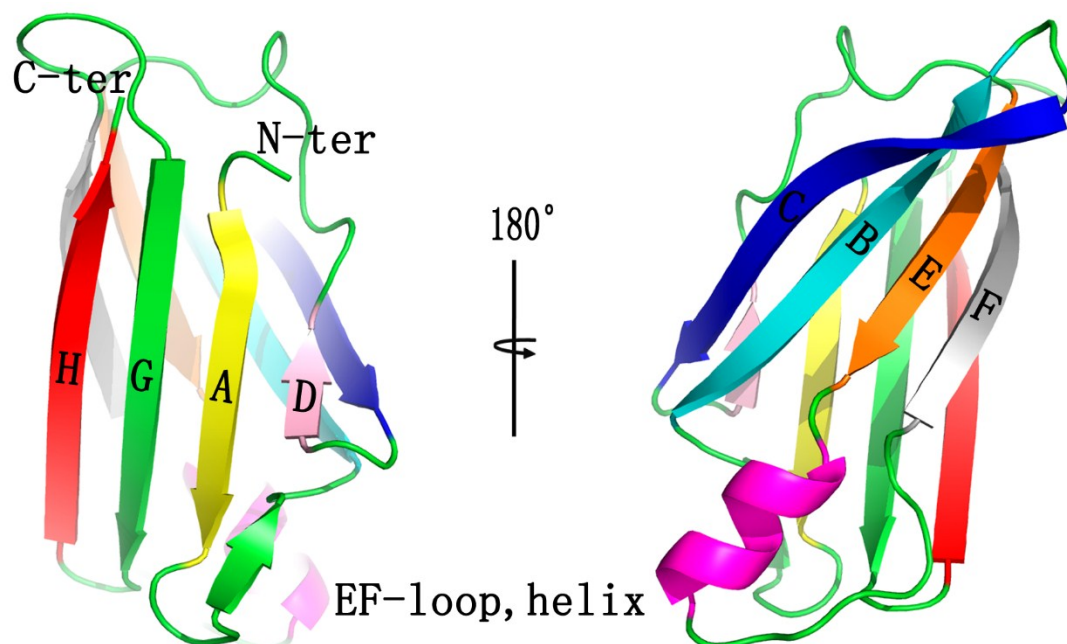


Fig. s2 a The 2D structure of Glab. b the 3D structure of Glab. c The potential surface energy of Glab. d The hydrophobicity of Glab.

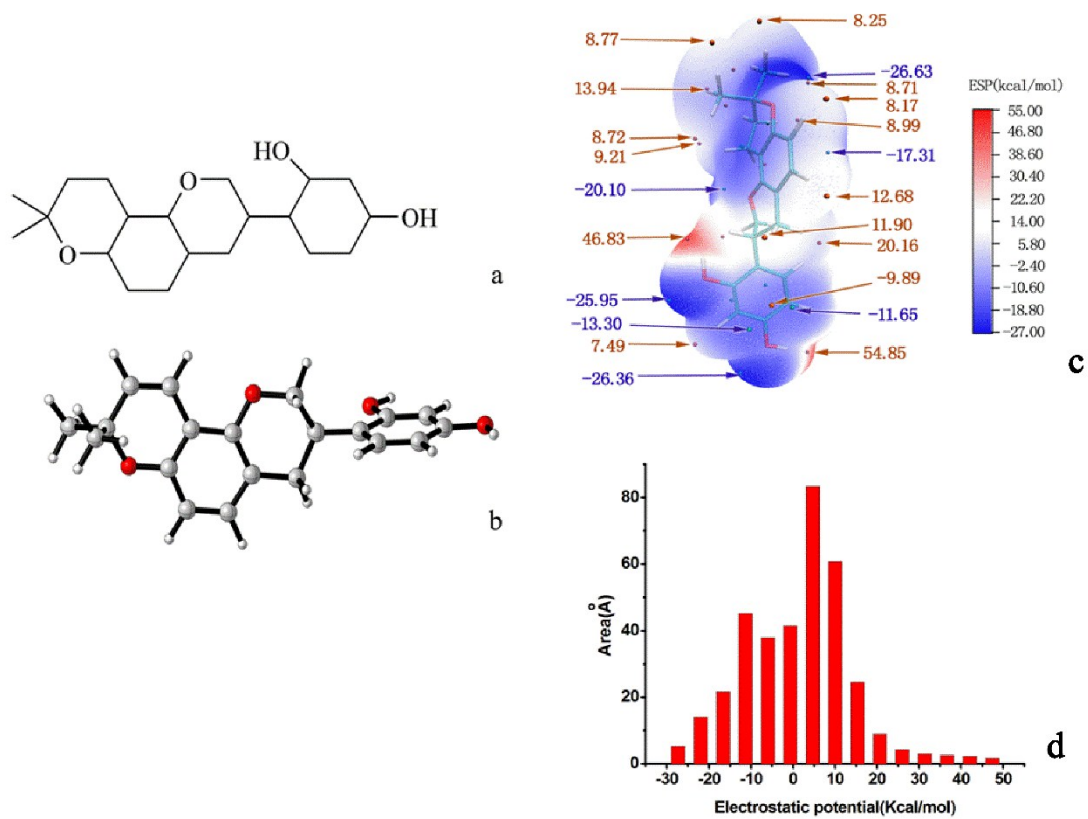


Fig. s3 The RMSD plot of WT and V30A during 20 ns MD simulations.

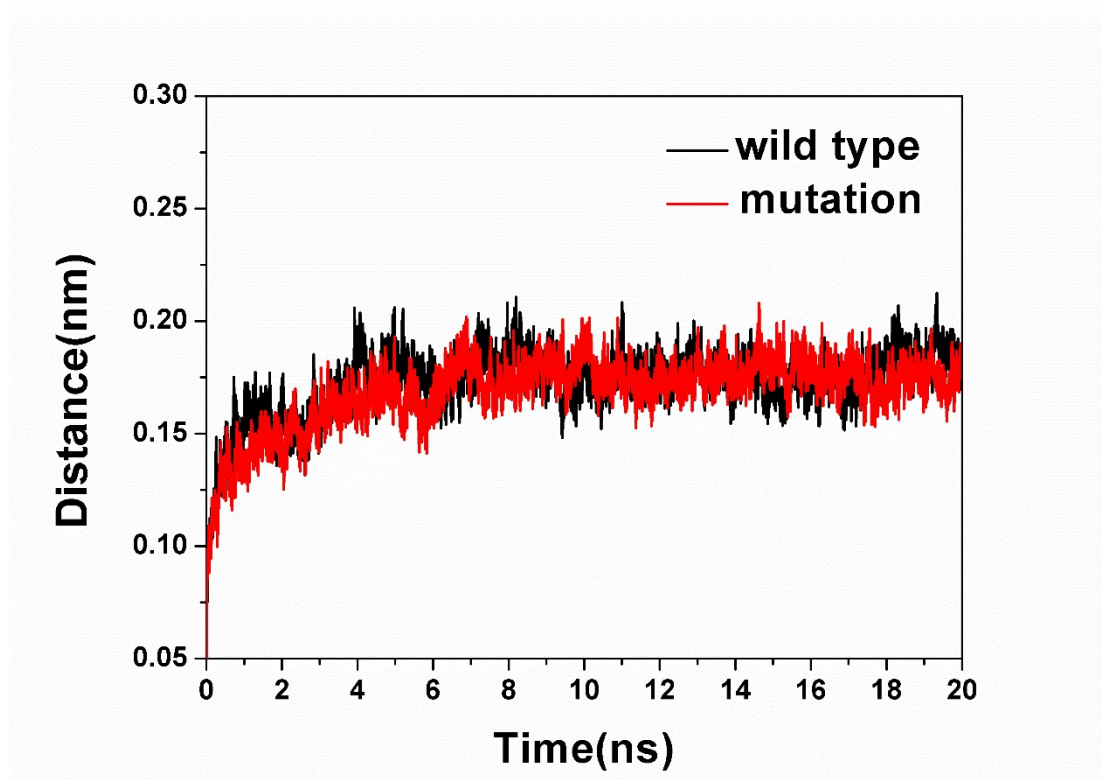


Fig. s4 a The important residues in the TTR channel. b Geometry of the channel in the sample snapshot calculated by CAVER 3.0 of the WT TTR. c Geometry of the channel in the sample snapshot calculated by CAVER 3.0 of the V30A TTR.

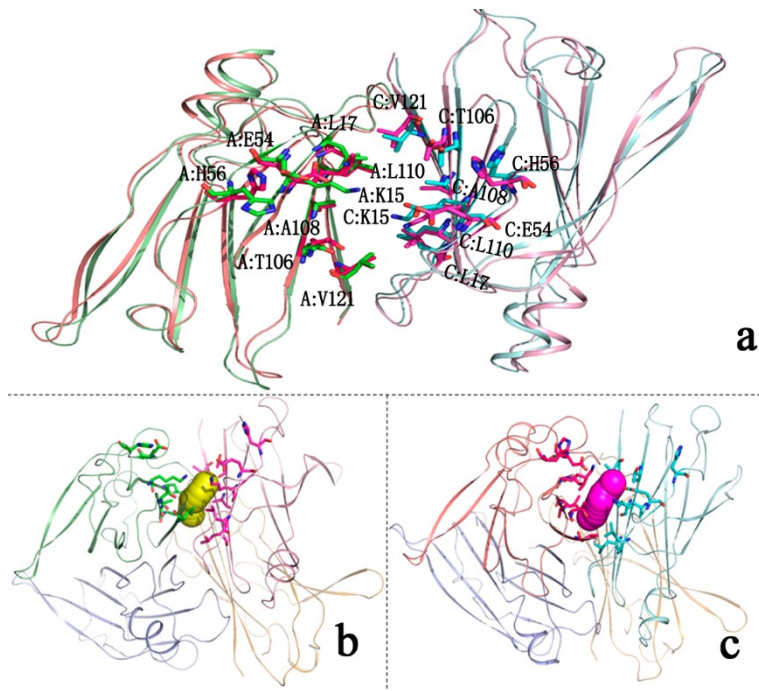


Fig. s5 The change of secondary structure of AB loop and CD loop

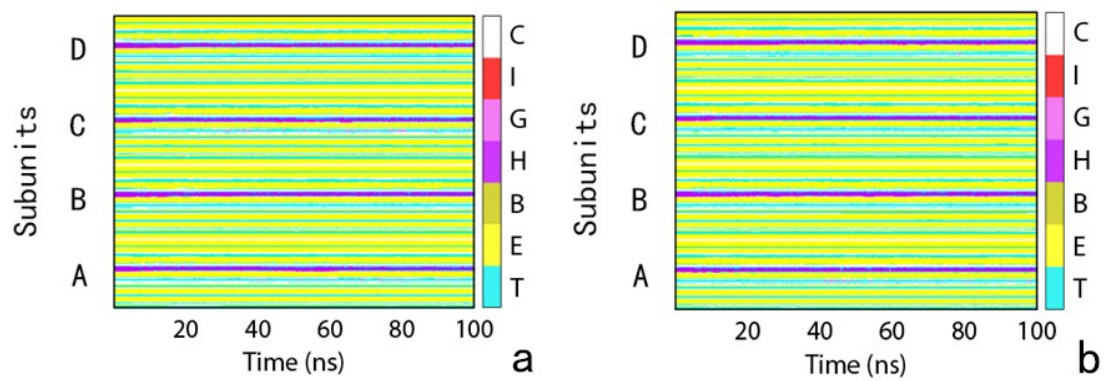


Fig. s6 The relative free energy surfaces along the first two principle components (PC-1, PC-2) of a TTR-Glab in A chain; b TTR-Glab in B chain; c TTR-Glab in C chain; d TTR-Glab in D chain; e V30A TTR-Glab in A chain; f V30A TTR-Glab in B chain; g V30A TTR-Glab in C chain; h V30A TTR-Glab in D chain.

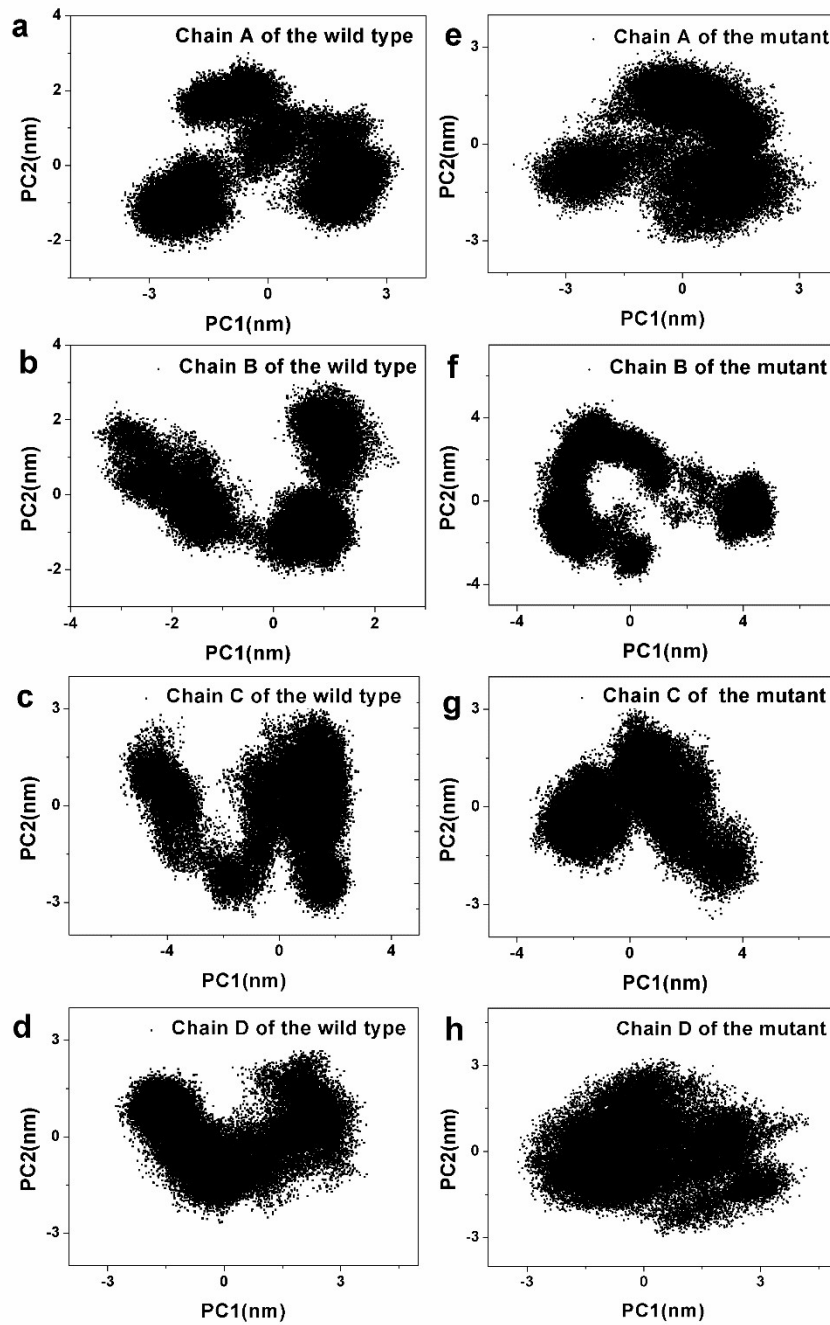


Fig. s7 The Turbidity of WT TTR and V30A TTR in different pH.

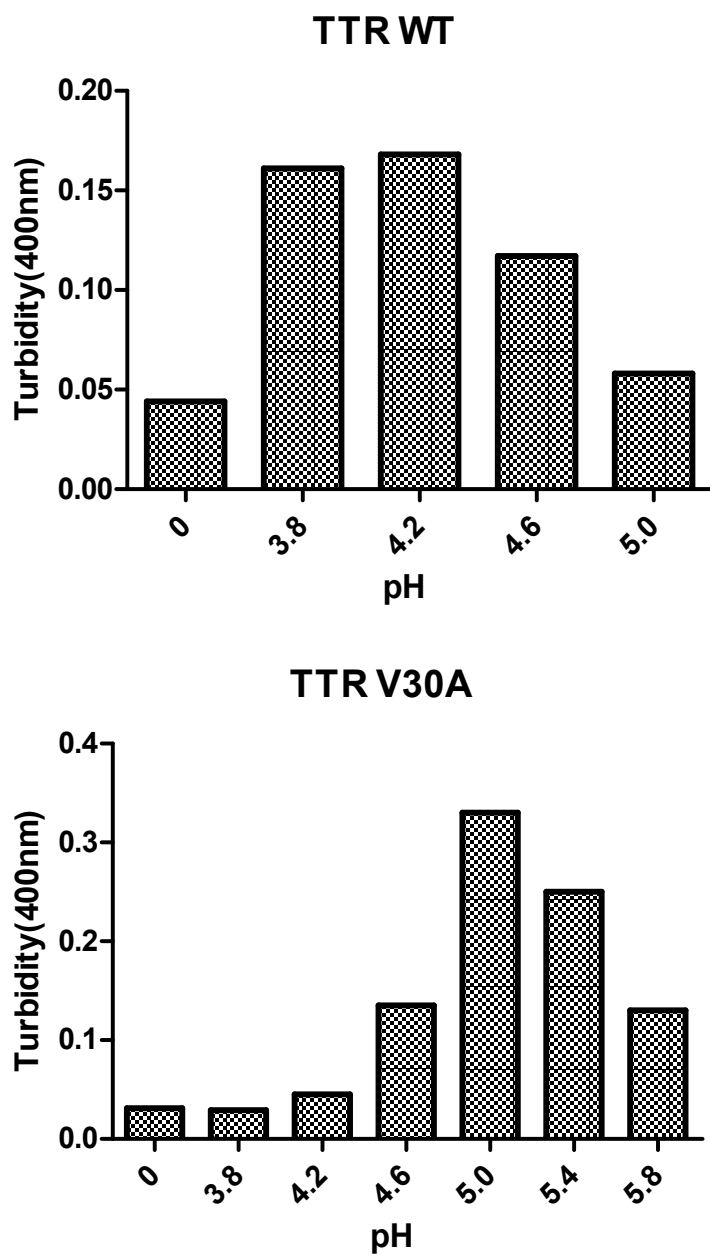


Table s1. Molecular Systems.

Simulations	Time(ns)	Solvent	Ions
WT-Glab1 (between chain A and chain C)	100	19253	20Na ⁺
WT-Glab2+Glab1	100	19307	20Na ⁺
V30A-Glab1 (between chain A and chain C)	100	19259	20Na ⁺
V30A-Glab 2+Glab1	100	19313	20Na ⁺
WT	20	19225	20Na ⁺
V30A	20	19217	20Na ⁺