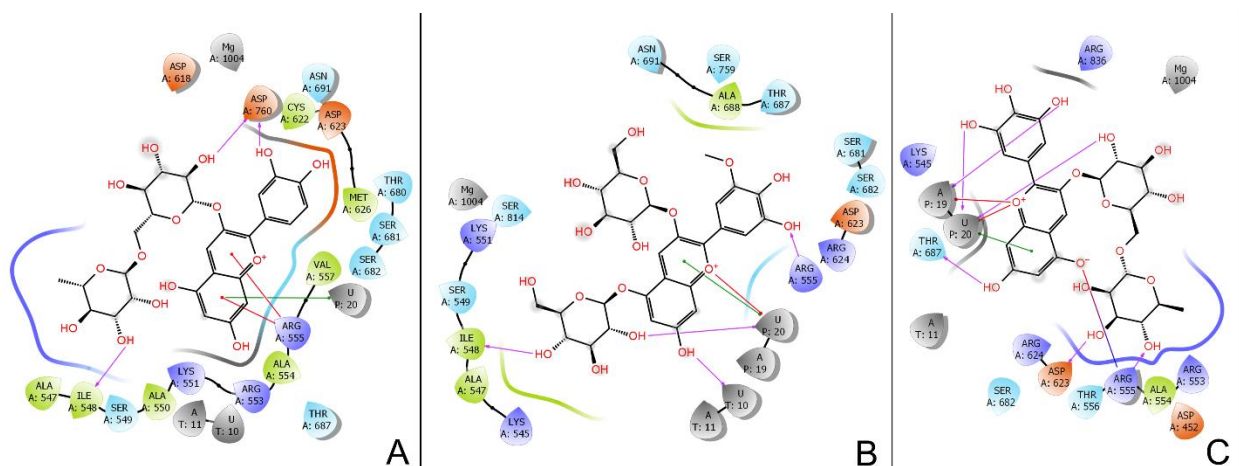
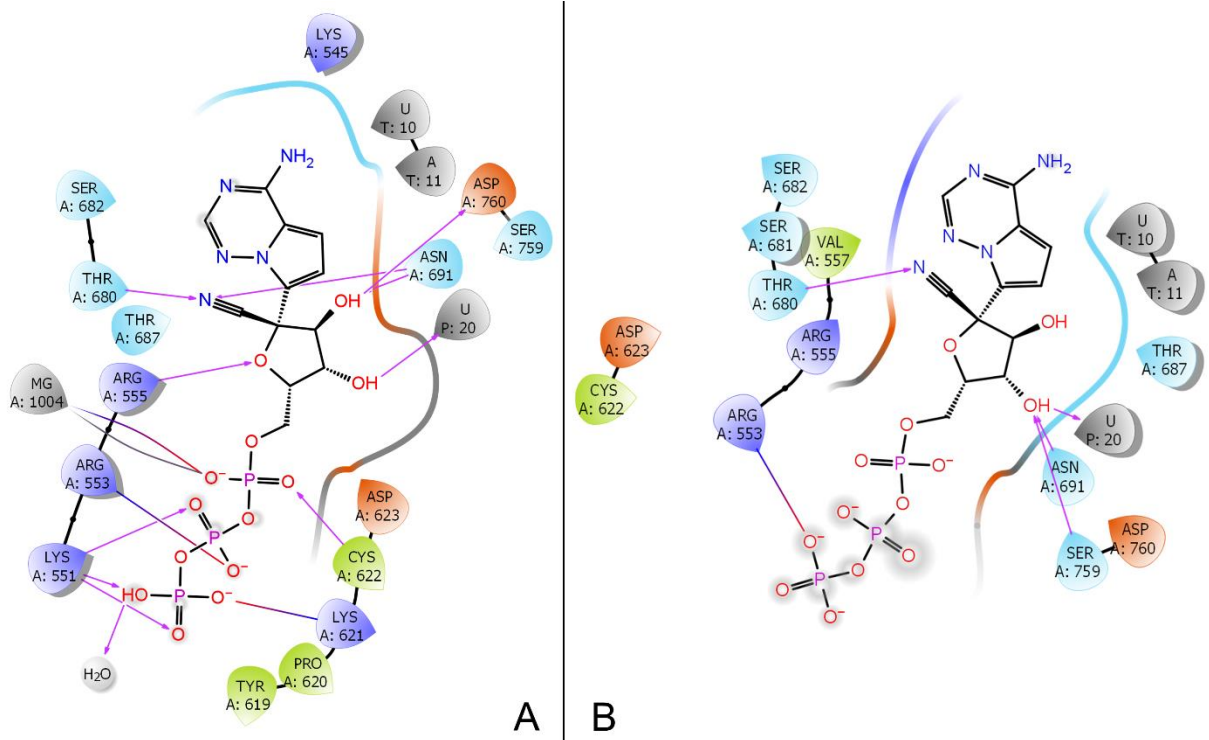


**Figure S1** The RMSD of 7BV2 before and after ligand-protein docking. The yellow line represents the RMSD of 7BV2 before ligand-protein docking; the blue line represents the RMSD of 7BV2 after binding of cyanidin 3-O-rutinoside; the red line represents the RMSD of 7BV2 after binding of petunidin 3,5-O-diglucoside; the green line represents the RMSD of 7BV2 after binding of delphinidin 3-O-rutinoside.



**Figure S2** 2D ligand-protein interaction diagrams of RdRp and the top three ligands after MD simulations: A, Cyanidin 3-O-rutinoside; B, Petunidin 3,5-O-diglucoside; C, Delphinidin 3-O-rutinoside. The pink spheres represent  $Mg^{2+}$  ions. The purple arrows indicate the hydrogen bonds; the green line represents  $\pi$ - $\pi$  stacking; the red line represents  $\pi$ -cation interaction; the blue-red line represents the salt bridge.



**Figure S3** 2D ligand-protein interaction diagrams of RdRp-remdesivir-TP before (A) and after (B) MD simulation. The purple arrows indicate the hydrogen bonds; the blue-red line represents the salt bridge; the gray line represents metal coordination.