

Fig. S1 The structure of human P-gp. (A) Two halves (TMD-NMD) of P-gp are connected by a flexible linker region (green). (B) Twelve transmembrane α -helices domains in TMDs. (C) The key and conserved motifs of P-gp ATPase in NBDs.

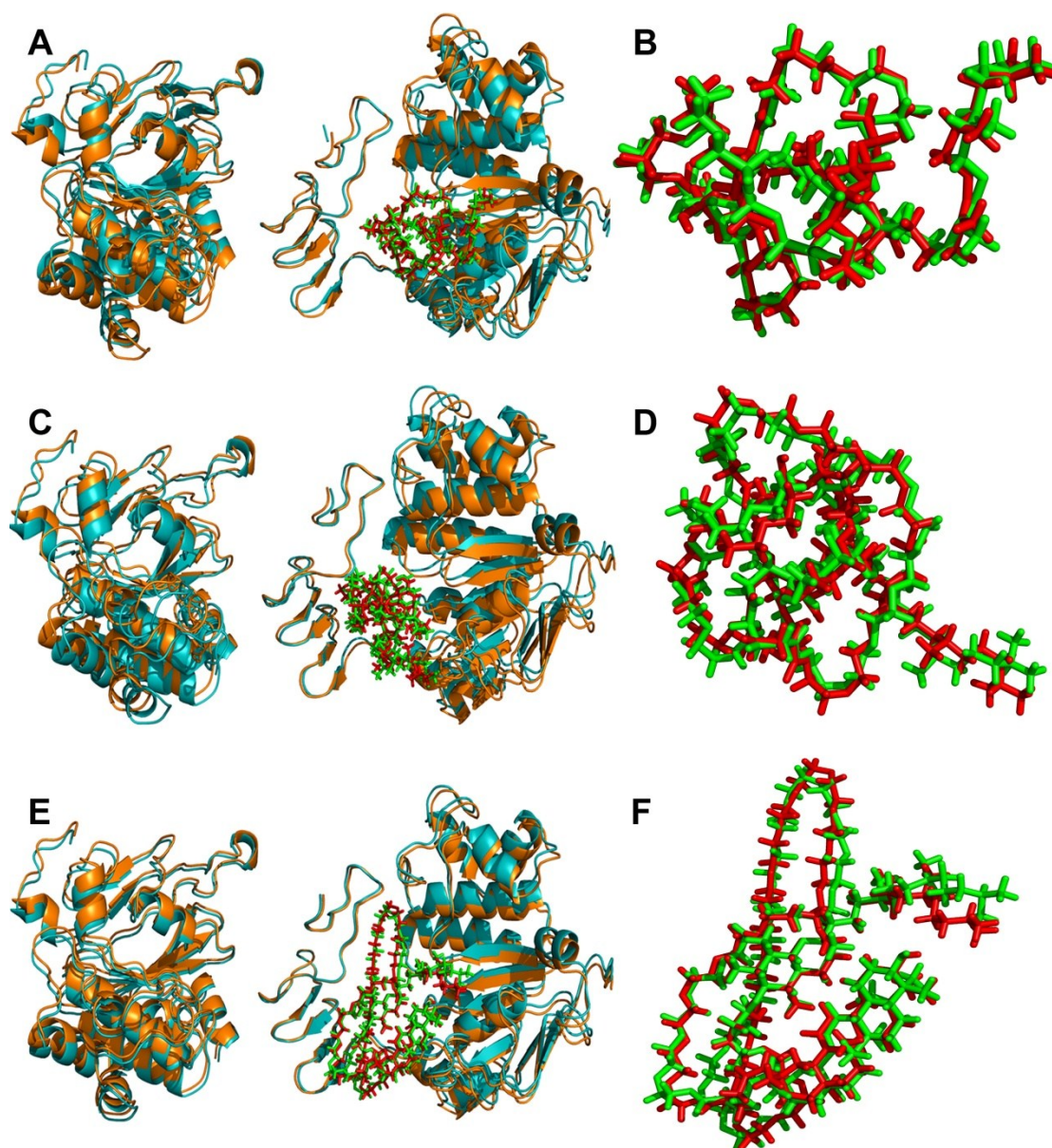


Fig. S2 The starting and lowest-energy conformations of P-gp-polymers complexes and polymers. (A) The superimposition of NBD-TPGS complexes; (B) The superimposition of TPGS; (C) The superimposition of NBD-TLA complexes; (D) The superimposition of TLA; (E) The superimposition of NBD-TGA complexes; (F) The superimposition of TGA. The structure of P-gp is not displayed for clear presentation, expect NBD.