

Supplementary Material

Pentagalloyl glucose targeted inhibition of P-glycoprotein and re-sensitization of multidrug-resistant leukemic cells (K562/ADR) to doxorubicin: in silico and functional studies

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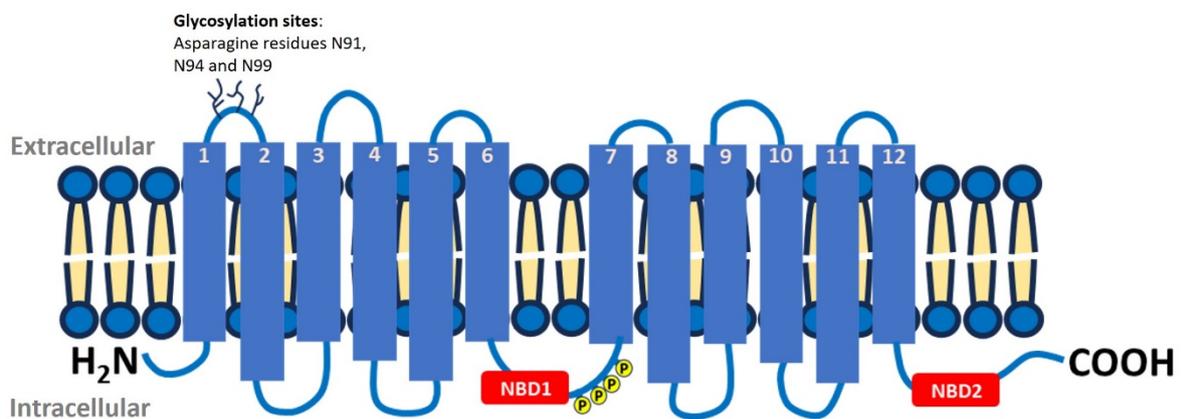
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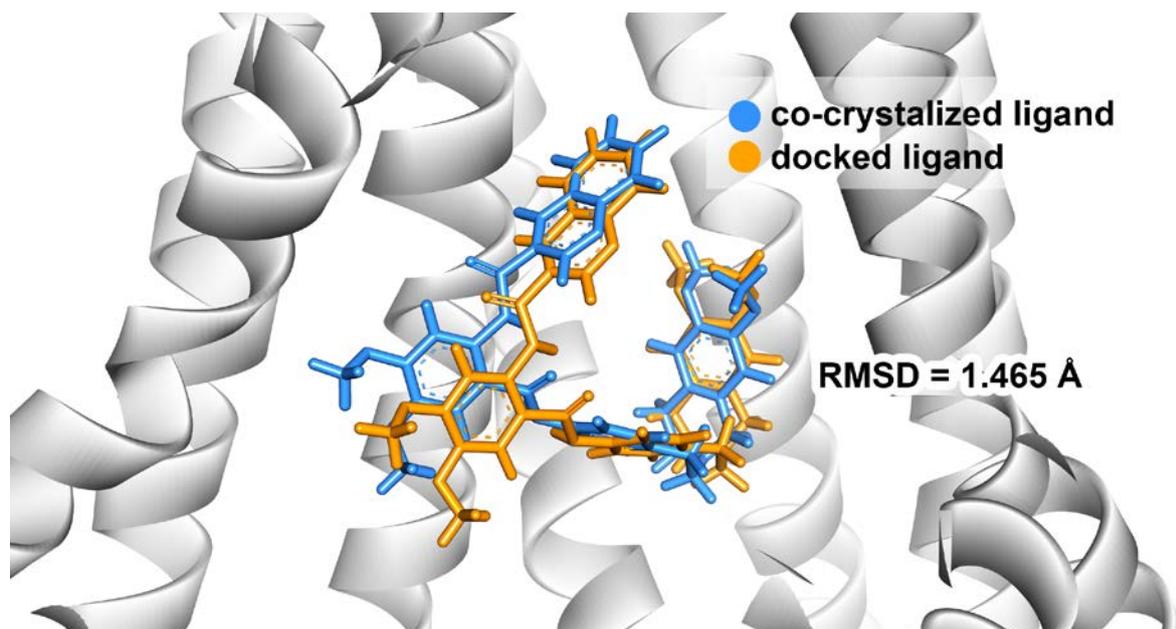
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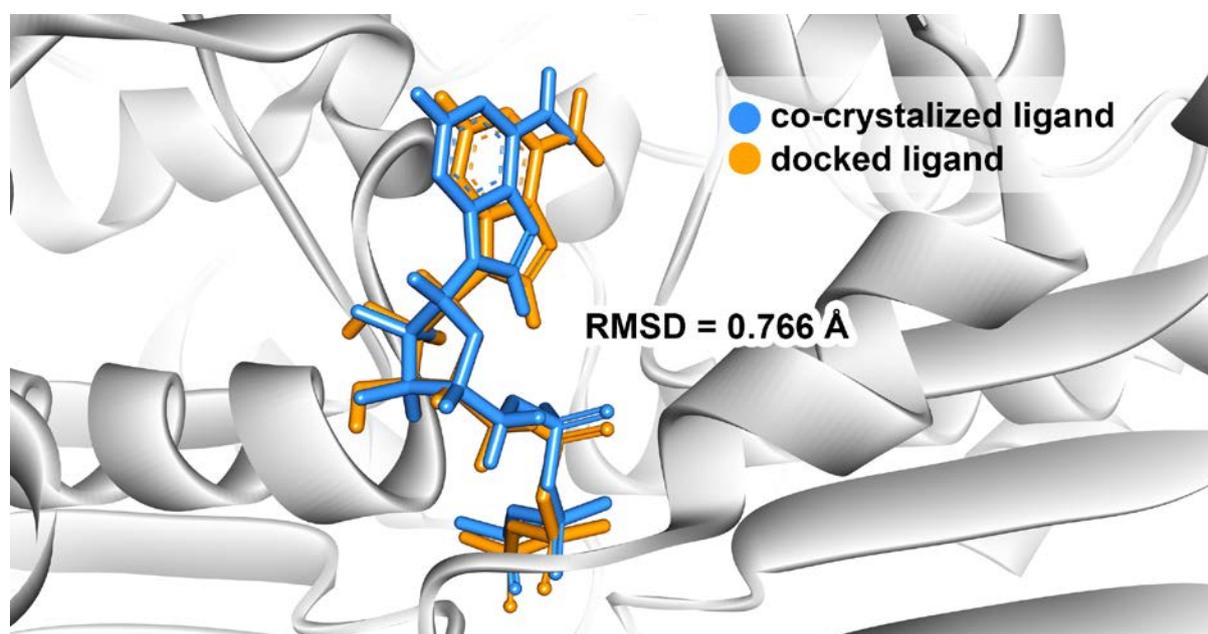
Supplementary Materials: Figure S1: P-glycoprotein (P-gp) structure consists of two transmembrane domains, each including six helices that transverse the cellular membrane. In addition, it contains two ATP-binding regions (nucleotide-binding domains, NBDs) within the cell; Figure S2: Tariquidar superimposed between docked and co-crystallized ligands at the substrate binding site for docking protocol validation (PDB ID: 7A6E). The result showed the RMSD value of 1.465 Å; Figure S3: Superimposed between the docked and co-crystallized ATP at the ATP binding site for docking protocol validation (PDB ID: 6C0V). The result showed the RMSD value of 0.766 Å; Figure S4: 3-Dimensional structures of PGG, tariquidar, verapamil and ATP together with the best fit of these structures; Figure S5: 3D structures of protein-ligand complex and free energy landscape (FEL) of three replica copies of verapamil at substrate binding site of P-gp; Figure S6: 3D structures of protein-ligand complex and free energy landscape (FEL) of three replica copies of tariquidar at substrate binding site of P-gp; Figure S7: 3D structures of protein-ligand complex and free energy landscape (FEL) of three replica copies of PGG at substrate binding site of P-gp; Figure S8: 3D structures of protein-ligand complex and free energy landscape (FEL) of three replica copies of ATP at ATP binding site of P-gp; Figure S9: 3D structures of protein-ligand complex and free energy landscape (FEL) of three replica copies of PGG at ATP binding site of P-gp Figure S10: The uncropped western blot images corresponding to Figure 3a.



Supplementary Figure S1. P-glycoprotein (P-gp) structure consists of two transmembrane domains, each including six helices that transverse the cellular membrane. In addition, it contains two ATP-binding regions (nucleotide-binding domains, NBDs) within the cell

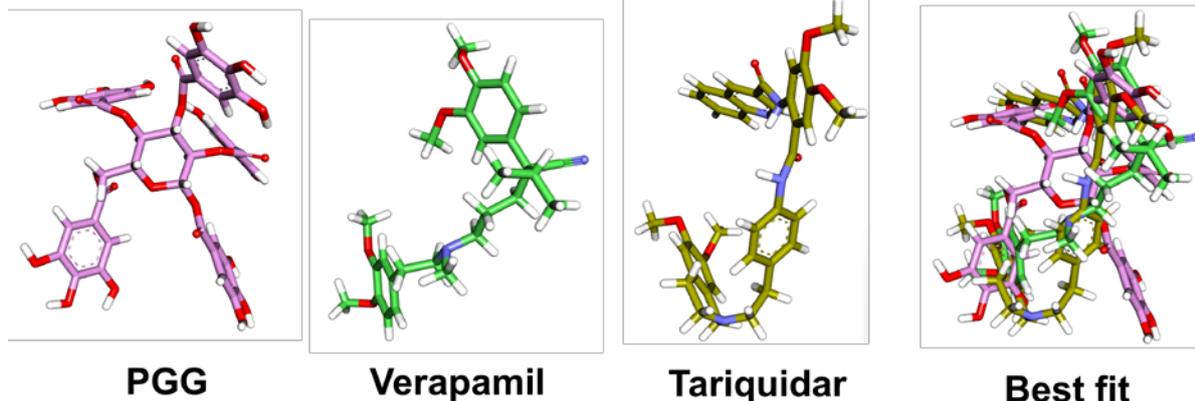


Supplementary Figure S2. Tariquidar superimposed between docked and co-crystallized ligands at the substrate binding site for docking protocol validation (PDB ID: 7A6E). The result showed the RMSD value of 1.465 Å.

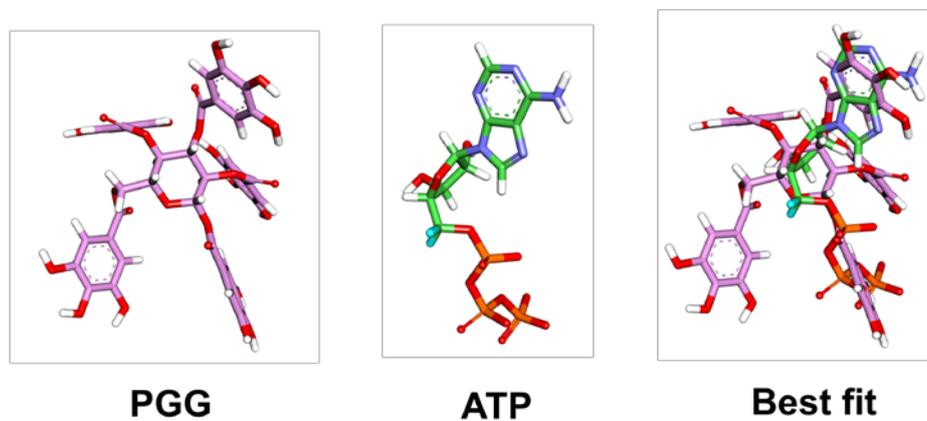


Supplementary Figure S3. Superimposed between the docked and co-crystallized ATP at the ATP binding site for docking protocol validation (PDB ID: 6C0V). The result showed the RMSD value of 0.766 Å.

3-Dimensional Structures of Ligands at the substrate binding site

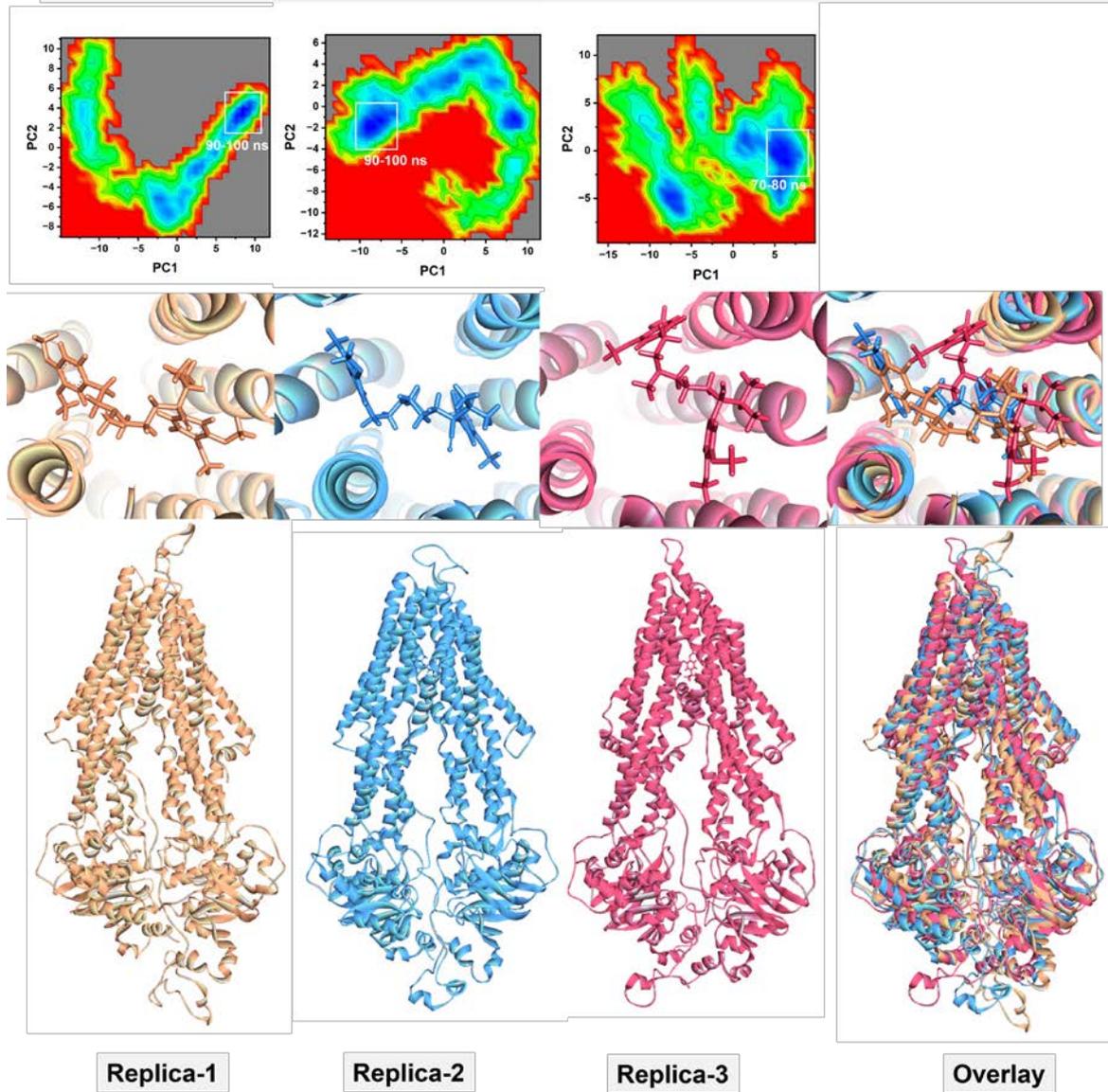


3-Dimensional Structures of Ligands at the ATP binding site



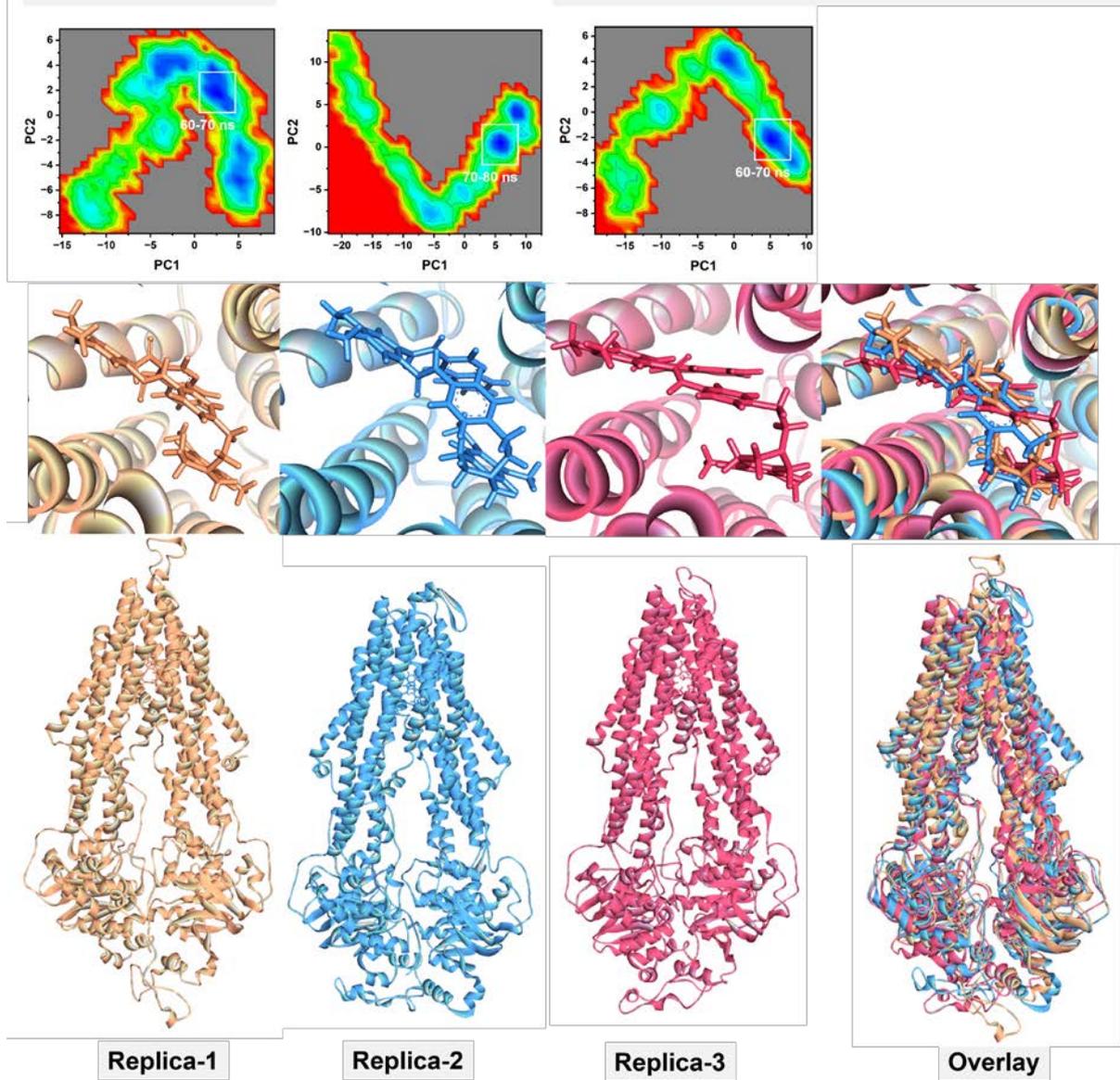
Supplementary Figure S4. 3-Dimensional structures of PGG, tariquidar, verapamil and ATP together with the best fit of these structures.

Three replica copies of verapamil bound with P-gp at substrate binding site



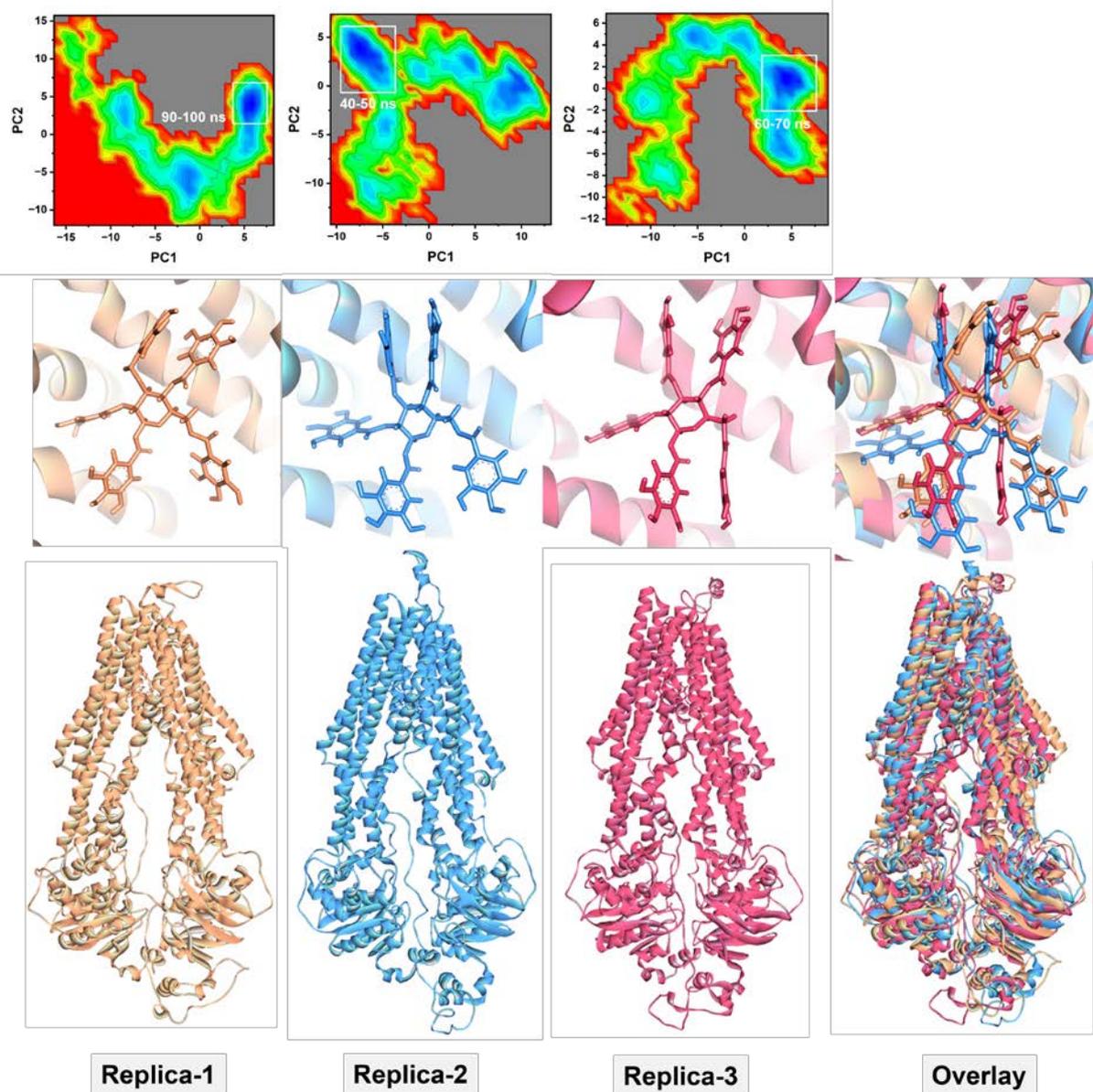
Supplementary Figure S5. 3D structures of protein-ligand complex and free energy landscape (FEL) of three replica copies of verapamil at substrate binding site of P-gp

Three replica copies of tariquidar bound with P-gp at substrate binding site



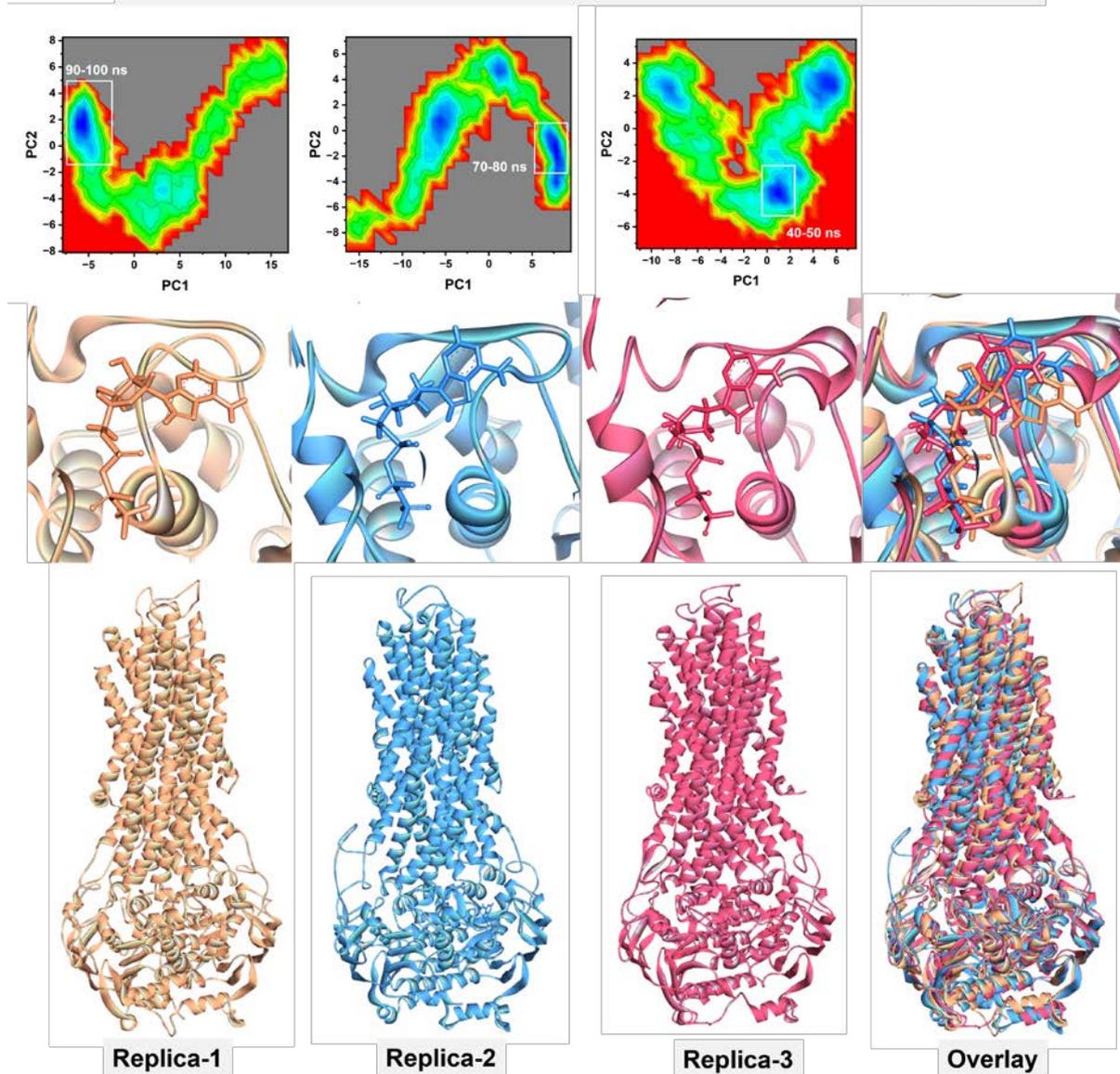
Supplementary Figure S6. 3D structures of protein-ligand complex and free energy landscape (FEL) of three replica copies of tariquidar at substrate binding site of P-gp

Three replica copies of PGG bound with P-gp at substrate binding site



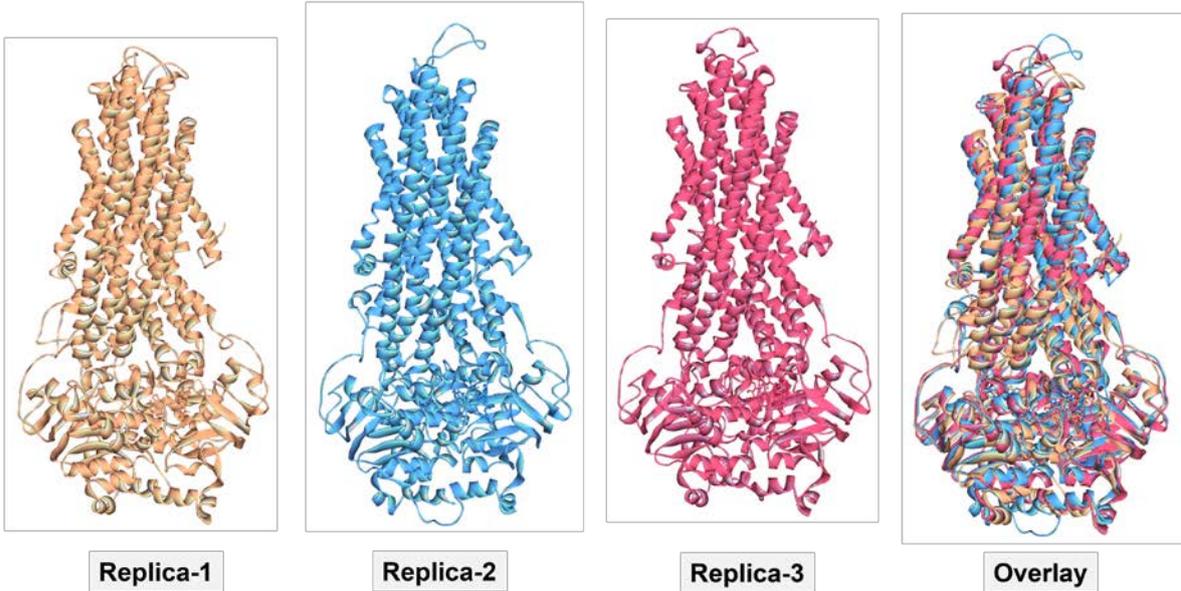
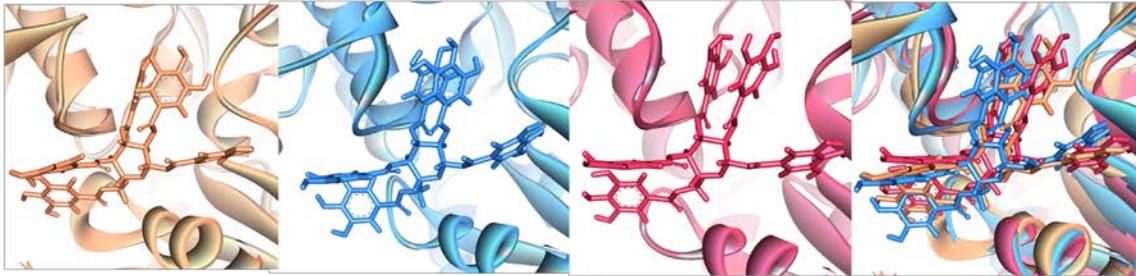
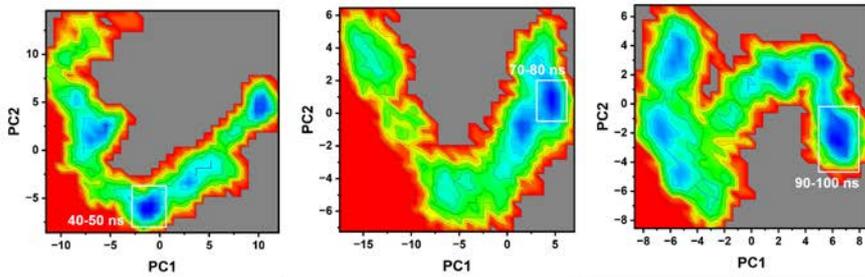
Supplementary Figure S7. 3D structures of protein-ligand complex and free energy landscape (FEL) of three replica copies of PGG at substrate binding site of P-gp

Three replica copies of ATP bound with P-gp at ATP binding site

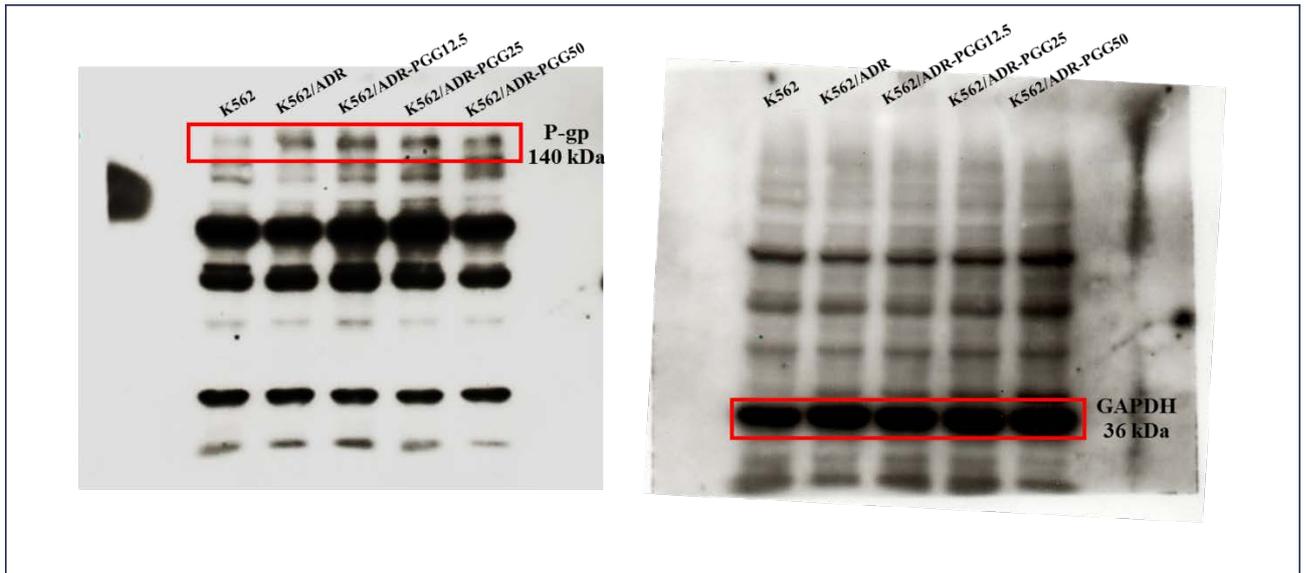


Supplementary Figure S8. 3D structures of protein-ligand complex and free energy landscape (FEL) of three replica copies of ATP at ATP binding site of P-gp

Three replica copies of PGG bound with P-gp at ATP binding site



Supplementary Figure S9. 3D structures of protein-ligand complex and free energy landscape (FEL) of three replica copies of PGG at ATP binding site of P-gp



Supplementary Figure S10. The uncropped Western blot images corresponding to Figure 3a showing all the bands. Red boxes indicate the samples of interest.