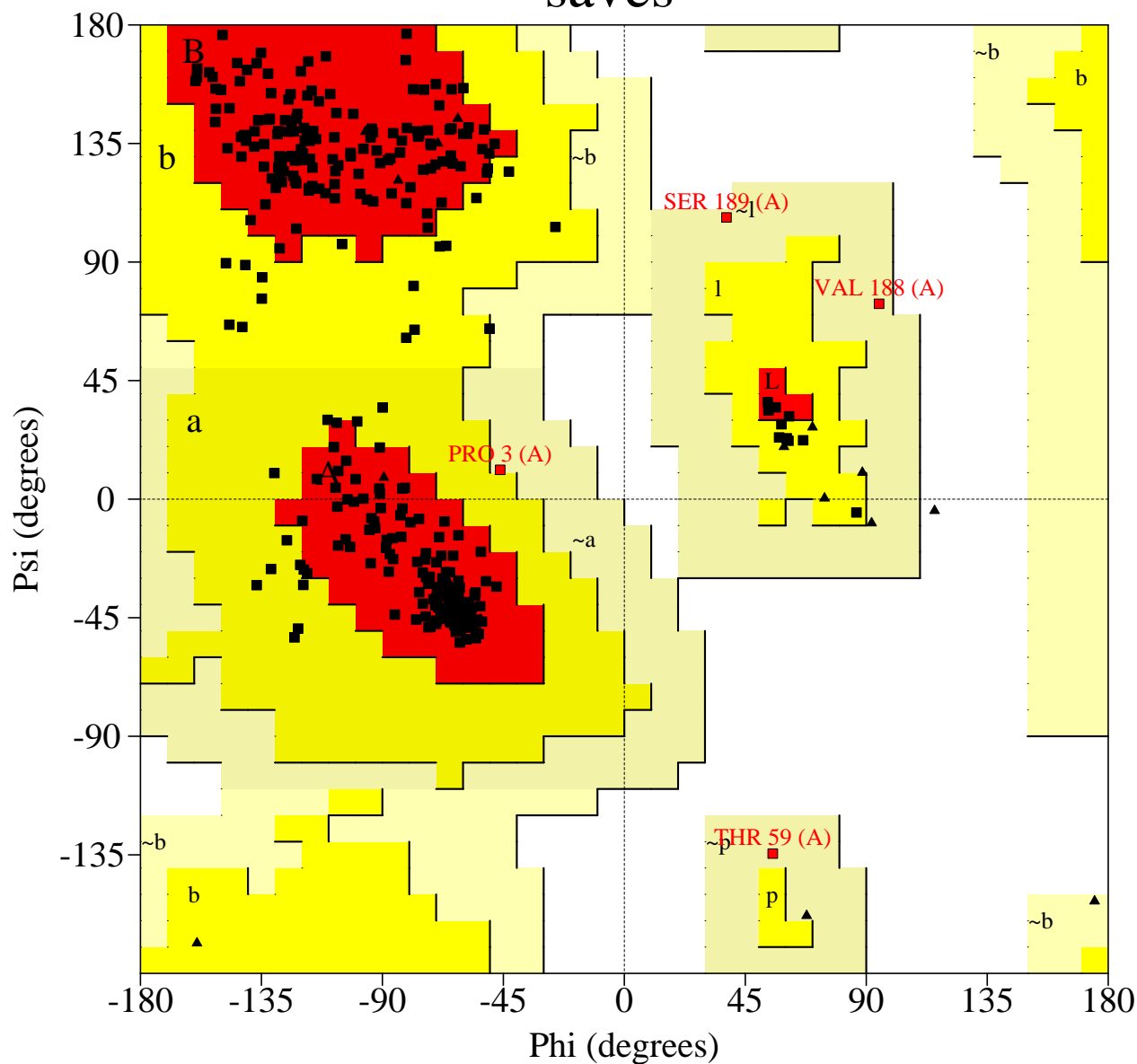


# Ramachandran Plot

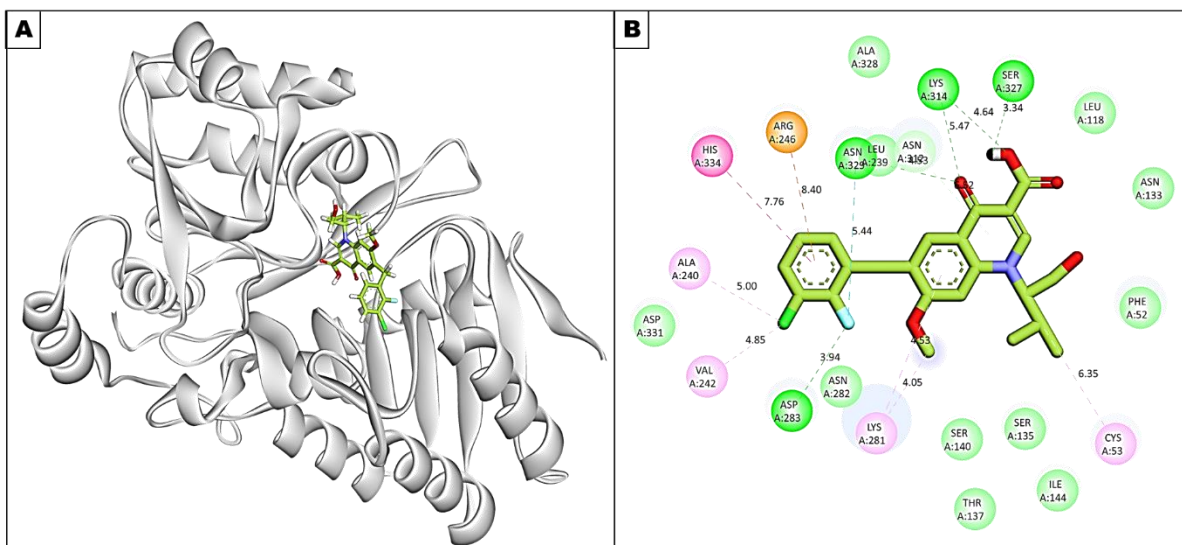
saves



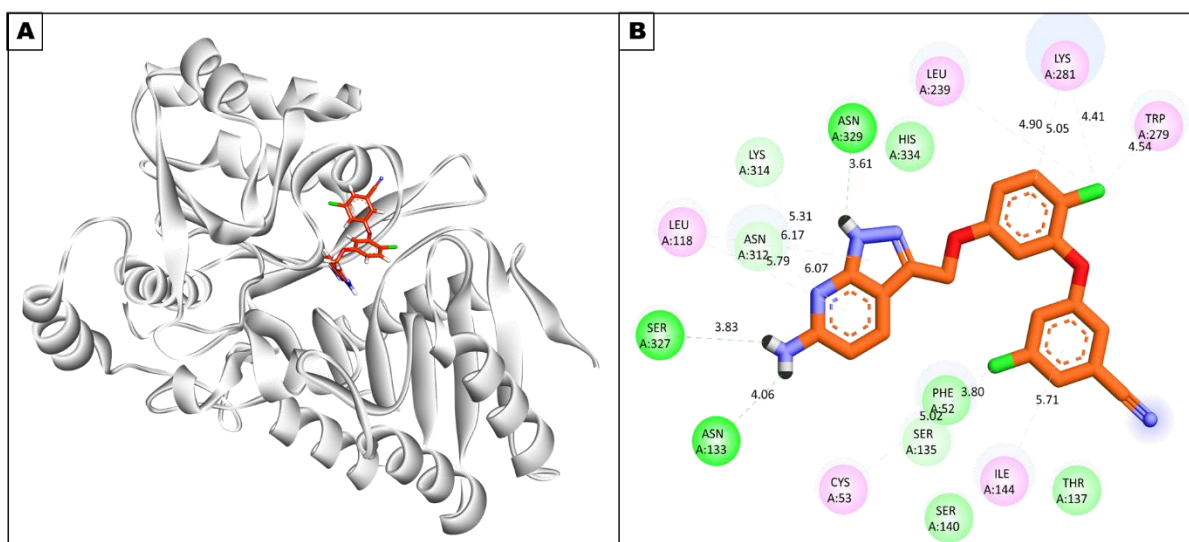
## Plot statistics

Residues in most favoured regions [A,B,L]	304	89.9%
Residues in additional allowed regions [a,b,l,p]	31	9.2%
Residues in generously allowed regions [~a,~b,~l,~p]	3	0.9%
Residues in disallowed regions	0	0.0%
-----		
Number of non-glycine and non-proline residues	338	100.0%
Number of end-residues (excl. Gly and Pro)	2	
Number of glycine residues (shown as triangles)	19	
Number of proline residues	12	
-----		
Total number of residues	371	

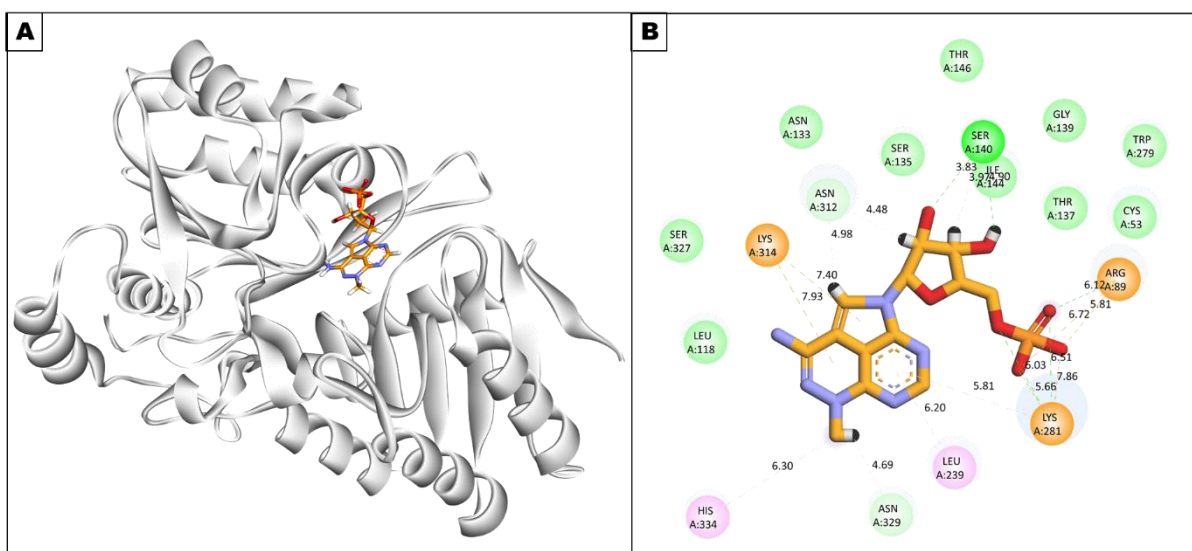
Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.



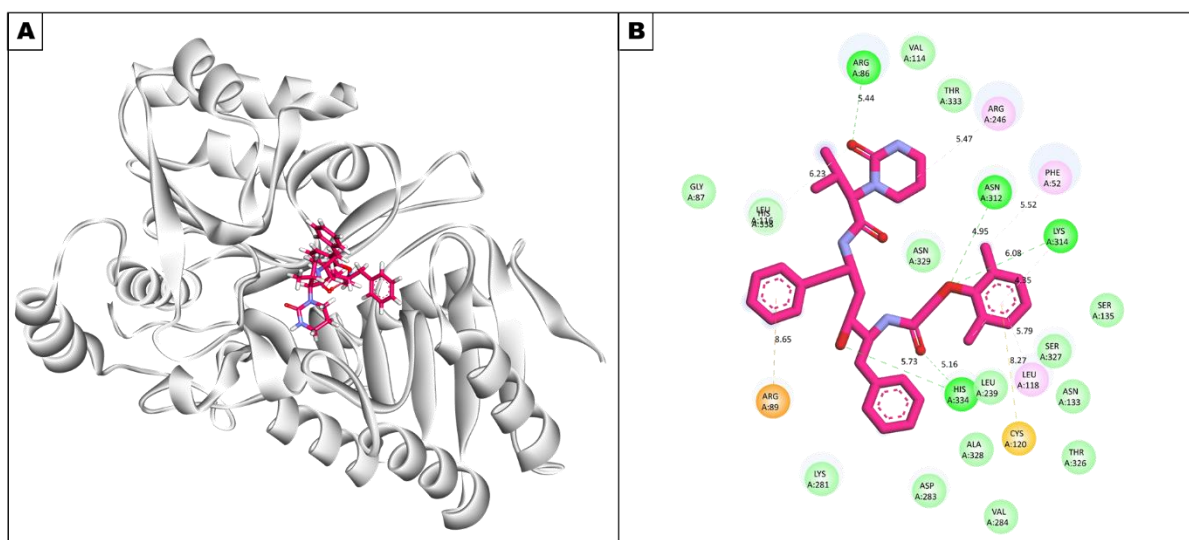
**Figure-S2 Three-dimensional representation of the Elvitegravir and Homology modelled structure. (A) 3 D representation and (B) 2 D representation (for clarity) describing ligands interactions by formation of various H-bonds and hydrophobic interactions with protein at the active site of the protein.**



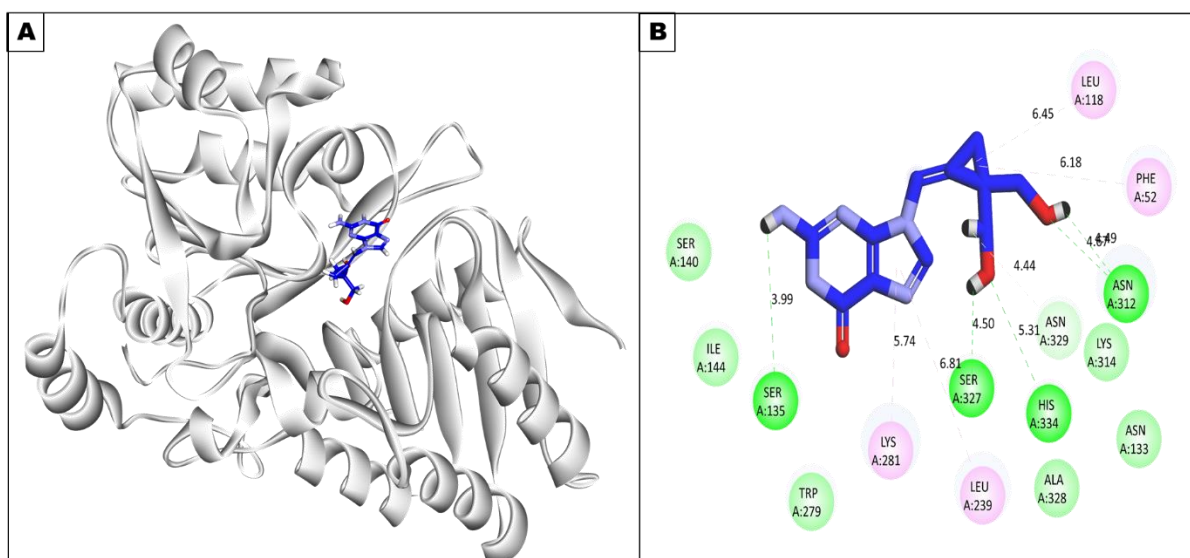
**Figure-S3 Three-dimensional representation of the MK-4965 and Homology modelled structure. (A) 3 D representation and (B) 2 D representation (for clarity) describing ligands interactions by formation of various H-bonds and hydrophobic interactions with protein at the active site of the protein.**



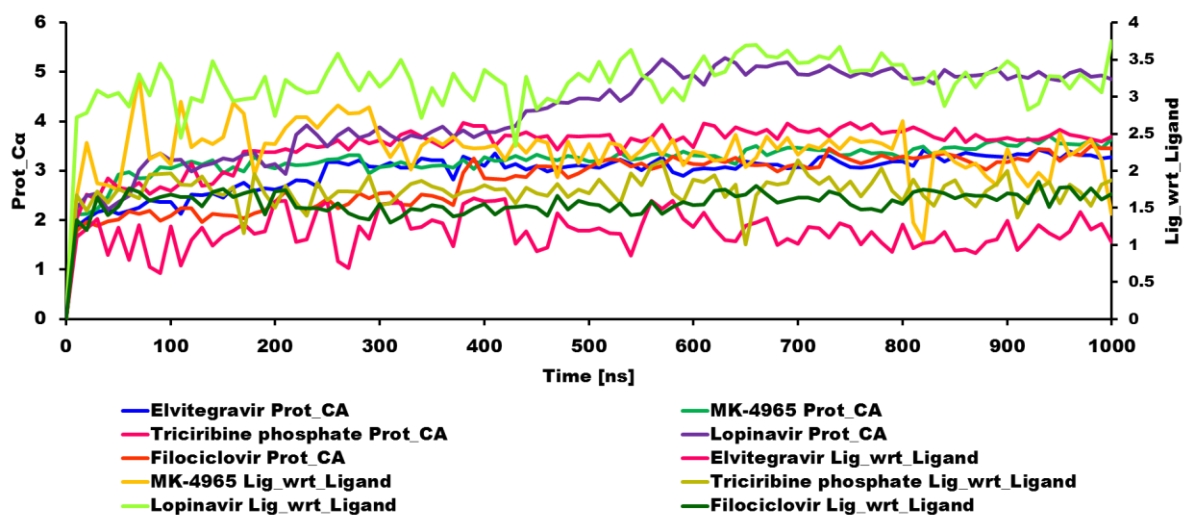
**Figure-S4 Three-dimensional representation of the Triciribine phosphate and Homology modelled structure. (A) 3 D representation and (B) 2 D representation (for clarity) describing ligands interactions by formation of various H-bonds and hydrophobic interactions with protein at the active site of the protein.**



**Figure-S5 Three-dimensional representation of the Lopinavir and Homology modelled structure. (A) 3 D representation and (B) 2 D representation (for clarity) describing ligands interactions by formation of various H-bonds and hydrophobic interactions with protein at the active site of the protein.**



**Figure-S6 Three-dimensional representation of the Filociclovir and Homology modelled structure. (A) 3 D representation and (B) 2 D representation (for clarity) describing ligands interactions by formation of various H-bonds and hydrophobic interactions with protein at the active site of the protein.**



**Figure-S7 RMSD plot of homology modelled protein with top ranked compounds from molecular dynamics simulated complexes. (Desmond Molecular Dynamics System, D. E. Shaw Research v6.1; [https://www.deshawresearch.com/resources\\_desmond.html](https://www.deshawresearch.com/resources_desmond.html)).**

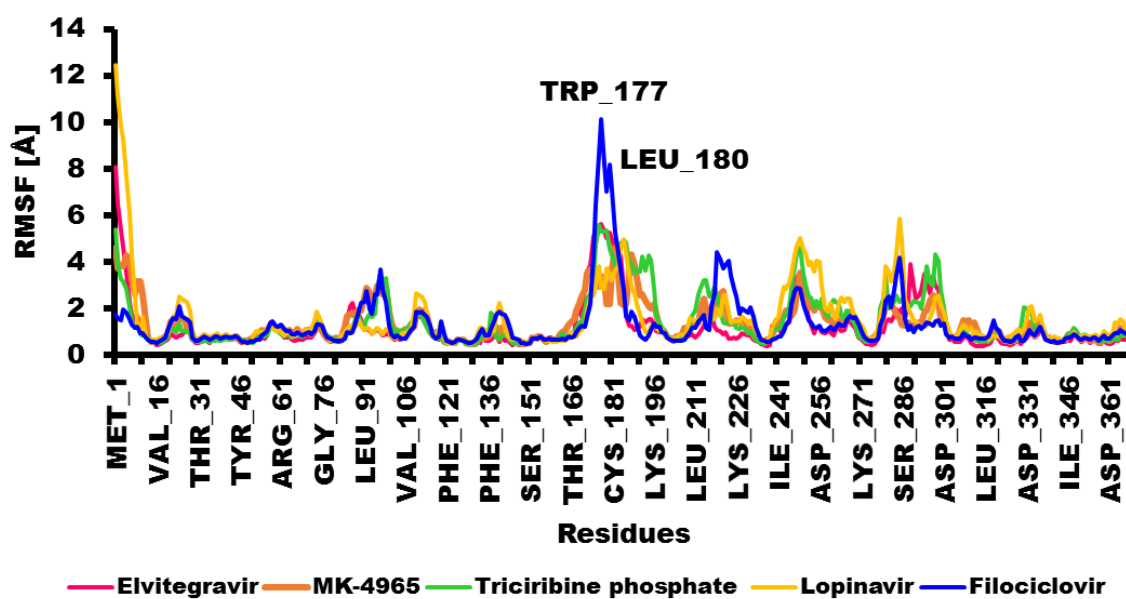
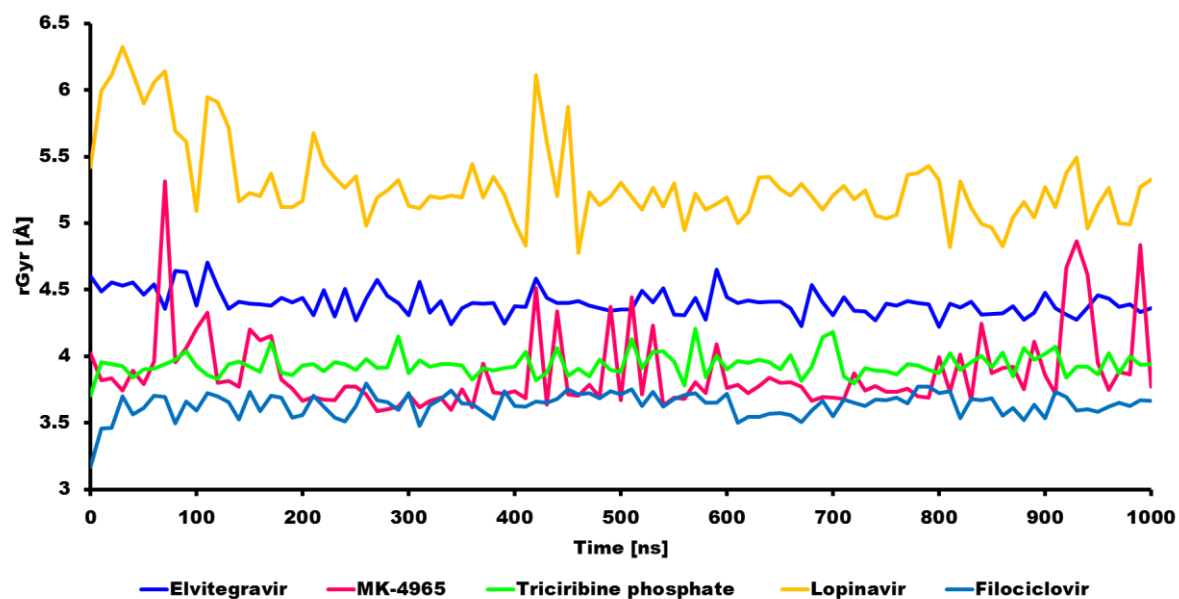
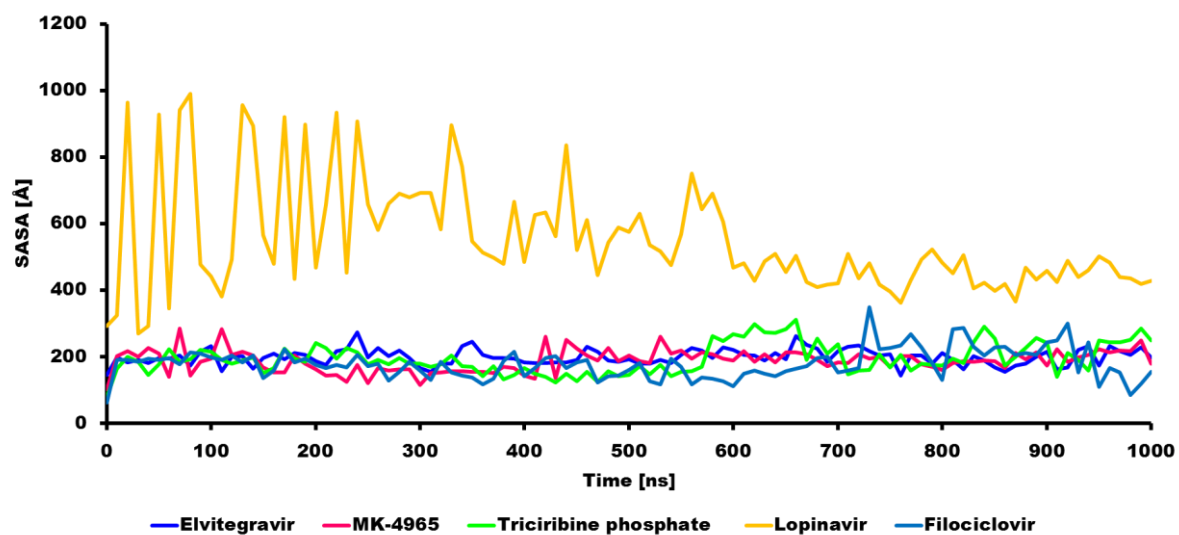


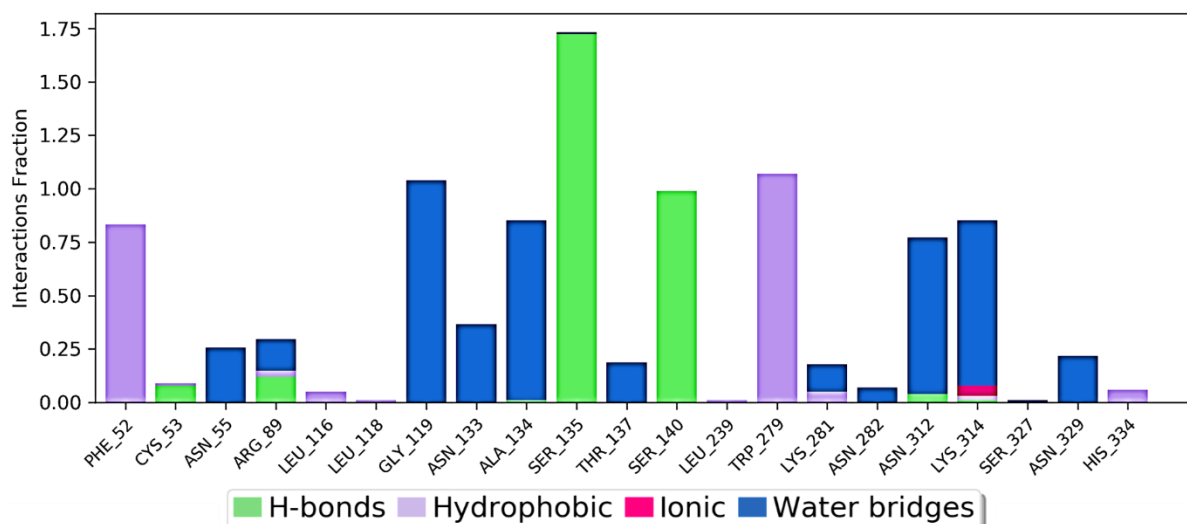
Figure-S8 RMSF plot of homology modelled protein with top ranked compounds from molecular dynamics simulated complexes.



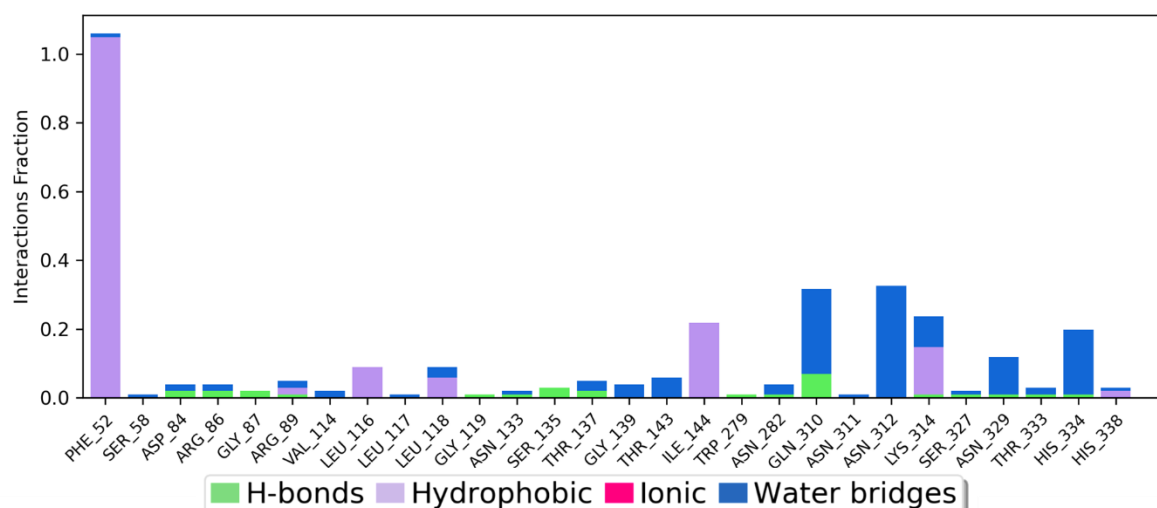
**Figure-S9 Ligand properties for top ranked compounds targeting homology modelled F13 envelope protein structure of monkey pox virus. Radius of gyration (rGyr) of molecular dynamics simulated complexes.**



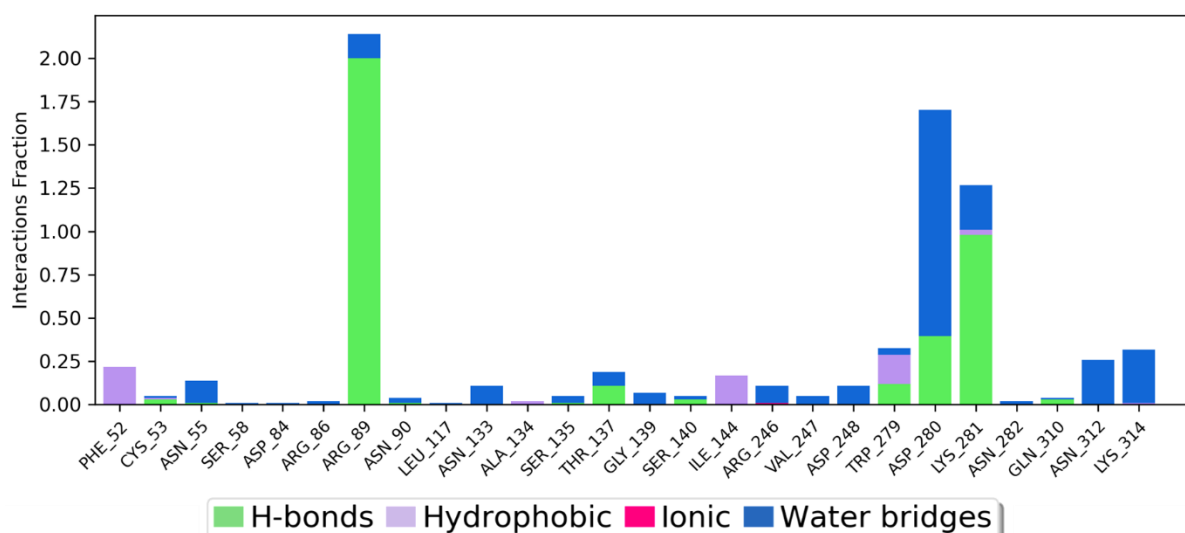
**Figure-S10 Ligand properties for top ranked compounds targeting homology modelled F13 envelope protein structure of monkey pox virus. Solvent accessible surface area (SASA) of molecular dynamics simulated complexes.**



**Figure-S11 Various intermolecular interactions made by homology modelled protein pocket residues Elvitegravir with captured during molecular dynamics simulations. (Desmond Molecular Dynamics System, D. E. Shaw Research v6.1; <https://www.deshawresearch.com/resourcesdesmond.html/>).**



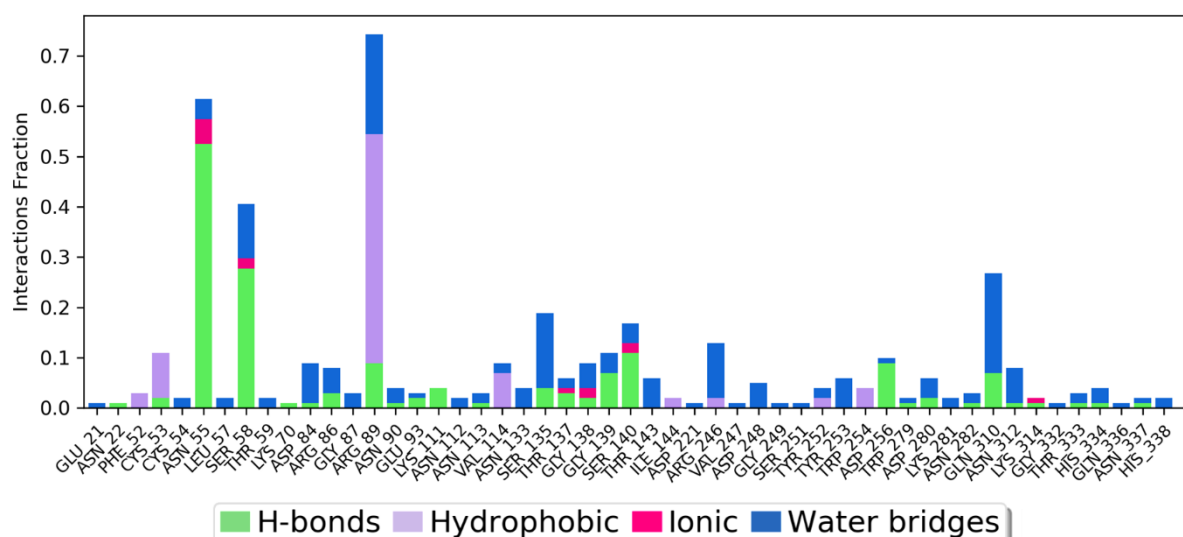
**Figure-S12 Various intermolecular interactions made by homology modelled protein pocket residues MK-4965 with captured during molecular dynamics simulations. (Desmond Molecular Dynamics System, D. E. Shaw Research v6.1; <https://www.deshawresearch.com/resourcesdesmond.html/>).**



**Figure-S13 Various intermolecular interactions made by homology modelled protein pocket residues Triciribine phosphate with captured during molecular dynamics simulations. (Desmond Molecular Dynamics System, D. E. Shaw Research v6.1; <https://www.deshawresearch.com/resourcesdesmond.html/>).**



**Figure-S14 Various intermolecular interactions made by homology modelled protein pocket residues Lopinavir with captured during molecular dynamics simulations. (Desmond Molecular Dynamics System, D. E. Shaw Research v6.1; <https://www.deshawresearch.com/resourcesdesmond.html>).**



**Figure-S15 Various intermolecular interactions made by homology modelled protein pocket residues Filociclovir with captured during molecular dynamics simulations. (Desmond Molecular Dynamics System, D. E. Shaw Research v6.1; <https://www.deshawresearch.com/resourcesdesmond.html/>).**