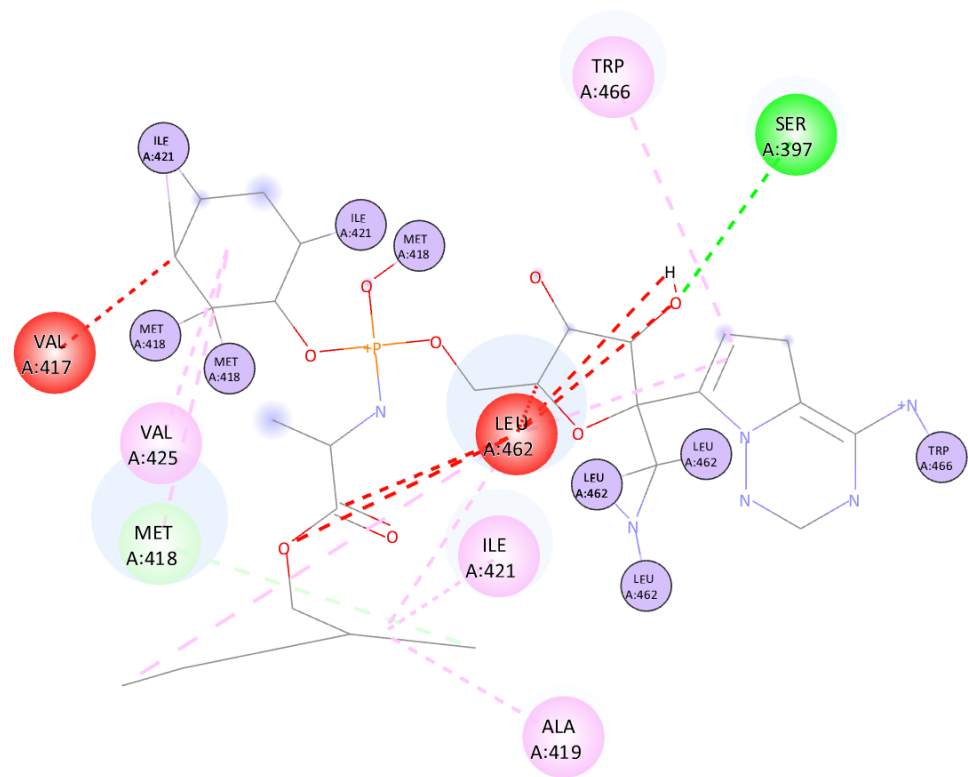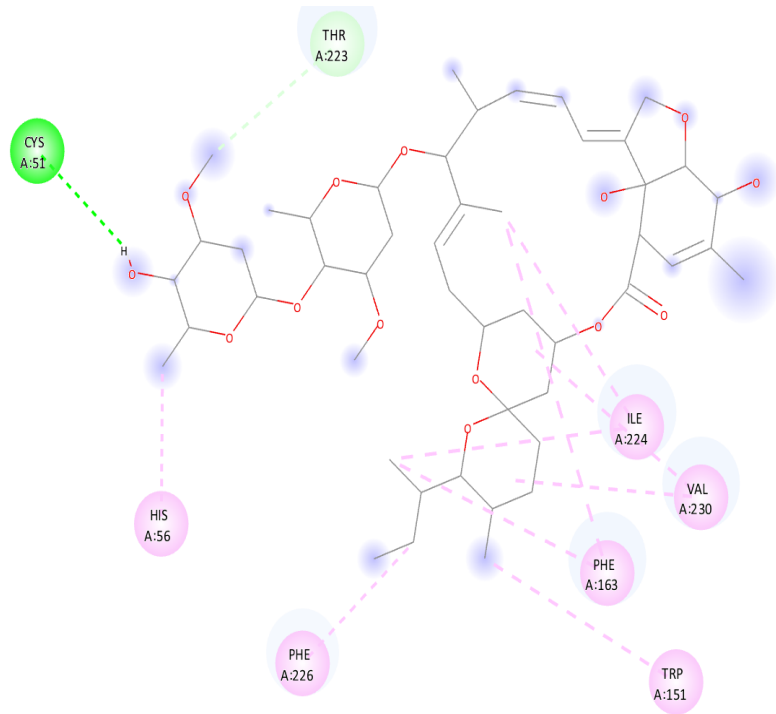Supplementary Figure 1: Drug-binding interactions
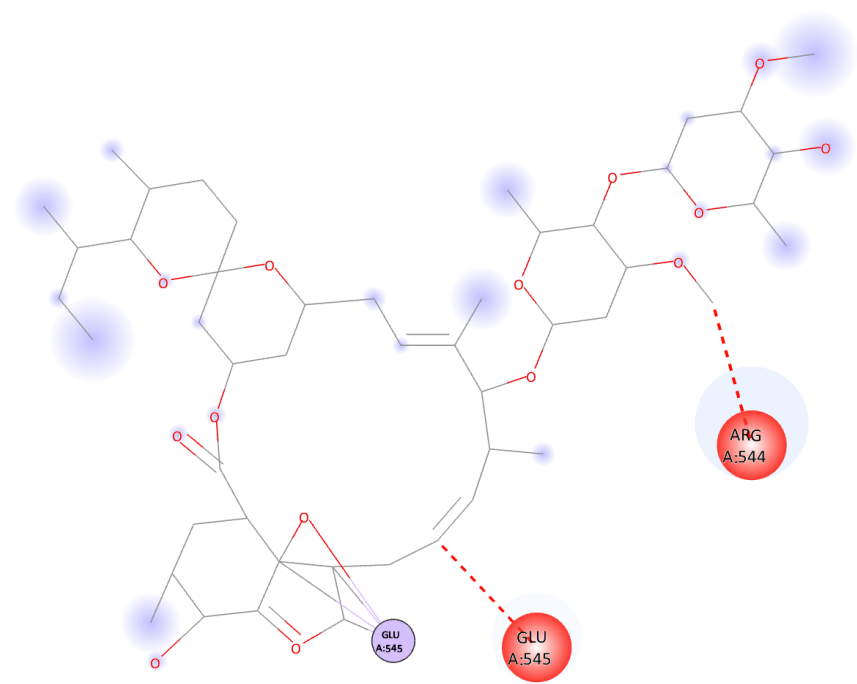

Wild type I120_Remdesivir (NSP1)

Mutant F120_Remdesivir (NSP1)

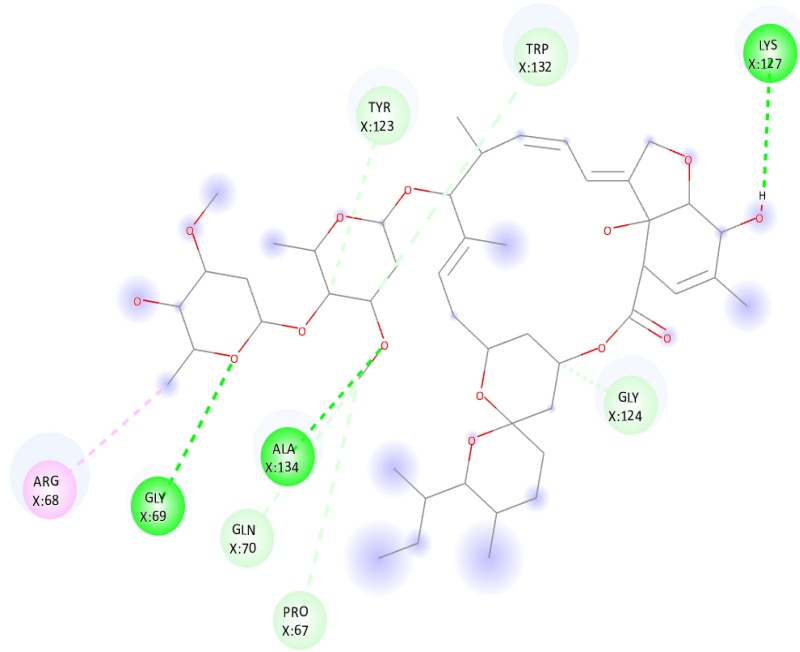Supplementary Figure 1: Drug-binding interactions
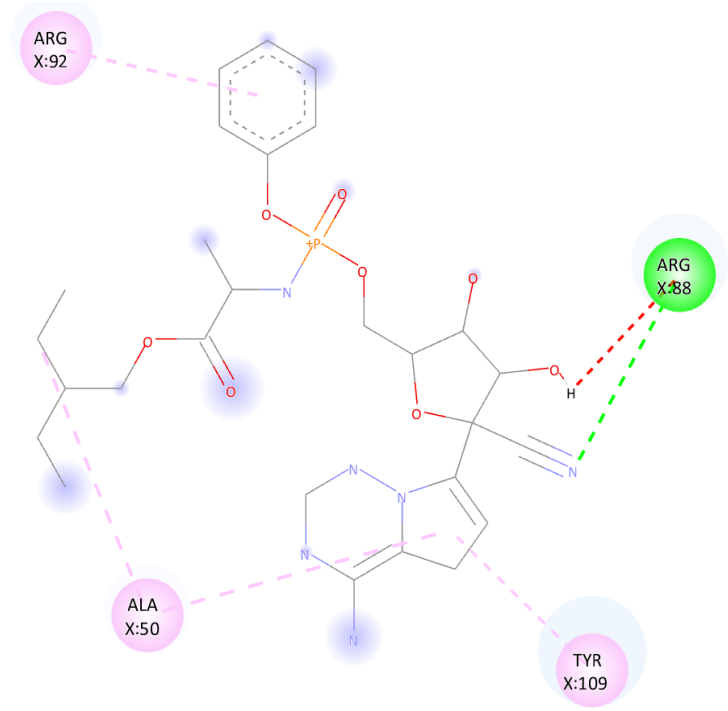
Wildtype I120_Ivermectin (NSP1)

Mutant F120_Ivermectin(NSP1)

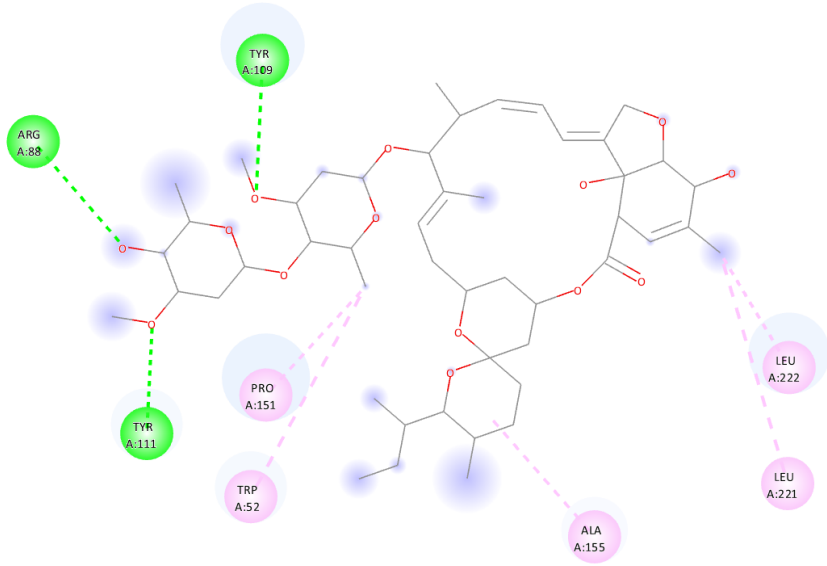# Supplementary Figure 1: Drug-binding interactions

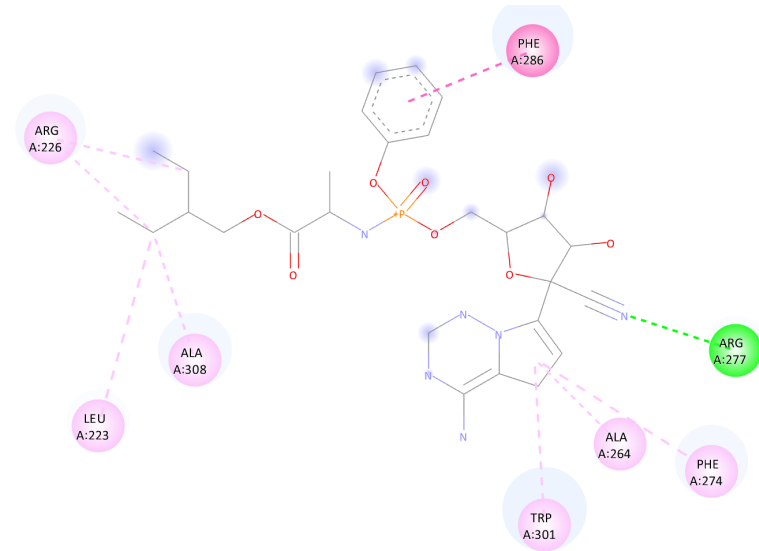Wild type 202_203_204_Ivermectin (N)

Wild type 202_203_204_Remdesivir (N)

Supplementary Figure 1: Drug-binding interactions
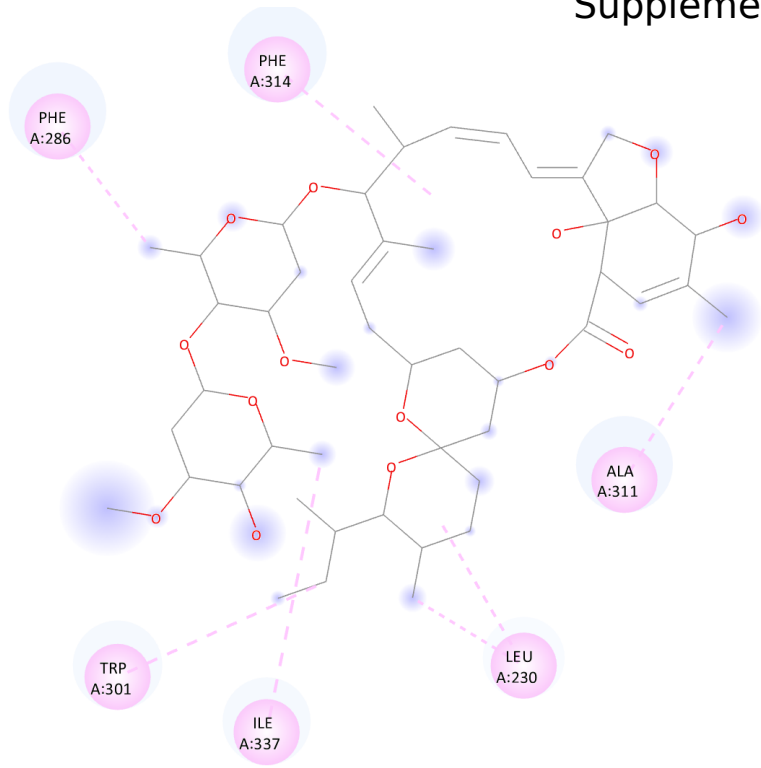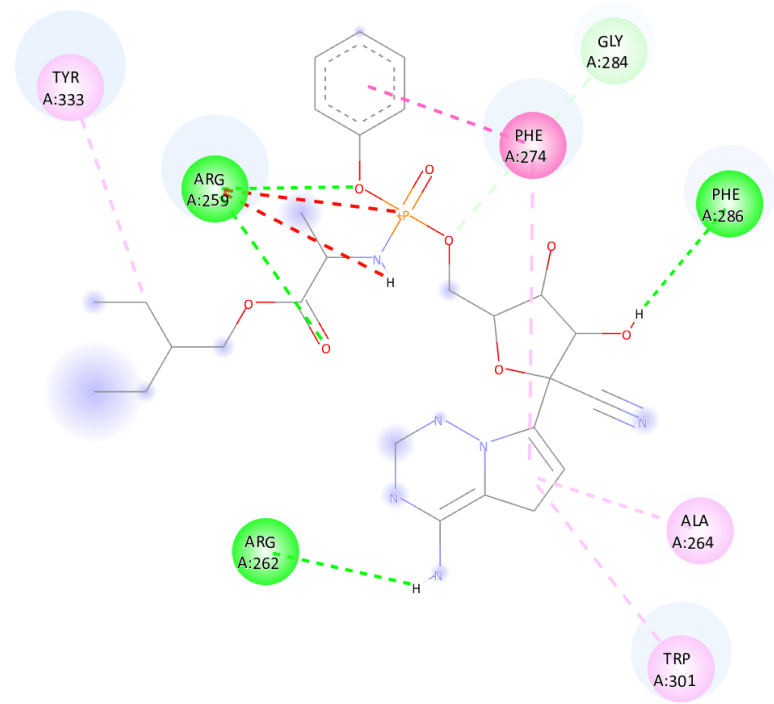

Mutant_203_Ivermectin (N)

Mutant_203_Remdesivir (N)

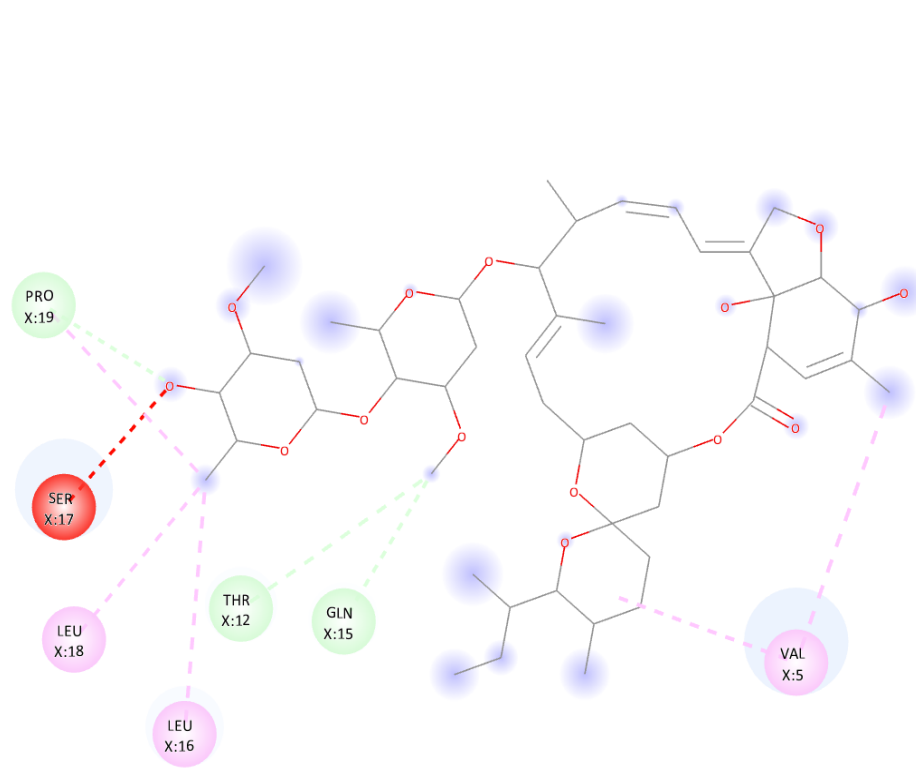Supplementary Figure 1: Drug-binding interactions

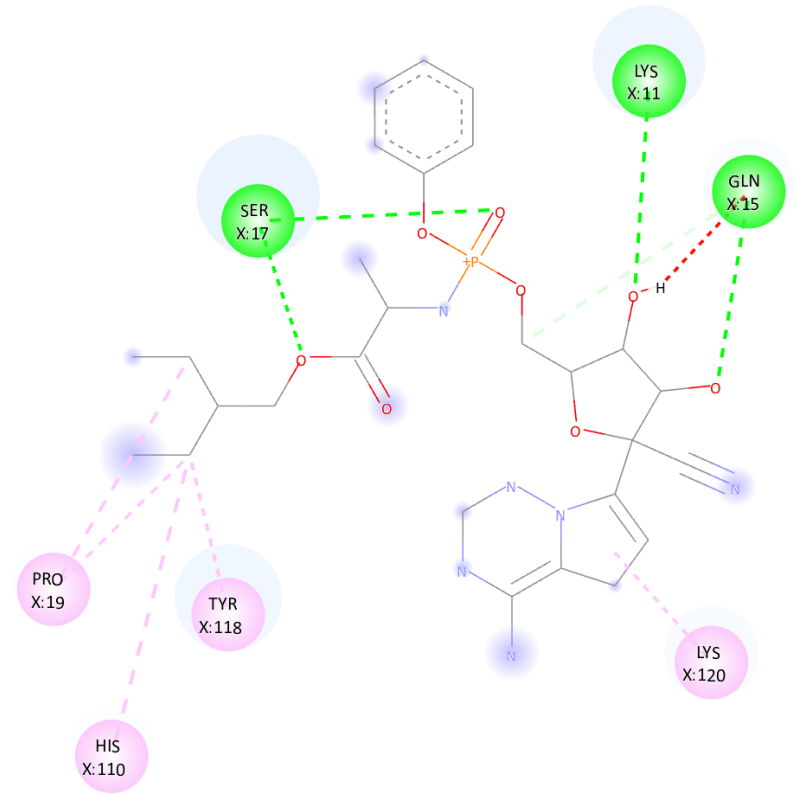Mutant_204_Ivermectin (N)

Mutant_204_Remdesivir (N)
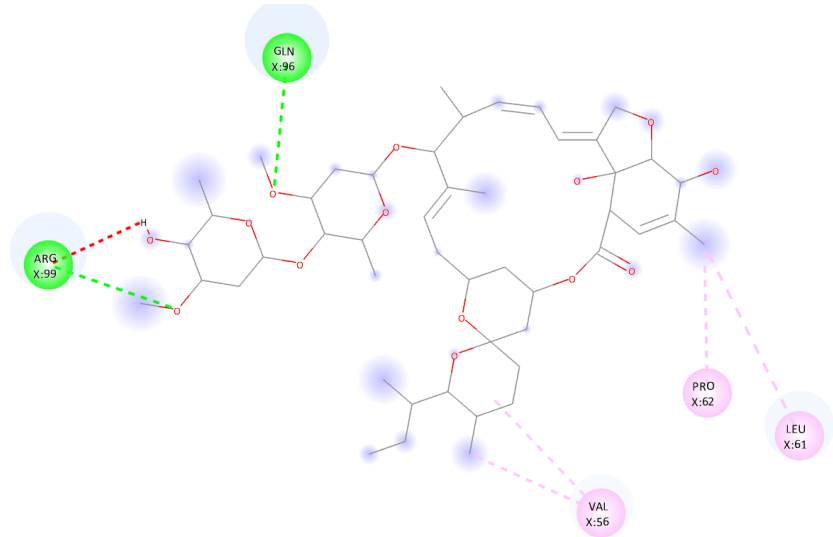
Supplementary Figure 1: Drug-binding interactions

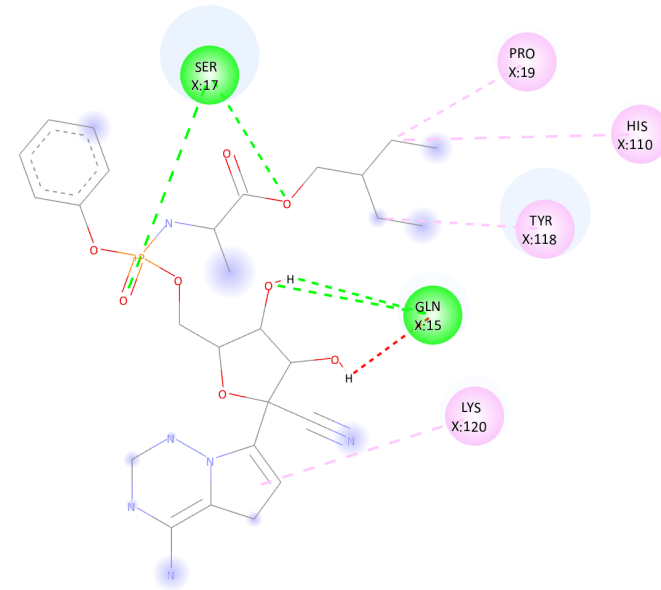Wild type Valine121_Ivermectin (NSP1)   Wild type Valine_121_Remdesivir (NSP1)

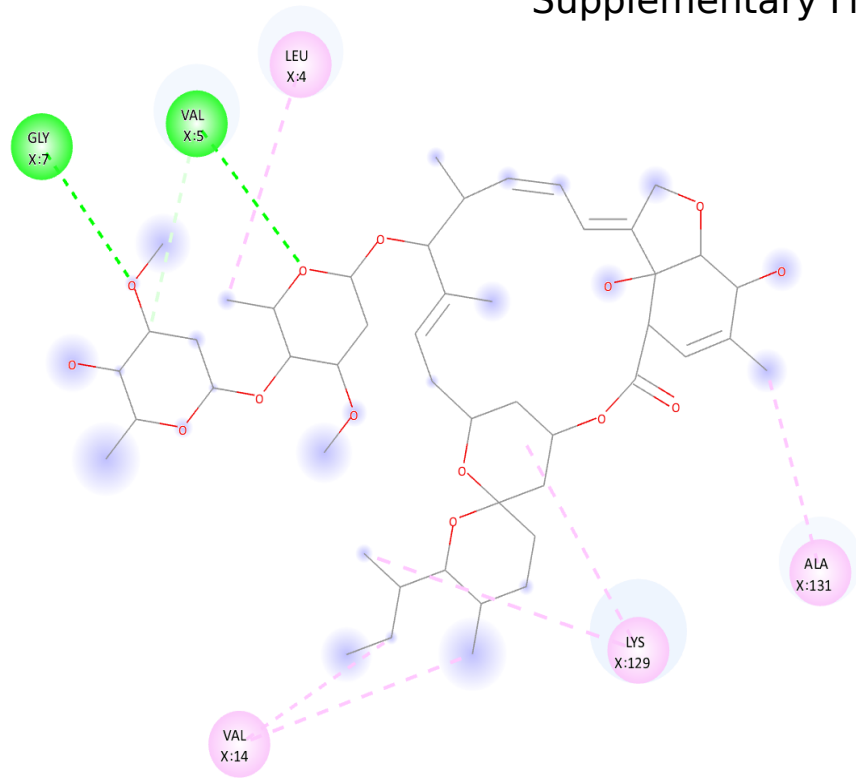# Supplementary Figure 1: Drug-binding interactions
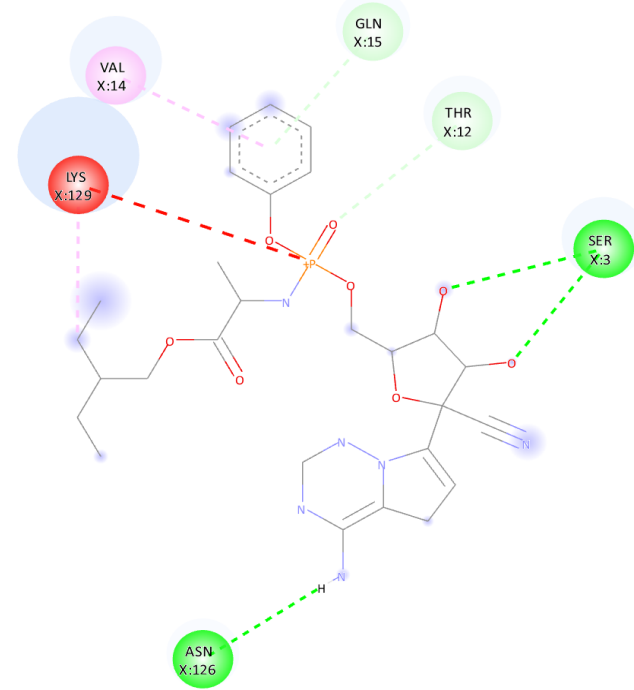

Wild type L122__Ivermectin (NSP1)

Wild type L122_Remdesivir (NSP1)

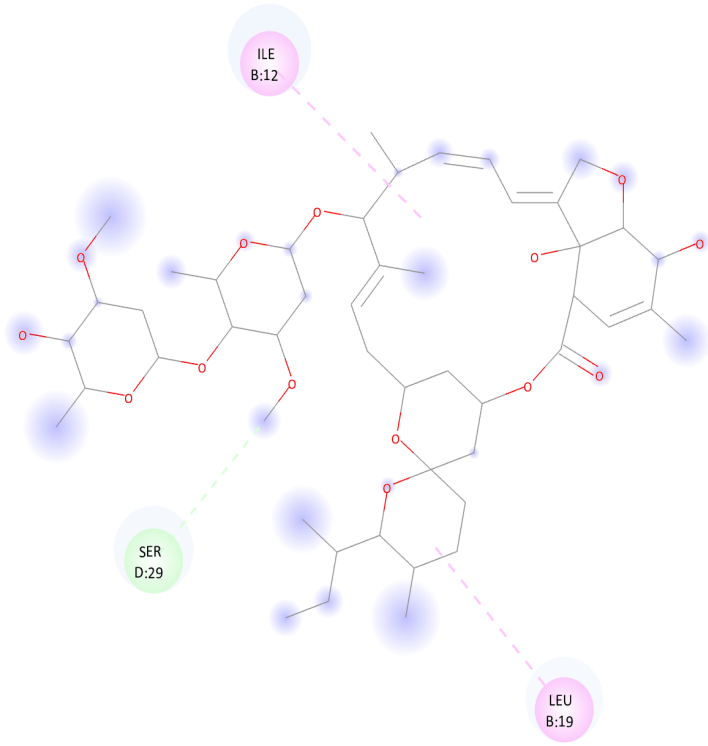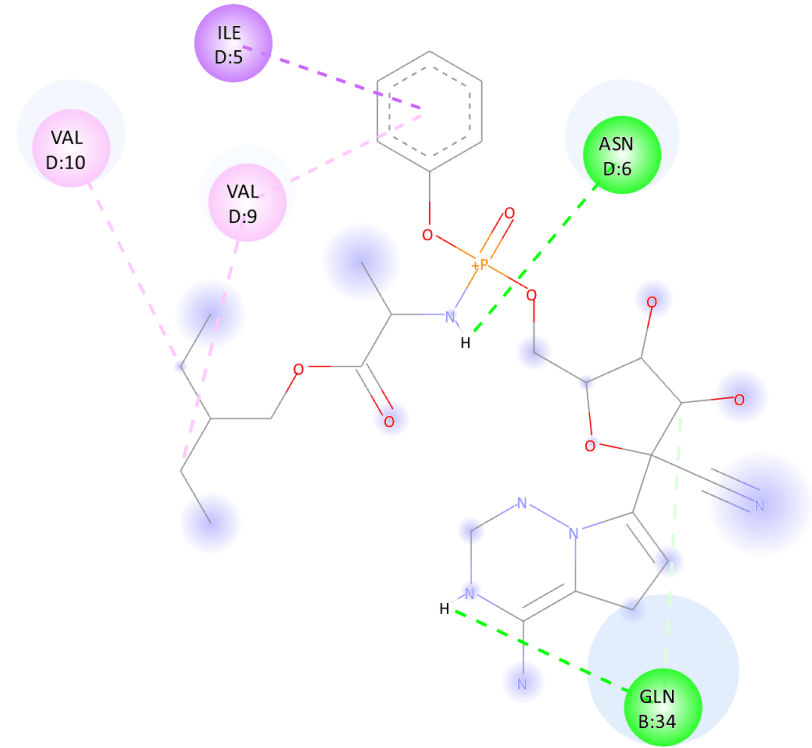Supplementary Figure 1: Drug-binding interactions

Mutant Ile122_Ivermectin (NSP1)

Mutant Ile122_Remdesivir (NSP1)

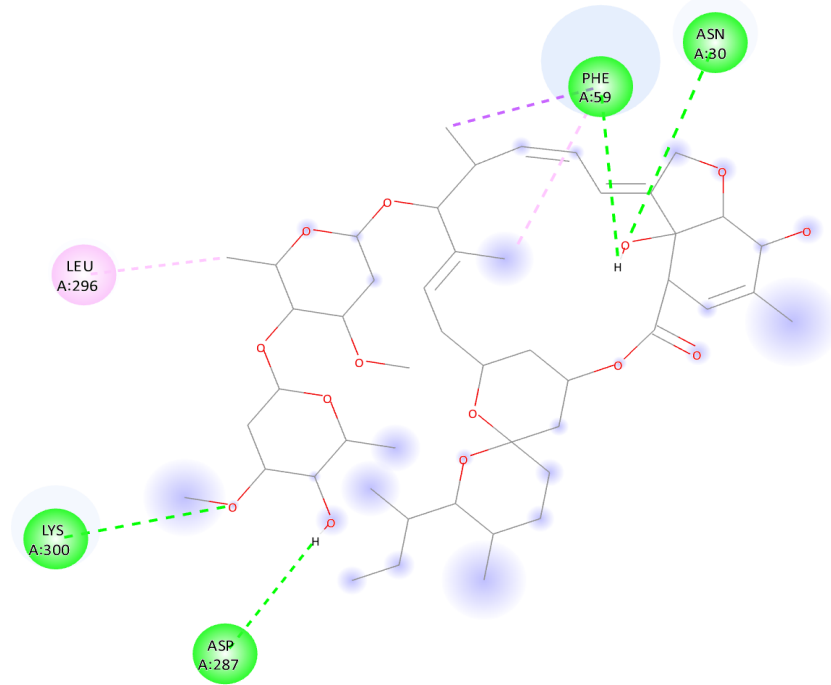# Supplementary Figure 1: Drug-binding interactions
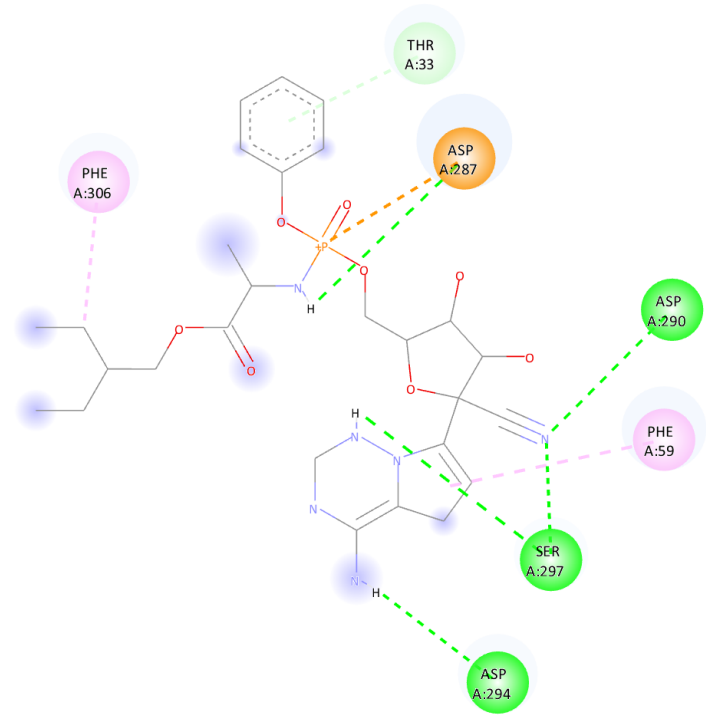

Wild ASP614_Ivermectin (S)

Wild ASP614_Remdesivir (S)

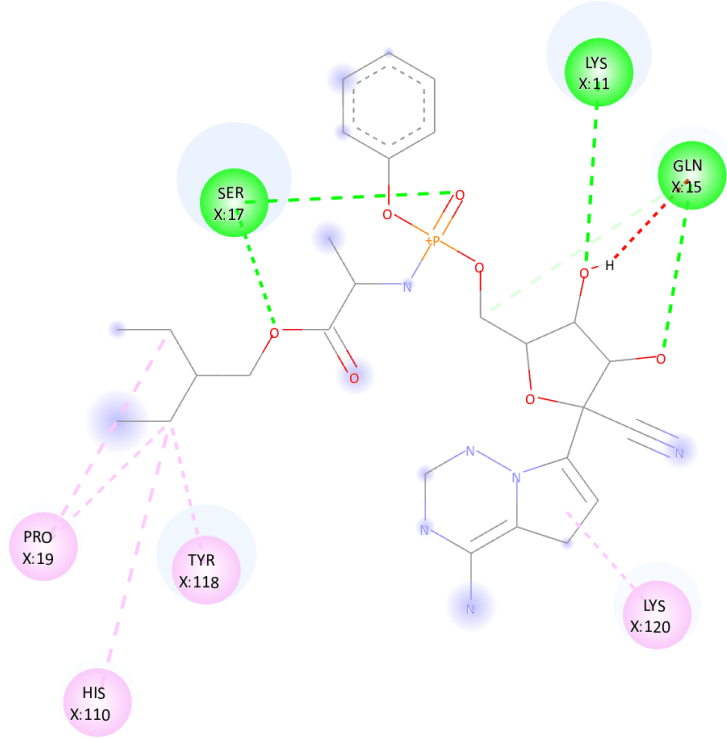Supplementary Figure 1: Drug-binding interactions

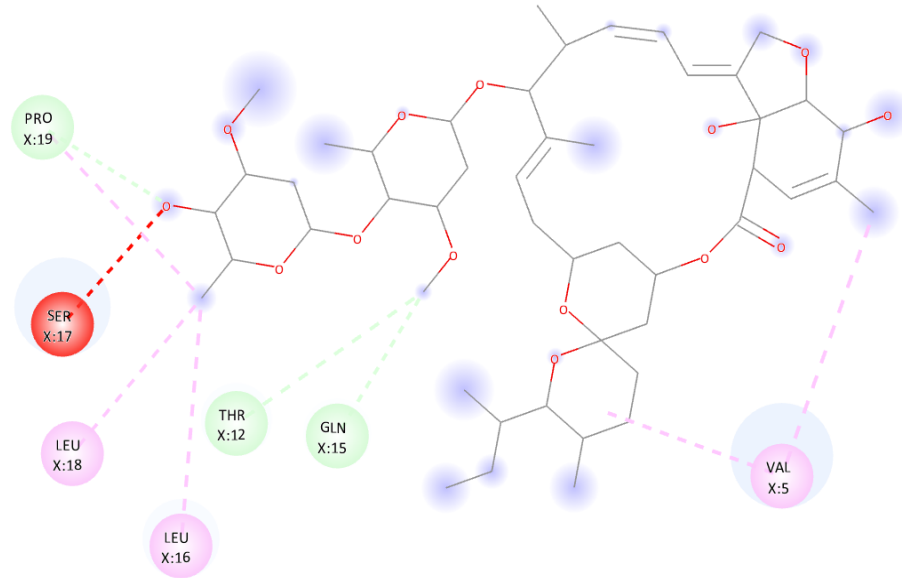Mutant D614G_Ivermectin (S)

Mutant D614G_Remdesivir (S)

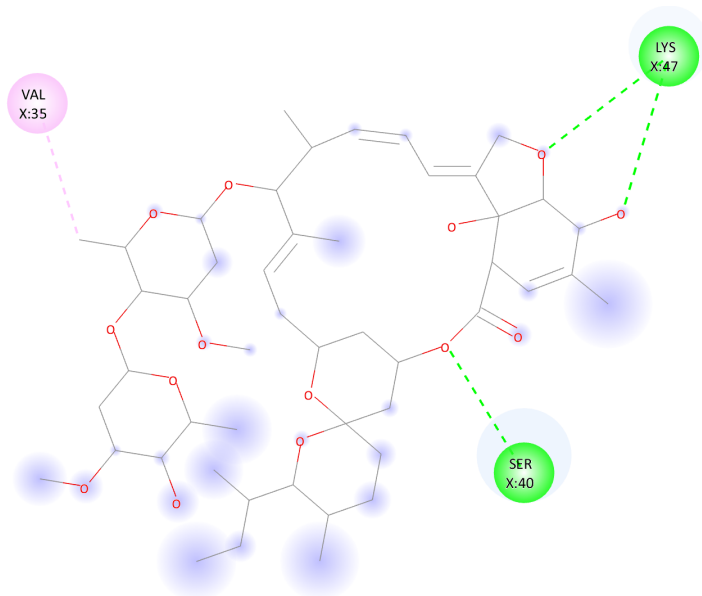Supplementary Figure 1: Drug-binding interactions
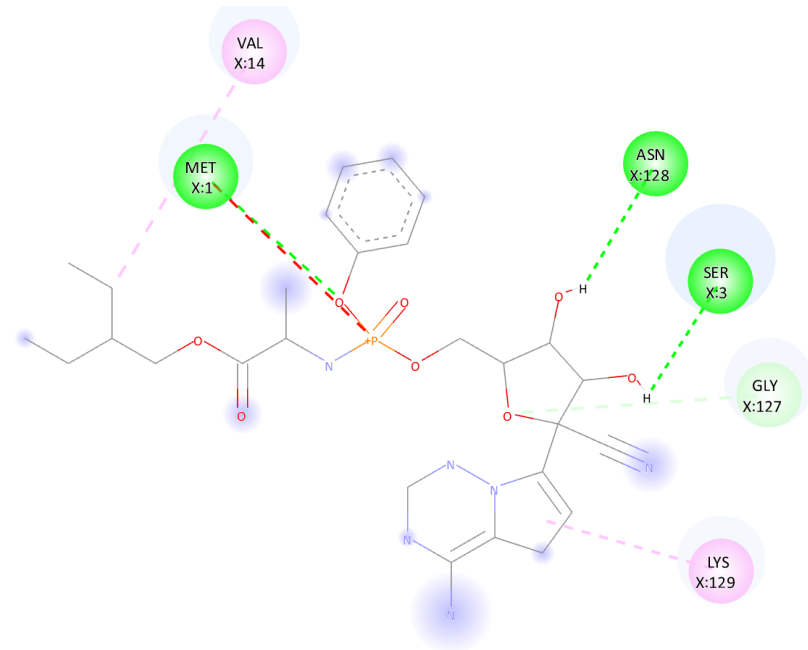
Wild type V_121_Remdesivir (NSP1)

Wild type V_121_Ivermectin (NSP1)
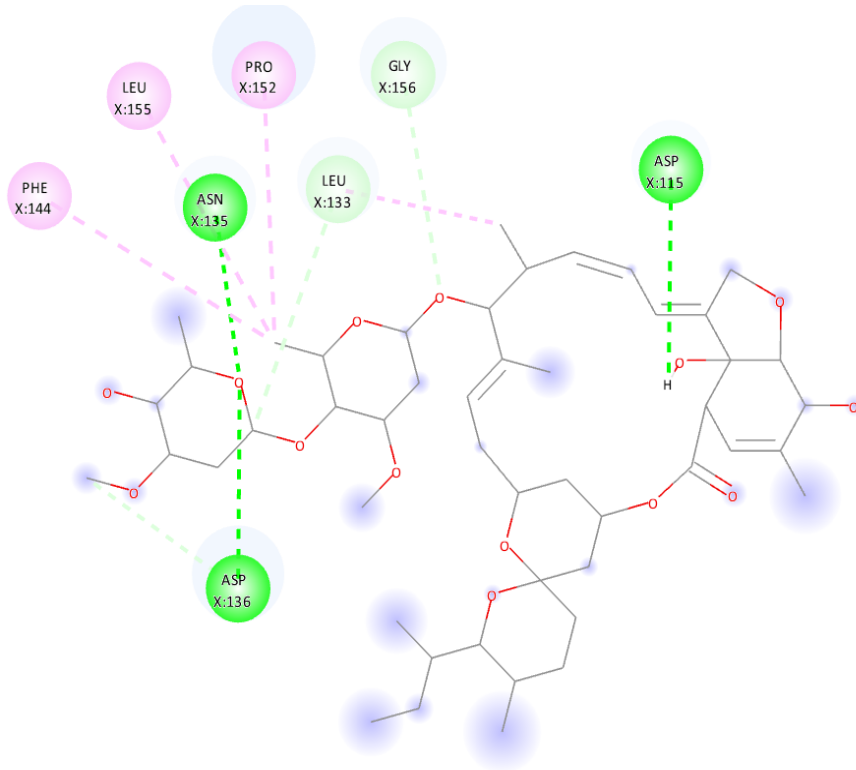
Supplementary Figure 1: Drug-binding interactions
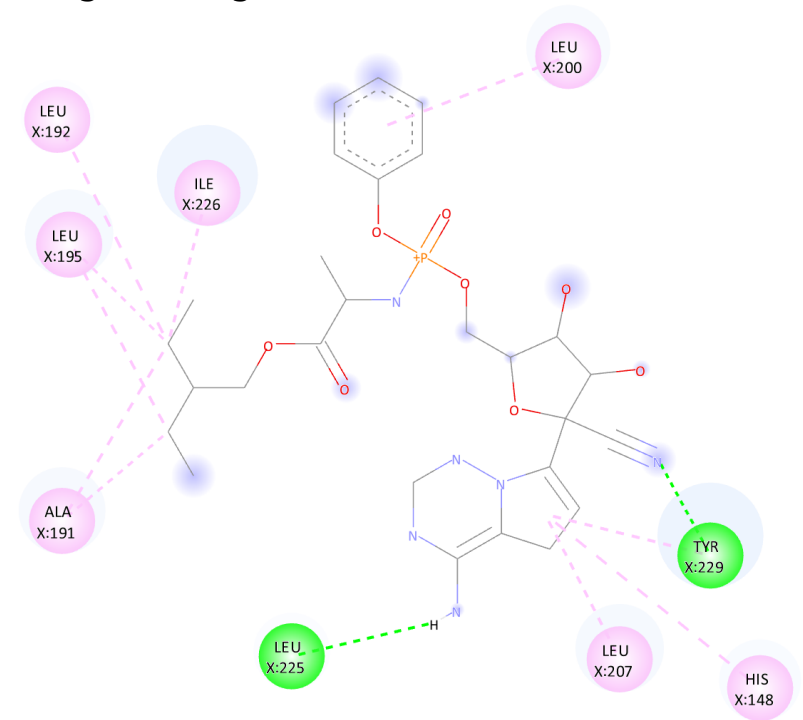

Mutant D_121_Ivermectin (NSP1)

Mutant D_121_Remdesivir (NSP1)

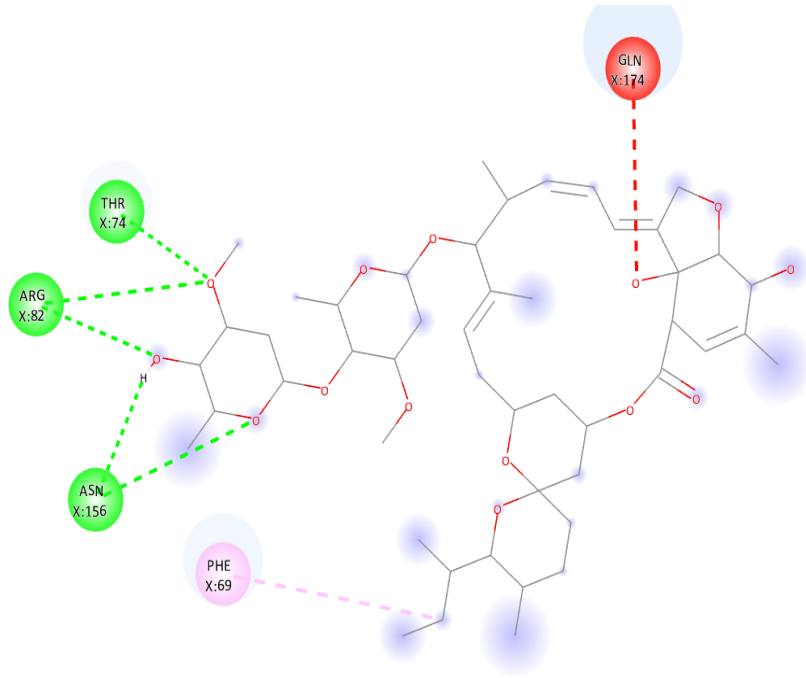# Supplementary Figure 1: Drug-binding interactions
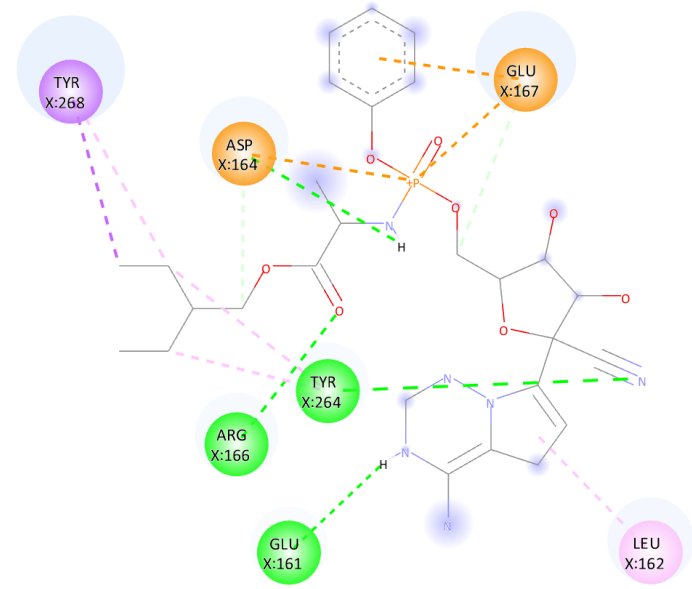

Wild type_843, 889_Ivermectin (NSP3)

Wild type_843, 889_Remdesivir (NSP3)

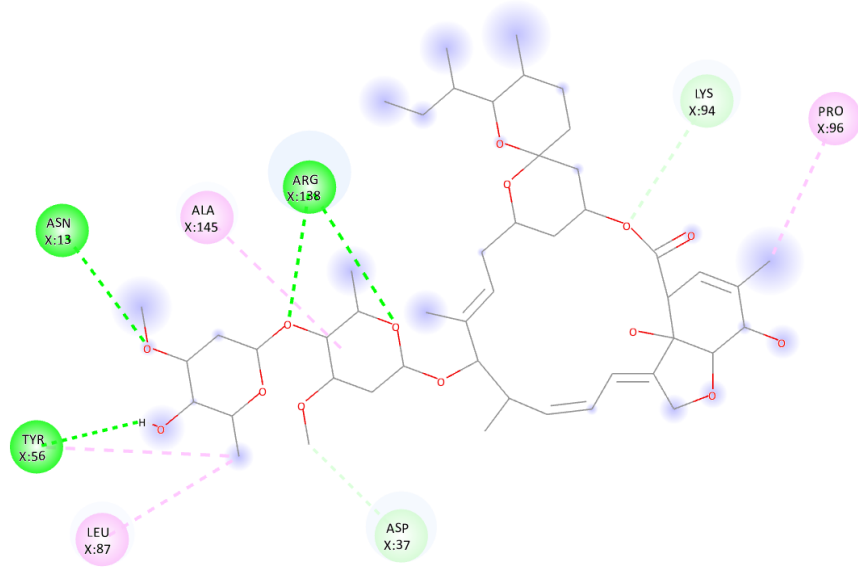Supplementary Figure 1: Drug-binding interactions
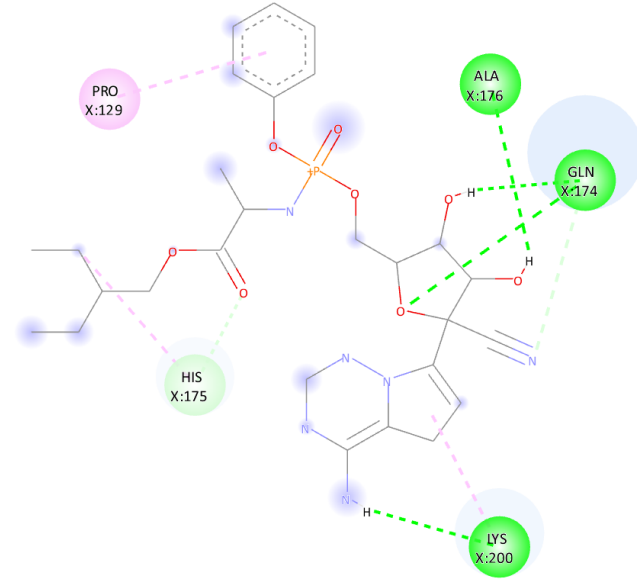
Mutant V843F_Ivermectin (NSP3)

Mutant V843F_Remdesivir (NSP3)
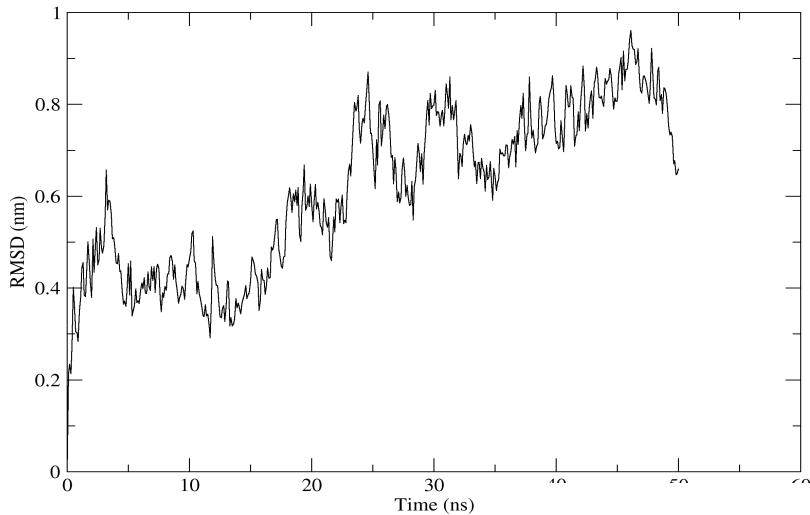
Supplementary Figure 1: Drug-binding interactions

Mutant type A889V Ivermectin (NSP3)
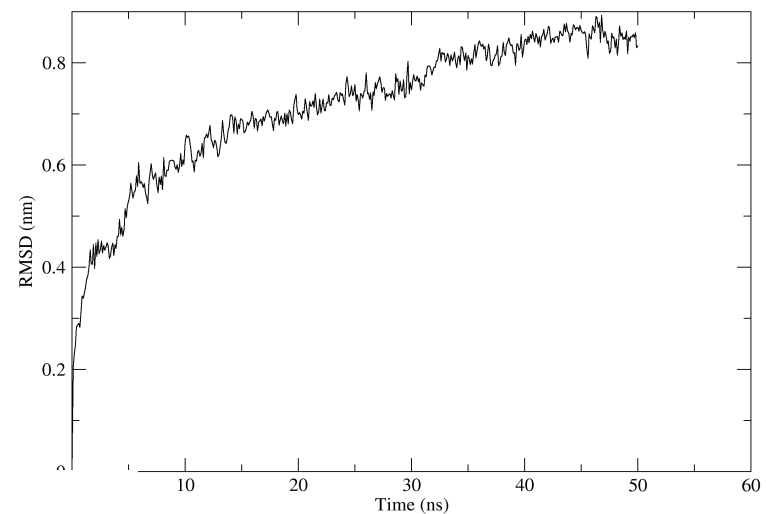

Mutant type A889V Remdesivir (NSP3)

Supplementary Figure 2: Results of Molecular Dynamic Simulation

NSP3 wild

NSP3 V843F

NSP3 A889V
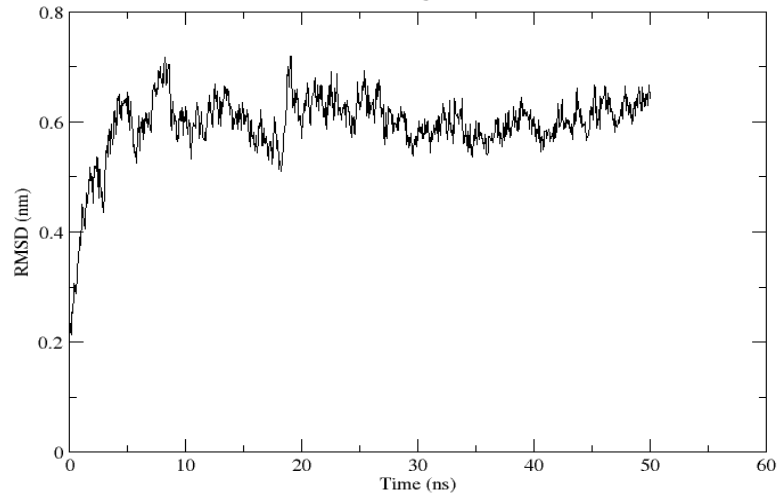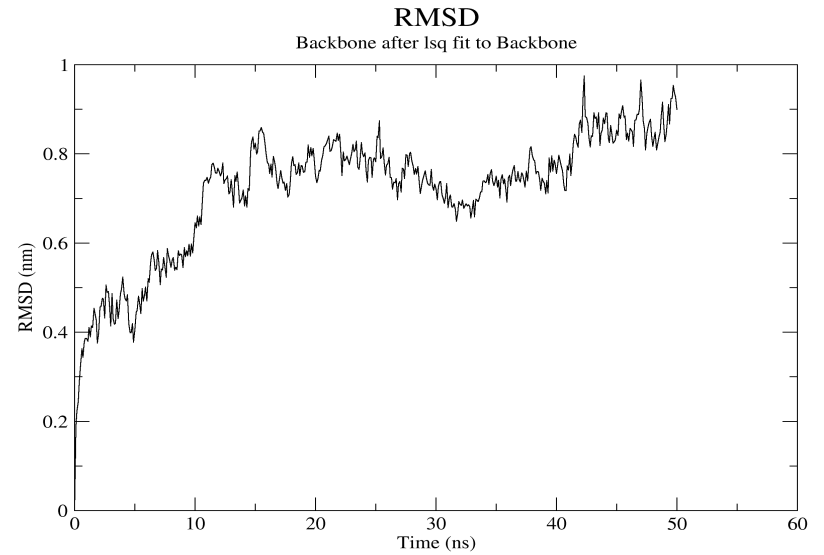
Supplementary Figure 2: Results of Molecular Dynamic Simulation
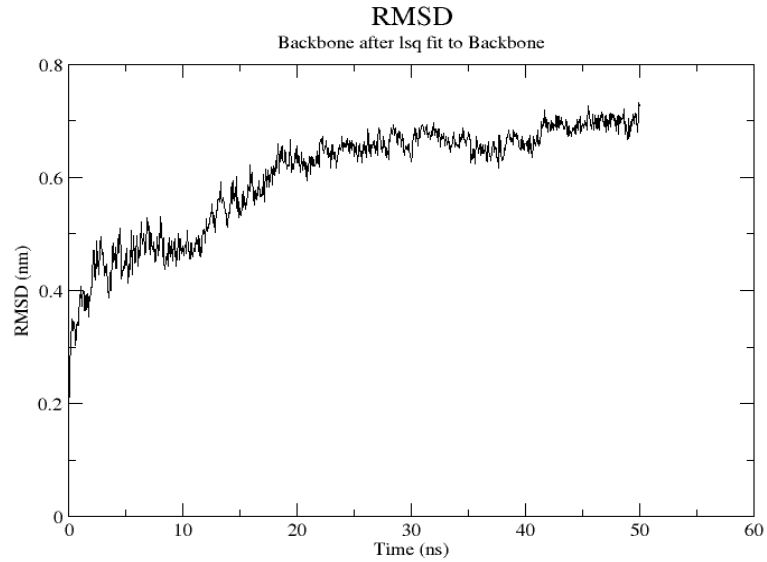
NSP1 wild

NSP1 V121D

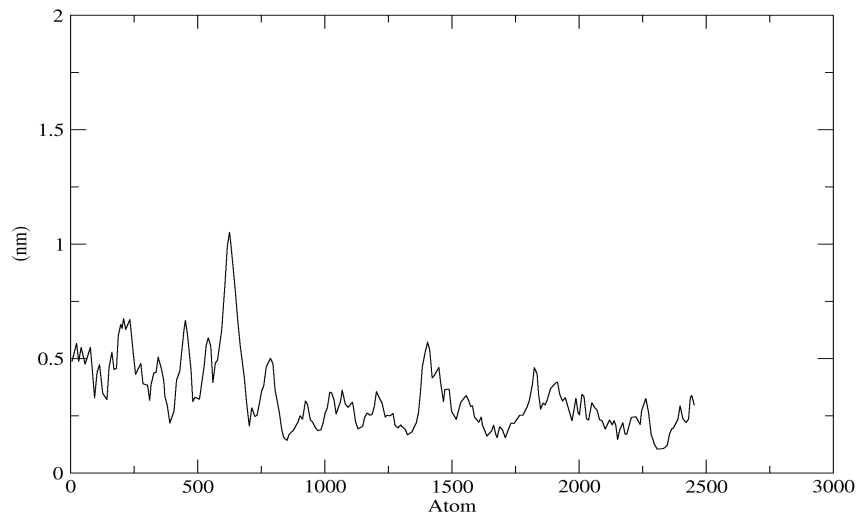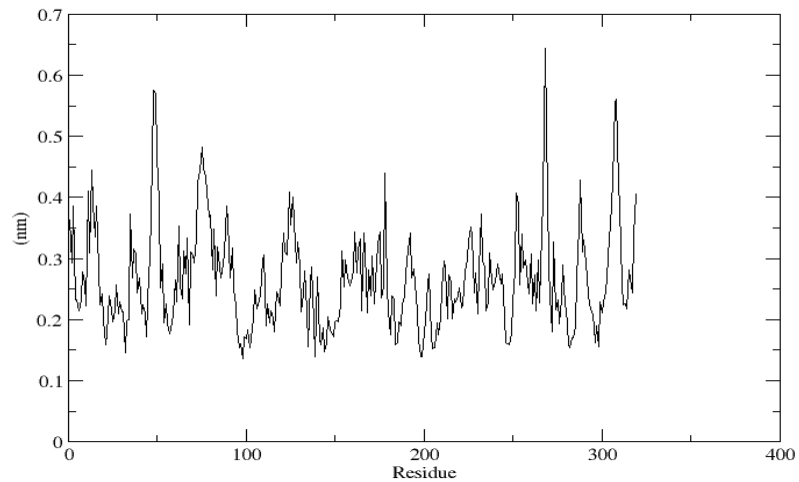# Supplementary Figure 2: Results of Molecular Dynamic Simulation
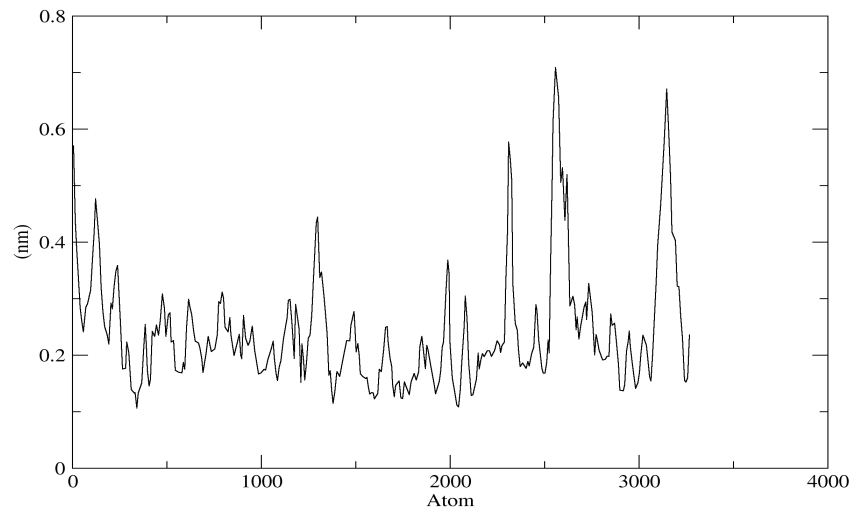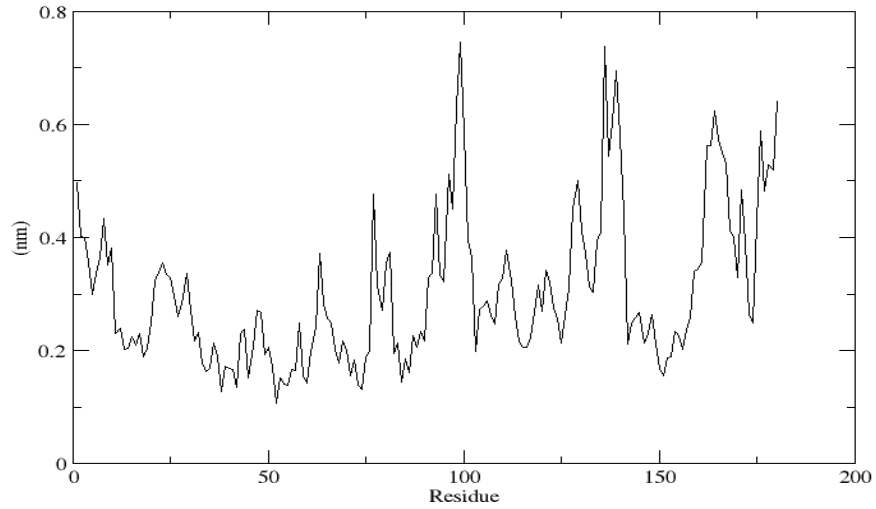

NSP3 wild

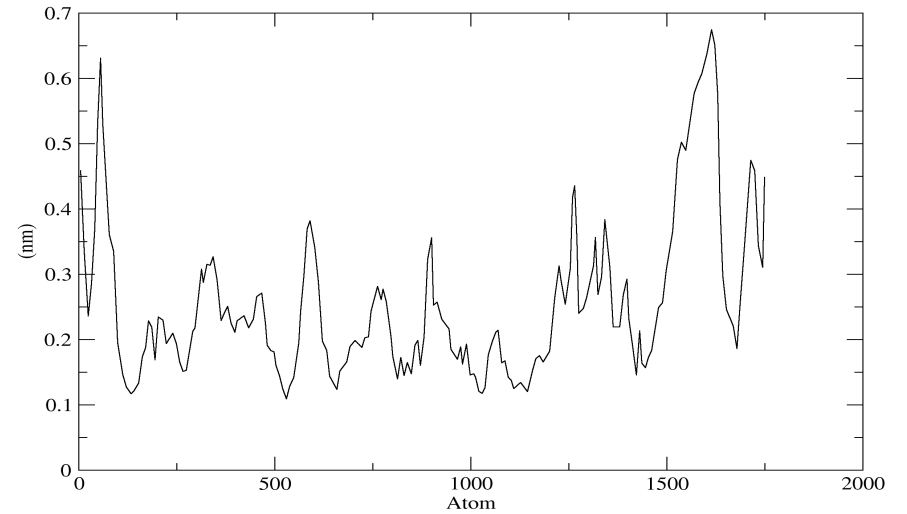NSP3 V843F

NSP3 A889V

Supplementary Figure 2: Results of Molecular Dynamic Simulation
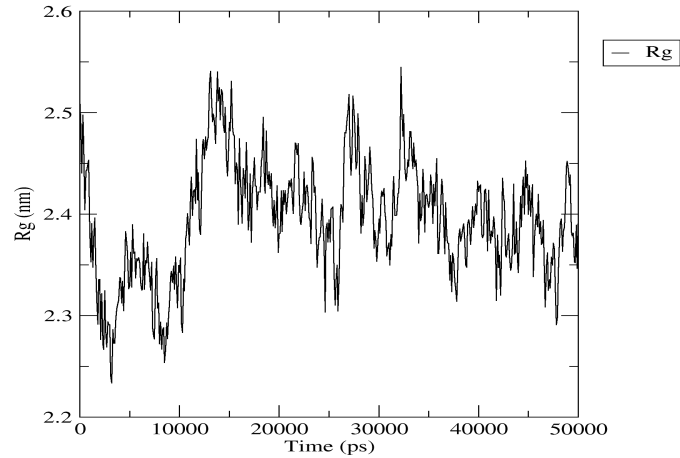

RMS fluctuation

NSP1 wild

RMS fluctuation
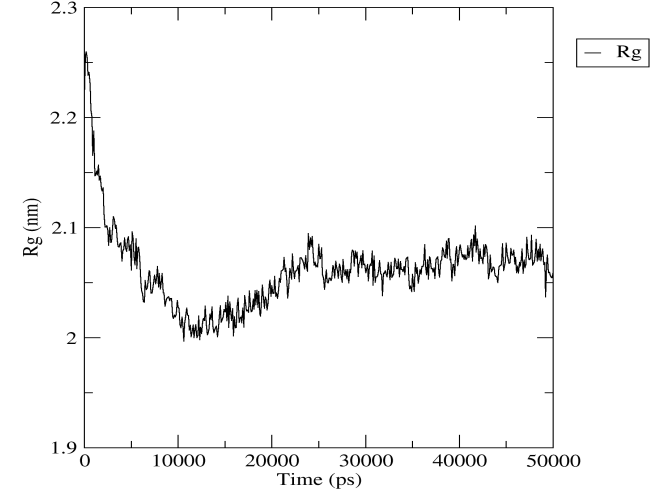
NSP1 V121D

Supplementary Figure 2: Results of Molecular Dynamic Simulation

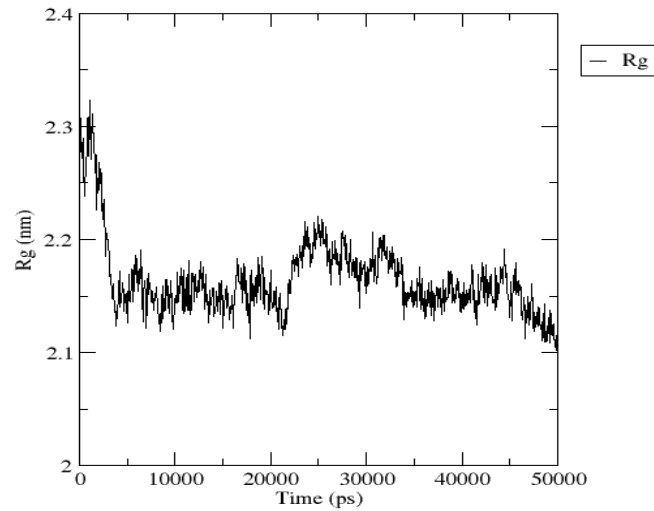Radius of gyration (total and around axes)

NSP3 wild

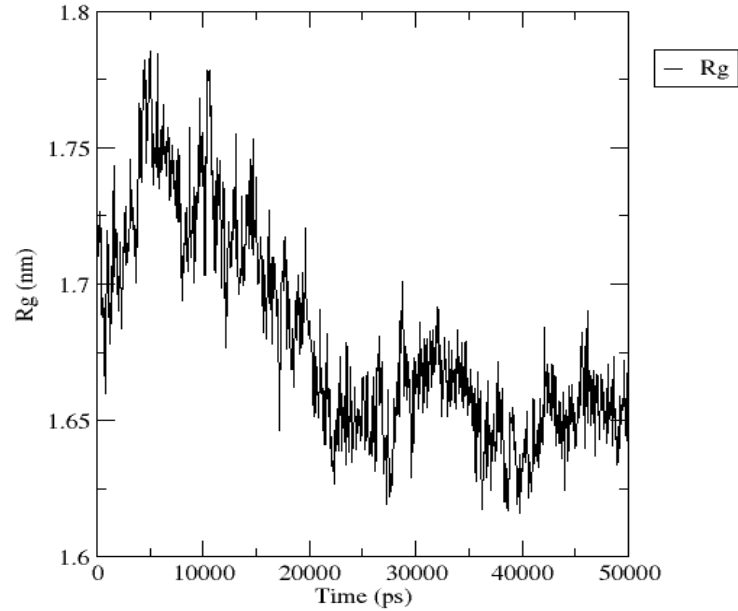Radius of gyration (total and around axes)

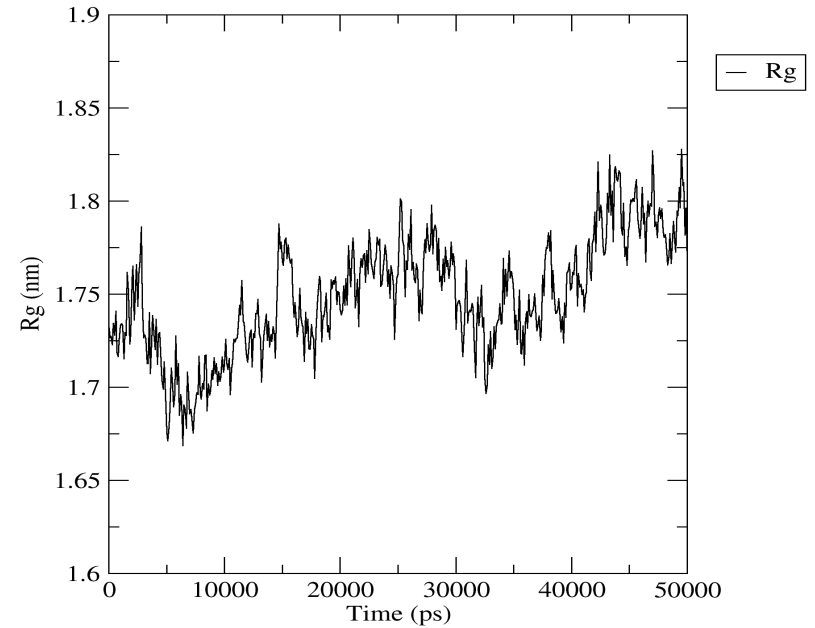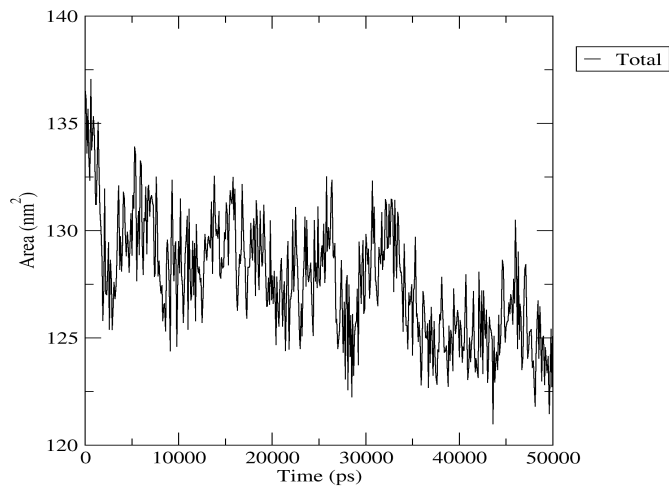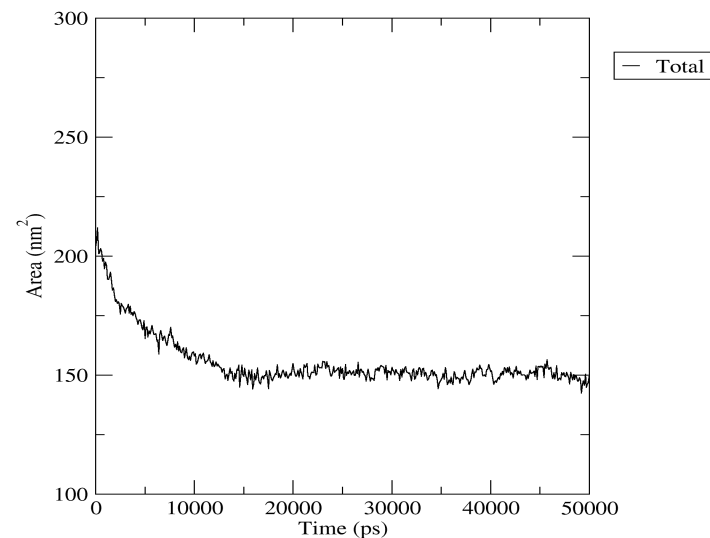NSP3 V843F

f gyration (total and around axes)

NSP3 A889V

Supplementary Figure 2: Results of Molecular Dynamic Simulation

NSP1 wild V121

NSP1 V121D

Supplementary Figure 2: Results of Molecular Dynamic Simulation

NSP3 wild

NSP3 V843F

NSP3 A889V

Supplementary Figure 2: Results of Molecular Dynamic Simulation

NSP1 Wild V121

NSP1 V121D