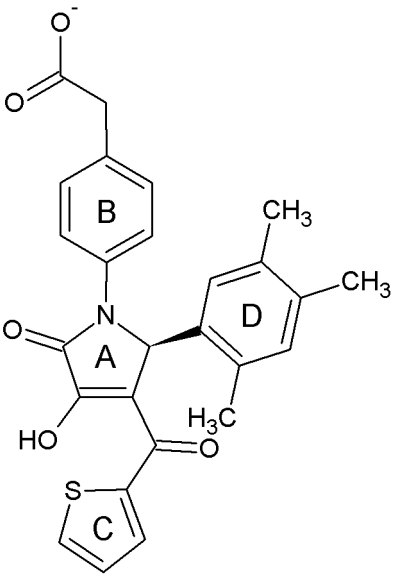
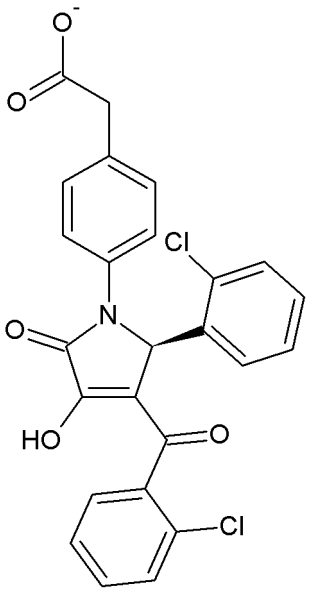
Supplementary Informations - *In Silico* study of VP35 inhibitors: from Computational Alanine Scanning to Essential Dynamics

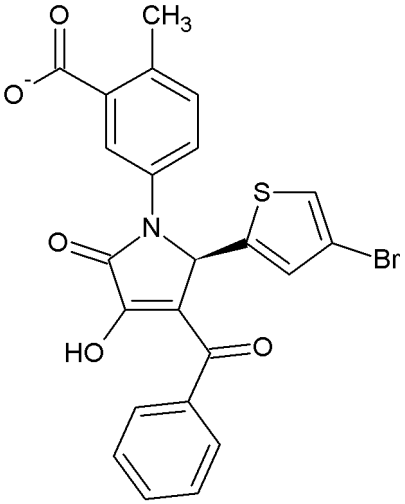
Molecular structures



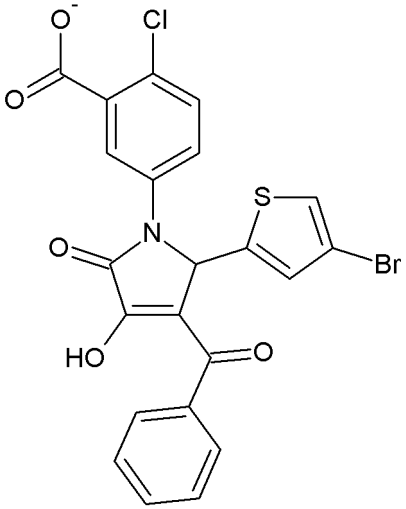
GA017



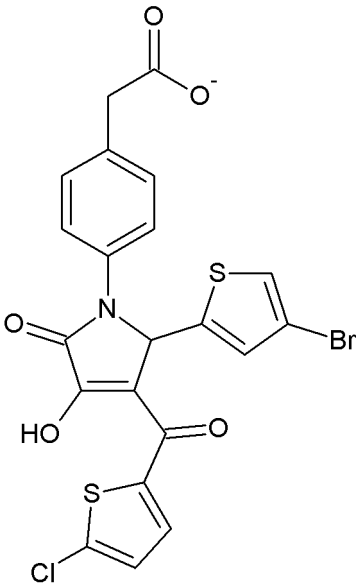
GA246



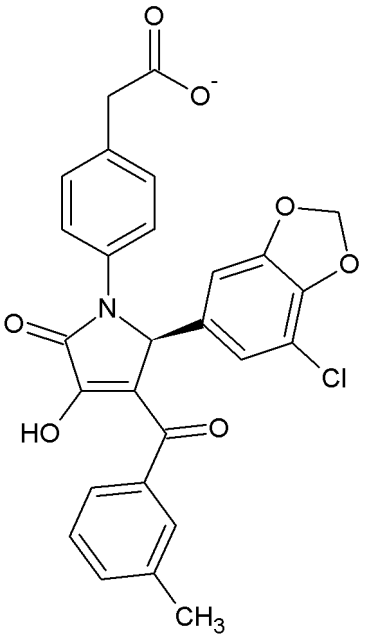
VPL27



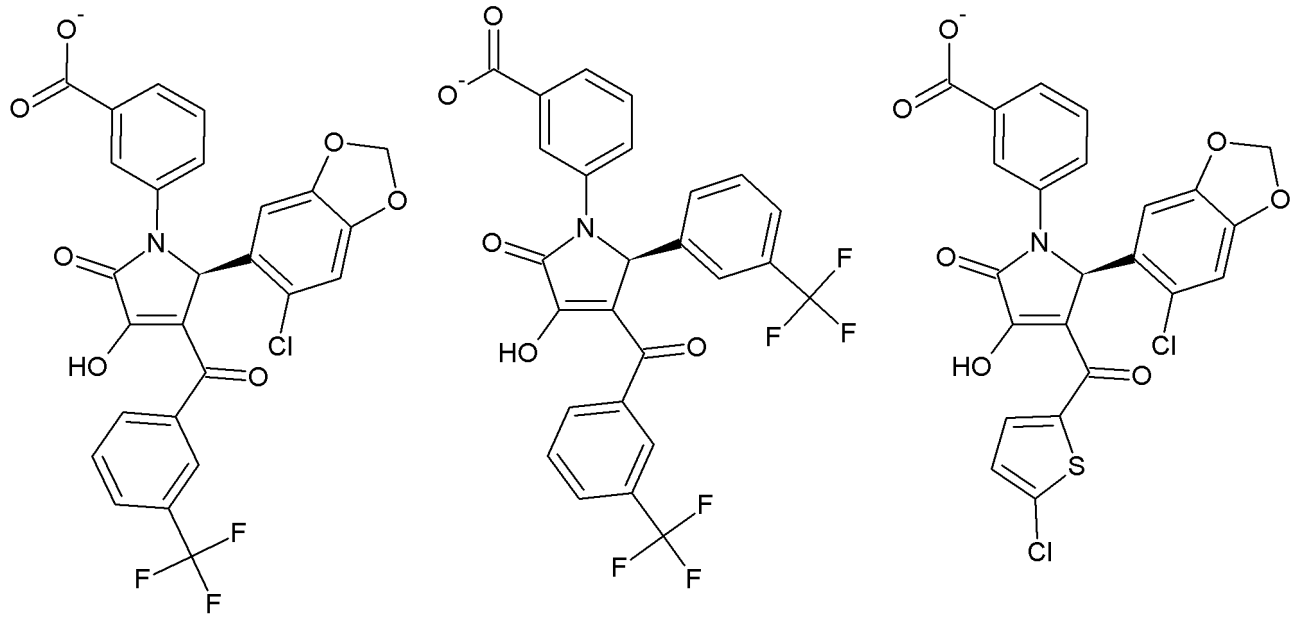
VPL29



VPL42



VPL48



VPL57 VPL58 VPL60

Figure S1: Molecular structures of the ligands

Binding Free Energies

Name	$\Delta G_{binding}$ / kcal mol^{-1}	σ / kcal mol^{-1}
GA246	-47.32	5.69
GA017	-41.46	2.36
VPL60	-40.72	5.28
VPL27	-40.42	4.48
VPL48	-40.40	4.98
VPL58	-39.23	4.27
VPL42	-39.15	5.05
VPL57	-38.15	5.28
VPL29	-37.00	4.72

Table 1: Binding free energies of ligands.

RMSD plots

In the following figures are shown the RMSD plots of ligands fitting protein C_α.

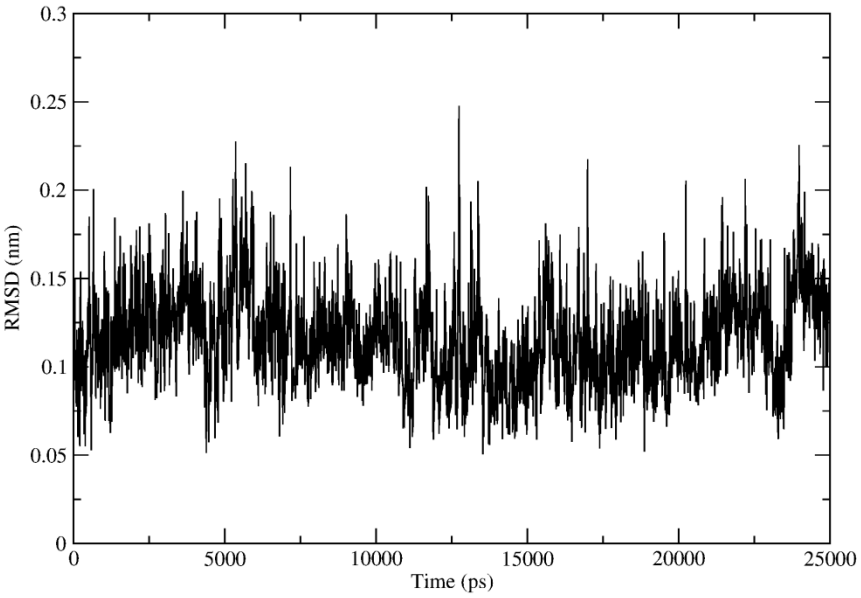


Figure S2: GA017

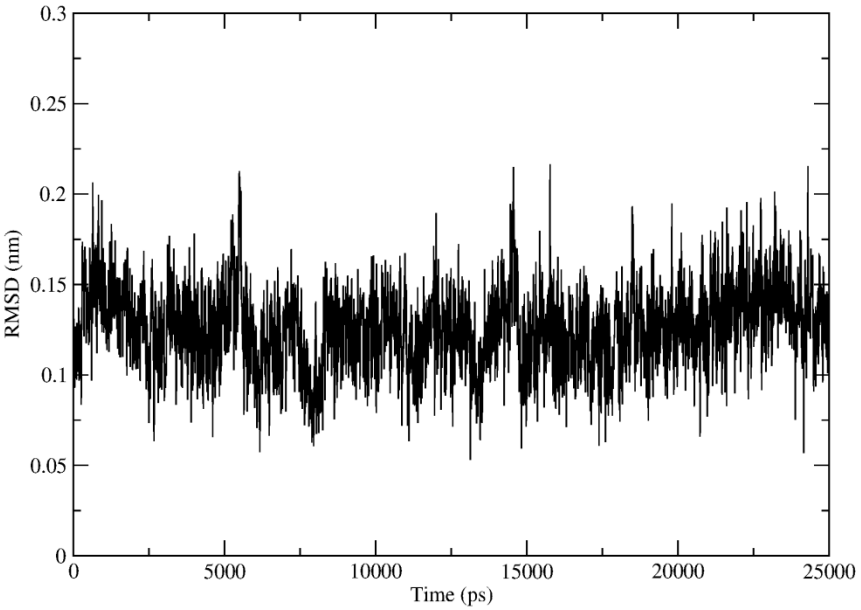


Figure S3: GA246

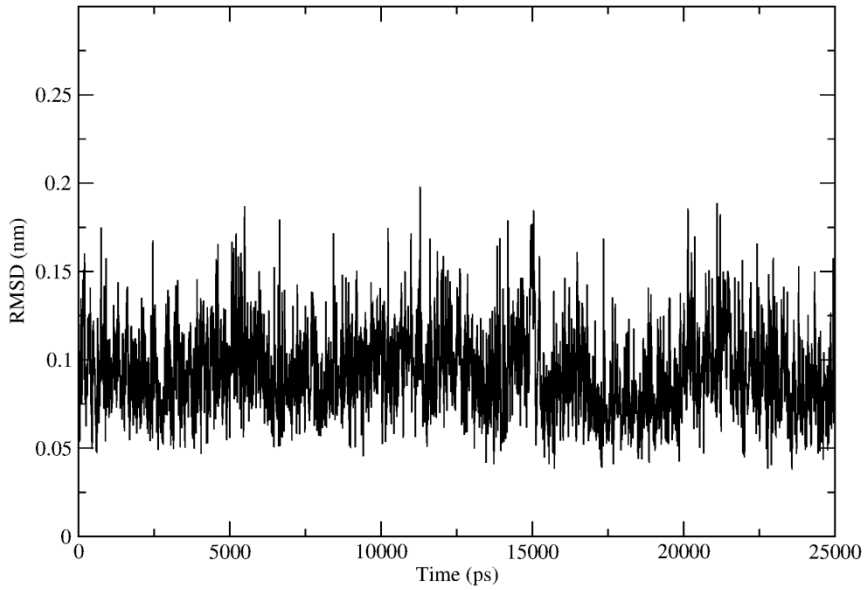


Figure S4: VPL27

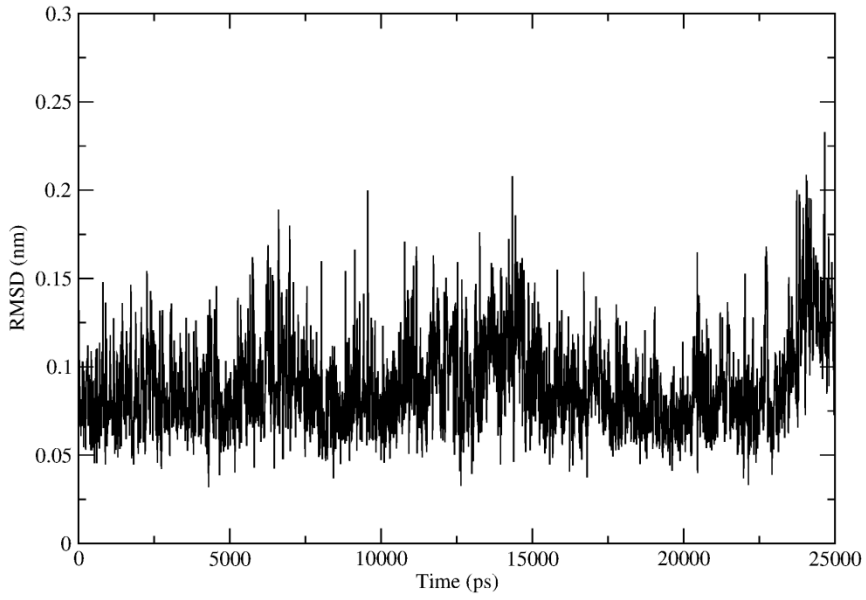


Figure S5: VPL29

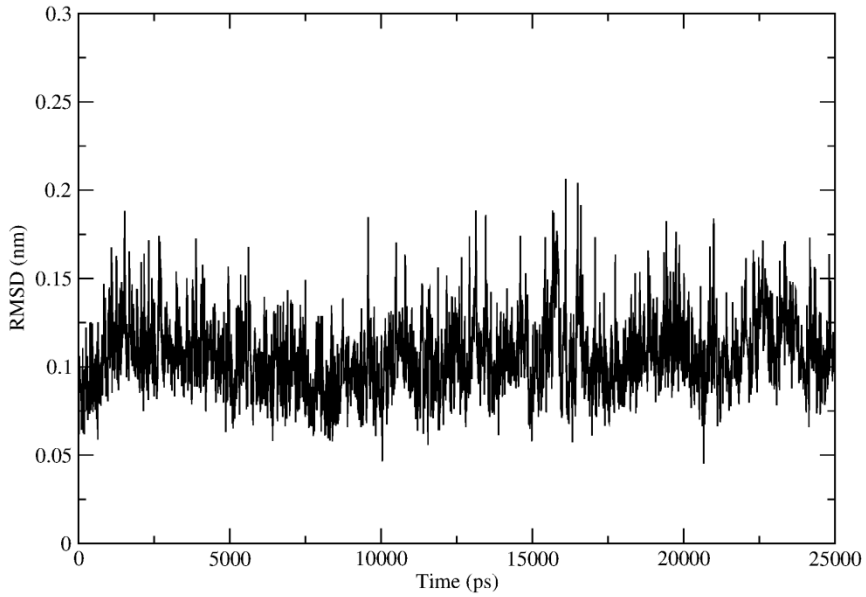


Figure S6: VPL42

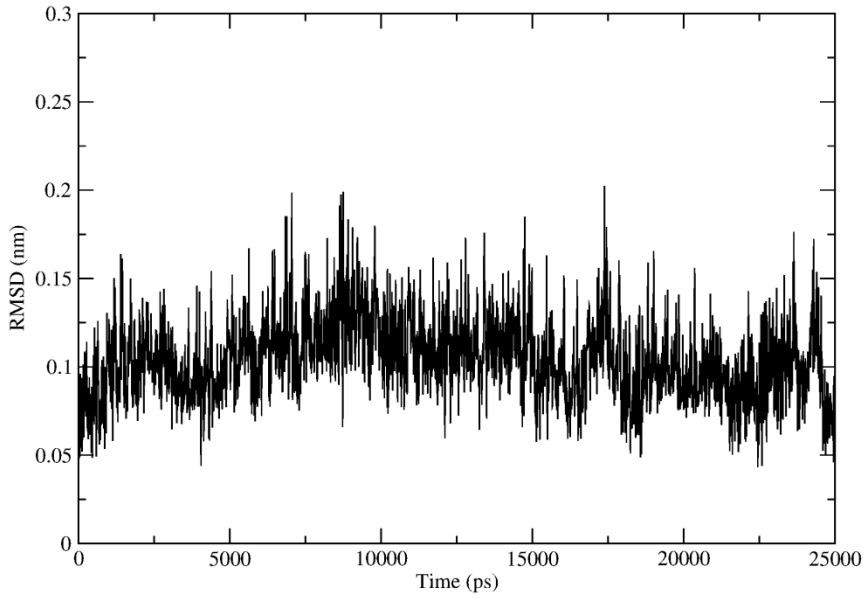


Figure S7: VPL48

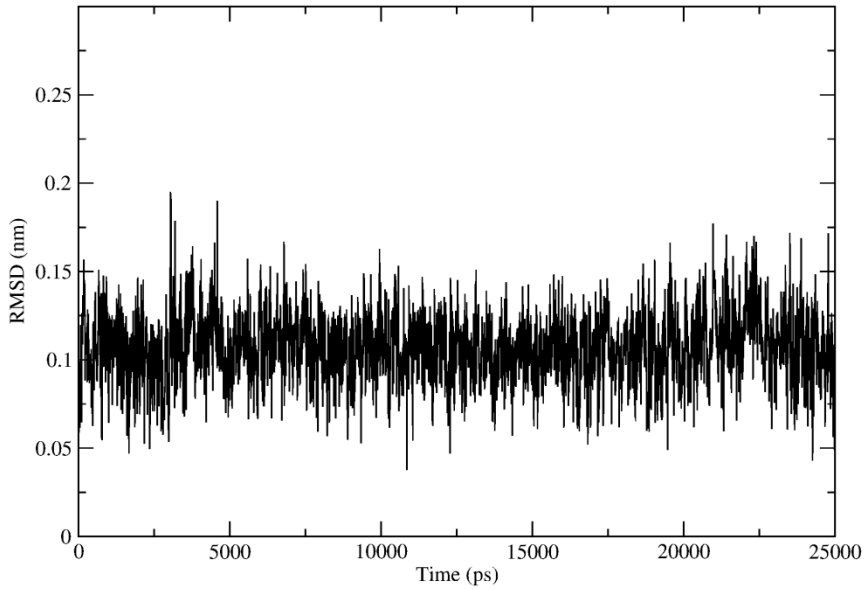


Figure S8: VPL57

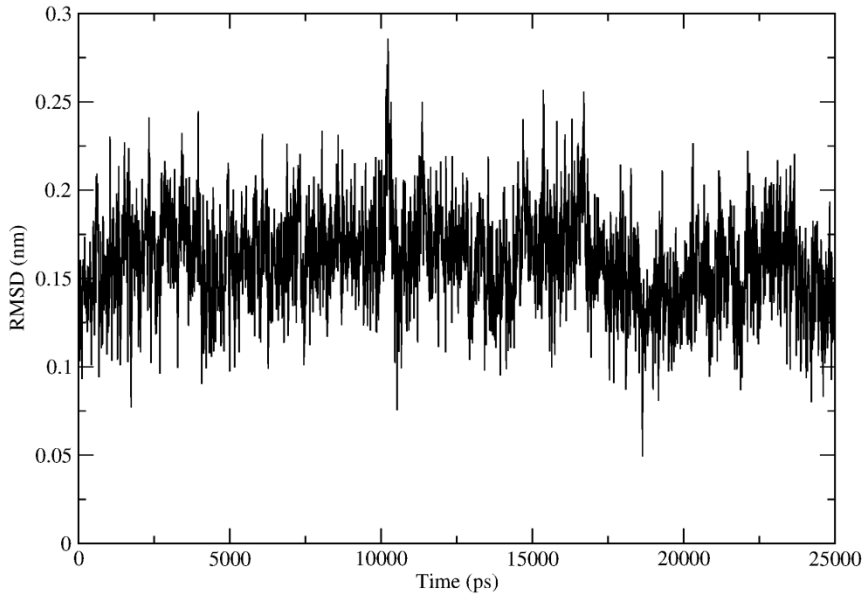


Figure S9: VPL58

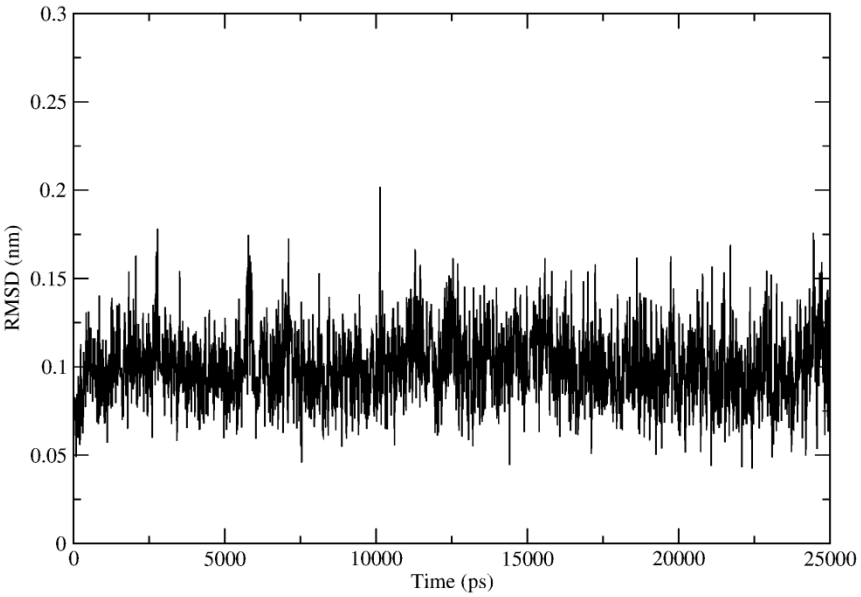


Figure S10: VPL60

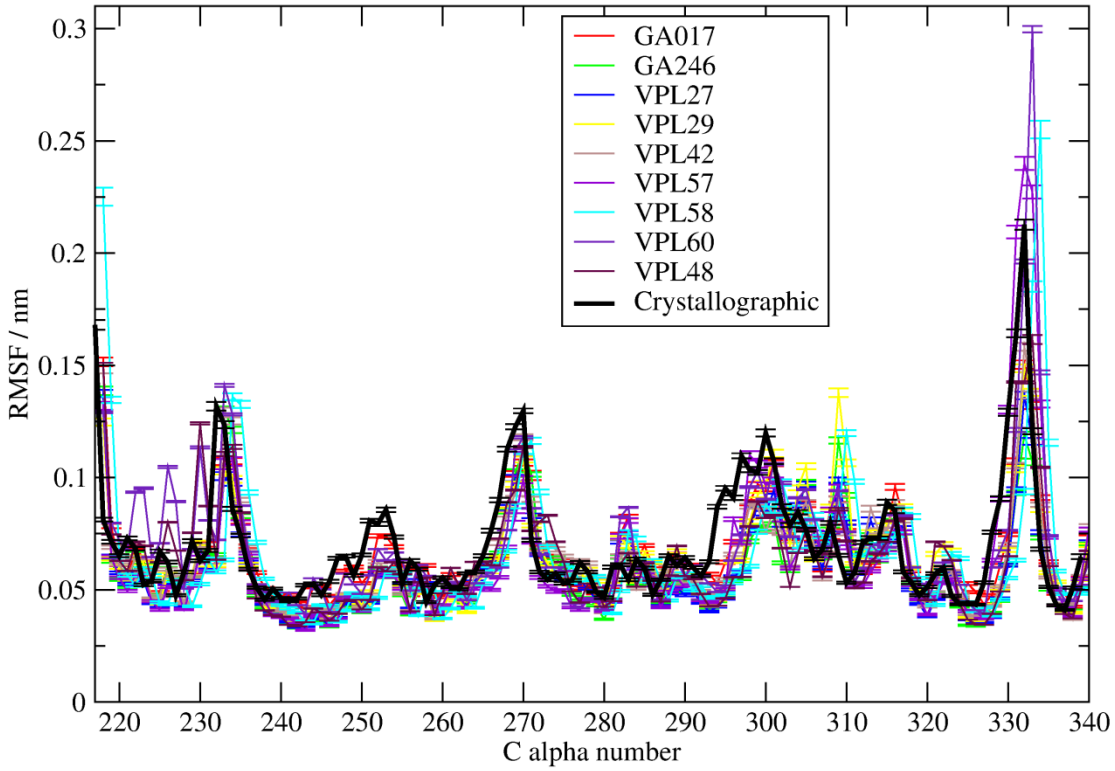


Figure S11: RMSF bootstrap analysis

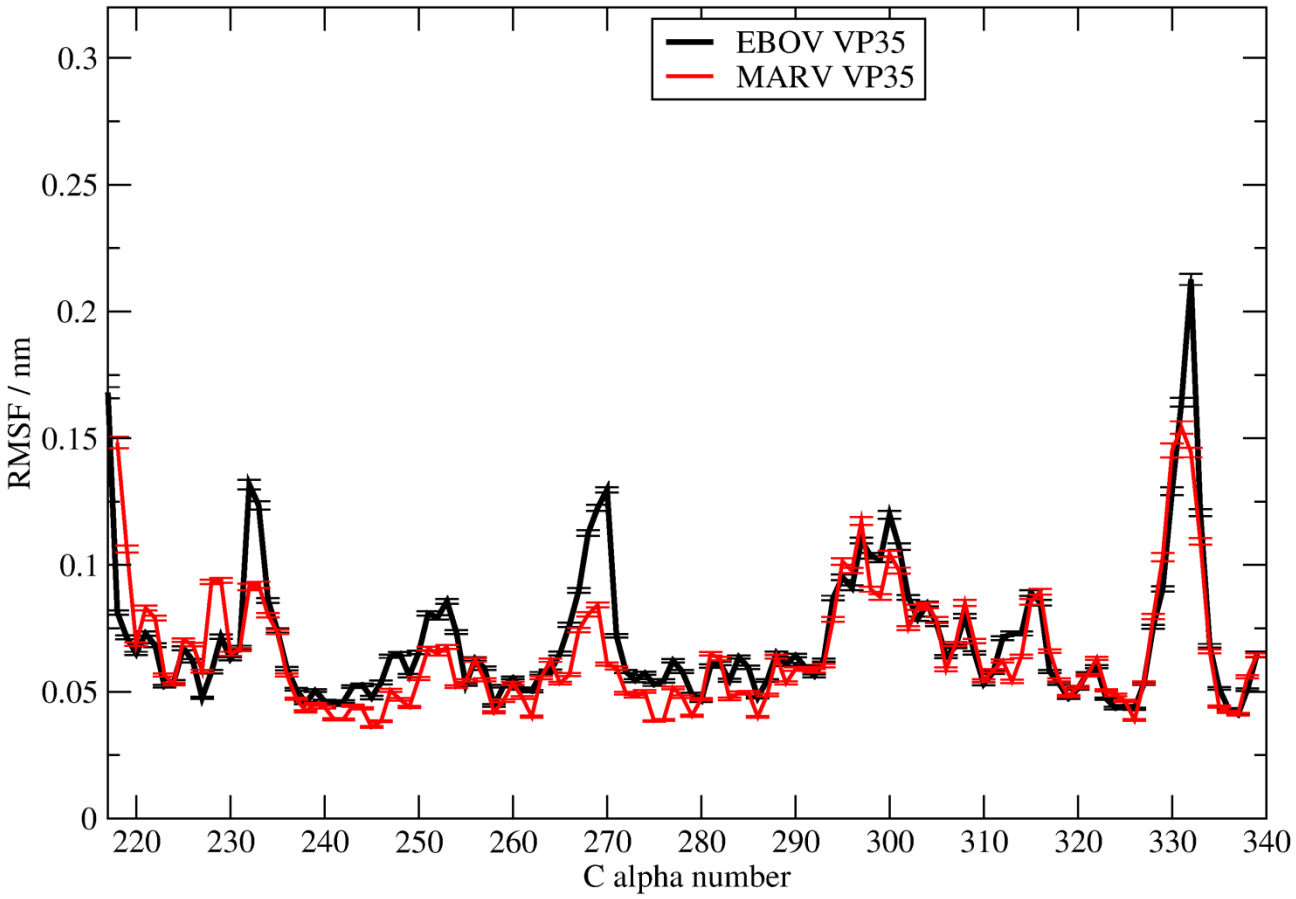


Figure S12: Comparison between MARV and EBOV VP35 RMSF.