

Fig S2 : i) Secondary structure analysis of predicted model (generated from PDBSum database). Magenta color shows helices present in the three-dimensional structure of coat protein. Arrow represents the β strand present in the structure. Presence of β turns and loops is labeled. ii) Three-dimensional structure of coat protein, all secondary structure components are labeled according to their presence from N-terminal to C-terminal. Blue color shows ARM region position in three-dimensional structure. Green color shows R Domain of coat protein which was not crystallized while magenta is showing S Domain.

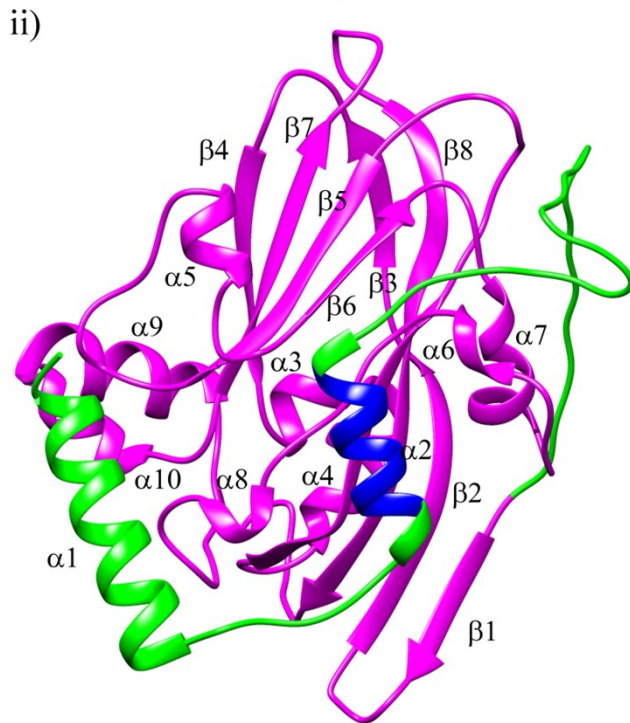
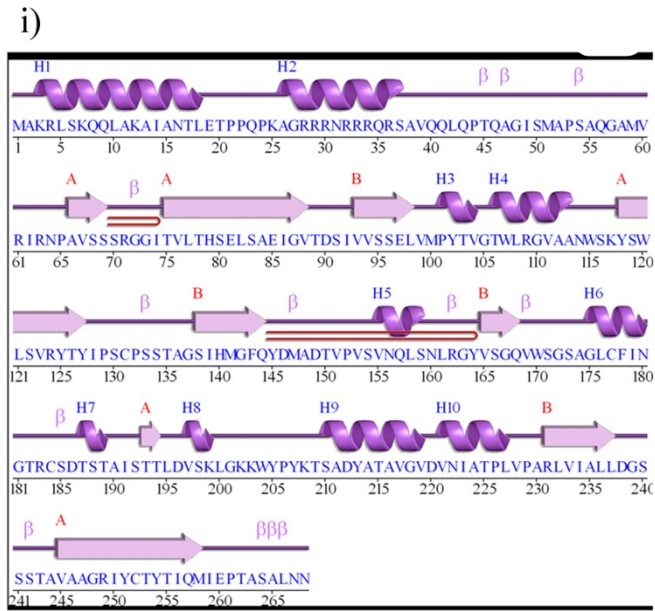


Fig S3 : Secondary structure of genome of SeMV virus predicted using RNAWeb server.

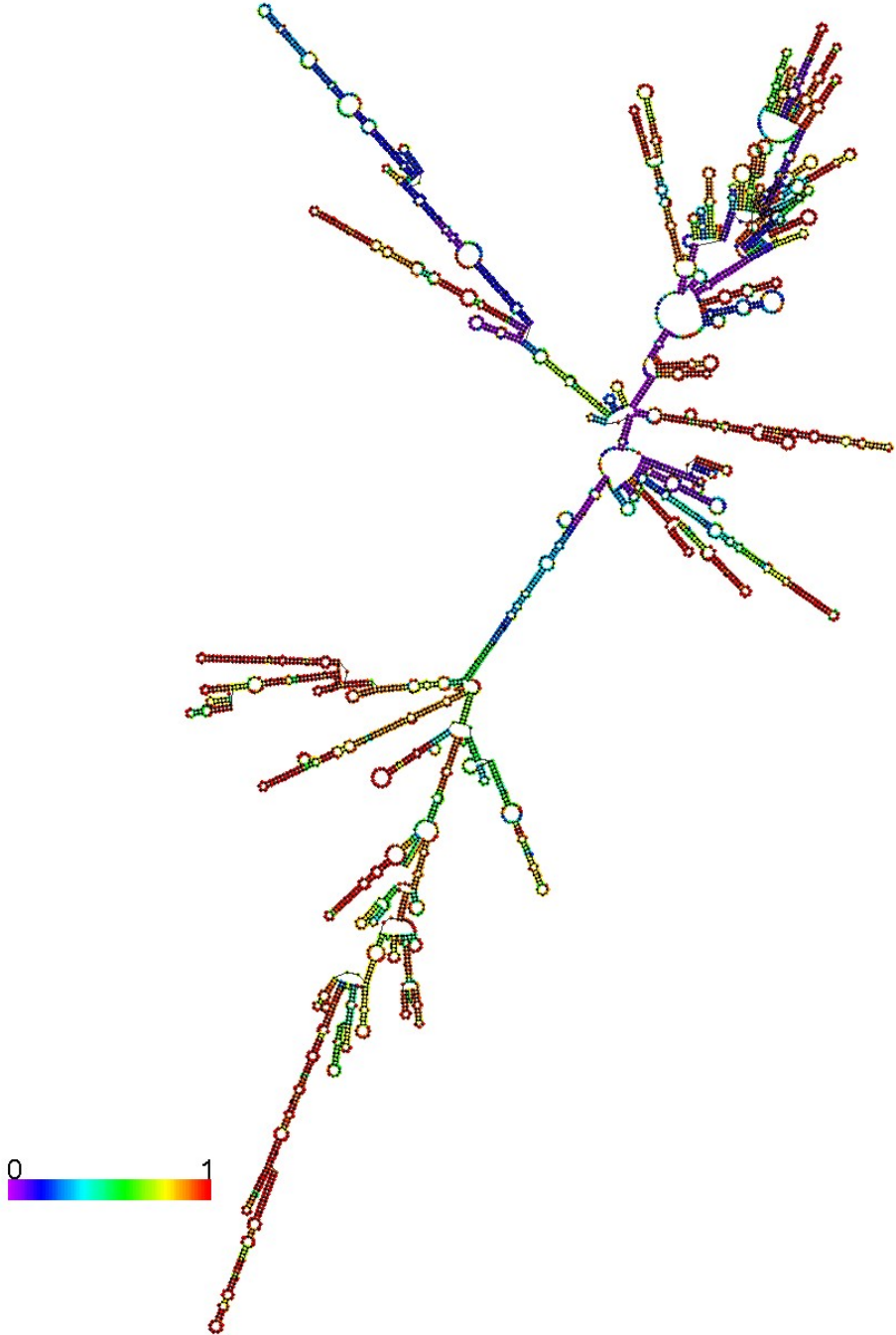


Fig S4: RMS fluctuation of coat protein alone and coat protein complex with Loop7. Black color shows complex while Red color shows coat protein. ARM region is boxed while R and S domain are represented by blue and green color lines, respectively.

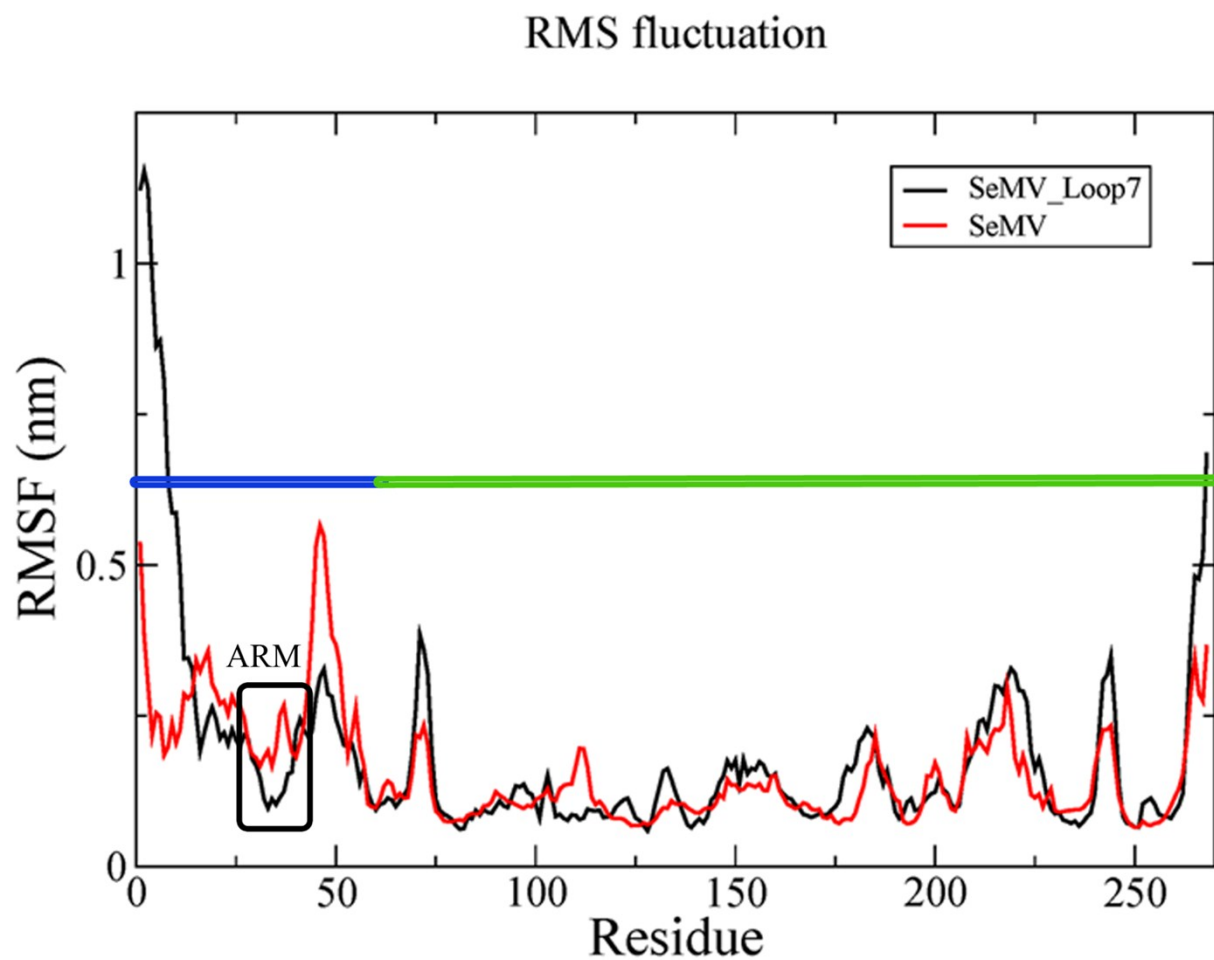


Fig S5 : Movement of N-terminal region throughout the simulation of coat protein alone. The first helix loses its helicity and turned to coil and bending downwards.

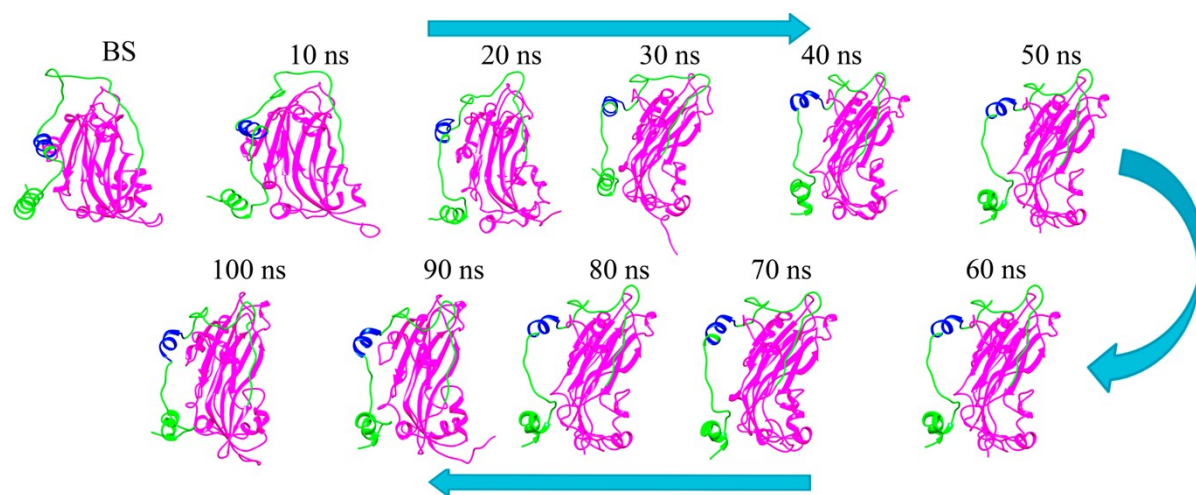


Fig S6 : Free energy landscape for coat protein alone and complex with RNA operator loop. i) Loop4, ii) Loop9, iii) Loop11, iv) Loop13 and v) Loop14.

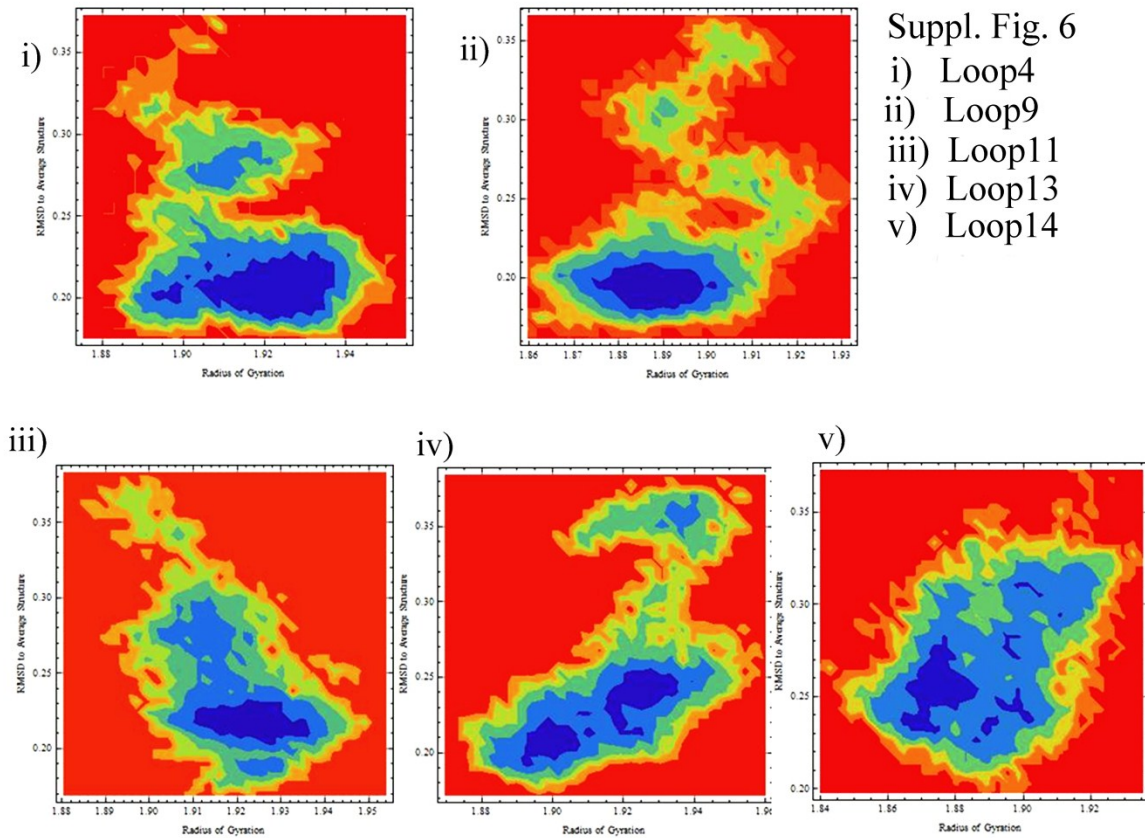


Fig S7 : H-bond existing graph of protein RNA complexes. i) SeMV coat protein-RNA operator Loop7 complex graph. ii) Mutated SeMV coat protein-RNA operator Loop7 complex. iii) SeMV coat protein-Mutated RNA operator loop complex graph. All graphs are generated for 10 ns simulation period. These graphs were generated between simulation time(X axis) and existence of H-bond(Y axis) throughout the simulation. The intensity of Red color line shows the existence of H-bond throughout the simulation. The number of Red line represents the number of H-bond of that complex.

