

The above results as obtained by protparam [13] annotate the peptide in detail. The length of the peptide is found to be 80 amino acids with the molecular weight of 8764.32 and isoelectric point 8.57. This is the pH at which the peptide becomes inactive in an electric field. The peptide was identified to be unstable with the Instability index being 47.53. The peptide is basic in nature.

9.5 Construction of Peptide 3D Structure in Argus Lab

The 3D structure of peptide predicted above was constructed in Argus lab. Argus lab [12] is downloadable software for protein and chemical annotation. It is specially used for targeted docking studies and molecule and protein building. It has an inbuilt programme of energy minimization and geometry optimization of the molecule. The energy of any molecule generated in the software can be calculated.

Figure 9.5 shows the 3D structure of the selected peptide which can be used as a potential vaccine candidate. The yellow highlighted site is amino acid K (Lys) which is the one with maximum antigenic propensity. The energy of the peptide was calculated to be 2523.94 kcal/mol.

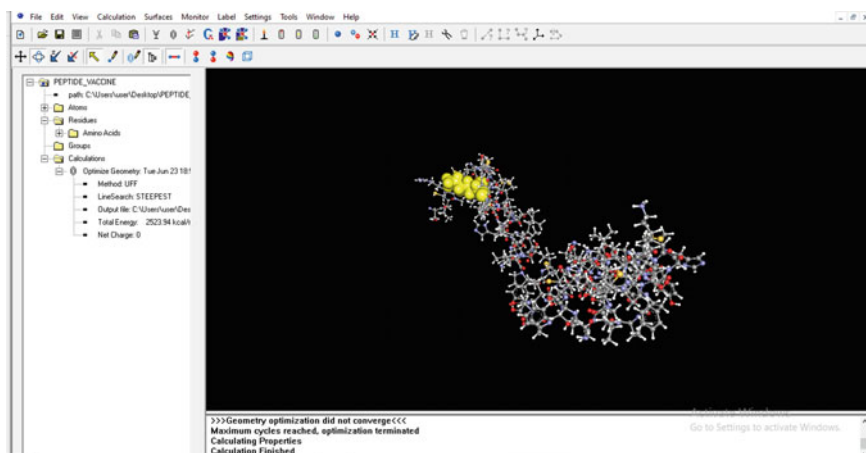


Fig. 9.5 The optimized structure of the vaccine candidate peptide designed in Argus lab