

Supplementary Materials

Table S1. Four vaccine constructs with antigenicity and allergenicity score.

| Vaccine construct | Adjuvant | Construct | Allergenicity | Antigenpro | Vaxijen | Solubility |
|-------------------|-------------------------|--|---------------|------------|------------------|------------|
| V1 | Hbha adjuvant | <p>EAAAKMAENPNIDDLAPLLAALGAADL ALATVNDLIANLRERAETRAETRTRVEE RRARLTKFQEDLPEQFIELRDKFTTEELRK AAEGYLEAATNRYNELVERGEAALQRLR SQAFEDASARAEGYVDQAVELTQEALGT VASQTRAVGERAAKLVGIELEAAAKTLNL FPLNF^{AYY}AKAKYPFSY^{AYYY}SNIGFLLY ^{AYY}SSRPTILIR^{AYY}RLSPVPSVK^{AYY}IYIK NIDEL^{AYY}EAKDIATTY^{AYY}AHYRNLVSL GPGPGNLFPLNFKSITNKRFGPGPGHYIRA GYNHKYPFRIGPGPGENTDSFYSNIGFLLY GPGPGKLPFRSSRPTILIRNGPGPGMNDIL RLSPVPSVKGPGPGGPLQYIYIKNIDELKK KDIATTYNFTQHLSFVKKAAFAHYRNLVS LIRLKKNTLNLFPLNFKSITNKKHKYPFRI CSIAKGTDLKKVELPEGLYCPRTEINLKKK LFRSSRPTILIRNTKKYSTKNTGMPVLR VLKKKLQNIYEKHMFFTNLTFGGGSAKFV AAWTLKAAAGGGSKKAKDIATTYNFTQH LSFHEYGAEALERAGKKVSLIRLVKRTISIS NLHEYGAEALERAGAKFVAAWTLKAAA GGGS</p> <p>EAAAKGIINTLQKYYCRVGGRCVLSCL PKEEQIGKCSTRGRKCCRRKKEAAAKTLN LFPLNF^{AYY}AKAKYPFSY^{AYYY}SNIGFL Y^{AYY}SSRPTILIR^{AYY}RLSPVPSVK^{AYY}IYI KNIDEL^{AYY}EAKDIATTY^{AYY}AHYRNLVS LGPGPGNLFPLNFKSITNKRFGPGPGHYIR AGYNHKYPFRIGPGPGENTDSFYSNIGFLL YGPGPGKLPFRSSRPTILIRNGPGPGMNDI LRLSPVPSVKGPGPGGPLQYIYIKNIDELK KKDIATTYNFTQHLSFVKKAAFAHYRNLV SLIRLKKNTLNLFPLNFKSITNKKHKYPF RICSIKGTDLKKVELPEGLYCPRTEINLK KKLPFRSSRPTILIRNTKKYSTKNTGMPV LRVLKKKLQNIYEKHMFFTNLTFGGGSAK FVAAWTLKAAAGGGSKKAKDIATTYNFT QHLSFHEYGAEALERAGKKVSLIRLVKRTI SISNLHEYGAEALERAGAKFVAAWTLKA AAGGGG</p> <p>EAAAKMAENSNIDDIKAPLLAALGAADLA LATVNELITNLRERAETRRSRVEESRRL TKLQEDLPEQLTELREKFTAEEELRKA AEGYLEAATSELVERGEAALERLRSQQSFEEVS ARAEGYVDQAVELTQEALGTVASQVEGR AAKLVGIELEAAAKTLNLFPLNF^{AYY}AKA KYPFSY^{AYYY}SNIGFLLY^{AYY}SSRPTILIRA YYRLSPVPSVK^{AYY}IYIKNIDEL^{AYY}EAKD IATTY^{AYY}AHYRNLVSLGPGPGNLFPLNF KSITNKRFGPGPGHYIRAGYNHKYPFRIGP PGENTDSFYSNIGFLLYGPGPGKLPFRSS RPTILIRNGPGPGMNDILRLSPVPSVKGPG PGGPLQYIYIKNIDELKKKDIATTYNFTQH LSFVKKAAFAHYRNLVSLIRLKKNTLNLFP LNFKSITNKKHKYPFRICSIKGTDLKKV ELPEGLYCPRTEINLKKKLPFRSSRPTILIRN TKKYSTKNTGMPVLRVLKKKLQNIYEKH MFFTNLTFGGGSAKFVAAWTLKAAAGGG SKKAKDIATTYNFTQHLSFHEYGAEALER AGKKVSLIRLVKRTISISNLHEYGAEALER AGAKFVAAWTLKAAAGGGG</p> | NON-ALLERGEN | 0.6842 | Probable ANTIGEN | |
| V2 | Beta definsin adjuvant | <p>EAAAKGIINTLQKYYCRVGGRCVLSCL PKEEQIGKCSTRGRKCCRRKKEAAAKTLN LFPLNF^{AYY}AKAKYPFSY^{AYYY}SNIGFL Y^{AYY}SSRPTILIR^{AYY}RLSPVPSVK^{AYY}IYI KNIDEL^{AYY}EAKDIATTY^{AYY}AHYRNLVS LGPGPGNLFPLNFKSITNKRFGPGPGHYIR AGYNHKYPFRIGPGPGENTDSFYSNIGFLL YGPGPGKLPFRSSRPTILIRNGPGPGMNDI LRLSPVPSVKGPGPGGPLQYIYIKNIDELK KKDIATTYNFTQHLSFVKKAAFAHYRNLV SLIRLKKNTLNLFPLNFKSITNKKHKYPF RICSIKGTDLKKVELPEGLYCPRTEINLK KKLPFRSSRPTILIRNTKKYSTKNTGMPV LRVLKKKLQNIYEKHMFFTNLTFGGGSAK FVAAWTLKAAAGGGSKKAKDIATTYNFT QHLSFHEYGAEALERAGKKVSLIRLVKRTI SISNLHEYGAEALERAGAKFVAAWTLKA AAGGGG</p> <p>EAAAKMAENSNIDDIKAPLLAALGAADLA LATVNELITNLRERAETRRSRVEESRRL TKLQEDLPEQLTELREKFTAEEELRKA AEGYLEAATSELVERGEAALERLRSQQSFEEVS ARAEGYVDQAVELTQEALGTVASQVEGR AAKLVGIELEAAAKTLNLFPLNF^{AYY}AKA KYPFSY^{AYYY}SNIGFLLY^{AYY}SSRPTILIRA YYRLSPVPSVK^{AYY}IYIKNIDEL^{AYY}EAKD IATTY^{AYY}AHYRNLVSLGPGPGNLFPLNF KSITNKRFGPGPGHYIRAGYNHKYPFRIGP PGENTDSFYSNIGFLLYGPGPGKLPFRSS RPTILIRNGPGPGMNDILRLSPVPSVKGPG PGGPLQYIYIKNIDELKKKDIATTYNFTQH LSFVKKAAFAHYRNLVSLIRLKKNTLNLFP LNFKSITNKKHKYPFRICSIKGTDLKKV ELPEGLYCPRTEINLKKKLPFRSSRPTILIRN TKKYSTKNTGMPVLRVLKKKLQNIYEKH MFFTNLTFGGGSAKFVAAWTLKAAAGGG SKKAKDIATTYNFTQHLSFHEYGAEALER AGKKVSLIRLVKRTISISNLHEYGAEALER AGAKFVAAWTLKAAAGGGG</p> | NON-ALLERGEN | 0.7289 | Probable ANTIGEN | |
| V3 | Hbha cons rved adjuvant | <p>EAAAKMAENPNIDDLAPLLAALGAADL ALATVNDLIANLRERAETRAETRTRVEE RRARLTKFQEDLPEQFIELRDKFTTEELRK AAEGYLEAATNRYNELVERGEAALQRLR SQAFEDASARAEGYVDQAVELTQEALGT VASQTRAVGERAAKLVGIELEAAAKTLNL FPLNF^{AYY}AKAKYPFSY^{AYYY}SNIGFLLY ^{AYY}SSRPTILIR^{AYY}RLSPVPSVK^{AYY}IYIK NIDEL^{AYY}EAKDIATTY^{AYY}AHYRNLVSL GPGPGNLFPLNFKSITNKRFGPGPGHYIRA GYNHKYPFRIGPGPGENTDSFYSNIGFLLY GPGPGKLPFRSSRPTILIRNGPGPGMNDIL RLSPVPSVKGPGPGGPLQYIYIKNIDELKK KDIATTYNFTQHLSFVKKAAFAHYRNLVS LIRLKKNTLNLFPLNFKSITNKKHKYPFRI CSIAKGTDLKKVELPEGLYCPRTEINLKKK LFRSSRPTILIRNTKKYSTKNTGMPVLR VLKKKLQNIYEKHMFFTNLTFGGGSAKFV AAWTLKAAAGGGSKKAKDIATTYNFTQH LSFHEYGAEALERAGKKVSLIRLVKRTISIS NLHEYGAEALERAGAKFVAAWTLKAAA GGGS</p> <p>EAAAKMAENSNIDDIKAPLLAALGAADLA LATVNELITNLRERAETRRSRVEESRRL TKLQEDLPEQLTELREKFTAEEELRKA AEGYLEAATSELVERGEAALERLRSQQSFEEVS ARAEGYVDQAVELTQEALGTVASQVEGR AAKLVGIELEAAAKTLNLFPLNF^{AYY}AKA KYPFSY^{AYYY}SNIGFLLY^{AYY}SSRPTILIRA YYRLSPVPSVK^{AYY}IYIKNIDEL^{AYY}EAKD IATTY^{AYY}AHYRNLVSLGPGPGNLFPLNF KSITNKRFGPGPGHYIRAGYNHKYPFRIGP PGENTDSFYSNIGFLLYGPGPGKLPFRSS RPTILIRNGPGPGMNDILRLSPVPSVKGPG PGGPLQYIYIKNIDELKKKDIATTYNFTQH LSFVKKAAFAHYRNLVSLIRLKKNTLNLFP LNFKSITNKKHKYPFRICSIKGTDLKKV ELPEGLYCPRTEINLKKKLPFRSSRPTILIRN TKKYSTKNTGMPVLRVLKKKLQNIYEKH MFFTNLTFGGGSAKFVAAWTLKAAAGGG SKKAKDIATTYNFTQHLSFHEYGAEALER AGKKVSLIRLVKRTISISNLHEYGAEALER AGAKFVAAWTLKAAAGGGG</p> | NON-ALLERGEN | 0.6838 | Probable ANTIGEN | |

Continued.

| Vaccine construct | Adjuvant | Construct | Allergenicity | Antigenpro | Vaxijen | Solubility |
|-------------------|----------------------------|--|---------------|------------|---------|------------------|
| V4 | Ribosomal protein adjuvant | <p> EAAAKMAENSNIDDIKAPLLAALGAADL ALATVNELITNLRERAEETRRSRVEESRA RLTKLQEDLPEQLTELREKFTAEELRKAA EGYLEAATSELVERGEAALERLRSQQSFE EVSARAEGYVDQAVELTQEALGTVASQV EGRAAKLVGIELEAAAKTLNLFPLNFAYY AKAKYPFSYAYYSNIGFLLYAYYSSRPT ILIRAYYRLSPVSVKAYYIYIKNIDELAY YEAKDIATTYAYYAHYRNLVSLGPGPGN LFPLNFKSITNKRFGPGPGHYIRAGYNHK YPFRIGPGPGENTDSFYSNIGFLLYGPGPG KLPFRSSRPTILIRNGPGPGPMDILRLSPV PSVKGPGPGPLQYIYIKNIDELKKDIAT TYNFTQHLSFVKAAFAHYRNLVSLIRLK KNTLNLFPLNFKSITNKKKHKYPFRICSIA KGTDLKKVELPEGLYCPRTEINLKKLPF RSSRPTILIRNTKKYSTKNTGPMPVLRVLK KLQNIYEKHMFFTNLTFGGSAKFVAA WLKAAAGGGSKKAKDIATTYNFTQHLS FHEYGAEALERAGKKVSLIRLVKRTISISN LHEYGAEALERAGAKFVAAWLKAAAG GS </p> | NON-ALLERGEN | 0.6706 | | Probable ANTIGEN |

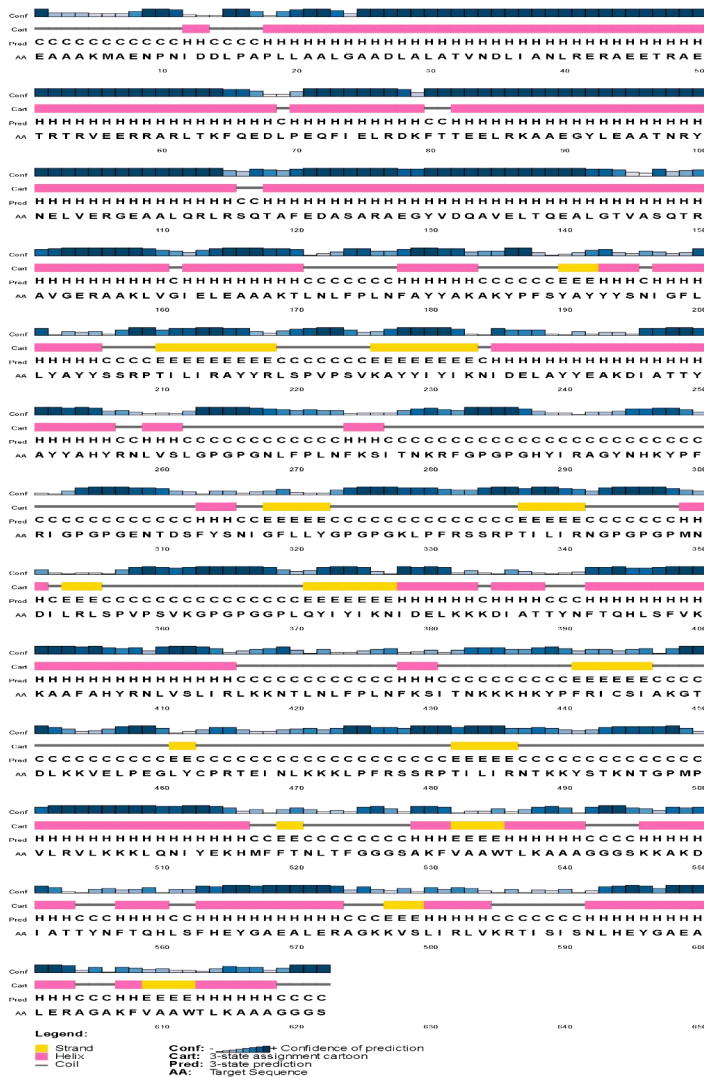


Figure S1. 2D structure of V1 construct, Yellow color in the structure represents Beta strands, the pinks color represents Alpha Helix and the black represents random coils in the structure.



Figure S2. 2D structure of V2 construct, yellow color in the structure represents Beta strands, the pinks color represents Alpha Helix and the black represents random coils in the structure.

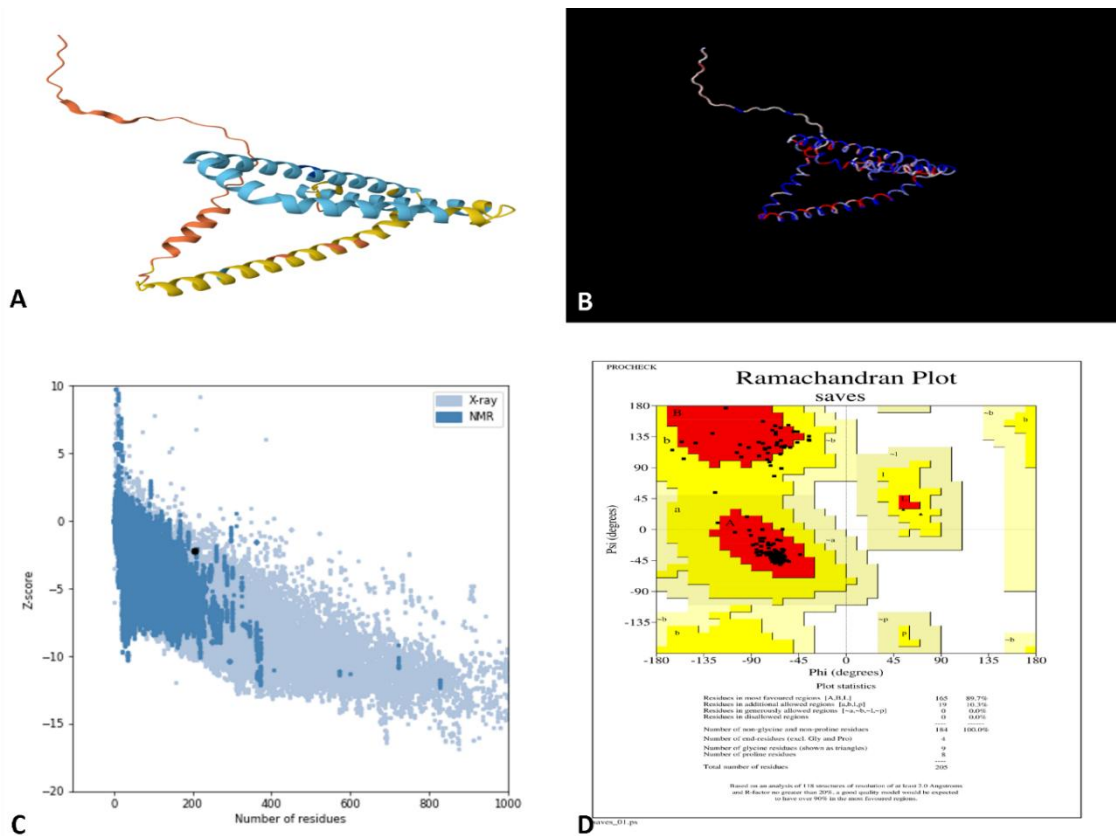


Figure S4. Vaccine construct V1. (A) 3D structure predicted on AlphaFold server. (B) Validated Structure of V1. (C) Z-score of V1 construct. (D) Ramachandran Plot of V1 construct scoring 89.7% of residues in most favored region, 10.3% of residues in additional allowed region, 0% in generously allowed region and 0% in disallowed regions.

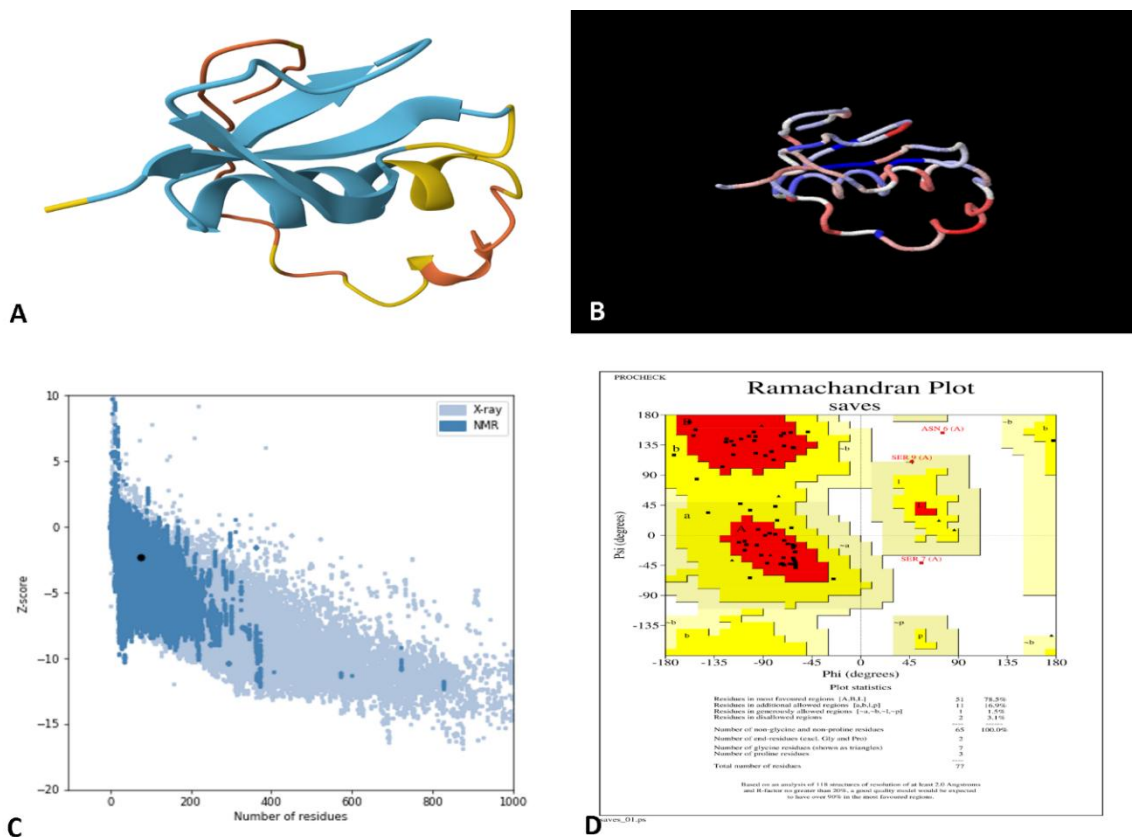


Figure S5. Vaccine construct V2. (A) 3D structure predicted on AlphaFold server. (B) Validated Structure of V2. (C) Z-score of V2 construct. (D) Ramachandran Plot of V2 construct scoring 78.5% of residues in most favored region, 16.9% of residues in additional allowed region, 1.5% in generously allowed region and 3.1% in disallowed regions.

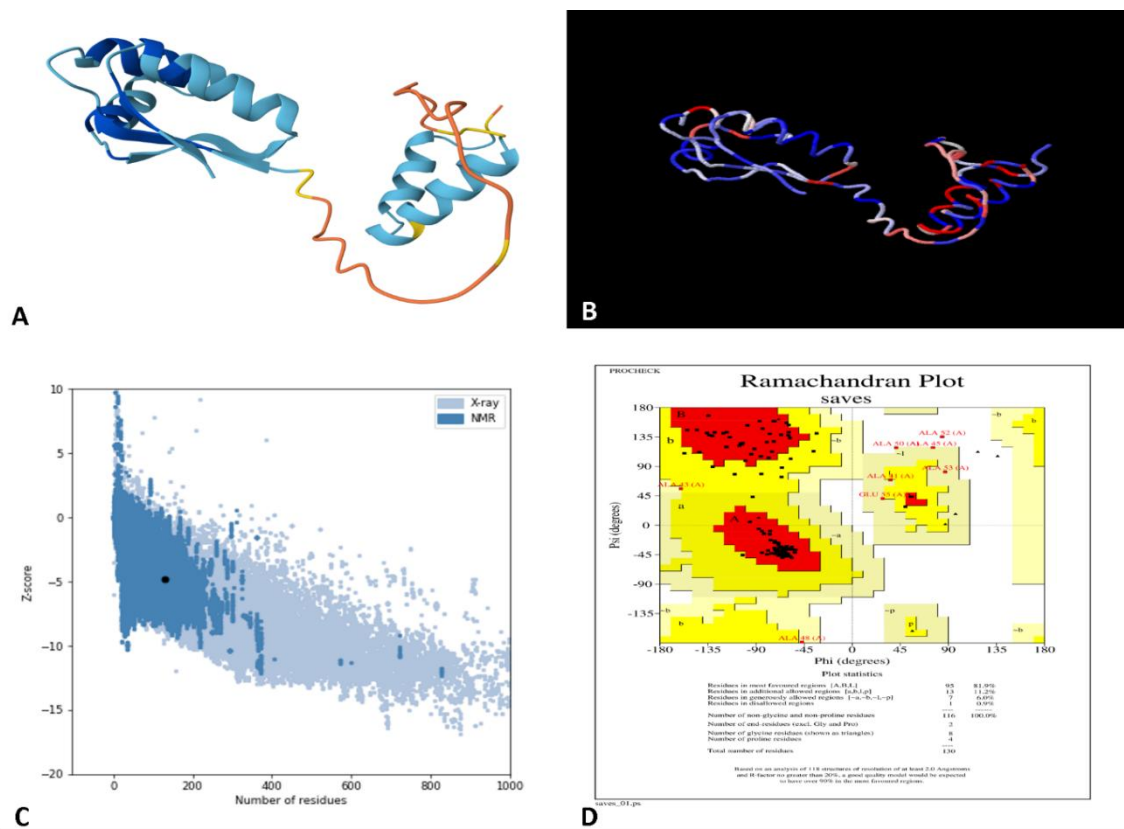


Figure S6. Vaccinate construct V4. (A) 3D structure predicted on AlphaFold server. (B) Validated Structure of V4. (C) Z-score of V4 construct. (D) Ramachandran Plot of V4 construct scoring 81.9% of residues in most favored region, 11.2% of residues in additional allowed region, 6.0% in generously allowed region and 0.9% in disallowed regions.