

Native pMHCII-TCR complex shows that the peptide was stabilized by eight HBs: side chain group of R71 α 2 and the carbonyl group of P(L314), side chain group of K75 α 1 and the carbonyl group of P(T318), side chain group of R76 α 1 and the carbonyl group of P(L316), side chain group of Y50V β and the carbonyl group of P(K315), the carbonyl group of G97V β and the side chain of P(T318), side chain groups of N82 α 2 and P(Y308), side chain groups of N82 α 2 and P(V309), side chain groups of N62 α 1 and P(V309), and the carbonyl group of Y50V β and the side chain of P(N312), and one SB: side chain groups of E56V β and P(Q311).

For p1MHCII-TCR complex seven HBs are formed between the MHCII-TCR and the peptide, eight HBs: side chain group of R71 α 2 and the carbonyl group of P(L314), side chain group of K75 α 1 and the carbonyl group of P(T318), side chain group of R76 α 1 and the carbonyl group of P(L316), side chain of N69 α 1 and P(K315), the carbonyl group of Y78 α 2 and the side chain of P(Q311), the carbonyl group of N82 α 2 and the side chain of P(Y308), and the carbonyl group of Y50V β and the side chain of P(N312).

For p2MHCII-TCR complex eight HBs are formed between the MHCII-TCR and the peptide, eight HBs: side chain group of R71 α 2 and the carbonyl group of P(L314), side chain group of K75 α 1 and the carbonyl group of P(T318), side chain group of R76 α 1 and the carbonyl group of P(L316), side chain groups of N82 α 2 and P(V309), side chain of Y83 α 2 and P(Q311), the carbonyl group of Y78 α 2 and the side chain of P(Q311), the side chain of H81 α 2 and the carbonyl group of P(K307), and between the side chains of Y50V β and P(N312), and two SBs: side chain groups of E56V β and P(K310), side chain groups of E71 α 1 and P(K315).

For p3MHCII-TCR complex eight HBs are formed between the MHCII-TCR and the peptide, eight HBs: side chain group of R71 α 2 and the carbonyl group of P(L314), side chain group of K75 α 1 and the carbonyl group of P(T318), side chain group of R76 α 1 and the carbonyl group of P(L316), side

chain group of N82 α 2 and the carbonyl group of P(V309), side chain of Y78 α 2 and the carbonyl group of P(K310), the carbonyl group of G97V β and the side chain of P(T318), the side chain of H81 α 2 and the carbonyl group of P(K307), the side chain of Y50V β and the carbonyl group of P(K315), and two SBs: side chain groups of E56V β and P(N312), side chain groups of E71 α 1 and P(K315).

For p4MHCII-TCR complex eight HBs are formed between the MHCII-TCR and the peptide, eight HBs: side chain group of R71 α 2 and the carbonyl group of P(L314), side chain group of K75 α 1 and the carbonyl group of P(T318), side chain group of R76 α 1 and the carbonyl group of P(L316), side chain of Y83 α 2 and P(Q311), side chain group of N82 α 2 and the carbonyl group of P(V309), the carbonyl group of Y50V β and the side chain of P(K315), the carbonyl group of H81 α 2 and the side chain P(Y308), the side chain of Y50V β and the carbonyl group of P(K315), and side chain groups of N62 α 1 and P(Q311).

For p5MHCII-TCR complex eight HBs are formed between the MHCII-TCR and the peptide, eight HBs: side chain group of R71 α 2 and the carbonyl group of P(L314), side chain group of K75 α 1 and the carbonyl group of P(T318), the carbonyl group of K75 α 1 and the side chain of P(T318), side chain group of R76 α 1 and the carbonyl group of P(L316), side chains of Y83 α 2 and P(Q311), side chain groups of E55 α 1 and P(Y308), side chain groups of N82 α 2 and the carbonyl group of P(Q311), the carbonyl group of Y78 α 2 and the side chain of P(Q311), and two SB: side chains of N69 α 1 and P(K315), side chain groups of E56V β and P(K307).

For p6MHCII-TCR complex five HBs are formed between the MHCII-TCR and the peptide, HBs: side chain group of R71 α 2 and the carbonyl group of P(L314), side chain group of K75 α 1 and the carbonyl group of P(T318), the carbonyl group of A68 α 1 and the side chain of P(K315), the carbonyl group of H81 α 2 and the side chain P(Y308), side chain group of R76 α 1 and the carbonyl

group of P(L316), and two SB: side chains of N69 α 1 and P(K315), side chain groups of E56V β and P(K307).

For p7MHCII-TCR complex eight HBs are formed between the MHCII-TCR and the peptide, eight HBs: side chain group of R71 α 2 and the carbonyl group of P(T313), side chain group of R71 α 2 and the carbonyl group of P(L314), side chain group of K75 α 1 and the carbonyl group of P(Q311), side chain group of K75 α 1 and the carbonyl group of P(T318), side chain of H81 α 2 and the carbonyl group of P(K307), side chain group of R76 α 1 and the carbonyl group of P(L316), two HBs between side chains of Y83 α 2 and P(Q311), side chain group of N82 α 2 and the carbonyl group of P(V309), side chain of Y78 α 2 and the carbonyl group of P(A312), and one SB: side chains of E71 α 1 and P(K315).

For p8MHCII-TCR complex five HBs are formed between the MHCII-TCR and the peptide, HBs: side chain group of R71 α 2 and the carbonyl group of P(L314), side chain group of K75 α 1 and the carbonyl group of P(T318), side chain group of R76 α 1 and the carbonyl group of P(L316), the carbonyl group of H81 α 2 and the side chain of P(Y308), side chain groups of N82 α 2 and the carbonyl group of P(V309), and one SB: side chain groups of E56V β and P(Q311).

For p9MHCII-TCR complex eight HBs are formed between the MHCII-TCR and the peptide, eight HBs: side chain group of R71 α 2 and the carbonyl group of P(L314), the carbonyl group of K75 α 1 and the side chain of P(T318), side chain group of R76 α 1 and the carbonyl group of P(L316), side chains of Y83 α 2 and P(Q311), side chain groups of E55 α 1 and P(Y308), side chain groups of N62 α 1 and P(Q311), the carbonyl group of V75 α 2 and the side chain of P(T313), side chain groups of N82 α 2 and the carbonyl group of P(V309), the carbonyl group of F13 α 2 and the side chain of P(Q311), and one SB: side chains of N69 α 1 and P(K315).

For p10MHCII-TCR complex eight HBs are formed between the MHCII-TCR and the peptide, eight HBs: the carbonyl group of R71 α 2 and the side group of P(T313), side chain group of R71 α 2 and the carbonyl group of P(L314), side chain group of R76 α 1 and the carbonyl group of P(A317), side chain group of K75 α 1 and the carbonyl group of P(T318), side chain groups of N62 α 1 and P(Q311), side chain group of R76 α 1 and the carbonyl group of P(L316), side chain of H81 α 2 and the carbonyl group of P(K307), side chain group of N82 α 2 and the carbonyl group of P(V309), side chain of Y83 α 2 and P(Q311), side chain group of Y50V β and the carbonyl group of P(A315), and one SB: side chains of E56V β and P(K310).

For p11MHCII-TCR complex eight HBs are formed between the MHCII-TCR and the peptide, eight HBs: the side chain groups of E71 α 1 and P(T318), side chain group of R71 α 2 and the carbonyl group of P(L314), side chain group of K75 α 1 and the carbonyl group of P(T318), carbonyl group of Y78 α 2 and the side chain group of P(Q311), side chain group of N82 α 2 and the carbonyl group of P(V309), side chain of E55 α 1 and P(Y308), side chain group of Y50V β and the carbonyl group of P(K315), side chains of E56V β and P(N312).

For p12MHCII-TCR complex eight HBs are formed between the MHCII-TCR and the peptide, eight HBs: side chain group of R71 α 2 and the carbonyl group of P(L314), side chain group of K75 α 1 and the carbonyl group of P(T318), side chain group of R76 α 1 and the carbonyl group of P(L316), the carbonyl group of F13 α 2 and the side chain of P(Q311), side chains of N69 α 1 and P(K315), side chain group of N82 α 2 and the carbonyl group of P(Q311), side chain group of N82 α 2 and the carbonyl group of P(V309), side chain of Y83 α 2 and P(Q311), carbonyl group of H81 α 2 and the side chain group of P(Y308), side chain group of H81 α 2 and the carbonyl group of P(K307), and one SB: side chains of E56V β and P(K310).

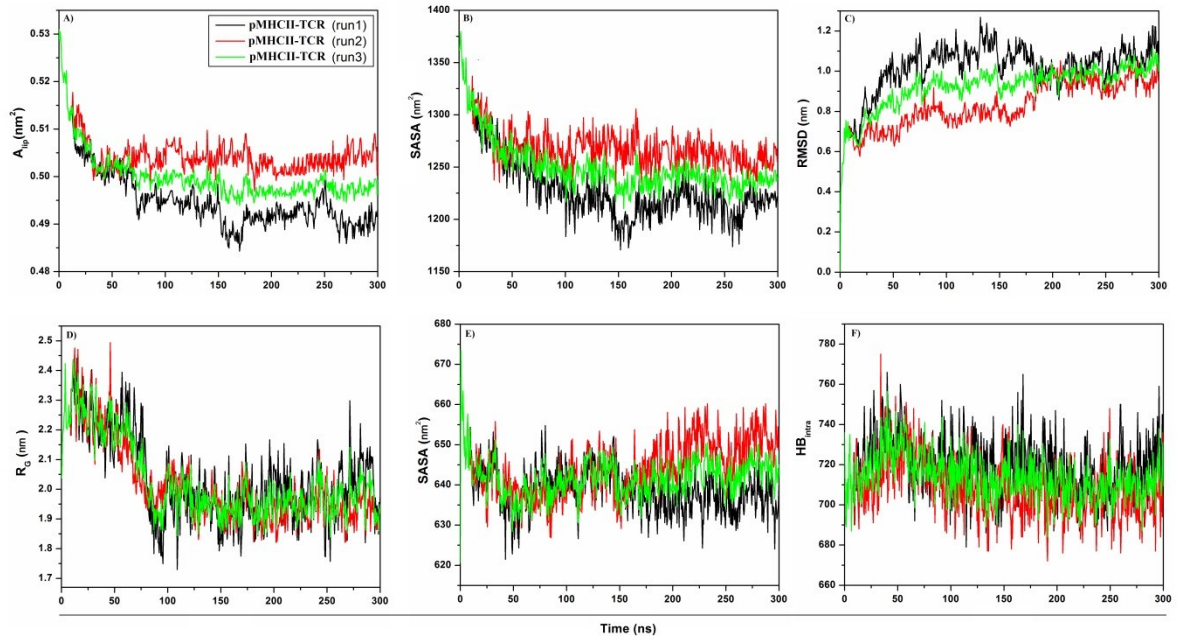


Fig. S1

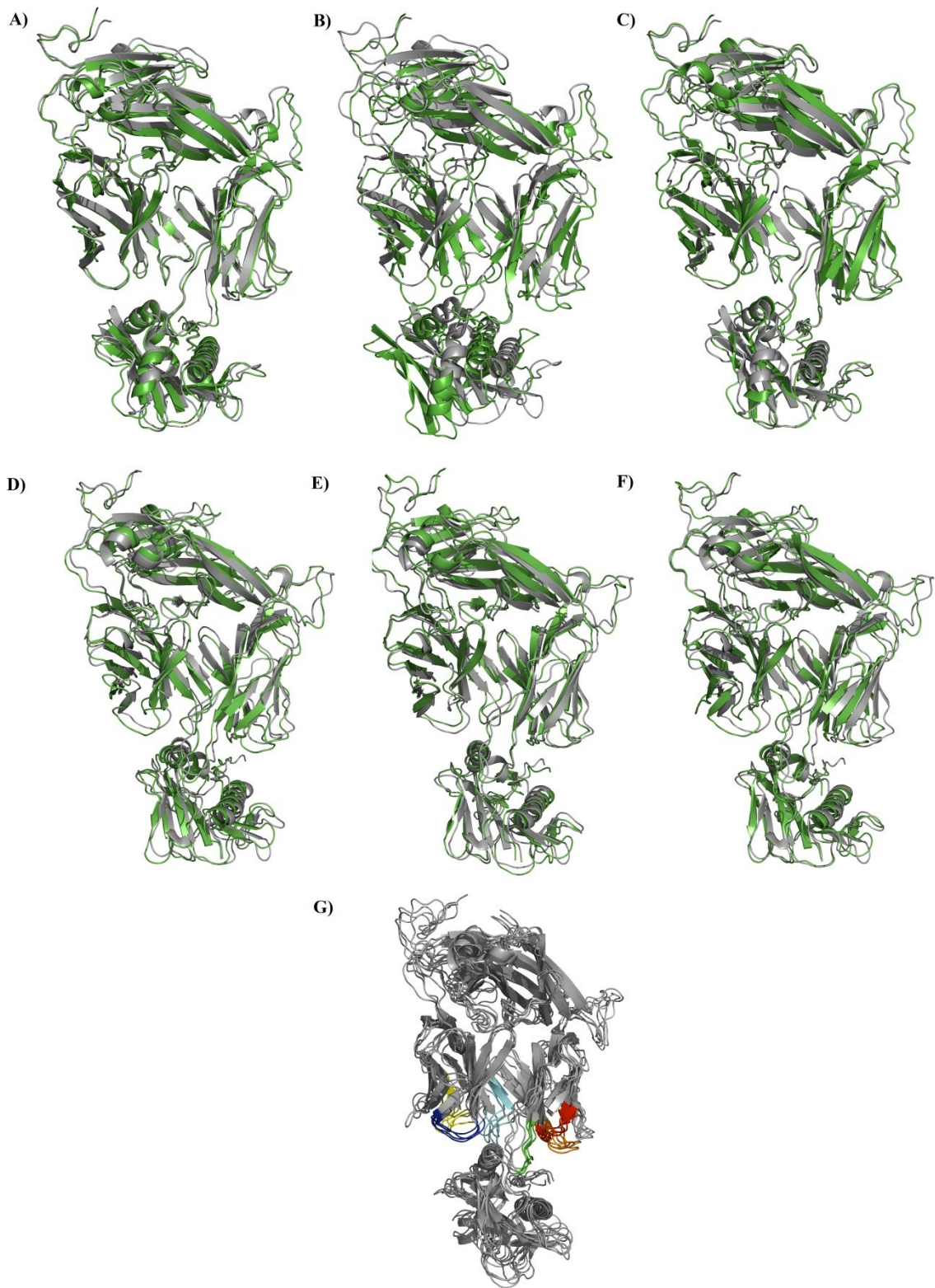


Fig. S2