

A

Amino acid in peptide	PITCR contacts with CD3 ζ	PITCR interaction distance	PITCRG41P contacts with CD3 ζ	PITCRG41P interaction distance
Asp1	ZA Tyr33*	3.37Å	none	-
Ser5	ZB Cys32*	3.60Å	none	-
Tyr6	ZB Asp28** ZB Leu26**	3.37Å 2.67Å	none	-
Tyr15	ZA Thr47*	2.76Å	ZA Thr47* ZB Tyr42*	2.61Å 2.79Å
Thr20	ZB Tyr42*	2.89Å	none	-
Glu30	ZB Arg57*	2.67Å	ZB Ser56*	2.72Å

*Interaction with sidechain atoms in TCR

**Interaction with backbone atoms in TCR

B

Model 1		Model 2	Maximum displacement of Zeta A α -carbon	Maximum displacement of Zeta B α -carbon	RMSD for Zeta A + Zeta B + TCR α
TCR	vs	TCR + PITCR	6.01Å	8.20Å	1.876Å
TCR	vs	TCR + PITCRG41P	3.72Å	3.62Å	1.179Å
TCR	vs	TCR + TYPE7	4.25Å	3.97Å	1.044Å
TCR	vs	TCR + pHLIP	2.49Å	1.86Å	0.438Å