

**Supplementary Table 1** Data collection and refinement statistics

	pCPA12/ H-2L <sup>d</sup> -42F3	pCPB7/ H-2L <sup>d</sup> -42F3	pCPB9/ H-2L <sup>d</sup> -42F3	pCPC5/ H-2L <sup>d</sup> -42F3	pCPE3/ H-2L <sup>d</sup> -42F3
<b>Data collection</b>					
Space group	<i>P</i> 6 <sub>1</sub> 22	<i>C</i> 2	<i>C</i> 2	<i>P</i> 6 <sub>1</sub> 22	<i>P</i> 3 <sub>1</sub> 21 (twinned)
Cell dimensions					
<i>a</i> , <i>b</i> , <i>c</i> (Å)	101.6, 101.6, 327.1	172.8, 60.4, 69.7	175.3, 60.6, 70.1	102.7, 102.7, 322.9	102.5, 102.5, 325.7
$\alpha$ , $\beta$ , $\gamma$ (°)	90, 90, 120	90, 98, 90	90, 96, 90	90, 90, 120	90, 90, 120
Resolution (Å)	59.90-3.06 (3.169-3.06)	34.49-3.09 (3.2-3.09)	34.85-1.92 (2.0-1.92)	43.33-2.60 (2.69-2.60)	59.99-2.90 (3.00-2.90)
<i>R</i> <sub>meas</sub> (%)	5.7 (22.2)	8.4 (32.2)	4.4 (24.5)	8.8 (51.9)	6.7 (53.1)
<i>I</i> / $\sigma$ <i>I</i>	12.0 (4.1)	7.3 (1.7)	8.2 (3.6)	7.9 (2.2)	6.5 (2.5)
Completeness (%)	98.9 (99.9)	90.0 (70.0)	94.4 (95.5)	96.7 (98.3)	99.6 (99.3)
Total reflections	140668 (20823)	66431 (6703)	134780 (19908)	166944 (24563)	310774 (29484)
Unique reflections	19619 (2793)	11969 (1283)	53037 (7753)	31125 (4521)	44993 (4385)
Redundancy	7.2 (7.5)	5.2 (5.2)	2.6 (2.6)	5.4 (5.4)	6.9 (6.7)
<b>Refinement</b>					
Resolution (Å)	59.90-3.06 (3.22-3.06)	34.49-3.09 (3.4-3.09)	34.85-1.92 (1.957-1.92)	43.34-2.60 (2.680-2.60)	42.81-2.90 (2.95-2.90)
<i>R</i> <sub>work</sub> / <i>R</i> <sub>free</sub>	0.194/ 0.227	0.231/ 0.279	0.180/ 0.219	0.211/ 0.240	0.196/ 0.247
No. atoms					
Protein	4947	4933	4835	4952	9790
Water	0	0	445	37	0
B-factors					
Protein	66.0	113.4	45.2	86.1	51.8
Water			47.3	63.4	
R.m.s deviations					
Bond lengths (Å)	0.005	0.002	0.016	0.003	0.006
Bond angles (°)	0.87	0.63	1.58	0.77	0.96
Ramachandran favored (%)	96	96	97	97	95
Ramachandran outliers (%)	0	0.16	0.17	0	0
PDB accession code	4N5E	4MVB	4MS8	4MXQ	4N0C

\*Highest resolution shell is shown in parenthesis.

**Supplementary Table 2.** TCR-pMHC Nomenclature

PBD	Peptide Clone	Peptide	Source*	TCR	MHC
3TF7	QL9	QLSPFPFDL	Mouse	42F3	H-2L <sup>d</sup>
3TFK	p4B10	QLSDVPMDL	Yeast Library 4	42F3	H-2L <sup>d</sup>
3TPU	p5E8	FLSPFWFDI	Yeast Library 5	42F3	H-2L <sup>d</sup>
4N5E	pCPA12	VPYMAEFGM	Yeast Library CP	42F3	H-2L <sup>d</sup>
4MXQ	pCPC5	SPAPRPLDL	Yeast Library CP	42F3	H-2L <sup>d</sup>
4N0C	pCPE3	MPAGRPWDL	Yeast Library CP	42F3	H-2L <sup>d</sup>
4MVB	pCPB7	WPAEGGFQL	Yeast Library CP	42F3	H-2L <sup>d</sup>
4MS8	pCPB9	SPAEAGFFL	Yeast Library CP	42F3	H-2L <sup>d</sup>
3TJH	p3A1	SPLDSLWWI	Yeast Library 3	42F3	H-2L <sup>d</sup>
2O19	QL9	QLSPFPFDL	Mouse	2C	H-2L <sup>d</sup>
3E3Q	QL9	QLSPFPFDL	Mouse	2C-m13	H-2L <sup>d</sup>
3E2H	QL9	QLSPFPFDL	Mouse	2C-m67	H-2L <sup>d</sup>
2E7L	QL9	QLSPFPFDL	Mouse	2C-m6	H-2L <sup>d</sup>
-	MCMV	YPHFMPDNL	Virus	-	H-2L <sup>d</sup>

\* Yeast Libraries 3-5 were previously described (Adams et al Immunity 2011)