

Supplementary Material for 'Quantifying conformational changes in the TCR:pMHC-I binding interface'

1 CORRELATION BETWEEN CONFORMATIONAL CHANGE AND AFFINITY

We were interested in whether there was a correlation between the amount of conformational change in the binding interface of T cell antigen receptor (TCR):class I peptide-MHCs (pMHC-Is) between *apo* and *holo* states and the affinity of the interaction. We combined the results of our analysis of crystal structures with affinity measures available in the ATLAS dataset Borrman et al. (2017). Shown in Fig. S9 and Fig. S10, we plotted the changes in conformation, measured as root mean squared deviation (RMSD), versus the affinity values, measured as the equilibrium dissociation (K_d), and measured the correlation. Only the CDR2 α , CDR3 α , and CDR3 β loops showed a small correlation to affinity ($R^2 > 0.00$). The other loops show very little to no correlation. On the pMHC-I side, neither the movement in peptide, major histocompatability complex (MHC) TCR contacting regions, nor the rest of the MHC antigen binding domain showed any correlation to affinity. This analysis suggests that although there are slight correlations between conformational change and affinity, the trends are subtle and one is not indicative of the other.

2 CORRELATION OF CDR LOOP AND PEPTIDE LENGTHS TO CONFORMATIONAL CHANGE

Probing the underlying causes of conformational change in the complementarity determining region (CDR) loops and peptides, we investigated the role length plays in allowing for conformational change. Shown in Fig. S11A, bulk CDR movements are weakly correlated to RMSD changes between *apo* and *holo* states ($R^2 = 0.11$). However, Fig. S11B shows a stronger correlation to the deformation effect of loops ($R^2 = 0.35$). The increased correlation makes sense since other parts of the protein can drive the conformational changes from the framework regions, but when the loops are aligned together, the only differences can be driven by changes in the loops themselves, implying the loop length has more of an effect. Looking at the correlation ($R^2 = 0.17$). From these results, it seems both loop and peptide lengths have some impact on the inherent flexibility of these entities, but other factors also likely modulate the flexibility such as amino acid composition and interactions with other domains Milighetti et al. (2024).

3 SUPPLEMENTARY TABLES AND FIGURES

Table S1: Breakdown of the data used in the analysis of *apo* and *holo* forms of TCR and pMHC structures. In total, 391 structures are coming from 301 PDB entries.

PDB ID	Structure Type	α-chain ID	β-chain ID	Antigen Chain II	MHC Chain ID
1b0g	pMHC-I	-	-	С	А
1b0g	pMHC-I	-	-	F	D
1bii	pMHC-I	-	-	Р	А
				Cor	tinued on next page

PDB ID	Structure Type	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
1ddh	pMHC-I	-	-	Р	А
1duz	pMHC-I	-	-	С	А
1duz	pMHC-I	-	-	F	D
1e28	pMHC-I	-	-	С	А
1ffn	pMHC-I	-	-	С	А
1ffn	pMHC-I	-	-	F	D
1fzj	pMHC-I	-	-	Р	А
1fzm	pMHC-I	-	-	Р	А
1hhi	pMHC-I	-	-	С	А
1hhi	pMHC-I	-	-	F	D
1hhk	pMHC-I	-	-	С	А
1hhk	pMHC-I	-	-	F	D
1hoc	pMHC-I	-	-	С	А
1i4f	pMHC-I	-	-	С	А
1jf1	pMHC-I	-	-	С	А
1jht	pMHC-I	-	-	С	А
1kj3	pMHC-I	-	-	Р	Н
1kj3	pMHC-I	-	-	Q	Ι
1kpu	pMHC-I	-	-	Р	А
1leg	pMHC-I	-	-	Р	А
11ek	pMHC-I	-	-	Р	А
1m05	pMHC-I	-	-	Е	А
1m05	pMHC-I	-	-	F	С
1n5a	pMHC-I	-	-	С	А
1n5a	pMHC-I	-	-	F	D
1n5a	pMHC-I	-	-	Ι	G
1n5a	pMHC-I	-	-	L	J
1nan	pMHC-I	-	-	М	Н
1s7u	pMHC-I	-	-	С	А
1s7u	pMHC-I	-	-	F	D
1s7u	pMHC-I	-	-	Ι	G
1s7u	pMHC-I	-	-	L	J
1s9w	pMHC-I	-	-	С	А
1t1w	pMHC-I	-	-	С	А
1t20	pMHC-I	-	-	С	А
1t21	pMHC-I	-	-	С	А
1t22	pMHC-I	-	-	С	А
1wby	pMHC-I	-	-	С	А
1yn6	pMHC-I	-	-	С	А
1zhk	pMHC-I	-	-	С	А
1zhl	pMHC-I	-	-	С	А
2av1	pMHC-I	-	-	С	А
2av1	pMHC-I	-	-	F	D
2av7	pMHC-I	-	-	С	А
2av7	pMHC-I	-	-	F	D
2bss	pMHC-I	-	-	С	А
2c7u	pMHC-I	-	-	С	А
2c7u	pMHC-I	-	-	F	D
				Cont	nued on next page

Table S1: Breakdown of the data used in the analysis of apo and holo forms of TCR and pMHC structures.

PDB ID	Structure Type	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
2clv	pMHC-I	-	-	С	А
2clv	pMHC-I	-	-	М	Н
2clz	pMHC-I	-	-	С	А
2clz	pMHC-I	-	-	М	Н
2f74	pMHC-I	-	-	С	А
2f74	pMHC-I	-	-	F	D
2gt9	pMHC-I	-	-	С	А
2gt9	pMHC-I	-	-	F	D
2gtz	pMHC-I	-	-	С	А
2gtz	pMHC-I	-	-	F	D
2guo	pMHC-I	-	-	С	А
2guo	pMHC-I	-	-	F	D
2mha	pMHC-I	-	-	Е	А
2mha	pMHC-I	-	-	F	С
2v2w	pMHC-I	-	-	С	А
2v2w	pMHC-I	-	-	F	D
2vaa	pMHC-I	-	-	Р	А
2vll	pMHC-I	-	-	C	A
2vll	pMHC-I	-	-	F	D
2x4r	pMHC-I	-	-	C	A
2x4r	pMHC-I	_	_	F	D
3dx8	pMHC-I			r C	Δ
3ech	pMHC-I	_	_	P	Δ
3000	pMHC-I	_	_	P	Δ
3h7h	pMHC I	-	-	ſ	A A
3h7b	pMHC I	-	-	E	A D
31170 2h0h	pMHC-I	-	-	r C	
3h0h	pMHC I	-	-	E	A D
2hni	pMHC-I	-	-	r C	
2hni	pMHC-I	-	-	E	A
3npj 2:	pMHC-I	-	-	F	D
2i	PMHC-I	-	-	E	A
31xa	pMHC-I	-	-	F	D
экрр	рмнс-і	-	-	C	A
3kpq	pMHC-I	-	-	C	A
3kww	pMHC-I	-	-	C	A
3mre	pMHC-I	-	-	P	A
3mrm	pMHC-I	-	-	P	A
3nfn	pMHC-I	-	-	С	A
3pwl	pMHC-I	-	-	C	А
3pwl	pMHC-I	-	-	F	D
3qfd	pMHC-I	-	-	C	А
3qfd	pMHC-I	-	-	F	D
3quk	pMHC-I	-	-	С	А
3quk	pMHC-I	-	-	F	D
3sko	pMHC-I	-	-	С	А
3tbs	pMHC-I	-	-	С	А
3tbs	pMHC-I	-	-	F	D
3tby	pMHC-I	-	-	С	Α
				Contir	ued on next page

PDB ID	Structure Type	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
3tby	pMHC-I	-	-	F	D
3tby	pMHC-I	-	-	Ι	G
3tby	pMHC-I	-	-	L	J
3utq	pMHC-I	-	-	С	А
3vfm	pMHC-I	-	-	С	А
3vfn	pMHC-I	-	-	С	А
3vfo	pMHC-I	-	-	С	А
3vfp	pMHC-I	-	-	С	А
3vxn	pMHC-I	-	-	С	А
3vxo	pMHC-I	-	-	С	А
3vxo	pMHC-I	-	-	F	D
3vxp	pMHC-I	-	-	С	А
3vxp	pMHC-I	-	-	F	D
3x13	pMHC-I	-	-	С	А
4g8i	pMHC-I	-	-	С	А
4g9d	pMHC-I	-	-	С	А
4hux	pMHC-I	-	-	С	А
4jfp	pMHC-I	-	-	С	А
4jfp	pMHC-I	-	-	F	D
4nsk	pMHC-I	-	-	С	А
4pr5	pMHC-I	-	_	С	А
4pra	pMHC-I	-	_	С	А
4ara	pMHC-I	-	_	С	А
4uli	pMHC-I	-	-	С	А
4u1j	pMHC-I	-	_	С	А
4wu5	pMHC-I	-	-	С	А
4wu5	pMHC-I	-	-	F	D
4wu7	pMHC-I	-	-	С	А
4wu7	pMHC-I	-	-	F	D
5c0d	pMHC-I	-	-	С	А
5c0e	pMHC-I	-	-	С	А
5c0f	pMHC-I	-	-	С	А
5c0g	pMHC-I	-	-	С	А
5c0i	pMHC-I	-	_	С	А
5c0j	pMHC-I	-	_	С	А
5hga	pMHC-I	-	-	С	А
5hga	pMHC-I	-	-	F	D
5hgb	pMHC-I	-	-	С	А
5hgb	pMHC-I	-	-	F	D
5hgb	pMHC-I	-	-	Ι	G
5hgb	pMHC-I	-	-	L	J
5hgd	pMHC-I	-	-	С	А
5hgd	pMHC-I	-	-	F	D
5hgh	pMHC-I	-	-	С	А
5hhn	pMHC-I	-	-	С	А
5hhp	pMHC-I	-	-	С	А
5n1y	pMHC-I	-	-	С	А
5nmh	pMHC-I	-	-	С	A
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PDB ID	Structure Type	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
5nmk	pMHC-I	-	-	С	А
5wjl	pMHC-I	-	-	С	А
5wjl	pMHC-I	-	-	F	D
5wjl	pMHC-I	-	-	Ι	G
5wjn	pMHC-I	-	-	С	А
5wjn	pMHC-I	-	-	F	D
5wjn	pMHC-I	-	-	Ι	G
5wli	pMHC-I	-	-	С	А
5wli	pMHC-I	-	-	F	D
5wli	pMHC-I	-	-	Ι	G
5wli	pMHC-I	-	-	L	J
5wmo	pMHC-I	-	-	С	А
5xos	pMHC-I	-	-	С	А
6amt	pMHC-I	-	-	С	А
6amt	pMHC-I	-	-	F	D
6at5	pMHC-I	-	-	С	А
6g9r	pMHC-I	-	-	I	С
6g9r	pMHC-I	-	-	J	E
6g9r	pMHC-I	-	-	K	G
6g9r	pMHC-I	-	-	Р	A
6øh1	pMHC-I	-	_	P	A
6gh1	pMHC-I	-	_	0	C
6gh1	pMHC-I	-	_	R	E
6gh1	pMHC-I	-	_	Z	G
6itn	pMHC-I	_	_	C C	A
6mt6	pMHC-I	_	_	B	A
6npr	pMHC-I	_	_	P	C C
6npr	pMHC-I	_	_	R	A
6a3k	pMHC-I	-	_	P	A
6ulk	pMHC-I		_	r C	Δ
6vr5	pMHC-I		_	P	Δ
6vr5	pMHC-I		_	0	D
7mkh	pMHC-I		_	Q C	Δ
7n1a	pMHC I	-	-	C C	A .
7n1a 7n1a	pMHC I	-	-	E	D
7n1b	pMHC-I			ſ	Δ
7n1b	pMHC I	-	-	E	A D
7n5a	pMHC-I			ſ	Δ
7n5q	pMHC I	-	-	U U	F
7n5q 7n6d	pMHC I	-	-	II C	1. A
7110u 7n6d	pMHC-I	-	-	C	A E
7110u 7n6d	pMIC-I	-	-	U V	L
7110u 7n6d	pMHC I	-	-	N O	1 M
71100 7n0:	pMHC I	-	-	C	1/1
/119] 7nm ¹	pMIC I	-	-	C	A .
/nmd	pMHC-I	-	-	C E	A
/nmd	рмнС-і «МИС І	-	-	Г	
70W3	рмнс-і	-	-		A
/ow3	рмнС-і	-	-	F	D
				Contir	nued on next page

PDB ID	Structure Type	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
7ow3	pMHC-I	-	-	L	J
7ow4	pMHC-I	-	-	С	А
7ow4	pMHC-I	-	-	F	D
7ow4	pMHC-I	-	-	Ι	G
7p0a	pMHC-I	-	-	С	А
7p0a	pMHC-I	-	-	F	D
7p0t	pMHC-I	-	-	С	А
7p0t	pMHC-I	-	-	F	D
7p3d	pMHC-I	-	-	С	А
7r7v	pMHC-I	-	-	С	А
7rtd	pMHC-I	-	-	С	А
1kgc	TCR	D	Е	-	-
1tcr	TCR	А	В	-	-
2bnu	TCR	А	В	-	-
2pyf	TCR	А	В	-	-
2vlm	TCR	D	Е	-	-
3dx9	TCR	A	B	-	-
3dx9	TCR	C	D	-	-
3geu	TCR	A	B	-	-
3geu	TCR	D	E	-	-
3ah3	TCR	A	B	_	-
3skn	TCR	A	B	_	-
3skn	TCR	C	D	_	-
3skn	TCR	E	F	_	-
3skn	TCR	G	н	_	
3utn	TCR	D	F	_	
3utn	TCR	K	I	_	
3vxa	TCR	Δ	B	_	
3779	TCR	D	F	_	
3vvt	TCR	Δ	B	_	_
3vxt	TCR	C C	D	-	-
JvAt Aifh	TCR	D D	D F	-	-
4jiii Aarn	TCR	р к	L	-	-
4qrp 5;1	TCR	к л	D	-	-
5im1	TCR	A	D	-	-
5im1	TCR	E	D	-	-
51W1	TCR		Г D	-	-
5mmd	TCR	A	D	-	-
	TCR		D	-	-
Gaio	TCR	A	Б	-	-
orp9 Guth		<u>к</u>	L	-	-
ovin Guitte		A	Б	-	-
ovin	TCD		E	-	-
/amp 7=1	TCD	A	в	-	-
/nic	TCR	D	E	-	-
/nld	ICK	A	В	-	-
/r/z	ICK	A	В	-	-
Tao7	TCR:pMHC-I	D	E	C	A
1bd2	TCR:pMHC-I	D	Е	C	А
				Contin	nued on next page

1fo0TCR:pMHC-IABPH1g6rTCR:pMHC-IABPH1kj2TCR:pMHC-IABPH1lp9TCR:pMHC-IEFCA1mi5TCR:pMHC-IDECA1mwaTCR:pMHC-IABPH1namTCR:pMHC-IABPH1ogaTCR:pMHC-IDECA1qrnTCR:pMHC-IDECA1qsfTCR:pMHC-IDECA2ak4TCR:pMHC-IDECA2bnqTCR:pMHC-IDECA	PDB ID	Structure Type	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
lg6rTCR:pMHC-IABPHlkj2TCR:pMHC-IABPHllp9TCR:pMHC-IEFCAlmi5TCR:pMHC-IDECAlmwaTCR:pMHC-IABPHlnamTCR:pMHC-IABPHlogaTCR:pMHC-IDECAlqrnTCR:pMHC-IDECAlqsfTCR:pMHC-IDECAlqsfTCR:pMHC-IDECAlqsfTCR:pMHC-IDECAlbnqTCR:pMHC-IDECAlbnqTCR:pMHC-IDECAlbnqTCR:pMHC-IDECA	1fo0	TCR:pMHC-I	А	В	Р	Н
1kj2TCR:pMHC-IABPH1lp9TCR:pMHC-IEFCA1mi5TCR:pMHC-IDECA1mwaTCR:pMHC-IABPH1namTCR:pMHC-IABPH1ogaTCR:pMHC-IDECA1qrnTCR:pMHC-IDECA1qseTCR:pMHC-IDECA1qsfTCR:pMHC-IDECA2ak4TCR:pMHC-IDECA2bnqTCR:pMHC-IDECA	1g6r	TCR:pMHC-I	А	В	Р	Н
1lp9TCR:pMHC-IEFCA1mi5TCR:pMHC-IDECA1mwaTCR:pMHC-IABPH1namTCR:pMHC-IABPHlogaTCR:pMHC-IDECAlqrnTCR:pMHC-IDECAlqsfTCR:pMHC-IDECAlqsfTCR:pMHC-IDECA2ak4TCR:pMHC-IDECA2bnqTCR:pMHC-IDECA	1kj2	TCR:pMHC-I	А	В	Р	Н
1mi5TCR:pMHC-IDECA1mwaTCR:pMHC-IABPH1namTCR:pMHC-IABPHlogaTCR:pMHC-IDECA1qrnTCR:pMHC-IDECA1qséTCR:pMHC-IDECA1qsfTCR:pMHC-IDECA2ak4TCR:pMHC-IDECA2bnqTCR:pMHC-IDECA	11p9	TCR:pMHC-I	Е	F	С	А
ImwaTCR:pMHC-IABPHInamTCR:pMHC-IABPHIogaTCR:pMHC-IDECAIqrnTCR:pMHC-IDECAIqseTCR:pMHC-IDECAIqsfTCR:pMHC-IDECA2ak4TCR:pMHC-IDECA2bnqTCR:pMHC-IDECA2bnrTCR:pMHC-IDECA	1mi5	TCR:pMHC-I	D	E	С	А
InamTCR:pMHC-IABPHlogaTCR:pMHC-IDECAlqrnTCR:pMHC-IDECAlqseTCR:pMHC-IDECAlqsfTCR:pMHC-IDECAlqsfTCR:pMHC-IDECA2ak4TCR:pMHC-IDECA2bnqTCR:pMHC-IDECA2bnrTCR:pMHC-IDECA	1mwa	TCR:pMHC-I	А	В	Р	Н
logaTCR:pMHC-IDECAlqrnTCR:pMHC-IDECAlqseTCR:pMHC-IDECAlqsfTCR:pMHC-IDECA2ak4TCR:pMHC-IDECA2bnqTCR:pMHC-IDECA2bnrTCR:pMHC-IDECA	1nam	TCR:pMHC-I	А	В	Р	Н
1qrnTCR:pMHC-IDECA1qseTCR:pMHC-IDECA1qsfTCR:pMHC-IDECA2ak4TCR:pMHC-IDECA2bnqTCR:pMHC-IDECA2bnrTCR:pMHC-IDECA	1oga	TCR:pMHC-I	D	Е	С	А
1qseTCR:pMHC-IDECA1qsfTCR:pMHC-IDECA2ak4TCR:pMHC-IDECA2bnqTCR:pMHC-IDECA2bnrTCR:pMHC-IDECA	1qrn	TCR:pMHC-I	D	Е	С	А
1qsfTCR:pMHC-IDECA2ak4TCR:pMHC-IDECA2bnqTCR:pMHC-IDECA2bnrTCR:pMHC-IDECA	1qse	TCR:pMHC-I	D	E	С	А
2ak4TCR:pMHC-IDECA2bnqTCR:pMHC-IDECA2bnrTCR:pMHC-IDECA	1qsf	TCR:pMHC-I	D	Е	С	А
2bnqTCR:pMHC-IDECA2bnrTCR:pMHC-IDECA	2ak4	TCR:pMHC-I	D	Е	С	А
2bnr TCR:pMHC-I D E C A	2bnq	TCR:pMHC-I	D	Е	С	А
1	2bnr	TCR:pMHC-I	D	E	С	А
2ckb TCR:pMHC-I A B P H	2ckb	TCR:pMHC-I	А	В	Р	Н
2f53 TCR:pMHC-I D E C A	2f53	TCR:pMHC-I	D	Е	С	А
2f54 TCR:pMHC-I D E C A	2f54	TCR:pMHC-I	D	Е	С	А
2j8u TCR:pMHC-I E F C A	2j8u	TCR:pMHC-I	Е	F	С	А
2jcc TCR:pMHC-I E F C A	2jcc	TCR:pMHC-I	Е	F	С	А
2013 TCR:pMHC-I A B P H	2013	TCR:pMHC-I	А	В	Р	Н
2p5e TCR:pMHC-I D E C A	2p5e	TCR:pMHC-I	D	Е	С	А
2p5w TCR:pMHC-I D E C A	2p5w	TCR:pMHC-I	D	Е	С	А
2pve TCR:pMHC-I D E C A	2pye	TCR:pMHC-I	D	Е	С	А
2uwe TCR:pMHC-I E F C A	2uwe	TCR:pMHC-I	Е	F	С	А
2vlj TCR:pMHC-I D E C A	2vlj	TCR:pMHC-I	D	Е	С	А
2vlk TCR:pMHC-I D E C A	2vlk	TCR:pMHC-I	D	Е	С	А
2vlr TCR:pMHC-I D E C A	2vlr	TCR:pMHC-I	D	Е	С	А
3d39 TCR:pMHC-I D E C A	3d39	TCR:pMHC-I	D	Е	С	А
3d3v TCR:pMHC-I D E C A	3d3v	TCR:pMHC-I	D	Е	С	А
3dxa TCR:pMHC-I D E C A	3dxa	TCR:pMHC-I	D	Е	С	А
3ffc TCR:pMHC-I D E C A	3ffc	TCR:pMHC-I	D	Е	С	А
3gsn TCR:pMHC-I A B P H	3gsn	TCR:pMHC-I	А	В	Р	Н
3h9s TCR:pMHC-I D E C A	3h9s	TCR:pMHC-I	D	Е	С	А
3hg1 TCR:pMHC-I D E C A	3hg1	TCR:pMHC-I	D	Е	С	А
3kpr TCR:pMHC-I D E C A	3kpr	TCR:pMHC-I	D	Е	C	А
3kps TCR:pMHC-I D E C A	3kps	TCR:pMHC-I	D	Е	С	А
3kxf TCR:pMHC-I D E Q A	3kxf	TCR:pMHC-I	D	Е	0	А
3041 TCR:pMHC-I D E C A	3041	TCR:pMHC-I	D	Е	C	А
3pay TCR:pMHC-I D E C A	3pav	TCR:pMHC-I	D	Е	С	А
3pwp TCR:pMHC-I D E C A	3pwp	TCR:pMHC-I	D	Е	C	А
3adg TCR:pMHC-I D E C A	3adg	TCR:pMHC-I	D	Е	C	А
3adi TCR:pMHC-I D E C A	3adi	TCR:pMHC-I	D	Е	C	А
3qdm TCR:pMHC-I D E C A	3qdm	TCR:DMHC-I	D	Е	С	А
Jaeq TCR:pMHC-I D E C A	3aea	TCR:pMHC-I	D	Е	C	А
3qfj TCR:pMHC-I D E C A	3qfj	TCR:pMHC-I	D	Е	С	А
3sjv TCR:pMHC-I D E C A	3sjv	TCR:pMHC-I	D	Е	С	А
3uts TCR:pMHC-I D E C A	3uts	TCR:pMHC-I	D	Ē	C	A
3utt TCR:pMHC-I D E C A	3utt	TCR:pMHC-I	D	Е	C	А
Continued on payt page			-	_	Contir	uled on next page

PDB ID	Structure Type	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
3vxm	TCR:pMHC-I	D	Е	С	А
3vxr	TCR:pMHC-I	D	Е	С	А
3vxs	TCR:pMHC-I	D	Е	С	А
3vxu	TCR:pMHC-I	D	Е	С	А
3w0w	TCR:pMHC-I	D	Е	С	А
4eup	TCR:pMHC-I	G	Н	F	D
4ftv	TCR:pMHC-I	D	Е	С	А
4g8g	TCR:pMHC-I	D	Е	С	А
4g9f	TCR:pMHC-I	D	Е	С	А
4jfd	TCR:pMHC-I	D	Е	С	А
4jfe	TCR:pMHC-I	D	Е	С	А
4jff	TCR:pMHC-I	D	Е	С	А
4jrx	TCR:pMHC-I	D	Е	С	А
4jry	TCR:pMHC-I	D	Е	С	А
413e	TCR:pMHC-I	D	Е	С	А
4mii	TCR:pMHC-I	D	Е	С	А
4prh	TCR:pMHC-I	D	E	C	A
4pm	TCR:pMHC-I	D	Ē	C	A
4aok	TCR:pMHC-I	D	E	C	A
4arp	TCR:pMHC-I	D	Ē	C	A
5c07	TCR [.] pMHC-I	D	E	C	A
5c08	TCR:pMHC-I	D	E	C	A
5c09	TCR:pMHC-I	D	E	C	A
5c0a	TCR:pMHC-I	D	E	C	A
5c0b	TCR:pMHC-I	D	F	C	Δ
5c0c	TCR:pMHC-I	I	I	C	A
5d2n	TCR:pMHC-I	r C	, F	G	н
5e9d	TCR:pMHC-I	D	F	C	A
5euo	TCR:pMHC-I	F	F	I	A
5hhm	TCR:pMHC I	D	F	, ,	A A
5hho	TCR:pMHC I	D	E	C	A A
5hvi	TCR:pMHC I	D	E	C	A A
51ez	TCR:pMHC I	D	E	C	A A
5182	TCR:pMHC I	D E	E	D	A A
5ibd	TCR:pMHC I	E D	Г Г	F C	A
5jnu 5jai	TCR:pMHC I	D	E	C	A
5jzi 5m00	TCR:pMHC I	D G	L U	P	A
5m01	TCR:pMHC-I	G C	п	P	A
5 02	TCR:pMHC-I	G	н	P	A
5m02	TCR:pMHC-I	G	н	P	A
5nnt 5	TCR:pMHC-I	A	Б	P	H
5nme	TCR:pMHC-I	D	E	C C	A
SUMI	TCK:PMHC-I	ע	E		A
5nmg	TCK:pMHC-I	D	E		A
Snqk	TCK:pMHC-I	A	Б	r	н
5sws	TCR:pMHC-I	D	E	C	A
JSWZ	TCR:pMHC-I	D	E		A
501	TCK:pMHC-I	ы С	н	C I	A
Stje	TCR:pMHC-I	G	Н	1	A
				Conti	nued on next page

Table S1: Breakdown of the data used in the analysis of apo and holo forms of TCR and pMHC structures.

PDB ID	Structure Type	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
5wkf	TCR:pMHC-I	D	Е	С	А
5wkh	TCR:pMHC-I	D	Е	С	А
5wlg	TCR:pMHC-I	D	E	С	А
5xot	TCR:pMHC-I	D	E	С	А
5xov	TCR:pMHC-I	Ι	J	С	А
5yxn	TCR:pMHC-I	А	В	Ι	С
6am5	TCR:pMHC-I	D	Е	С	А
6amu	TCR:pMHC-I	D	Е	С	А
6avf	TCR:pMHC-I	А	В	Р	Н
6avg	TCR:pMHC-I	С	D	Р	G
6bj2	TCR:pMHC-I	D	Е	С	А
6bj3	TCR:pMHC-I	D	Н	С	А
6d78	TCR:pMHC-I	D	Е	С	А
6dkp	TCR:pMHC-I	D	Е	С	А
6eqa	TCR:pMHC-I	D	Е	С	А
6eab	TCR:pMHC-I	D	Е	С	А
6g9a	TCR:pMHC-I	G	Н	Р	А
6mtm	TCR:pMHC-I	D	E	C	A
6a3s	TCR:pMHC-I	D	E	C	A
6rp9	TCR:pMHC-I	D	E	C	A
6rsv	TCR:pMHC-I	D	E	C	A
6tmo	TCR:pMHC-I	D	E	C	A
6tro	TCR:pMHC-I	D	E	C	A
6110n	TCR:pMHC-I	G	н	F	D
6uz1	TCR:pMHC-I	D	F	ſ	Δ
6vmv	TCR:pMHC-I	D	E	C C	Δ
6vao	TCR:pMHC-I	D	F	P	Δ
6vrm	TCR:pMHC-I	D	E	P	Δ
6vrn	TCR:pMHC-I	D	E	P	Δ
67kw	TCR:pMHC I	D	E	ſ	A A
7dam	TCR:pMHC I	D F	D	C	A A
7dzn	TCR:pMHC I	E	D	C	A A
7uzii 7iwi	TCR:pMHC I	D	D F	C	A A
7jwi 7jwi	TCR:pMHC I	D	E E	C	A
7jwj 7n1o	TCR.pMHC I	D	E	C	A
7n1f	TCR.pMHC I	D	E	C	A
/1111 7 n 5a	TCR:pMHC-I	D	с г	C	A
71150	TCR.pMHC I	D	E	C	A
7115p	TCR:pMHC-I	D I		C C	A
/noe 7	TCR:pMHC-I	I D	J	C C	A
71185	TCR:pMHC-I	D	с г	C	A
/nme	TCR:pMHC-I	D	E	C C	A
/nmI	TCR:pMHC-I	ע	E E		A
/ow5	TCR:pMHC-I	D	E		A
/ow6	TCK:pMHC-I	D D	E	C	A
/po2	TCR:pMHC-I	D	E		A
/pbe	TCR:pMHC-I	D ^	E D		A
/r80	TCR:pMHC-I	A	В	E	C
/rm4	тск:рМНС-Г	E	D	C	A
				Contir	nued on next page

PDB ID	Structure Type	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
7rtr	TCR:pMHC-I	D	Е	С	А
8gvb	TCR:pMHC-I	А	В	Р	Н
8gvg	TCR:pMHC-I	А	В	Р	Н
8gvi	TCR:pMHC-I	А	В	Р	Н

Table S1: Breakdown of the data used in the analysis of *apo* and *holo* forms of TCR and pMHC structures.

Table S2: TCR comparisons made in the analysis. For each TCR, pair-wise combinations of all structures are computed. All results in the paper are normalised by taking the mean of the measurement per TCR so that TCRs with higher numbers of structures do not bias the results. TCRs are denoted by the sequence of all their CDR loops.

State	PDB ID	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID			
ATGYPSATKADDKALSDPVNDMR,SGHATFQNNGVASSLRGRGDQPQH								
аро	4qrp	Κ	L	-	-			
holo	4qrp	D	Е	С	A			
DRG	SQSIYSN	IGDALTRG	PGNQFY,	SGHVSFNYEAQ	.ASSSPGGVSTEAF			
аро	6rp9	Κ	L	-	-			
holo	6rp9	D	E	С	А			
DRC	SQSIYSN	IGDAVNFG	GGKLI,N	IRHNASNTAGTA	ASSLSFGTEAF			
аро	3qeu	А	В	-	-			
аро	3qeu	D	Е	-	-			
holo	3qdg	D	E	С	А			
holo	3qdj	D	E	С	А			
holo	6am5	D	E	С	А			
holo	6amu	D	E	С	Α			
DRC	SQSIYSN	IGDAVNRD	DKII,SEH	INRFQNEAQAS	SPDIEQY			
аро	7n1d	А	В	-	-			
holo	7n1f	D	E	С	А			
holo	7rtr	D	E	С	A			
DRC	SQSIYSN	IGDAVNVA	GKST,GT	SNPNSVGIGAW	SETGLGTGELF			
holo	3hg1	D	E	С	А			
holo	4qok	D	E	С	A			
holo	6eqa	D	E	С	A			
DRC	SQSIYSN	IGDAVRTN	SGYALN,	QGHDTYYEEEE	ASSDTVSYEQY			
apo	5nmd	А	В	-	-			
apo	5nmd	С	D	-	-			
holo	5nme	D	E	С	A			
holo	5nmf	D	E	C	Α			
holo	5nmg	D	E	С	A			
DRC	SQSIYSN	IGDAVTTD	SWGKLQ, .	MNHEYSVGAGI	ASRPGLAGGRPEQY			
аро	3qh3	А	В	-	-			
аро	7amp	А	В	-	-			
holo	1ao7	D	E	С	A			
holo	1qrn	D	E	С	A			
holo	1qse	D	Е	C	A			
holo	1qsf	D	E	С	A			
holo	3d39	D	Е	C	A			
					Continued on next page			

State	PDB ID	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
holo	3d3v	D	Е	С	А
holo	3h9s	D	Е	С	А
holo	3pwp	D	Е	С	А
holo	3qfj	D	Е	С	А
DRG	SQSIYSI	NGDGTYNO	QGGKLI,N	MNHEYSMNVEV	ASSGASHEQY
apo	3vxt	А	В	-	-
apo	3vxt	С	D	-	-
holo	3vxu	D	Е	С	A
holo	3w0w	D	Е	С	А
DSA	IYNIQSS	QREAQLN	QAGTALI,	MNHEYSVGAGI.	ASSYGTGINYGYT
apo	7r7z	А	В	-	-
holo	7r80	А	В	Е	С
DSA	IYNIQSS	QREAVRM	DSSYKLI,	SEHNRFQNEAQ.	ASSSWDTGELF
apo	3vxq	А	В	-	-
apo	3vxq	D	Е	-	-
holo	3vxr	D	Е	С	А
holo	3vxs	D	Е	С	А
DSA	IYNIQSS	QREAVRPL	LDGTYIPT	,MNHEYSVGAC	TASSYLGNTGELF
apo	2pyf	А	В	-	-
holo	2pye	D	Е	С	А
DSA	IYNIQSS	QREAVRPT	SGGSYIPT	,MNHEYSVGAG	IASSYVGNTGELF
apo	2bnu	А	В	-	-
holo	2bnq	D	Е	С	A
holo	2bnr	D	Е	С	A
holo	2f54	D	Е	С	А
holo	6q3s	D	Е	С	A
DSS	STYIFSN	MDMAEPS	GNTGKLI, .	SEHNRFQNEAQ	ASSLHHEQY
holo	7nme	D	Е	С	A
holo	7nmf	D	Е	С	A
DST	FNYILSV	SDKAALY	GNEKIT,N	NNHDYSYVADS	ASSDAGGRNTLY
holo	5m00	G	Н	Р	А
holo	5m01	G	Н	Р	А
holo	5m02	G	Н	Р	А
holo	5til	G	Н	С	А
holo	5tje	G	Н	Ι	А
holo	6g9q	G	Н	Р	А
DST	FNYIRSV	SDKAASE	rsgswqli,	MNHDTYYDKI	LASSRDLGRDTQY
holo	5swz	D	Е	С	А
holo	7jwi	D	Е	С	А
FLG	SQSTYR	EGDAVNDO	GGRLT,G	ISNPNWGPFGA	WSETGLGMGGWQ
аро	4jfh	D	Е	-	-
holo	4jfd	D	Е	С	А
holo	4jfe	D	Е	С	А
holo	4jff	D	Е	С	А
holo	6eqb	D	Е	С	А
holo	6tmo	D	Е	С	А
KAL	YSLLKG	GEQGLGD	AGNMLT	SGHATFONNGV	ASSLGQGLLYGYT
holo	5wkf	D	E	C	A
					Continued on next page

Table S2:	TCR	comparisons	made	in	the	analysis.

State	PDB ID	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
holo	5wkh	D	Е	С	А
NIAT	INDYGYI	KTKLVGEII	.DNFNKFY,	MDHENSYDVK	XMASSQRQEGDTQY
apo	6at6	А	В	-	-
holo	6avf	А	В	Р	Н
NSA	FDYILSV	SNKAASAS	SFGDNSKLI	.,MSHETSYDVI	DSASSLGHTEVF
apo	5iw1	А	В	-	-
apo	5iw1	С	D	-	-
apo	5iw1	E	F	-	-
holo	5ivx	Е	F	Р	Α
NSA	FQYTYS	SGNAMRGI	DSSYKLI,	SGHDYFNNNVP	.ASSLWEKLAKNIQY
apo	3utp	D	Е	-	-
apo	3utp	Κ	L	-	-
holo	3uts	D	Е	С	А
holo	3utt	D	Е	С	А
holo	5c07	D	Е	С	А
holo	5c08	D	E	С	А
holo	5c09	D	E	С	A
holo	5c0a	D	E	С	A
holo	5c0b	D	Е	С	Α
holo	5c0c	Ι	J	С	Α
holo	5hyj	D	E	С	A
NSA	SQSVYS	SGVVQPGC	GYQKVT,	MNHNSSASEGT	ASSEGLWQVGDEQY
apo	6vth	А	В	-	-
apo	6vth	D	Е	-	-
holo	6vrm	D	Е	Р	А
NSA	SQSVYS	SGVVRAGH	KLI,MNHI	EYSVGEGTASG	QGNFDIQY
apo	3skn	А	В	-	-
apo	3skn	С	D	-	-
apo	3skn	Е	F	-	-
apo	3skn	G	Н	-	-
holo	3sjv	D	E	С	А
SIFN	TLYKAG	ELAGGTG	NQFY,ENI	HRYSYGVKDAI	SEVGVGQPQH
holo	3qdm	D	Е	С	А
holo	3qeq	D	Е	С	А
STY	SPFSFTD	NKRALFLA	SSSFSKLV,	NNHDYSYVAD	SASSDWVSYEQY
holo	11p9	Е	F	С	Α
holo	2j8u	Е	F	С	А
holo	2jcc	Е	F	С	А
holo	2uwe	Е	F	С	А
SVFS	SSVVTG	GEVAGAGS	QGNLI,L	NHDASQIVNDA	SSSRSSYEQY
apo	2vlm	D	Е	-	-
holo	1oga	D	Е	С	А
holo	2vlj	D	Е	С	Α
holo	2vlk	D	Е	С	Α
holo	5hhm	D	Е	С	Α
TISC	NEYGLK	NNIVRGL	NNAGNMLT	,SGHNSFNNNV	PASSLGIDAIY
holo	7dzm	Е	D	С	Α
holo	7dzn	Е	D	С	А
					Continued on a set
					Continued on next page

Table S2: TCR comparisons made in the analysis.

State	PDB ID	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
TISC	GNEYGLF	KNNIVWGG	YQKVT,	SEHNRFQNEAQ	ASRYRDDSYNEQF
apo	3dx9	А	В	-	-
apo	3dx9	С	D	-	-
holo	3dxa	D	E	С	А
TISC	GNEYGLQ	QNILSGGS	NYKLT,N	ASHETSYDVDS	ASSFGREQY
holo	3pqy	D	Е	С	А
holo	7n5p	D	Е	С	Α
TISC	GTDYGLT	SNILPLAG	GTSYGKLT,	,SGHVSFQNEA	QASSLGQAYEQY
apo	1kgc	D	E	-	-
holo	1mi5	D	E	С	А
holo	3kpr	D	E	С	А
holo	3kps	D	Е	С	Α
TQD	SSYFQD	SYKKENAN	ARGDYGGSC	SNKLI,NSQYPW	LRSPGDTCSADRVGNTLY
holo	1fo0	А	В	Р	Н
holo	1nam	А	В	Р	Н
holo	2013	А	В	Р	Н
TRD	TAYYQP	WWGEQNA	MSVPSGDG	SYQFT,MNHEY	SVGEGTASKVGPGQHNSPLH
holo	7ow5	D	Е	С	А
holo	7ow6	D	E	С	A
TRD	TTYYRN	SFDEQNAL	SGFYNTDKI	LI,MNHNSSAS	SEGTASPGLAGEYEQY
holo	2ak4	D	E	С	A
holo	3kxf	D	E	Q	Α
TSD	QSYGQG	SYDEQNA	MRDLRDNFN	NKFY,MNHEY	SVGAGIASREGLGGTEAF
holo	4g8g	D	E	С	А
holo	4g9f	D	E	С	Α
TSE	SDYYQE	AYKQQNAY	GEDDKII,	MGHDKSYGVN	SASRRGPYEQY
holo	5jzi	D	E	С	А
holo	5yxn	А	В	Ι	С
TSW	WSYYQ	GSDEQNAL	GEGGAQKLV	V,MNHNSSAS	EGTASRTRGGTLIEQY
holo	5xot	D	E	С	А
holo	6bj3	D	Н	С	А
VSG	LRGLYS	AGEEAVQE	LGTSGSRLT	,SGDLSYYNG	EEASSARSGELF
holo	4prh	D	E	С	А
holo	4prp	D	E	С	А
YGA	TPYYFS0	GDTLVAVG	FTGGGNKLT	,SEHNRFQNE	AQASSDRDRVPETQY
holo	8gvb	А	В	Р	Н
holo	8gvg	А	В	Р	Н
YRC	SQSIYS	NGDAVNFG	GGKLI,N	IRHNASNTAGT	ASSWSFGTEAF
holo	413e	D	Е	С	А
holo	6d78	D	Е	С	Α
YSA	TPYYYS	GDPVVAVS	GFASALT,	NNHNNSYGAGS	ASGGGGTLY
apo	1tcr	А	В	-	-
holo	1g6r	А	В	Р	Н
holo	1mwa	А	В	Р	Н
holo	2ckb	А	В	Р	Н
YSG	SPEHISR	ALSGFNNA	GNMLT,	SGHATFQNNGV	ASSLGGAGGADTQY
apo	7n1c	D	Е	-	-
holo	7n1e	D	Е	С	A

Table S2: TCR	comparisons	made in the	analysis.
	1		~



Comparison of amino acids in CDR loops between selected structures and OTS

Figure S1. Comparison of the composition of amino acid residues in each CDR loop between the structures in this analysis and a comparative background of TCRs randomly sampled from Observed TCR Space (OTS) Raybould et al. (2024).

Table S3: pMHC-I comparisons made in the analysis. For each pMHC-I, pair-wise combinations of all structures are computed. All results in the paper are normalised by taking the mean of the measurement per pMHC-I so that pMHC-Is with higher numbers of structures do not bias the results. The pMHC-Is are denoted by their peptide sequence and allele code.

State	PDB ID	α-chain ID	β -chain ID	Antigen Chain II	MHC Chain ID			
ASNENMETM, H2-Db								
аро	1hoc	-	-	С	А			
аро	4hux	-	-	С	А			
holo	5sws	D	E	С	А			
holo	5swz	D	Е	С	А			
holo	7jwi	D	Е	С	А			
holo	7jwj	D	Е	С	А			
				Cor	tinued on next page			

State	PDB ID	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
KAPA	NFATM, H2	2-Db			
аро	3tbs	-	-	С	А
аро	3tbs	-	-	F	D
holo	5m01	G	Н	Р	А
KAPF	NFATM, H2	2-Db			
аро	3tby	-	-	С	А
аро	3tby	-	-	F	D
аро	3tby	-	-	Ι	G
аро	3tby	-	-	L	J
holo	5m02	G	Н	Р	А
KAPY	DYAPI, H2	-Db			
аро	6g9r	-	-	Ι	С
аро	6g9r	-	-	J	E
аро	6g9r	-	-	Κ	G
apo	6g9r	-	-	Р	А
holo	6g9q	G	Н	Р	А
KAPY	NFATM, H	2-Db			
apo	4nsk	-	-	С	А
apo	7p0a	-	-	С	А
apo	7p0a	-	-	F	D
holo	5til	G	Н	С	А
KAVA	NFATM, H2	2-Db			
apo	3quk	-	-	С	А
apo	3quk	-	-	F	D
holo	5m00	G	Н	Р	Α
KAVY	NFATM, H	2-Db			
аро	1ffn	-	-	С	А
аро	1ffn	-	-	F	D
аро	1n5a	-	-	С	А
аро	1n5a	-	-	F	D
аро	1n5a	-	-	Ι	G
apo	1n5a	-	-	L	J
apo	1s7u	-	-	С	А
apo	1s7u	-	-	F	D
apo	1s7u	-	-	Ι	G
аро	1s7u	-	-	L	J
аро	2f74	-	-	С	А
аро	2f74	-	-	F	D
аро	7p0t	-	-	С	Α
аро	7p0t	-	-	F	D
holo	5tje	G	Н	Ι	А
SQLLI	NAKYL, H	2-Db		-	
аро	5wli	-	-	C	А
аро	5wli	-	-	F	D
аро	5wli	-	-	1	G
apo	5wli	-	-	L	J
holo	5wlg	D	Е	C	А
SSLCI	NFRAYV, H	2-Db			
				Contin	nued on next page

-1 and -3 . -1 with -1 control -1 solution in a dominant -1 and -1 in the analysis.

State	PDB ID	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
аро	7n5q	-	-	С	А
аро	7n5q	-	-	Н	F
holo	7n5c	D	Е	С	А
holo	7n5p	D	Е	С	А
SSLE	NFRAYV, H	2-Db			
apo	1wby	-	-	С	А
apo	1vn6	-	-	С	А
holo	3pgy	D	Е	С	А
YGFR	NVVHI, H2	2-Db		-	
аро	7n9i	_	-	С	А
holo	7na5	D	Е	C	А
RGPG	RAFVTLH			-	
ano	1bii	_	_	Р	А
ano	1ddh	_	_	P	A
ano	3ech		_	P	Δ
apo	6npr			P	A C
apo	6npr	-	-	P	۵ ۵
upo kolo	5iuv	- E	- E	R D	A
FOVE			Г	P	A
EQIK	11 IF 15 V, H2-1	KD		D	
аро	Tieg	-	-	P	A
apo	1 lek	-	- D	P	A
holo	Imwa	A	В	P	H
holo	2ckb	A	В	Р	H
INFDI	-'NTI, H2-K	b			
аро	1nan	-	-	М	Н
аро	2clz	-	-	C	А
аро	2clz	-	-	М	Н
holo	1fo0	A	В	Р	Н
KVITI	FIDL, H2-K	b			
аро	1kj3	-	-	Р	Н
аро	1kj3	-	-	Q	Ι
holo	1kj2	А	В	Р	Н
RGYV	YQGL, H2	-Kb			
аро	1fzj	-	-	Р	А
аро	1fzm	-	-	Р	А
аро	1kpu	-	-	Р	А
аро	2mha	-	-	E	А
аро	2mha	-	-	F	С
аро	2vaa	-	-	Р	А
holo	1nam	Α	В	Р	Н
SQYY	YNSL, H2-	Kb			
аро	2clv	-	-	С	А
аро	2clv	-	-	М	Н
holo	2013	А	В	Р	Н
AAGI	GILTV, HLA	A-A*02:01			
аро	2guo	-	-	С	А
аро	2guo	-	-	F	D
аро	3qfd	-	-	С	А
-					
				Conti	nued on next page

Table S3: pMHC-I comparisons made in the analysis.

State	PDB ID	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
apo	3qfd	-	-	F	D
holo	3qdj	D	Е	С	А
holo	3qeq	D	Е	С	А
holo	6d78	D	Е	С	А
holo	6eqa	D	Е	С	А
holo	6eqb	D	Е	С	А
ALGI	GILTV, HLA	A-A*02:01			
apo	1 jht	-	-	С	А
apo	2gtz	-	-	С	А
apo	2gtz	-	-	F	D
holo	4eup	G	Н	F	D
ALWO	JEFFPVL, HI	LA-A*02:01			
аро	1b0g	-	-	С	А
apo	1b0g	-	-	F	D
holo	11p9	Е	F	С	А
holo	2j8u	Е	F	С	А
holo	2jcc	Е	F	С	А
holo	2uwe	Е	F	С	А
ALWO	GPDPAAA,	HLA-A*02:01			
apo	3utq	-	-	С	А
holo	3uts	D	Е	С	А
holo	3utt	D	Е	С	А
AOWO	GPDPAAA.	HLA-A*02:01		-	
apo	5c0d	-	-	С	А
holo	5hvi	D	Е	С	А
EAAG	IGILTV, HI	LA-A*02:01			
аро	2gt9	-	-	С	А
apo	2gt9	-	-	F	D
holo	4qok	D	Е	С	А
holo	6tmo	D	Е	С	А
ELAA	IGILTV. HI	A-A*02:01			
apo	4jfp	-	-	С	А
аро	4ifp	-	-	F	D
holo	4jfd	D	Е	С	А
ELAG	IGILTV. HI	A-A*02:01			
apo	1jf1	-	-	С	А
holo	3hg1	D	Е	С	А
holo	3qdg	D	Е	С	А
holo	3qdm	D	Е	С	А
holo	4jff	D	Е	С	А
holo	413e	D	Е	С	А
holo	5e9d	D	Е	С	А
holo	5nht	А	В	Р	Н
holo	5ngk	А	В	Р	Н
holo	6dkp	D	Е	С	А
GILEF	VFTL. HL	A-A*02:01			
apo	5hhp	-	-	С	А
holo	5hho	D	Е	С	А
				Contin	nued on next page

Table S3: pMHC-I comparisons made in the analysis.

GILGFVFTL, HLA-A*02:01 apo hhi - F D apo $2vll$ - C A qpo $2vll$ - C A qpo $2vll$ - F D $holo$ $10ga$ D E C A $holo$ $2vll$ D E C A $holo$ $2vll$ D E C A $holo$ $2vlr$ D E C A $holo$ $5uv$ E F J A $holo$ $5ivd$ D E C A $holo$ $5ivd$ D E C A $GUCTUVFTL, HLA-A*02:01 ago Shim D E C A dvo blo E P A A A A dvo fr -$	State	PDB ID	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
apo 1hii - - C A apo 1hii - - C A apo 2vil - - F D apo 2vil - - F D holo loga D E C A holo 2vil D E C A holo 2vil D E C A holo 2vil D E C A holo Siuo E F J A holo Simo - C A holo Sihm D E C A GUCTLVATL, HLA-A*02:01 - P A apo 1áf - - C A holo 6tro D E C A holo 6tro D E P A holo 6tro D E P A holo 6tro<	GILG	FVFTL, HL	A-A*02:01			
apo 1hhi - - F D apo 2vII - - F D apo 2vII - - F D holo loga D E C A holo loga D E C A holo 2vIr D E C A holo 2vIr D E C A holo Siz D E C A holo Sihm D E C A holo Sihm D E C A GUCTVAML, HLA-A*02:01 T P A A holo 3off D E C A GVYDGREHTV, HLA-A*02:01 T P A A apo 6vr5 - - P A holo 6vr5 - - P A holo 6vr5 - - P A	аро	1hhi	-	-	С	А
apo 2vII - - C A apo 2vII - - F D holo 10ga D E C A holo 2vII D E C A holo 2vIr D E C A holo 5uo E F J A holo 5jhd D E C A holo 5jhd D E C A GILGLYFTL, HLA-A*02:01 - C A qo 3mre - P A holo 3c41 D E C A GVYDGREHTV, HLA-A*02:01 - P A qo 1i4f - - C A holo 6vr5 - - P A apo 6vr5 - - P A apo 6vr5 - - P A bolo form D	apo	1hhi	-	-	F	D
app 2vII - F D holo loga D E C A holo 2vIj D E C A holo 2vIk D E C A holo 5ux D E C A holo 5ixz D E C A holo 5ihd D E C A out 5ihm D E C A out 5ihm D E C A out 3mre - - P A holo 3thm D E C A out 3atif D E C A out 3atif D E C A holo for D E P A holo for D E P A<	аро	2vll	-	-	С	А
holo loga D E C A holo 2vlj D E C A holo 2vlk D E C A holo 2vlr D E C A holo Seuo E F J A holo Sisz D E C A holo Sihm D E C A holo Sihm D E C A GUCTUVETL, HLA-A*02:01 T T A A holo 3o41 D E C A GVTUCREHTV, HLA-A*02:01 T T A A apo 1i4f - - C A holo 6vr5 - - P A apo 6vr5 - - Q D holo 6vrn D E P A holo 6vrn D E C A <t< td=""><td>аро</td><td>2vll</td><td>-</td><td>-</td><td>F</td><td>D</td></t<>	аро	2vll	-	-	F	D
holo 2vij D E C A holo 2vik D E C A holo Seuo E F J A holo Siz D E C A holo Siz D E C A molo Siz D E C A GUCTULTANCA*02:01 - C A qo Shhn - - P A holo 3of4 D E C A GVYDGREHTV, HLA-A*02:01 - P A A qo 1i4f - - C A holo 6vr5 - - Q D holo 6vr5 - - Q D holo 6vro D E P A holo 6vro D E P A holo 6vro D E P A holo	holo	1oga	D	Е	С	А
holo 2vik D E C A holo 2vir D E C A holo Seuo E F J A holo Sizt D E C A holo Sjhd D E C A aloo Sjhn - - C A holo Shhn - - C A holo Shhn D E C A holo Shhn D E C A holo Shhn D E C A dolo Shhn D E C A holo 3041 D E C A dolo 6tro D E P A holo 6tro D E P A holo 6tro D E P A holo 6tro D E P A	holo	2vlj	D	Е	С	А
holo 2vir D E C A holo Size D E C A holo Size D E C A holo Size D E C A old Size D E C A GUCILVETL, HLA-A*02:01 apo Shhm D E C A dolo 3old D E C A holo 3old D E C A holo 3old D E C A dolo 6tro D E C A dolo 6tro D E C A dolo 6tro D E P A apo 6vr5 - - Q D holo 6vrn D E P A holo 6vrn D E P A holo 5yri D E <t< td=""><td>holo</td><td>2vlk</td><td>D</td><td>Е</td><td>С</td><td>А</td></t<>	holo	2vlk	D	Е	С	А
holo Seuo E F J A $holo$ Sisz D E C A $holo$ Sipid D E C A apo Shhn - - C A $holo$ Shhn D E C A $dolo$ Shhn D E C A $holo$ Shhn D E C A $dolo$ Shm D E C A $holo$ 3o41 D E C A $dolo$ 3o41 D E C A $dolo$ 6uro D E C A $holo$ 6uro D E C A $holo$ 6uro D E P A $holo$ 6vr5 - - Q Q $holo$ 6vro D E P A $holo$ fyrm D E C <td>holo</td> <td>2vlr</td> <td>D</td> <td>Е</td> <td>С</td> <td>А</td>	holo	2vlr	D	Е	С	А
holo Sisz D E C A holo Sjhd D E C A GILGLVFTL, HLA-A*02:01 aqo Shhn D E C A go Shhn D E C A holo Sohn D E C A dolo Shhn D E C A GUCTIVAML, HLA-A*02:01 aqo Sold D E C A dolo Sold D E C A holo Sold D E C A dolo ftro - - P A holo ftro D E P A apo fvirb - - Q D apo fvirb - - P A holo fvirb D E P A holo fvirb D E C A holo fyirb	holo	5euo	Е	F	J	А
holo Sjhd D E C A GILGLVFTL, HLA-A*02:01 - - C A $holo$ 5hhn D E C A $holo$ 5hhn D E C A $dolo$ 3hne - - P A $holo$ 3o41 D E C A goo 3mre - - C A $holo$ 3o41 D E C A goo 3mre - - C A $dolo$ 6vr5 - - C A $holo$ 6vr5 - - Q D $holo$ 6vr5 - - Q D $holo$ 6vr5 - - Q D $holo$ 6vr6 D E P A $holo$ 6vr7 D E C A $holo$ 5yr A B I	holo	5isz	D	Е	С	А
GILGLVFTL, HLA-A*02:01 apo 5hhn - - C A holo 5hhn D E C A GLCTLVAML, HLA-A*02:01 - - P A holo 3o41 D E C A GVYDGREHTV, HLA-A*02:01 - - C A apo li4f - - C A holo foro D E C A HMTEVVRHC, HLA-A*02:01 - Q D D A apo 6vr5 - - P A holo 6vr5 - - Q D holo 6vr0 D E P A holo 6vrm D E P A holo 6vrm D E C A kolo 6yrm D E C A holo fyrn D E C A holo fyrn A <td>holo</td> <td>5jhd</td> <td>D</td> <td>Е</td> <td>С</td> <td>А</td>	holo	5jhd	D	Е	С	А
apo Shhn D E C A $holo$ Shhn D E C A GLCTLVAML, HLA-A*02:01 apo 3mre - - P A $holo$ 3041 D E C A GVYDGREHTV, HLA-A*02:01 apo 1i4f - - C A apo 1i4f - - C A A $holo$ 6 tro D E C A A apo 6 tr5 - - P A A A A A A A A A A A B D C A A A A A A A A B D C A	GILGI	VFTL, HL	A-A*02:01			
holo Shhm D E C A GLCTLVAML, HLA-A*02:01 - - P A holo 3o41 D E C A GVYDGREHTV, HLA-A*02:01 - C A holo 6tro D E C A holo 6tro D E C A holo 6tro D E C A hmolo 6tro D E C A halo 6tro D E P A apo 6vr5 - - Q D holo 6vrgo D E P A holo 6vrm D E C A holo 6vrm D E C A holo 5yix D E C A holo 3pwl - - F D	аро	5hhn	-	-	С	А
GLCTLVAML, HLA-A*02:01 Image: Heat of the system of the syst	holo	5hhm	D	Е	С	А
apo 3mre - P A holo 3o41 D E C A GVYDGREHTV, HLA-A*02:01 apo li4f - - C A holo 6tro D E C A HMTEVVRHC, HLA-A*02:01 apo 6vr5 - - P A apo 6vr5 - - P A A holo 6vop D E P A holo 6vrfs - - P A holo 6vrm D E P A holo 6vrm D E P A holo 6vrm D E C A holo fyzi D E C A holo fyzi D E C A holo fyzi D E C A <td< td=""><td>GLCT</td><td>LVAML HI</td><td></td><td>=</td><td>-</td><td></td></td<>	GLCT	LVAML HI		=	-	
r_{eff} $holo$ $3o4l$ D E C A go $1i4f$ $ C$ A $holo$ $6tro$ D E C A apo $6tro$ D E C A apo $6tro$ D E C A apo $6vr5$ $ Q$ D $holo$ $6vr5$ $ Q$ D $holo$ $6vro$ D E P A $holo$ $6vro$ D E C A $holo$ $5vro$ D E C A $holo$ $5yro$ A B I C $Lorder 3pwl -$	ano	3mre	-	-	Р	А
GVYDGREHTV, HLA-A*02:01 A apo 1i4f - - C A $holo$ $6tro$ D E C A HMTEVVRHC, HLA-A*02:01 apo $6vr5$ - - P A apo $6vr5$ - - Q D D A $holo$ $6vr5$ - - Q D A $holo$ $6vr5$ - - Q D A $holo$ $6vr5$ - - Q D A $holo$ $6vrn$ D E P A A $holo$ $6vrn$ D E P A $holo$ $7rm4$ E D C A $holo$ $5jzi$ D E C A $holo$ $5yxn$ A B I C LGYGFVNYI, HLA-A*02:01 - - C A $holo$ $3dy$ D E C A </td <td>holo</td> <td>3041</td> <td>D</td> <td>Е</td> <td>C</td> <td>A</td>	holo	3041	D	Е	C	A
apo li4f - C A $holo$ $broto$ D E C A HMTEVVRHC, HLA-A*02:01 apo $6vr5$ - P A apo $6vr5$ - - Q D $holo$ $6vrn$ D E P A $holo$ $6vrn$ D E D A $holo$ $7rm4$ E D C A $holo$ $5jzi$ D E C A $holo$ $5yxn$ A B I C $LGYGFVNYI, HLA-A*02:01 - - C A holo 3gy D E C A holo 3d3y D$	GVYF	GREHTV		-	-	
apo $helo$ $brow$ D E C A $holo$ $6tro$ D E C A apo $6vr5$ $ Q$ D $holo$ $6vqo$ D E P A $holo$ $6vqo$ D E P A $holo$ $6vqo$ D E P A $holo$ $6vrn$ D E P A $holo$ $7rm4$ E D C A $holo$ $5yrn$ A B I C apo $3mrm$ $ P$ A $holo$ $5yrn$ A B I C $LGYGFVNYI, HLA-A*02:01$ apo $3pwl$ $ C$ apo $3pwl$ $ C$ A $holo$ $3d39$ D E C A $holo$ $3d3y$ D E C A <	ano	1i/f	-	_	C	Δ
Indice D D E C A HMTEVVRHC, HLA-A*02:01 apo $6vr5$ - - P A apo $6vr5$ - - Q D D $holo$ </td <td>holo</td> <td>6tro</td> <td>D</td> <td>F</td> <td>C C</td> <td>Α Δ</td>	holo	6tro	D	F	C C	Α Δ
apo $6vr5$ - - P A apo $6vr5$ - - Q D $holo$ $6vqo$ D E P A $holo$ $6vqo$ D E P A $holo$ $6vrn$ D E P A $holo$ $7rm4$ E D C A $klVALGINAV, HLA-A*02:01 apo 3mrm - - P A holo 5yxn A B I C L LGYGFVNYI, HLA-A*02:01 apo apo apo apo apo apo aqo apo ada apo ada ada ada adaa adaa adaa adaaa adaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaa$	ните	VVPHC H	U A A*02.01	L	c	A
apo $bvis$ - - - P A apo $6vr5$ - - Q D $holo$ $6vqo$ D E P A $holo$ $6vrm$ D E P A $holo$ $6vrm$ D E P A $holo$ $6vrm$ D E P A $holo$ $frmd$ E D C A $holo$ $7rm4$ E D C A $holo$ $5jzi$ D E C A $holo$ $5yxn$ A B I C LGYGFVNYI, HLA-A*02:01 apo $3pwl$ - - F D $holo$ $3d39$ D E C A $holo$ $3d39$ D E C A $holo$ $3d37$ D E C A $holo$ $3qfj$ D E C A <	ano	ал л л л л л л л л л л л л л л л л л л	LA-A 02.01		D	•
apo $bvis$ QD $holo$ $6vqo$ DEPA $holo$ $6vrm$ DEPA $holo$ $6vrm$ DEPA $holo$ $7rm4$ EDCAKLVALGINAV, HLA-A*02:01 apo $3mrm$ P apo $3mrm$ PA $holo$ $5yxn$ ABICLGYGFVNYI, HLA-A*02:01 apo $3pwl$ C apo $3pwl$ CA $holo$ $3pwl$ DECA $holo$ $3pwl$ DECA $holo$ $3qvp$ DECA $holo$ $3d39$ DECA $holo$ $3d39$ DECA $holo$ $3d39$ DECA $holo$ $3qfj$ DECA apo IduzCA apo IhhkFD apo 2av1 <td>apo</td> <td>6115</td> <td>-</td> <td>-</td> <td>F</td> <td>A</td>	apo	6115	-	-	F	A
holo $bvqo$ DEPA $holo$ $6vrm$ DEPA $holo$ $6vrn$ DEPA $holo$ $7rm4$ EDCAKLVALGINAV, HLA-A*02:01 apo $3mrm$ P apo $3mrm$ PA $holo$ $5jzi$ DECA $holo$ $5yxn$ ABICLGYGFVNYI, HLA-A*02:01 apo $3pwl$ C apo $3pwl$ CA $holo$ $3pwp$ DECA $holo$ $3pwp$ DECA $holo$ $3d39$ DECA $holo$ $3d3y$ DECA $holo$ $3d3y$ DECA $holo$ $3d3y$ DECA $holo$ $3d3y$ DECA $holo$ $3dif$ DECA $holo$ $3dif$ DECA $holo$ $3qif$ DECA $holo$ $3qif$ DECA $holo$ $3qif$ DECA $holo$ $3qif$ DECA apo IduzCA apo IhhkCA apo 2av1 <td>apo</td> <td>6v15</td> <td>-</td> <td>-</td> <td>Q</td> <td>D</td>	apo	6v15	-	-	Q	D
noloovrmDEPAholo $6vrn$ DEPAholo $7rm4$ EDCAKLVALGINAV, HLA-A*02:01 apo $3mrm$ P apo $3mrm$ PAholo $5jzi$ DECAholo $5yxn$ ABICLGYGFVNYI, HLA-A*02:01CA apo $3pwl$ FDholo $3pyp$ DECALLFGFPVYV, HLA-A*02:01FDholo $3d3y$ DECAholo $3d3y$ DECAholo $3dqfj$ DECAholo $3qqfj$ DECAholo $3qqfj$ DECAholo $3qqy$ DFapoIduzCAapoIduzFDa	holo	ovqo	D	E	P	A
noloovinDEPAholo $7rm4$ EDCAKLVALGINAV, HLA-A*02:01 apo $3mrm$ P apo $3mrm$ PAholo $5jzi$ DECAholo $5jxi$ ABICLGYGFVNYI, HLA-A*02:01 apo $3pwl$ C apo $3pwl$ FDholo $3pwp$ DECALLFGFPVYV, HLA-A*02:01 A CAholo $3d3y$ DECAholo $3qfj$ DECAholo $3dqfj$ DECAholo $3qtj$ DFDAholo $3qtj$ CAholo $3qtj$ FDholo $2av1$ FD <td>noio</td> <td>ovrm</td> <td>D</td> <td>E</td> <td>P</td> <td>A</td>	noio	ovrm	D	E	P	A
noiorm4EDCAKLVALGINAV, HLA-A*02:01 apo 3mrmPAholo5jziDECAholo5jziDECAholo5yxnABICLGYGFVNYI, HLA-A*02:01 apo 3pwlC apo 3pwlCA apo 3pwpDECALLFGFPVYV, HLA-A*02:01 $holo$ 3d39DEC $holo$ 3qfjDECA $holo$ 3qfjDECA $holo$ 3qfjDECA $holo$ 3qtfjDECA $holo$ 3qtfjDECA apo 1duzCA apo 1duzCA apo 1hhkCA apo 1hhkCA apo 2av1CA apo 2av1CA apo 2av1CA apo 2av1CA	noio	ovrn 74	D	E	P	A
RLVALGINAV, HLA-A*02:01 apo 3mrmPA $holo$ 5jziDECA $holo$ 5yxnABICLGYGFVNYI, HLA-A*02:01CA apo 3pwlFD $holo$ 3pwpDECALLFGFPVYV, HLA-A*02:01FD $holo$ 3d39DECA $holo$ 3d37DECA $holo$ 3d19DECA $holo$ 3d19DECA $holo$ 3d2vDECA $holo$ 3d19DECA $holo$ 3d19DECA $holo$ 3d19DECA $holo$ 3d19DECA $holo$ 3d19DECA $holo$ 3d19DECA $holo$ 3d2vDECA $holo$ 3qfiDECA $holo$ 3qfiDECA $holo$ 3qfiDECA $holo$ 3qfiDFDA apo 1duzCA apo 1hhkFD apo 2av1C<	noio	/rm4	E	D	t	А
apo $simm$ $ P$ A $holo$ $5jzi$ D E C A $holo$ $5yxn$ A B I C $LGYGFVNYI, HLA-A*02:01$ apo $3pwl$ $ C$ A apo $3pwl$ $ F$ D $holo$ $holo$ $3pwp$ D E C A $LLFGFPVYV, HLA-A*02:01$ $holo$ $3d3y$ D E C $holo$ $3d3y$ D E C A $holo$ $3qfj$ D E C A apo $1duz$ $ C$ A apo $1duz$ $ F$ D apo $1hhk$ $ F$ D apo $2av1$ $ C$ A apo $2av1$ $ -$	KLVA	LGINAV, H	LA-A*02:01		D	
holoSjziDECAholoSyxnABICLGYGFVNYI, HLA-A*02:01apo $3pwl$ CAapo $3pwl$ FDholo $3pwp$ DECALLFGFPVYV, HLA-A*02:01holo $3d39$ DECAholo $3d39$ DECAholo $3d39$ DECAholo $3d39$ DECAholo $3qfj$ DECAholo $3qfj$ DECAholo $3qfj$ DECAholo $3qtj$ DECAapo1duzCAapo1duzCAapo1hhkFDapo2av1FDapo2av1CAapo2av1CA </td <td>apo</td> <td>3mrm</td> <td>-</td> <td>-</td> <td>P</td> <td>A</td>	apo	3mrm	-	-	P	A
holoSyxnABICLGYGFVNYI, HLA-A*02:01 apo $3pwl$ CA apo $3pwl$ FD $holo$ $3pwp$ DECALLFGFPVYV, HLA-A*02:01 $holo$ $3d39$ DECA $holo$ $3d3y$ DECA $holo$ $3d3y$ DECA $holo$ $3d3y$ DECA $holo$ $3qfj$ DECA $holo$ $3qfj$ DECA $holo$ $3qfj$ DECA $holo$ $3qtj$ DECA apo IduzCA apo IduzCA apo IhhkFD apo 2av1CA apo 2av1CA apo 2av1CA	holo	5jzi	D	E	C	A
LGYGFVNYI, HLA-A*02:01 apo $3pwl$ C A apo $3pwl$ F D holo $3pwp$ D E C A LLFGFPVYV, HLA-A*02:01 holo $3d39$ D E C A holo $3d39$ D E C A holo $3d3v$ D E C A holo $3qfj$ D E C A holo $3qfj$ D E C A holo $3qfj$ D F D C A holo $3qfj$ D F F D A holo $3qfj$ C A holo $3qfj$ C A holo $3qfj$ C A holo $3qfj$ C A holo $3qfj$	holo	5yxn	Α	В	1	С
apo $3pwl$ CA apo $3pwl$ FD $holo$ $3pwp$ DECALLFGFPVYV, HLA-A*02:01ECA $holo$ $3d39$ DECA $holo$ $3d39$ DECA $holo$ $3d3y$ DECA $holo$ $3d3y$ DECA $holo$ $3qfj$ DECA apo IduzCA apo	LGYG	FVNYI, HI	LA-A*02:01		-	
apo $3pwl$ FD $holo$ $3pwp$ DECALLFGFPVYV, HLA-A*02:01 $holo$ $3d39$ DECA $holo$ $3d3v$ DECA $holo$ $3qfj$ DECA $LLFGYPVYV, HLA-A*02:01$ </td <td>аро</td> <td>3pwl</td> <td>-</td> <td>-</td> <td>С</td> <td>А</td>	аро	3pwl	-	-	С	А
holo $3pwp$ DECALLFGFPVYV, HLA-A*02:01holo $3d39$ DECAholo $3d3v$ DECAholo $3qfj$ DECAholo1duzCAapo1duzCAapo1hhkFDapo2av1FDapo2av7CA	аро	3pwl	-	-	F	D
LLFGFPVYV, HLA-A*02:01 holo $3d39$ D E C A holo $3d3v$ D E C A holo $3qfj$ D E C A LLFGYPVYV, HLA-A*02:01 apo $1duz$ C A apo $1duz$ F D apo $1hhk$ C A apo $1hhk$ - C A apo $1hhk$ - C A apo $2av1$ - C A c C A apo $2av1$ - C C A Continued on next page	holo	3pwp	D	Е	С	А
holo $3d39$ DECAholo $3d3v$ DECAholo $3qfj$ DECALLFGYPVYV, HLA-A*02:01 apo 1duzC apo 1duzCA apo 1duzCA apo 1hhkCA apo 1hhkCA apo 1hhkCA apo 2av1CA apo 2av1CA apo 2av7CA	LLFGI	FPVYV, HL	A-A*02:01			
holo $3d3v$ DECAholo $3qfj$ DECALLFGYPVYV, HLA-A*02:01apo $1duz$ CAapo $1duz$ CAapo $1duz$ CAapo $1duz$ CAapo $1hhk$ CAapo $1hhk$ CAapo $2av1$ CAapo $2av1$ CAapo $2av7$ CAContinued on next page	holo	3d39	D	E	С	А
holo $3qfj$ DECALLFGYPVYV, HLA-A*02:01 apo $1duz$ CA apo $1duz$ FD apo $1duz$ CA apo $1hhk$ CA apo $1hhk$ CA apo $1hhk$ CA apo $2av1$ CA apo $2av1$ CA apo $2av7$ CA	holo	3d3v	D	E	С	А
LLFGYPVYV, HLA-A*02:01 apo 1duzCA apo 1duzFD apo 1hhkCA apo 1hhkCA apo 2av1CA apo 2av1CA apo 2av1CA apo 2av7CAContinued on next page	holo	3qfj	D	Е	С	Α
apo $1duz$ CA apo $1duz$ FD apo $1hhk$ CA apo $1hhk$ FD apo $2av1$ CA apo $2av1$ CA apo $2av1$ CA apo $2av7$ CA	LLFG	YPVYV, HL	LA-A*02:01			
apo $1duz$ FD apo 1hhkCA apo 1hhkFD apo 2av1CA apo 2av1FD apo 2av7CAContinued on next page	аро	1duz	-	-	С	А
apo1hhkCAapo1hhkFDapo2av1CAapo2av1FDapo2av7CA	аро	1duz	-	-	F	D
apo1hhkFDapo2av1CAapo2av1FDapo2av7CA	аро	1hhk	-	-	С	А
apo2av1CAapo2av1FDapo2av7CA	аро	1hhk	-	-	F	D
apo 2av1 - - F D apo 2av7 - - C A	аро	2av1	-	-	С	А
apo 2av7 C A Continued on next page	аро	2av1	-	-	F	D
Continued on next page	аро	2av7	-	-	С	А
					Conti	nued on next page

Table S3: pMHC-I comparisons made in the analysis.

apo 2av7 . . F D apo 3ixa - - F D $holo$ 1ac7 D E C A $holo$ 1bd2 D E C A $holo$ 1bd2 D E C A $holo$ 6uz1 D E C A $holo$ 6uz1 D E C A $mbolo$ 6uz1 D E C A $mbolo$ 6uz1 D E C A mpo 3h7b - - C A apo 3h7b - - F D $holo$ 3h9h - - F D $holo$ 6amt - - C A mo Samu D E C A mo Salph -	State	PDB ID	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID
apo $3ixa$ - - F D aqo $3ixa$ - - F D $holo$ $1ao7$ D E C A $holo$ $1bd2$ D E C A $holo$ $bulo$ D E C A $holo$ $bulo$ D E C A $mulower 3h7b - - C A apo 3h7b - - C A apo 3h9h - - C A apo 6amt - - C A apo 6amt - - C A holo 6amt - - C A holo 6amt -$	ano	2017		•	F	D
apo $5xa$ - F D $holo$ $1ao7$ D E C A $holo$ $1bd2$ D E C A $holo$ $6uz1$ D E C A $mbdo$ $6uz1$ D E C A $mbdo$ $6uz1$ D E C A $mbdo$ $3h7b$ - - F D apo $3h7b$ - - F D apo $3h7b$ - - F D apo $3h9h$ - - C A apo $3h9h$ - - C A $mwwwwwwwwwwwwwwwwwwwwwwwwwwwwwwwwwwww$	apo	Zav / Bixa	-	-	ſ	Δ
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	ano	3ixa	_	_	F	D
nolo 1bd2 D E C A holo 4ftv D E C A holo 6uz1 D E C A mailer D E C A mailer - C A apo 3h7b - - F D apo 3h9h - - F D holo 3h9b - - F D holo 3h9b - - F D holo 3h9b - - F D holo 6amt - - C A mode 6amt - - C A holo 5cda D E C A holo 5cda D E C A holo 5cda D E C A holo 5cda C F D A holo 5cda <	holo	1207	D	F	ſ	Δ
nolo 100 D D E C A holo 6uzl D E C A muse Gaul D E C A muse State C A apo 3h7b - - C A apo 3h9h - - C A apo 3h9h - - F D holo 3h9h - - C A apo 6amt - - F D holo 6amt - - F D holo 6amt - - F D holo 6amt D E C A molo 6amt D E C A molo 5c0a D E C A holo 5c0a D E C A apo 5x1 - - C A apo </td <td>holo</td> <td>1bd2</td> <td>D</td> <td>F</td> <td>C</td> <td>Δ</td>	holo	1bd2	D	F	C	Δ
Ando Guz1 D E C A $holo$ Guz1 D E C A apo $3h7b$ - - C A apo $3h7b$ - - F D apo $3h9h$ - - C A apo $6amt$ - - F D $holo$ $6amt$ - - F D $holo$ $6amt$ - - C A mo $6amt$ - C A A mo $5amt$ - C A A mo $5atr$ - C A A mo $5atr$ - F D A mo $5atr$ - F	holo	4ftv	D	F	C	Δ
mill D D D C N MLWGYLQV, HLA-A*02:01 apo $3h7b$ - - C A apo $3h7b$ - - F D A apo $3h9h$ - - F D A apo $3h9h$ - - F D A apo $3h9h$ - - C A apo $6amt$ - C A $moio$ $6amt$ - C A $moio$ $5c0a$ D E C A $moio$ $5c0a$ D E C A apo $2x4r$ - C C A apo $2x4r$	holo	6uz1	D	F	C	Δ
apo $3h7b$ - - C A apo $3h7b$ - - F D apo $3h9h$ - - C A apo $3h9h$ - - F D $holo$ $3h9s$ D E C A $molo$ $3h9s$ D E C A $molo$ $6antt$ - - C A apo $6antt$ - - C A $holo$ $6antt$ - - C A $holo$ $5antt$ - - C A $holo$ $5c0a$ D E C A apo $3t4t$ - - C A apo $2x4t$ - - C A apo $3gso$ - - P A $holo$ $3gsn$ A B P H $holo$ $5d2n$ C	MIW	JVLOVV F	H A_A*02·01	Ľ	0	
apo $3h7b$ - - F D apo $3h9h$ - - F D $holo$ $3h9h$ - - F D $holo$ $3h9h$ - - F D $holo$ $6amt$ - - C A apo $6amt$ - - F D $holo$ $6amt$ - - F D $holo$ $6amt$ D E C A $MVWGPDPLYV, HLA-A*02:01 apo 5n1y - C A apo 5x0a D E C A nlob 5c0a D E C A apo 5x0a - F D D apo 5x14r - - C A apo 5x38r - P A apo 5x38r - P A apo 5x38r - Pano3h7b--СА$	ano	3h7b	-	-	С	А
apo Sh9h - - C A apo Sh9h - - F D $holo$ Sh9h - - F D apo 6amt - - C A apo 6amt - - F D $holo$ 6amu D E C A $MVWGPDPLYV, HLA-A*02:01$ - C A apo 5n1y - - C A $holo$ 5c0a D E C A mo 2x4r - - C A apo 5q3k - - P A $holo$ 3gsn A B P H $holo$ 5d2n C F D holo apo 7n1b - C A A apo 7n1b - C	apo	3h7b	-	-	F	D
apo $3h9h$ $ F$ D $holo$ $3h9s$ D E C A $MMWDRGLGMM, HLA-A*02:01$ apo $6antt$ $ C$ A apo $6antt$ $ C$ A $mbolo$ $6anu$ D E C A $mbolo$ $6anu$ D E C A $mbolo$ $5c0a$ D E C A $mbolo$ $5c0a$ D E C A $mbolo$ $2x4r$ $ C$ A apo $2x4r$ $ P$ A apo $3gso$ $ P$ A apo $3gso$ $ P$ A apo $3gso$ A B P H $holo$ apo $nholo$ ago $nholo$ ago $nholo$ $nholo$ $nholo$	apo	3h9h	-	-	C	A
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MMWDRGLGMM, HLA-A*02:01 Image: Constraint of the second seco	holo	3h9s	D	Е	C	A
apo 6amt - - C A apo 6amt - - F D holo 6amu D E C A MVWGPDPLYV, HLA-A*02:01 apo 5n1y - - C A holo 5c0a D E C A A NLVPMVATV, HLA-A*02:01 apo 2x4r - C A apo 2x4r - - C A apo 3gso - - P A apo 6q3k - - P A holo 3gsn A B P H holo 5d2n C F G H RLQSLQTYV, HLA-A*02:01 apo 7n1b - C A apo 7n1b - - C A holo 7n1e D E C A apo 3hpj - - F D holo f	MMW	DRGLGM	M HLA-A*02	·01		
apo $6amt$ - - F D $holo$ $6amu$ D E C A $MVWGPDPLYV, HLA-A*02:01$ apo $5n1y$ - - C A $holo$ $5c0a$ D E C A $nlvPMVATV, HLA-A*02:01$ apo $2x4r$ - - C A apo $2x4r$ - - F D apo $3gso$ - - P A apo $3gso$ - - P A A apo $3gso$ - - P A apo $3gso$ - - P A A apo apo $agso$ - - C A apo ago <	ano	6amt	-	-	C	А
polo Gamu D E C A MVWGPDPLYV, HLA-A*02:01 apo 5nly - C A holo 5c0a D E C A NLVPMVATV, HLA-A*02:01 apo 2x4r - C A apo 2x4r - - F D apo 3gso - - P A apo 6q3k - - P A A apo 6q3k - - P A apo 6q3k - - P A	ano	6amt	_	_	F	D
Image D <td>holo</td> <td>6amu</td> <td>D</td> <td>E</td> <td>C</td> <td>A</td>	holo	6amu	D	E	C	A
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holo 5C0a D E C A NLVPMVATV, HLA-A*02:01 apo 2x4r - - C A apo 2x4r - - F D apo 3gso - - P A apo 6q3k - - P A A holo 3gsn A B P H holo 3gsn A B P H H holo 5d2n C F G H RLQSLQTYV, HLA-A*02:01 apo 7n1b - - C A apo 7n1b - - C A A A D b D holo 7n1b - F D holo A A A A A D A A A A A A A A A A A A A A <td< td=""><td>apo</td><td>5n1v</td><td>-</td><td>_</td><td>С</td><td>А</td></td<>	apo	5n1v	-	_	С	А
NLVPMVATV, HLA-A*02:01 Image Product Image Product <th< td=""><td>holo</td><td>5c0a</td><td>D</td><td>Е</td><td>C</td><td>A</td></th<>	holo	5c0a	D	Е	C	A
apo $2x4r$ - - C A apo $2x4r$ - - F D apo $3gso$ - - P A apo $6q3k$ - - P A $holo$ $3gsn$ A B P H $RLQSLQTYV, HLA-A*02:01$ apo $7n1b$ - C A apo $7n1b$ - - C A $RMFPNAPYL, HLA-A*02:01$ apo $3hpj$ - - C A apo $3hpj$ - - C A A $RQFGPDFPTI, HLA-A*02:01$ apo $5c0j$ - -	NLVP	MVATV. HI	A-A*02:01		-	
apo $2x4r$ - - F D apo $3gso$ - - P A apo $6q3k$ - - P A $holo$ $3gsn$ A B P H $holo$ $5d2n$ C F G H RLQSLQTYV, HLA-A*02:01 apo 7n1b - C A apo $7n1b$ - - C A apo $3hpj$ - - C A apo $3hpj$ - - C A apo $3bpj$ - - C A $RQFGPDFPTI, HLA-A*02:01 - - C A apo 5c0b Dapo2x4r--СА$	apo	2x4r	-	-	С	А
apo $3gso$ $ P$ A apo $6q3k$ $ P$ A $holo$ $3gsn$ A B P H $holo$ $5d2n$ C F G H $RLQSLQTYV, HLA-A*02:01$ apo $7n1b$ $ C$ A apo $7n1b$ $ C$ A apo apo $7n1b$ $ C$ A apo $3hpj$ $ C$ A apo $5c0i$ $ C$ A $RQFGPDFPTI, HLA-A*02:01apo5c0bDECARQFGPDWIVA, HLA-A*02:01apo5c0f CAholo5c06DECARQWGPDPAAV, HLA-A*02:01apo5c06DECAapo1t1w CAapo2c7u CAapo2c7u CA<$	аро	2x4r	-	-	F	D
apo $6q_{3}k$ $ P$ A $holo$ $3gsn$ A B P H $holo$ $5d2n$ C F G H $RLQSLQTYV, HLA-A*02:01$ apo $7n1b$ $ C$ apo $7n1b$ $ C$ A apo $7n1b$ $ F$ D $holo$ $7n1e$ D E C A $RMFPNAPYL, HLA-A*02:01$ apo $3hpj$ $ C$ apo $3hpj$ $ C$ A $nobo$ $6rsy$ D E C A $RQFGPDFPTI, HLA-A*02:01$ apo $5c0i$ $ C$ apo $5c0b$ D E C A $holo$ $5c0c$ I J C A $nolo$ $5c0c$ I J C A $nolo$ $5c0s$ D E C A $nolo$ $5c0s$ D E C A $nolo$ $5c0f$ $ C$ A $nolo$ $5c08$ D E C A $sLFNTIAVL, HLA-A*02:01$ apo $1t1w$ $ C$ apo $2c7u$ $ C$ A apo $2c7u$ $ C$ A apo $2c7u$ $ C$ A apo $2c7u$ $-$ <t< td=""><td>apo</td><td>3gso</td><td>-</td><td>-</td><td>Р</td><td>А</td></t<>	apo	3gso	-	-	Р	А
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	apo	6q3k	-	-	Р	А
holo5d2nCFGHRLQSLQTYV, HLA-A*02:01 apo 7n1bCA apo 7n1bFD $holo$ 7n1eDECARMFPNAPYL, HLA-A*02:01 apo 3hpjCA apo 3hpjCA apo 3hpjFD $holo$ fersyDECARQFGPDFPTI, HLA-A*02:01 apo 5c0iCA $holo$ 5c0bDECARQFGPDWIVA, HLA-A*02:01 </td <td>holo</td> <td>3gsn</td> <td>А</td> <td>В</td> <td>P</td> <td>Н</td>	holo	3gsn	А	В	P	Н
RLQSLQTYV, HLA-A*02:01 apo 7n1b - - C A apo 7n1b - - F D $holo$ 7n1e D E C A RMFPNAPYL, HLA-A*02:01 apo 3hpj - - C A apo 3hpj - - C A A apo 3hpj - - C A apo 5c0i - - C A $holo$ 5c0b D E C A $nolo$ 5c0j - - C A $nolo$ 5c0c I J C A $nolo$ 5c0f - - C A $nolo$ 5c08 D E C A <td>holo</td> <td>5d2n</td> <td>С</td> <td>F</td> <td>G</td> <td>Н</td>	holo	5d2n	С	F	G	Н
apo $7n1b$ CA apo $7n1b$ FD $holo$ $7n1e$ DECARMFPNAPYL, HLA-A*02:01 apo $3hpj$ C apo $3hpj$ CA apo $3hpj$ FD $holo$ $6rsy$ DECARQFGPDFPTI, HLA-A*02:01 apo $5c0i$ C apo $5c0i$ CA $holo$ $5c0b$ DECARQFGPDWIVA, HLA-A*02:01 apo $5c0j$ C apo $5c0c$ IJCA $RQWGPDPAAV, HLA-A*02:01$ apo $5c08$ DEC apo $5c06$ CA $holo$ $5c08$ DECA $sLFNTIAVL, HLA-A*02:01$ apo $2c7u$ -CA apo $2c7u$ CA apo $2c7u$ CA apo $2c7u$ FDContinued on next page	RLOS	LOTYV, HI	LA-A*02:01			
apo $7n1b$ FD $holo$ $7n1e$ DECARMFPNAPYL, HLA-A*02:01 apo $3hpj$ CA apo $3hpj$ FD $holo$ $6rsy$ DECARQFGPDFPTI, HLA-A*02:01 apo $5c0i$ CA $holo$ $5c0b$ DECARQFGPDWIVA, HLA-A*02:01 apo $5c0j$ CA $holo$ $5c0c$ IJCARQWGPDPAAV, HLA-A*02:01 apo $5c0f$ CA $holo$ $5c08$ DECARQWGPDPAAV, HLA-A*02:01 apo $5c06$ CA $holo$ $5c08$ DECASLFNTIAVL, HLA-A*02:01 apo $1t1w$ CA apo $2c7u$ -FDContinued on next page	apo	7n1b	-	-	С	А
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RQFGPDFPTI, HLA-A*02:01 apo $5c0i$ CA $holo$ $5c0b$ DECARQFGPDWIVA, HLA-A*02:01 apo $5c0j$ CA $holo$ $5c0c$ IJCA $RQWGPDPAAV, HLA-A*02:01$ apo $5c0f$ CA $holo$ $5c08$ DECA $holo$ $5c08$ DECA $sLFNTIAVL, HLA-A*02:01$ apo $1t1w$ CA apo $2c7u$ CA apo $2c7u$ CA apo $2c7u$ FD	holo	6rsy	D	Е	С	А
apo $5c0i$ CA $holo$ $5c0b$ DECA $RQFGPDWIVA, HLA-A*02:01$ apo $5c0j$ CA $holo$ $5c0c$ IJCA $RQWGPDPAAV, HLA-A*02:01$ apo $5c0f$ CA $holo$ $5c0g$ DECA $holo$ $5c0g$ DECA $holo$ $5c08$ DECA $SLFNTIAVL, HLA-A*02:01$ apo 1t1wC apo $2c7u$ CA apo $2c7u$ FDContinued on next page	RQFG	PDFPTI, HI	LA-A*02:01			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	аро	5c0i	-	-	С	А
RQFGPDWIVA, HLA-A*02:01 apo $5c0j$ CA $holo$ $5c0c$ IJCARQWGPDPAAV, HLA-A*02:01 apo $5c0f$ CA $holo$ $5c08$ DECASLFNTIAVL, HLA-A*02:01 apo $1t1w$ CA apo $2c7u$ CA apo $2c7u$ FDContinued on next page	holo	5c0b	D	Е	С	А
apo $5c0j$ CA $holo$ $5c0c$ IJCARQWGPDPAAV, HLA-A*02:01 apo $5c0f$ CA $holo$ $5c08$ DECASLFNTIAVL, HLA-A*02:01 apo $1t1w$ CA apo $2c7u$ FD	RQFG	PDWIVA, H	HLA-A*02:01			
holo5c0cIJCARQWGPDPAAV, HLA-A*02:01 apo 5c0fCAholo5c08DECASLFNTIAVL, HLA-A*02:01 apo 1t1wCA apo 2c7uCA apo 2c7uFDContinued on next page	apo	5c0j	-	-	С	А
RQWGPDPAAV, HLA-A*02:01 apo 5c0f - - C A holo 5c08 D E C A SLFNTIAVL, HLA-A*02:01 - - C A apo 1t1w - - C A apo 2c7u - - C A apo 2c7u - - F D	holo	5c0c	Ι	J	С	А
apo $5c0f$ CA $holo$ $5c08$ DECASLFNTIAVL, HLA-A*02:01 apo $1t1w$ CA apo $2c7u$ CA apo $2c7u$ CA apo $2c7u$ FDContinued on next page	RQWO	GPDPAAV, I	HLA-A*02:01			
holo5c08DECASLFNTIAVL, HLA-A*02:01 apo 1t1wCA apo 2c7uCA apo 2c7uFDContinued on next page	apo	5c0f	-	-	С	А
SLFNTIAVL, HLA-A*02:01 apo 1t1w - - C A apo 2c7u - - C A apo 2c7u - - C A apo 2c7u - - F D	holo	5c08	D	Е	С	А
apo1t1wCAapo2c7uCAapo2c7uFD	SLFN	FIAVL, HL	A-A*02:01			
apo 2c7u - C A apo 2c7u - - F D Continued on next page	apo	1t1w	-	-	С	А
apo 2c7u F D Continued on next page	apo	2c7u	-	-	С	А
Continued on next page	apo	2c7u	-	-	F	D
					Cont	inued on next page

Table S3: pMHC-I comparisons made in the analysis.

State	PDB ID	α-chain ID	β-chain ID	Antigen Chain II	O MHC Chain ID
аро	5nmk	-	-	С	А
holo	5nmg	D	Е	С	А
SLLM	WITQC, HI	LA-A*02:01			
аро	1s9w	-	-	С	А
holo	2bnr	D	Е	С	А
holo	2f53	D	Е	С	А
holo	2f54	D	Е	С	А
holo	2p5e	D	Е	С	А
holo	2p5w	D	Е	С	А
holo	2pye	D	Е	С	А
SLLM	WITOV. HI	A-A*02:01			
holo	2bna	D	Е	С	А
holo	<u>−</u> 011q 6a3s	D	E	C	A
holo	6rn9	D	F	C	Δ
SLVN		A *02·01	L	c	Δ
	1t20		_	C	Δ
apo	1120 5nmh	-	-	C	л л
	5nmn	-	-	C	A
holo	5nmi	D	E	C	А
SLYN	IVAIL, HL	A-A*02:01		-	
аро	1t21	-	-	С	А
аро	1t22	-	-	C	А
аро	2v2w	-	-	C	А
аро	2v2w	-	-	F	D
holo	5nme	D	E	С	А
YLGG	PDFPTI, H	LA-A*02:01			
аро	5c0g	-	-	С	А
holo	5c09	D	E	С	А
YLQP	RTFLL, HL	A-A*02:01			
аро	7mkb	-	-	С	А
apo	7n1a	-	-	С	А
apo	7n1a	-	-	F	D
аро	7n6d	-	-	С	А
apo	7n6d	-	-	G	Е
apo	7n6d	-	-	K	Ι
аро	7n6d	-	-	0	М
аро	7p3d	-	-	С	А
аро	7rtd	-	-	С	А
holo	7n1f	D	Е	С	А
holo	7n6e	Ι	J	С	А
holo	7pbe	D	Е	С	А
holo	7rtr	D	Е	С	А
YQFG	PDFPIA, H	LA-A*02:01			
apo	5c0e	-	-	С	А
holo	5c07	D	Е	С	А
GTSG	SPIINR. HI	A-A*11:01			
аро	5win	-	-	С	А
apo	5win	-	-	F	D
apo	5win	-	_	I	G
r ·-					-
				Cor	ntinued on next page

Table S3: pMHC-I comparisons made in the analysis.

State	PDB ID	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID		
holo	5wkh	D	Е	С	А		
GTSG	GTSGSPIVNR, HLA-A*11:01						
аро	5wjl	-	-	С	А		
apo	5wjl	-	-	F	D		
apo	5wjl	-	-	Ι	G		
holo	5wkf	D	Е	С	А		
VVVC	GADGVGK,	, HLA-A*11:0	1				
apo	7ow4	-	-	С	А		
apo	7ow4	-	-	F	D		
аро	7ow4	-	-	Ι	G		
holo	7ow6	D	Е	С	А		
holo	7pb2	D	Е	С	А		
VVVC	GAGGVGK,	HLA-A*11:0	1				
apo	7ow3	-	-	С	А		
аро	7ow3	-	-	F	D		
apo	7ow3	-	-	L	J		
holo	7ow5	D	Е	С	А		
OLPR	LFPLL, HL	A-A*24:02					
apo	7nmd	-	-	С	А		
apo	7nmd	-	-	F	D		
holo	7nme	D	Е	С	А		
holo	7nmf	D	Е	C	А		
RFPLI	FGW. HLA	-A*24:02					
apo	4wu7	_	-	С	А		
apo	4wu7	-	-	F	D		
apo	5hga	-	-	C	A		
apo	5hga	-	-	F	D		
holo	8gvg	А	В	P	H		
RFPLT	FGWCF. H	LA-A*24:02					
apo	3vxo	-	-	С	А		
ano	3vx0	_	_	F	D		
ano	5hød	_	_	C	A		
ano	5hød	_	_	F	D		
holo	3vxm	D	Е	C	A		
holo	37811	D	E	C	A		
holo	3w0w	D	E	C	A		
RYPI	FGW. HI	- A-A*24:02	_	-			
ano	4w115	_	_	С	А		
ano	4w15	_	_	F	D		
ano	5høb	-	-	- C	A		
ano	5høb	-	-	F	D		
apo	5hgh	_	-	I	G		
ano	5høh	_	_	- L	I		
holo	8gyh	А	В	P	н		
holo	8ovi	A	B	Р	н		
RADI	FGWCF F	Π.Δ-Δ*24·02	<u> </u>	-	**		
ano	3nfn	-	-	С	А		
ano	3vxn	_	-	č	A		
upo	5, 11			~			
				Conti	inued on next page		

Table S3: pMHC-I comparisons made in the ar	alvsis

State	PDB ID	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID			
аро	5hgh	-	-	С	А			
holo	3vxr	D	Е	С	А			
holo	5xov	Ι	J	С	А			
RYPL	RYPLTLGWCF, HLA-A*24:02							
аро	3vxp	-	-	С	А			
apo	3vxp	-	-	F	D			
holo	3vxs	D	Е	С	А			
APRG	APRGPHGGAASGL HLA-B*07:02							
аро	6at5	-	-	С	А			
holo	6avf	А	В	Р	Н			
holo	6avg	С	D	Р	G			
RPPIF	IRRL, HLA	-B*07:02						
apo	5wmo	-	-	С	А			
holo	6vmx	D	Е	С	А			
FLRG	RAYGL, HI	LA-B*08:01		-				
apo	1m05	-	-	Е	А			
apo	1m05	-	-	F	С			
ano	3sko	-	-	C	A			
ano	3x13	_	_	C	A			
holo	1mi5	D	E	C	A			
holo	3ffc	D	E	C	A			
holo	3siv	D	E	C	A			
някк	KCDFL H	LA_B*08.01	<u> </u>		11			
ano	4ara		_	C	Δ			
holo	4 dam	D	F	C	A A			
KDWI		U A B*27.05	L	c	А			
	ILULINK, П	ILA-D ⁺ 27.05		C				
apo	2088 4g9d	-	-	C C	A A			
holo	4g9a	D	F	C	A A			
VDWI	TEOS	JI A D*27.05	L	c	А			
	100LINK, 1	пLA-D ⁺ 27.05		C	٨			
holo	4g01	- D	- E	C	A			
	4g91	U A D*25.0	1	t	A			
HPVG	DADIFEI,	, HLA-B*35:0	1	C	•			
apo	4pr5	- D	- E	C C	A			
nolo	4prn	D	E	t	A			
HPVG	QADYFEY.	, пla-в*35:0	1	C	•			
apo h e l e	4pra	- D	- E	C	A			
nolo	4prp	D #25.01	E	L	А			
IPLTE	EAEL, HLA	ч-в∗32:01		6				
apo	5xos	- D	- F		A			
nolo	5xot	D	E		A			
nolo	60j2	D	E		A			
nolo	0013		H	C	А			
LPEPI	LPQGQLTA	1, HLA-B*35	:01	6				
аро	Izhk	-	-	C	A			
apo	3kww	-	-	C	A			
apo	3vto	-	-	C	A			
holo	3kxf	D	Е	Q	A			
				Contin	nued on next page			

Table S3: pMHC-I comparisons made in the analysis.

State	PDB ID	α-chain ID	β-chain ID	Antigen Chain ID	MHC Chain ID		
LPEPL	LPEPLPQGQLTAY, HLA-B*35:08						
apo	1zhl	-	-	С	А		
apo	3vfm	-	-	С	А		
apo	3vfn	-	-	С	А		
apo	3vfp	-	-	С	А		
holo	2ak4	D	Е	С	А		
holo	4jrx	D	Е	С	А		
holo	4jry	D	Е	С	А		
FEDLI	RVLSF, HL	A-B*37:01					
apo	6mt6	-	-	В	А		
holo	6mtm	D	Е	С	А		
TPQD	LNTML, H	LA-B*42:01					
apo	4u1j	-	-	С	А		
holo	7dzn	Е	D	С	А		
EENL	LDFVRF, H	ILA-B*44:05					
apo	3dx8	-	-	С	А		
holo	3dxa	D	Е	С	А		
EEYL	KAWTF, HI	LA-B*44:05					
apo	3kpq	-	-	С	А		
holo	3kpr	D	Е	С	А		
EEYL	QAFTY, HI	A-B*44:05					
apo	3kpp	-	-	С	А		
holo	3kps	D	Е	С	А		
TAFTI	PSI, HLA-I	3*51:01					
apo	1e28	-	-	С	А		
holo	4mji	D	Е	С	А		
QASQ	EVKNW, H	ILA-B*53:01					
apo	7r7v	-	-	С	А		
holo	7r80	А	В	Е	С		
TPQD	LNTML, H	LA-B*81:01					
apo	4u1i	-	-	С	А		
holo	7dzm	E	D	С	Α		
GADG	WGKSAL,	HLA-C*08:02		-			
apo	6jtn	-	-	С	А		
apo	6ulk	-	-	С	А		
holo	6uon	G	Н	F	D		
RLPAI	KAPLL, HL	A-E*01:03					
apo	6gh1	-	-	Р	А		
apo	6gh1	-	-	Q	С		
apo	6gh1	-	-	R	Е		
apo	6gh1	-	-	Z	G		
holo	6zkw	D	Е	С	А		

Table S3: pMHC-I comparisons made in the analysis.

REFERENCES

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Figure S2. Proportion of the species of origin for the TCRs in the selected STCRDab structures and the randomly sampled OTS background.

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CDR Movement from Framework Alignment

Figure S3. Percentage of different movement categories from ech CDR type after alignment on TCR framework region.



Figure S4. Comparison of different movement types for each CDR loop after alignment on loop backbones. *apo:apo* refers to changes between different *apo* structures of the same TCR, *apo:holo* refers to changes between *apo* and *holo* structures, and *holo:holo* refers to changes between different *holo* structures of the same TCR. There are significant differences between the movement types based on a p-value of 3.61×10^{-18} from a Kruskal-Wallis test (significance level < 0.05). Significant *post hoc* results have been added to the plot.



Figure S5. D-scores between different conformational states. **A.** Comparison of CDR D-scores between *apo:apo, apo:holo*, and *holo:holo* interactions. There are significant differences between the movement types based on a p-value of 3.57×10^{-18} from a Kruskal-Wallis test (significance level < 0.05). Significant *post hoc* results have been added to the plot. **B.** Comparison of CDR D-scores and anchor D-scores (for five anchor residues on either side of the CDR loop). There are significant differences between the regions based on a p-value of 1.51×10^{-16} from a Kruskal-Wallis test (significance level < 0.05).



Figure S6. Describing the movement of each CDR loop in more detail after alignment on loop backbones. **A.** C_{α} movement between *apo* and *holo* conformations. **B.** Residue centre-of-mass changes between *apo* and *holo* conformations. **C.** χ_1 -angle changes between *apo* and *holo* conformations. **D.** D-scores (backbone dihedral angle differences) between *apo* and *holo* conformations.



TCR Contacts on the non-nonamer-peptides

Figure S7. Distribution of contacts made between CDR loops and non-nonamer peptides from the STCRDab Leem et al. (2018) structures.



Figure S8. Comparison of *apo:apo, apo:holo*, and *holo:holo* changes for pMHC-Is. Significant differences exist between the different comparisons based on the results of a Kruskal-Wallis test at a 0.05 significance level (p-value 5.64×10^{-21}).



Figure S9. Correlating RMSD changes of CDR loops to affinity.



Figure S10. Correlating affinity changes of pMHC-Is to RMSD.



Figure S11. Correlation of CDR loop and peptide lengths (by number of amino acids) to conformational change. **A.** Correlation of CDR loops when RMSD conformational changes are measured after TCRs are aligned on framework regions. **B.** Correlation of CDR loops when RMSD conformational changes are measured after CDR loops are aligned before comparison. **C.** Correlation of the loop apex (C_{α} of middle residue for odd length loops or the average of the two middle C_{α} distances for even length loops) when CDR loops are aligned before comparison. **D.** Correlation of lengths and RMSD for peptides aligned on the floors of the MHC antigen binding domain.