

Figure S1. Peptide $2F_{o}$ - F_{c} electron density in the native and anchor modified HuD/HLA-A2 structures. Mol1 (chain C) is for the first molecule in each asymmetric unit; Mol2 (chain F) is for the second molecule in each asymmetric unit.



Figure S2. Peptide (left) and CDR3 α/β loop (right) 2F_o-F_c electron density in the A6-HuD/HLA-A2 structure.



Figure S3. $2F_{o}$ - F_{c} electron density for the α 2 helix linker region in the free HuD/HLA-A2 complex (left; for Mol 1) and in the A6-HuD/HLA-A2 complex (center).







B		HLA-A2 α1 helix							HLA-A2 α2 helix										
		E58	R65	K66	K68	A69	Q72	K146	A149	A150	H151	E154	Q155	A158	Y159	T163	E166	W167	R170
	Tax	8	13	6	1	4	1		2	17	1		6	1	1	2	7	3	4
	HuD	2	15	4	2	4	4	1		1		8	14	2	1	3	3	7	1

	peptides											
Tax	L1	L1 L2		Y5	P6	V7	Y8					
	1	1	12	18	3	5	13					
HuD	L1	G2	G4	F5	V6	N7	Y8					
	2	1	16	13	1	3	16					

Figure S4. Comparison of the A6-peptide/HLA-A2 interfaces with Tax and HuD. A) Contacts to the TCR binding loops in the two interfaces. Loop sequence is shown across the center. The number of contacts to each amino acid is in blue, with Tax contacts above the sequence and HuD contacts below. HLA-A2 or peptide amino acids forming contacts are also shown, with the number of contacts given in parentheses. Yellow highlights indicate the amino acid participates in a single hydrogen bond or salt bridge; red highlights indicate two hydrogen bonds or salt bridges; and green indicates three hydrogen bonds or salt bridges. Loops are truncated at both ends for clarity. Superscripts on the first number of each loop sequence give the amino acid number according to the numbering in the A6-HuD/HLA-A2 PDB file. B) Number of contacts to amino acids in the HLA-A2 α 1 and α 2 helices and the peptides. Highlights are defined as in panel A. Contacts defined as interatomic distances \leq 4 Å and include all backbone and sidechain atoms.