

Fig. S1: ROC curves obtained by MJ and BT pair potential matrices for HLA-DRB1*0101.

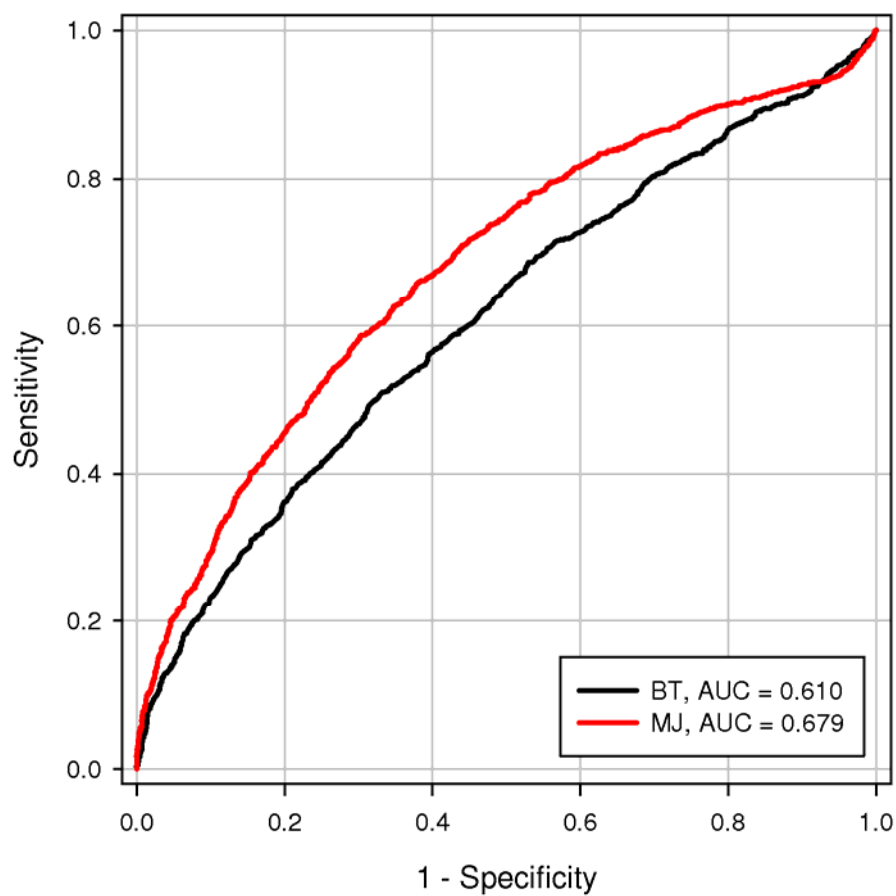


Table S1: List of alleles considered in this study for prediction of binding peptides by pair potential. The table lists the PDB IDs of the template used for prediction and whether it was a crystal structure or a structural model. Class II alleles are shown in bold fonts.

S. No	Allele	Template	Crystal Structure / model
1	HLA-A*0201 (10)	1HHH	Crystal Structure
2	HLA-A*0201 (9)	1AKJ	Crystal Structure
3	HLA-A*1101 (9)	1Q94	Crystal Structure
4	HLA-A*2402 (9)	2BCK	Crystal Structure
5	HLA-A*2601 (9)	1Q94	Model
6	HLA-A*6801 (9)	1AKJ	Model
7	HLA-B*0702 (9)	1M05	Model
8	HLA-B*0801 (9)	1M05	Crystal Structure
9	HLA-B*1501 (9)	1A9B	Model
10	HLA-B*1801 (9)	1A9B	Model
11	HLA-B*2703 (9)	1HSA	Model
12	HLA-B*2704 (9)	1HSA	Model
13	HLA-B*2705 (9)	1OGT	Crystal Structure
14	HLA-B*2705 (10)	1JGD	Model
15	HLA-B*2706 (9)	1K5N	Model
16	HLA-B*2709 (9)	1K5N	Crystal Structure
17	HLA-B*3701 (9)	1SYV	Model
18	HLA-B*3901 (9)	1M05	Model
19	HLA-B*4001 (9)	1M05	Model
20	HLA-B*4402 (9)	1M6O	Crystal Structure
21	HLA-B*4701 (9)	1N2R	Model
22	HLA-B*4901 (9)	1E27	Model
23	HLA-B*5101 (9)	1E27	Crystal Structure
24	HLA-Cw*0401 (9)	1QQD	Crystal Structure
25	HLA-DRB1*0401 (14)	1BX2	Model
26	H2-Db (9)	1BZ9	Crystal Structure
27	H2-Kb (8)	1BQH	Crystal Structure
28	H2-Kd (9)	1BZ9	Model
29	H2-Kk (8)	1BQH	Model
30	H2-Ab (15)	1MUJ	Crystal Structure
31	DRB1_0101	1KLG	Crystal Structure
32	DRB1_0301	1A6A	Crystal Structure
33	DRB1_0401	1J8H	Crystal Structure
34	DRB1_0404	1BX2	Model
35	DRB1_0405	1BX2	Model
36	DRB1_0701	1BX2	Model
37	DRB1_0802	1A6A	Model
38	DRB1_0901	1H15	Model

39	DRB1_1101	1A6A	Model
40	DRB1_1302	1A6A	Model
41	DRB1_1501	1BX2	Crystal Structure
42	DRB3_0101	1A6A	Model
43	DRB4_0101	1BX2	Model
44	DRB5_0101	1H15	Crystal Structure

Table S2: List of human class I MHC allele sequences obtained from IMGT/HLA database.

Serial Number	Class I MHC Allele	Number of Alleles
1	HLA-A	494
2	HLA-B	833
3	HLA-C	264
Total		1591

Table S3: List of human class II MHC allele sequences obtained from IMGT/HLA database.

Serial Number	Class II MHC Allele	Number of Alleles
1	DRA	2
2	DRB	524
3	DQA1	25
4	DQB1	66
5	DPA1	15
6	DPB1	114
Total		746

Table S4: List of human class I MHC-peptide complexes obtained from PDB.

Serial Number	Class I MHC Allele	Number of Structures
1	A*0101	1
2	A*0201	66
3	A*0265	7
4	A*0312	2
5	A*0326	5
6	A*1101	4
7	A*6801	1
8	B*0733	1
9	B*0801	2
10	B*0802	1
11	B*1505	3
12	B*2705	1
13	B*2709	4
14	B*2713	4
15	B*3501	1
16	B*3508	5
17	B*3542	11
18	B*3709	2
19	B*4402	1
20	B*4403	2
21	B*4405	1
22	B*5101	2
23	B*5301	2
24	B*5703	3
25	B*5711	1
26	B*5815	1
27	Cw*0304	1
28	Cw*0401	2
29	Cw*0602	1
30	Cw*0741	2
31	Cw*1202	7
32	Cw*1802	1
Total		148

Table S5: List of human class II MHC-peptide complexes obtained from PDB.

Serial Number	Class II MHC Allele	Number of Structures
1	HLA-DRB1*0301	1
2	HLA-DRB1*0101	23
3	HLA-DRB1*1501	2
4	HLA-DRB1*0401	2
5	HLA-DRB3*0101	1
6	HLA-DRB5*0101	4
7	HLA-DQA1*0501_HLA-DQB1*0201	1
8	HLA-DQA1*0302_HLA-DQB1*0302	3
9	HLA-DQA1*0102_HLA-DQB1*0602	1
10	HLA_DQA1*0303_HLA_DQB1*0310	4
Total		42

Table S6: List of mouse class I and class II MHC-peptide complexes obtained from PDB.

Serial Number	Mouse Allele	MHC Class	No of Structures
1	H2-D	Class I	1
2	H2-Db	Class I	16
3	H2-Dd	Class I	3
4	H2-Kb	Class I	34
5	H2-Ab	Class II	2
6	H2-Ad	Class II	2
7	H2-Ak	Class II	4
8	H2-A-nod	Class II	2
9	H2-Ek	Class II	8
10	H2-E	Class II	1
Total			73

Table S7: List of crystal structures of class I MHC alleles which bind a peptide whose source protein could be identified in the SWISSPROT database.

Serial Number	MHC Allele	Number of structures
1	A*0101	1
2	A*0201	17
3	A*0265	1
4	A*0312	1
5	A*0326	2
6	A*1101	4
7	A*2402	1
8	A*6801	1
9	B*0733	1
10	B*0801	1
11	B*1505	3
12	B*2705	1
13	B*2709	3
14	B*2713	2
15	B*3501	1
16	B*3508	4
17	B*3542	3
18	B*3709	1
19	B*4402	1
20	B*4403	1
21	B*4405	1
22	B*5101	2
23	B*5301	2
24	B*5703	3
25	B*5711	1
26	Cw*0304	1
27	Cw*0602	1
28	Cw*0741	3
29	Cw*1202	3
30	Cw*1802	1
31	E*0101	1
32	G*0101	1
33	G*0104	1
34	H2-Db	5
35	H2-Dd	1
36	H2-Kb	7
Total		84

Table S8: List of crystal structures of class II MHC alleles which bind a peptide whose source protein could be identified in the SWISSPROT database.

Serial Number	Class II MHC allele	Number of structures
1	H2-Ad	1
2	H2-Ak	3
3	H2-Ek	2
4	HLA-DQA1*0102_HLA-DQB1*0602	1
5	HLA-DQA1*0302_HLA-DQB1*0302	3
6	HLA-DRB1*0101	7
7	HLA-DRB1*0401	1
8	HLA-DRB1*1501	1
9	HLA-DRB5*0101	3
Total		22