Supplementary material

MHC Class I allele/peptide length	PDB ID	Peptide sequence	Peptide source/ Uniport accession no.	Resolution (A^0)	Gap Index (A^0)	Interface area (A^{02})	Total Hydrogen bonds in pMHC
H2-Kb/8	1KJ3	KVITFIDL	Naturally processed	2.3	0.6	905.3	14
	1FO0	INFDFNTI	pBM1 peptide [Mouse]	2.50	0.9	902.8	18
	1VAC	SIINFEKL	P01012	2.5	0.8	876.9	14
	1S7S	ALYNFATM	P07399	1.99	0.8	877.5	10
	1S7T	AVFNFATM	Lcmv-Peptide	2.30	0.8	852.3	11
	1G6R	SIYRYYGL	Syir protein	2.80	1.2	865.2	13
	1N59	AVYNFATM	P07399	2.95	0.9	864.7	9
	1LK2	GNYSFYAL	Synthetic	1.35	1.1	776.2	15
	1OSZ	RGYLYQGL	P11212	2.1	0.8	909.5	18
	1BQH	RGYVYQGL	P11212	2.80	0.8	882.6	12
	1LEG	EQYKFYSV	Q62425	1.75	0.9	880.6	15
H2-Db/9	1JUF	SSVIGVWYL	AAB81863	2.0	0.7	865.1	16
	1INQ	SSVVGVWYL	AAB81863	2.20	0.6	870.2	16
	1S7W	KALYNFATM	P07399	2.40	0.5	993.0	18
	1S7X	KAVFNFATM	P07399	2.41	0.5	950.0	18
	1FFO	AAVYNFATM	P07399	2.65	0.6	878.4	17
	1BZ9	FAPGVFPYM	P04857	2.8	0.8	1164.2	10
	1FFN	KAVYNFATM	P07399	2.70	0.7	946.8	18
	1FFP	SAVYNFATM	SRC2066(IEDB)	2.60	0.4	905.2	21
	1JPG	FQPQNGQFI	M20869	2.20	0.7	947.8	19
	1FG2	KAVYNFATC	P07399	2.75	0.6	928.4	17
	1CE6	FAPGNYPAL	SV nucleoprotein	2.90	0.9	867.7	15
	1QLF	FAPSNYPAL	P04857	2.65	0.7	879.5	13
HLA-A*0201/9	1QRN	LLFGYAVYV	Tax peptide P6A	2.8	1.1	871.5	10
	1AO7	LLFGYPVYV	Q82235	2.6	1.2	883.3	10
	1QSF	LLFGYPVAV	Tax peptide	2.80	1.2	828.6	10
	1HHI	GILGFVFTL	Q66PA1	2.5	0.5	842.0	9
	1QEW	FLWGPRALV	P43357	2.20	1	843.2	12
	1QSE	LLFGYPRYV	Tax peptide	2.80	1.3	873.0	11
	1B0G	ALWGFFPVL	Self peptide P1049]	2.5	0.5	860.2	12
	1I7T	ALWGVFPVL	Self peptide P1049	2.8	0.7	847.9	9
	1I7U	ALWGFVPVL	Self peptide [Human]	1.8	0.7	845.2	11
	1QR1	IISAVVGIL	P04626	2.4	0.9	827.1	9
	1EEY	ILSALVGIV	P04626	2.25	1.1	787.1	11
	1JHT	ALGIGILTV	NP_005502	2.15	0.8	781.0	12
	1I7R	FAPGFFPYL	P04857	2.20	0.9	902.5	11
	1I1F	FLKEPVHGV	HIV- reverse transcriptase	2.80	0.9	850.9	11
	1AKJ	ILKEPVHGV	HIV-reverse transcriptase	2.65	0.9	857.2	13
	1I1Y	YLKEPVHGV	HIV-reverse transcriptase	2.20	0.9	877.9	13
	1HHG	TLTSCNTSV	HIV-1 gp 120	2.6	1.4	765.8	12
HLA-A*0201/10	2CLR	MLLSVPLLLG	Calreticulin peptide	2.0	1.0	896.5	10
	1HHH	FLPSDFFPSV	HBV Nucleocapsid protein	3.0	0.6	918.4	11
	1JF1	ELAGIGILTV	melan-A [Homo sapiens]	1.85	0.6	870.4	11
	1I4F	GVYDGREHTV	P43358	1.40	1.1	820.1	15

Table1: MHC-peptide complexes used in the study.

MHC Class I allele/peptide length	Peptide ID	Peptide sequence	Category	Swiss Prot Accession no.	IC_{50} (nM)
H2-Kb/8	1	NTVVFDAL	SYNTHETIC	P23700	155000
	2	DDEEYVIL	SYNTHETIC	P31682	124000
	3	QPQNYLRL	SYNTHETIC	O86164	51667
	4	ANEGYDAL	SYNTHETIC	P31681	11923
	5	IIFLFILL	VIRAL	P03140	7500
	6	MWYWGPSL	VIRAL	P03140	7500
	7	LMSGFRQM	SYNTHETIC	Q9Z7H7	6889
	8	CLIFLLVL	VIRAL	P03140	6000
	9	FIIFLFIL	VIRAL	P03140	5000
H2-Db/9	1	AEDTNVSLI	SYNTHETIC	P23700	440000
	2	GFKSNFNKI	SYNTHETIC	Q9Z7H7	440000
	3	QLPPNSLLI	BACTERIAL	Q9Z7P3	293333
	4	VENPGGYCL	VIRAL	P09991	33500
	5	TAGANPMDL	SYNTHETIC	P31681	22000
	6	TGKLNLENL	SYNTHETIC	Q9Z6X8	17600
	7	SGVENPGGY	VIRAL	P09991	13155
	8	KAVYNFATC	VIRAL	P09991	5429
	9	LLVFNYPGI	SYNTHETIC	Q9Z6X9	5167
HLA-A*0201/9	1	VVHFFKNIV	SELF PEPTIDE	P02686	50000
	2	KIFGSLAFL	SELF PEPTIDE	P04626	27000
	3	TLPRARRRV	CANCER	Q01726	25000
	4	SLLMWITQC	SELF PEPTIDE	P78358	21070
	5	FLFGSLAFL	SELF PEPTIDE	P04626	19000
	6	FLYAALLLA	SELF PEPTIDE	P06905	17177
	7	NGMLIMCNA	CANCER	Q01718	16667
	8	SLYITVAVL	VIRAL	P05889	16667
	9	RLCVQSTHV	VIRAL	P03129	16666
	10	FLFESLAFL	SELF PEPTIDE	P04626	15000
	11	HLSLRGLPV	VIRAL	P20977	12500
	12	ALVARAAVL	CANCER	Q01726	11111
	13	SLCFLGAIA	CANCER	Q01726	10000
	14	HLEGKVILV	VIRAL	P03368	8333
	15	VALVGLFVL	SELF PEPTIDE	P40126	8333
	16	RVMAPRALL	CANCER	P43355	7667
	17	VCMTVDSLV	SELF PEPTIDE	P40126	7143
	18	ILLGIFFLC	CANCER	Q01726	5556
	19	KLPQLCTEL	VIRAL	P03126	5556

	20	ALGLVCVQM	CANCER	P43355	5000
	21	FLHLTLIVL	CANCER	Q01726	5000
	22	HLESLFTAV	VIRAL	P03156	5000
	23	LLGCAANWI	VIRAL	P12900	5000
HLA-A*0201/10	1	AAGIGILTVI	CANCER	Q16655	5555
	2	ELCCQHLWQI	ALLERGEN	P04721	5555
	3	FLPRHRDTGI	SELF PEPTIDE	P02686	5000

Table 2: MHC non binding peptide dataset used in the study.

MHC Class I allele/peptide length	**Nearest atom < 4.0 Å**				**C-beta< 7.0 Å**			
	PDB ID/Peptide ID	**MJ**	**PDB ID/Peptide ID**	**BT**	**PDB ID/Peptide ID**	**MJ**	**PDB ID/Peptide ID**	**BT**
H2-Kb/8	5	-196.3	6	-6.4	5	-90.5	3	-0.2
	9	-195.8	7	-6.3	9	-89.3	1FO0	-1.2
	8	-187.2	1FO0	-5.5	8	-84.6	6	-1.2
	1KJ3	-157.3	1S7S	-4.8	1FO0	-68.8	1OSZ	0.0
	1FO0	-157.0	1LEG	-4.8	6	-67.8	1BQH	0.0
	7	-154.9	5	-4.7	7	-66.2	7	0.2
	1VAC*	-154.8	9	-4.4	1KJ3	-65.7	2	0.3
	1S7S	-154.3	1KJ3	-4.3	1S7S	-65.2	1LK2	0.5
	1S7T	-153.6	1G6R	-4.2	1S7T	-65.1	1VAC*	0.6
	1G6R	-150.2	1N59	-4.2	1VAC*	-64.7	1S7S	0.6
	6	-149.2	1LK2	-4.2	1	-64.4	1S7T	0.6
	1N59	-147.5	1S7T	-4.0	1G6R	-64.3	4	0.6
	1	-146.0	1VAC*	-3.7	2	-63.0	1KJ3	0.7
	1LK2	-144.8	1OSZ	-3.7	1OSZ	-62.9	1N59	0.8
	1OSZ	-137.3	1BQH	-3.6	1N59	-62.4	1G6R	0.9
	2	-136.7	3	-3.4	1LK2	-62.2	1LEG	0.9
	1BQH	-135.4	8	-3.4	1BQH	-61.1	5	0.9
	1LEG	-133.4	1	-3.3	3	-57.2	1	1.1
	3	-131.7	4	-3.0	4	-56.7	8	1.3
	4	-127.8	2	-2.8	1LEG	-54.5	9	1.3
H2-Db/9	9	-166.6	1BZ9	-9.3	9	-101.2	1BZ9	-9.3
	3	-158.1	1CE6	-7.1	3	-100.4	1S7W	-7.0
	1BZ9	-155.6	1QLF	-7.0	1INQ*	-97.0	1FFN	-6.7
	1JUF	-153.8	1S7W	-7.0	1S7W	-91.1	1FG2	-2.6
	1JPG	-153.0	9	-7.0	1S7X	-90.1	8	-2.6
	1INQ*	-151.5	4	-6.9	1FFO	-87.9	4	-2.6
	1CE6	-148.6	1FFN	-6.7	1JUF	-87.8	1INQ*	-2.3
	4	-148.6	1JPG	-6.5	1FFN	-87.1	1JUF	-2.1
	1QLF	-148.1	1S7X	-6.2	1BZ9	-87.1	1CE6	-2.1
	1	-140.2	3	-6.1	1FFP	-87.0	1JPG	-2.0
	1FFO	-138.4	1FG2	-5.9	1FG2	-85.5	1S7X	-1.8
	1S7X	-137.3	8	-5.9	8	-85.5	3	-1.8
	1S7W	-135.6	1FFO	-5.4	4	-85.2	1QLF	-1.7
	1FFP	-134.6	1INQ*	-5.2	1	-84.0	1FFO	-1.4
	5	-134.5	1JUF	-5.2	1CE6	-83.4	1FFP	-1.2
	6	-134.5	1FFP	-4.1	1JPG	-83.4	1	-1.2
	1FFN	-132.6	1	-4.0	1QLF	-82.7	9	-1.0
	1FG2	-128.6	5	-3.9	6	-81.4	2	-0.8
	8	-128.6	7	-3.3	2	-80.0	6	-0.7
	2	-128.1	2	-2.5	5	-79.8	7	-0.5
	7	-117.6	6	-2.5	7	-73.6	5	0.7
HLA-	18	-209.2	1AO7	-10.6	18	-110.7	16	-7.4

A*0201/9	10	-201.6	1QRN	-10.3	21	-108.0	14	-4.4
	5	-200.9	6	-9.9	10	-107.8	6	-3.7
	21	-200.2	1QEW	-9.8	5	-107.1	10	-3.6
	1QRN	-195.7	18	-9.7	6	-104.4	1QRN	-3.5
	1AO7	-195.1	1QSF	-9.6	2	-100.0	1AO7	-3.5
	6	-193.9	10	-9.6	15	-99.0	18	-3.5
	15	-192.0	1B0G	-9.4	1B0G	-98.8	1QSF	-3.3
	1QSF	-190.6	1I7T	-9.2	14	-98.7	2	-3.0
	1HHI*	-190.1	1I7U	-9.1	1QRN	-97.9	21	-3.0
	1QEW	-184.1	1QSE	-8.9	1HHI*	-97.9	1QEW	-2.8
	1QSE	-182.5	1I7R	-8.7	1I7T	-97.8	1B0G	-2.8
	1B0G	-181.1	5	-8.6	1AO7	-96.7	22	-2.7
	2	-179.7	21	-8.5	1I7U	-96.1	1I7T	-2.6
	1I7T	-179.3	14	-8.2	1QR1	-95.9	5	-2.6
	1I7U	-179.1	2	-7.3	8	-95.8	11	-2.6
	1QR1	-177.4	19	-7.3	1EEY	-95.2	1I7U	-2.5
	14	-176.3	15	-7.1	1QEW	-94.5	1I1Y	-2.4
	1EEY	-174.5	1HHI*	-6.9	1QSF	-93.7	1HHI*	-2.3
	12	-173.1	22	-6.7	1JHT	-93.4	8	-2.3
	8	-172.5	1I1F	-6.3	12	-91.6	1JHT	-2.2
	23	-171.3	20	-6.1	1QSE	-90.2	1I7R	-2.1
	16	-170.2	11	-5.8	16	-89.4	1I1F	-2.1
	1JHT	-169.8	1I1Y	-5.5	23	-89.3	15	-2.1
	17	-168.0	12	-5.5	20	-88.9	20	-2.1
	1I7R	-167.9	1AKJ	-5.4	22	-88.5	1AKJ	-2.0
	11	-165.9	8	-5.3	1I7R	-87.5	19	-1.9
	20	-165.7	17	-5.1	4	-87.2	1QSE	-1.8
	1	-163.5	23	-5.0	13	-87.2	12	-1.8
	4	-162.3	9	-4.7	11	-87.1	1EEY	-1.1
	1I1F	-161.3	1JHT	-4.5	1I1F	-85.6	9	-1.1
	13	-159.9	1EEY	-4.3	1AKJ	-85.0	13	-1.0
	22	-159.0	1QR1	-4.1	17	-84.8	7	-0.9
	1AKJ	-158.8	1	-4.0	1	-83.9	1QR1	-0.7
	19	-155.6	3	-3.8	19	-83.5	4	-0.6
	9	-154.5	7	-3.4	1I1Y	-83.4	3	-0.5
	1I1Y	-152.9	13	-3.4	9	-81.1	23	-0.5
	1HHG	-146.1	4	-3.3	1HHG	-76.1	17	-0.1
	7	-143.0	16	-2.5	3	-74.4	1HHG	-0.0
	3	-142.7	1HHG	-2.4	7	-74.3	1	0.3
HLA-A*0201/10	2CLR	-176.8	3	-7.8	2CLR	-121.8	2CLR	-4.0
	1HHH	-158.6	2CLR	-7.3	1JF1	-108.0	1HHH	-2.6
	2	-157.0	1HHH	-6.7	2	-107.9	1JF1	-2.4
	3	-155.7	2	-5.6	1HHH	-102.2	2	-1.9
	1JF1	-148.9	1I4F*	-4.6	1	-101.7	3	-1.6
	1	-145.9	1JF1	-4.4	3	-95.8	1I4F*	-1.5
	1I4F*	-135.0	1	-1.9	1I4F*	-87.9	1	-0.0

Table 3 : Ranking of MHC binding and non peptides according to their predicted binding affinity by threading using a scoring matrix (MJ & BT) and two distance criteria (Nearest atom < 4.0 Å & C-beta< 7.0 Å). * Structure used as template.

MHC Class I allele/peptide length	**Nearest atom < 4.0 A^0**				**C-beta< 7.0 A^0**			
	PDB ID/Peptide	**MJ**	**PDB ID/Peptide**	**BT**	**PDB ID/Peptide**	**MJ**	**PDB ID/Peptide**	**BT**

	ID		ID		ID		ID	
H2-Kb/8	9	-185.0	1LEG*	-5.5	5	-105.3	6	-2.1
	5	-184.0	6	-6.8	9	-104.4	1FO0	-1.9
	8	-175.1	1FO0	-4.8	8	-100.1	1VAC	-0.6
	1FO0	-151.6	2	-4.0	1S7S	-81.0	1S7S	-0.6
	7	-145.6	1S7S	-3.6	1VAC	-79.9	1S7T	-0.5
	1VAC	-145.5	1LK2	-3.5	1KJ3	-79.3	3	-0.5
	1KJ3	-144.9	1OSZ	-3.5	1FO0	-79.1	1N59	-0.3
	1S7T	-144.8	3	-3.5	1S7T	-79.0	2	-0.2
	1S7S	-144.0	1BQH	-3.4	7	-79.0	4	-0.2
	6	-142.2	7	-3.3	6	-78.8	1KJ3	-0.1
	1N59	-137.3	1N59	-3.0	1G6R	-77.2	1LK2	-0.1
	1G6R	-136.3	9	-2.5	1N59	-76.3	1	-0.1
	1	-133.9	1G6R	-2.4	1	-75.7	5	-0.0
	1LK2	-131.6	4	-2.4	1LK2	-72.4	1OSZ	0.1
	1OSZ	-127.2	1KJ3	-2.2	2	-71.8	1BQH	0.1
	1BQH	-124.5	1VAC	-2.2	1OSZ	-71.5	1LEG*	0.2
	1LEG*	-123.9	5	-2.1	1BQH	-69.7	7	0.2
	3	-117.8	1S7T	-1.7	3	-65.9	9	0.2
	2	-116.9	1	-1.7	4	-65.9	8	0.3
	4	-112.6	8	-0.8	1LEG*	-64.9	1G6R	0.5
H2-Db/9	9	-190.3	1BZ9	-8.7	3	-112.8	1S7W	-3.5
	3	-177.7	1S7W	-7.6	9	-109.9	1FFN	-3.2
	1BZ9	-177.5	1FFN	-7.2	1JUF	-102.6	1BZ9	-3.1
	1JUF	-167.9	1S7X	-6.5	1INQ	-101.5	1FG2	-2.9
	1INQ	-166.2	8	-6.0	1BZ9	-96.6	8	-2.9
	1JPG*	-165.7	4	-5.4	1FFN	-96.6	4	-2.6
	1CE6	-165.3	3	-5.2	1S7W	-95.3	1S7X	-2.5
	1QLF	-165.0	9	-5.2	1S7X	-94.2	3	-2.4
	4	-160.8	1FFO	-4.1	1FFO	-93.1	1CE6	-2.3
	2	-156.3	1JUF	-4.0	2	-93.1	1QLF	-2.3
	1S7W	-156.0	1INQ	-4.0	1JPG*	-93.0	1JUF	-2.2
	1FFO	-156.0	1FFP	-3.7	4	-92.5	1INQ	-2.2
	1S7X	-155.2	1	-3.6	1FFP	-92.3	1JPG*	-2.2
	1	-153.4	6	-3.3	1CE6	-91.6	1FFO	-2.0
	1FFP	-153.2	2	-3.2	1QLF	-91.3	1FFP	-1.9
	1FFN	-152.0	7	-3.0	1	-90.6	9	-1.9
	6	-151.4	1FG2	-2.9	1FG2	-90.0	2	-1.6
	5	-149.1	5	-2.7	8	-90.0	1	-1.3
	1FG2	-147.3	1CE6	-2.3	5	-88.1	6	-1.1
	8	-147.3	1QLF	-2.3	6	-87.6	7	-1.0
	7	-133.9	1JPG*	0.1	7	-79.1	5	-0.0
HLA-A*0201/9	5	-191.5	1QRN	-10.1	18	-113.5	10	-4.7
	10	-191.5	1AO7*	-10.1	21	-110.4	1QRN	-4.6
	18	-188.1	1QEW	-9.8	10	-108.6	1AO7*	-4.6
	1QRN	-181.4	5	-9.4	5	-107.9	18	-4.5
	1AO7*	-181.0	10	-9.4	6	-	1QSF	-4.3

					106.5			
	21	-179.3	6	-9.2	15	-104.0	6	-4.0
	1QEW	-177.2	1QSE	-9.0	1HHI	-101.2	21	-3.9
	6	-176.3	2	-8.8	2	-100.0	5	-3.7
	1QSF	-175.5	1QSF	-8.7	1QRN	-99.9	14	-3.7
	1QSE	-175.2	16	-8.1	14	-99.4	1HHI	-3.6
	15	-166.4	1B0G	-8.0	1B0G	-99.0	1B0G	-3.6
	1QR1	-166.2	1I7U	-8.0	1AO7*	-98.6	1QEW	-3.5
	2	-164.7	18	-8.0	1I7T	-98.0	1I7T	-3.4
	1B0G	-164.2	21	-7.9	1QR1	-96.3	1I1F	-3.4
	23	-164.0	1I7T	-7.8	1I7U	-96.2	1I7U	-3.3
	1EEY	-163.7	14	-7.5	1JHT	-95.9	15	-3.3
	1I7U	-163.4	19	-7.1	1QSF	-95.6	1AKJ	-3.2
	1I7T	-163.2	1I7R	-7.0	8	-95.6	1I7R	-3.1
	1HHI	-162.5	12	-6.3	1EEY	-95.2	1I1Y	-3.1
	12	-160.8	8	-6.2	1QEW	-94.9	1JHT	-2.9
	17	-157.6	23	-6.1	12	-92.3	2	-2.9
	16	-157.4	9	-6.0	1QSE	-90.7	1QSE	-2.8
	14	-157.3	1I1F	-5.9	20	-90.5	20	-2.8
	8	-156.5	1I1Y	-5.8	16	-90.2	12	-2.7
	1I7R	-152.1	1HHI	-5.7	1I7R	-89.9	16	-2.7
	1	-151.6	11	-5.7	23	-89.2	11	-2.6
	1I1F	-150.2	15	-5.6	11	-88.9	8	-2.4
	1AKJ	-147.3	22	-5.3	13	-87.7	22	-2.0
	4	-145.5	1AKJ	-5.0	4	-87.6	7	-1.9
	13	-145.4	20	-4.9	22	-87.4	13	-1.7
	1JHT	-144.4	3	-4.8	1I1F	-86.7	19	-1.7
	11	-142.3	1EEY	-4.4	17	-86.4	1EEY	-1.6
	20	-141.8	1JHT	-4.4	1AKJ	-86.1	4	-1.4
	9	-141.7	13	-4.4	1	-85.1	1QR1	-1.3
	22	-141.1	17	-4.4	1I1Y	-83.9	3	-1.1
	1I1Y	-139.9	4	-4.1	19	-82.8	17	-1.1
	19	-136.5	1QR1	-4.0	9	-80.5	23	-1.1
	1HHG	-132.5	1	-3.9	7	-78.1	9	-1.0
	3	-131.6	1HHG	-2.6	1HHG	-75.7	1	-0.6
	7	-117.7	7	-2.4	3	-74.4	1HHG	-0.1
HLA-A*0201/10	2CLR*	-191.1	2CLR *	-9.7	1	-83.4	2CLR*	-4.3
	1HHH	-159.1	1HHH	-8.0	1HHH	-84.0	1JF1	-2.7
	2	-151.9	2	-7.0	1I4F	-75.6	2	-1.7
	3	-150.7	3	-5.4	1JF1	-95.2	1HHH	-1.5
	1JF1	-150.1	1JF1	-4.9	2	-89.1	1I4F	-1.0
	1	-138.9	1I4F	-4.2	2CLR*	-106.6	1	-0.6
	1I4F	-129.4	1	-3.0	3	-83.2	3	-0.5

Table 4: Ranking of MHC binding and non binding peptides according to their predicted binding affinity by threading using a scoring matrix (MJ & BT) and two distance criteria (Nearest atom < 4.0 A^0 & C-beta< 7.0 A^0). * Structure used as template.

MHC Class I allele/peptide length	Nearest atom < 4.0 A^0				C-beta< 7.0 A^0			
	PDB ID/Peptide ID	MJ	PDB ID/Peptide ID	BT	PDB ID/Peptide ID	MJ	PDB ID/Peptide ID	BT

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H2-Kb/8	5	-196.3	6	-6.60	5	-97.90	6	-1.65
	9	-195.8	1LEG*	-5.15	9	-96.85	1FO0	-1.55
	8	-187.2	1FO0	-5.15	8	-92.35	3	-0.35
	1KJ3	-157.3	7	-4.80	1FO0	-73.95	1VAC*	0.0
	1FO0	-157.0	1S7S	-4.20	6	-73.30	1S7S	0.0
	7	-154.9	1LK2	-3.85	1S7S	-73.10	1S7T	0.05
	1VAC*	-154.8	1OSZ	-3.60	7	-72.60	2	0.05
	1S7S	-154.3	1N59	-3.60	1KJ3	-72.50	1OSZ	0.05
	1S7T	-153.6	1BQH	-3.50	1VAC*	-72.30	1BQH	0.05
	1G6R	-150.2	3	-3.45	1S7T	-72.05	4	0.20
	6	-149.2	9	-3.45	1G6R	-70.75	1LK2	0.20
	1N59	-147.5	2	-3.40	1	-70.05	7	0.20
	1	-146.0	5	-3.40	1N59	-69.35	1N59	0.25
	1LK2	-144.8	1G6R	-3.30	2	-67.40	1KJ3	0.30
	1OSZ	-137.3	1KJ3	-3.25	1LK2	-67.30	5	0.45
	2	-136.7	1VAC*	-2.95	1OSZ	-67.20	1	0.50
	1BQH	-135.4	1S7T	-2.85	1BQH	-65.40	1LEG*	0.55
	1LEG*	-133.4	4	-2.70	3	-61.55	1G6R	0.70
	3	-131.7	1	-2.50	4	-61.30	9	0.75
	4	-127.8	8	-2.10	1LEG*	-59.70	8	0.80
H2-Db/9	9	-178.45	1BZ9	-9	3	-106.6	1BZ9	-6.2
	3	-167.9	1S7W	-7.3	9	-105.55	1S7W	-5.25
	1BZ9	-166.55	1FFN	-6.95	1INQ*	-99.25	1FFN	-4.95
	1JUF	-160.85	1S7X	-6.35	1JUF	-95.2	1FG2	-2.75
	1JPG*	-159.35	4	-6.15	1S7W	-93.2	8	-2.75
	1INQ*	-158.85	9	-6.1	1S7X	-92.15	4	-2.6
	1CE6	-156.95	8	-5.95	1BZ9	-91.85	1INQ*	-2.25
	1QLF	-156.55	3	-5.65	1FFN	-91.85	1CE6	-2.2
	4	-154.7	1FFO	-4.75	1FFO	-90.5	1S7X	-2.15
	1FFO	-147.2	1CE6	-4.7	1FFP	-89.65	1JUF	-2.15
	1	-146.8	1QLF	-4.65	4	-88.85	3	-2.1
	1S7X	-146.25	1JUF	-4.6	1JPG*	-88.2	1JPG*	-2.1
	1S7W	-145.8	1INQ*	-4.6	1FG2	-87.75	1QLF	-2
	1FFP	-143.9	1FG2	-4.4	8	-87.75	1FFO	-1.7
	6	-142.95	1FFP	-3.9	1CE6	-87.5	1FFP	-1.55
	1FFN	-142.3	1	-3.8	1	-87.3	9	-1.45
	2	-142.2	5	-3.3	1QLF	-87	1	-1.25
	5	-141.8	1JPG*	-3.2	2	-86.55	2	-1.2
	1FG2	-137.95	7	-3.15	6	-84.5	6	-0.9
	8	-137.95	6	-2.9	5	-83.95	7	-0.75
	7	-125.75	2	-2.85	7	-76.35	5	0.35
HLA-A*0201/9	18	-198.65	1AO7*	-10.35	18	-112.1	16	-5.05
	10	-196.55	1QRN	-10.2	21	-109.2	10	-4.15
	5	-196.2	1QEW	-9.8	10	-108.2	1QRN	-4.05
	21	-189.75	6	-9.55	5	-107.5	1AO7*	-4.05
	1QRN	-188.55	10	-9.5	6	-105.45	14	-4.05
	1AO7*	-188.05	1QSF	-9.15	15	-101.5	18	-4
	6	-185.1	5	-9	2	-100	6	-3.85
	1QSF	-183.05	1QSE	-8.95	1HHI*	-99.55	1QSF	-3.8
	1QEW	-180.65	18	-8.85	14	-99.05	21	-3.45
	15	-179.2	1B0G	-8.7	1QRN	-98.9	1B0G	-3.2
	1QSE	-178.85	1I7U	-8.55	1B0G	-98.9	5	-3.15
	1HHI*	-176.3	1I7T	-8.5	1I7T	-97.9	1QEW	-3.15
	1B0G	-172.65	21	-8.2	1AO7*	-97.65	1I7T	-3
	2	-172.2	2	-8.05	1I7U	-96.15	1HHI*	-2.95
	1QR1	-171.8	14	-7.85	1QR1	-96.1	2	-2.95
	1I7U	-171.25	1I7R	-7.85	8	-95.7	1I7U	-2.9
	1I7T	-171.25	19	-7.2	1EEY	-95.2	1I1F	-2.75

	1EEY	-169.1	15	-6.35	1QEW	-94.7	1I1Y	-2.75
	23	-167.65	1HHI*	-6.3	1JHT	-94.65	15	-2.7
	12	-166.95	1I1F	-6.1	1QSF	-94.65	1AKJ	-2.6
	14	-166.8	22	-6	12	-91.95	1I7R	-2.6
	8	-164.5	12	-5.9	1QSE	-90.45	11	-2.6
	16	-163.8	8	-5.75	16	-89.8	1JHT	-2.55
	17	-162.8	11	-5.75	20	-89.7	20	-2.45
	1I7R	-160	1I1Y	-5.65	23	-89.25	8	-2.35
	1	-157.55	23	-5.55	1I7R	-88.7	22	-2.35
	1JHT	-157.1	20	-5.5	11	-88	1QSE	-2.3
	1I1F	-155.75	9	-5.35	22	-87.95	12	-2.25
	11	-154.1	16	-5.3	13	-87.45	19	-1.8
	4	-153.9	1AKJ	-5.2	4	-87.4	7	-1.4
	20	-153.75	17	-4.75	1I1F	-86.15	13	-1.35
	1AKJ	-153.05	1JHT	-4.45	17	-85.6	1EEY	-1.35
	13	-152.65	1EEY	-4.35	1AKJ	-85.55	9	-1.05
	22	-150.05	3	-4.3	1	-84.5	4	-1
	9	-148.1	1QR1	-4.05	1I1Y	-83.65	1QR1	-1
	1I1Y	-146.4	1	-3.95	19	-83.15	3	-0.8
	19	-146.05	13	-3.9	9	-80.8	23	-0.8
	1HHG	-139.3	4	-3.7	7	-76.2	17	-0.6
	3	-137.15	7	-2.9	1HHG	-75.9	1	-0.15
	7	-130.35	1HHG	-2.5	3	-74.4	1HHG	-0.05
HLA-A*0201/10	2CLR*	-183.95	2CLR*	-8.5	2CLR*	-121.8	2CLR*	-4.15
	1HHH	-158.85	1HHH	-7.35	1JF1	-108	1JF1	-2.55
	2	-154.45	3	-6.6	2	-107.9	1HHH	-2.05
	3	-153.2	2	-6.3	1HHH	-102.2	2	-1.8
	1JF1	-149.5	1JF1	-4.65	1	-101.7	1I4F*	-1.25
	1	-142.4	1I4F*	-4.4	3	-95.8	3	-1.05
	1I4F*	-132.2	1	-2.45	1I4F*	-87.9	1	-0.3

Table 5 : Ranking of MHC binding and non binding peptides according to their average predicted binding affinity by threading using a scoring matrix (MJ & BT) and two distance criteria (Nearest atom < 4.0 A^0 & C-beta< 7.0 A^0). * Structure used as template.

MHC Class I allele/peptide length	**Nearest atom < 4.0 A^0**				**C-beta< 7.0 A^0(Rank)**			
	PDB ID	**MJ**	**PDB ID**	**BT**	**PDB ID**	**MJ**	**PDB ID**	**BT**
H2-Kb/8	1VAC	13	1LEG	4	1LEG	42	1LEG	40
	1LEG	29	1BQH	59	1VAC	66	1BQH	126
	1BQH	96	1VAC	87	1BQH	92	1VAC	165
H2-Db/9	1INQ	17	1INQ	31	1INQ	6	1INQ	19
	1JPG	79	1JPG	143	1JPG	135	1JPG	89
HLA-A*0201/9	1AO7	1	1AO7	1	1HHI	1	1AO7	4
	1HHI	1	1QEW	5	1QEW	6	1QEW	22
	1QEW	2	1HHI	22	1AO7	8	1HHI	35
	1QR1	5	1QR1	430	1QR1	14	1QR1	325
HLA-A*0201/10	1I4F	104	1I4F	105	1I4F	147	1I4F	142

Table 6: Ranking of MHC binding peptides according to their predicted binding affinity by threading using own template in their source protein sequence for scoring matrices (MJ & BT) and two distance criteria (Nearest atom < 4.0 A^0 & C-beta< 7.0 A^0).