

Supplementary Table 3. Average RMSD (Å) value of the docked complexes according to CABS-dock server. The complexes with average RMSD < 3Å are highlighted in yellow. The complexes highlighted in green did not have the docking prediction succeeded.

allele	pdb	peptide	code	%Rank	OPA prediction	average RMSD
HLA-A*01:01	4NQX	LIDLQELGKY	pep1	0.0943	0.7076	1.4055
HLA-A*01:01	4NQX	NLDSKVGGNV	pep2	0.1041	0.7882	2.5624
HLA-A*01:01	4NQX	GWTAGAAAYY	pep3	0.2305	0.5358	2.6896
HLA-A*01:01	4NQX	QTGKIADYNY	pep4	0.2558	1.5116	5.0924
HLA-A*01:01	4NQX	IGAELVNNNSY	pep5	0.2775	1.2671	1.8515
HLA-A*02:01	4L29	KLNDLCFTNV	pep6	0.2287	2.6927	1.1479
HLA-A*02:01	4L29	FELLHAPATV	pep7	0.3513	0.5982	1.1796
HLA-A*03:01	6O9B	RQIAPGQTGK	pep8	0.0281	1.7893	0.2197
HLA-A*03:01	6O9B	HVTYVPAQEK	pep9	0.1565	1.0786	1.3426
HLA-A*03:01	6O9B	TEILPVSMTK	pep10	0.1664	1.4160	4.3437
HLA-A*03:01	6O9B	SLIDLQELGK	pep11	0.2065	1.0275	1.6195
HLA-A*03:01	6O9B	RASANLAATK	pep12	0.3043	0.6339	3.8388
HLA-A*03:01	6O9B	VTLADAGFIK	pep13	0.3220	0.8702	1.8588
HLA-A*11:01	1X7Q	TEILPVSMTK	pep14	0.0899	1.4160	1.7311
HLA-A*11:01	1X7Q	VTLADAGFIK	pep15	0.1366	0.8702	2.1979
HLA-A*11:01	1X7Q	HVTYVPAQEK	pep16	0.2111	1.0786	1.7008
HLA-A*11:01	1X7Q	RQIAPGQTGK	pep17	0.2413	1.7893	1.9430
HLA-A*11:01	1X7Q	SLIDLQELGK	pep18	0.2777	1.0275	1.9232
HLA-A*11:01	1X7Q	RASANLAATK	pep19	0.3951	0.6339	3.0145
HLA-A*24:02	2BCK	TYVPAQEKNF	pep24	0.0424	0.7276	2.0925
HLA-A*24:02	2BCK	GYLQPRTFLL	pep25	0.2671	0.7535	2.9333
HLA-A*24:02	2BCK	CYFPLQSYGF	pep27	0.4313	0.7776	2.2579
HLA-B*07:02	5EO0	TPCSFGGVSV	pep59	0.3909	1.7080	2.7139
HLA-B*07:02	5EO0	LPIGINITRF	pep60	0.4512	1.3027	1.2501
HLA-B*07:02	5EO0	QPYRVVLSF	pep61	0.4916	0.8458	0.4823
HLA-A*68:01	6PBH	STGSNVFQTR	pep64	0.2211	0.5411	1.7305
HLA-A*68:01	6PBH	HVTYVPAQEK	pep65	0.2517	1.0786	1.1007
HLA-A*68:01	6PBH	HVSGTNGTKR	pep66	0.3046	0.8315	4.9815
HLA-A*68:01	6PBH	DLPIGINITR	pep67	0.3285	1.8171	2.2309
HLA-A*68:01	6PBH	NTQEVFAQVK	pep68	0.3695	0.5676	0.4723
HLA-A*68:01	6PBH	DIADTTDAVR	pep69	0.4165	0.8147	2.9764
HLA-B*51:01	5VUE	VAYSNNSIAI	pep70	0.4565	1.0545	1.2241
HLA-B*18:01	6MT3	DGEWVLLSTF	pep71	0.3204	0.6551	2.2091
HLA-B*35:01	1XH3	LPIGINITRF	pep72	0.0959	1.3027	2.2773
HLA-B*35:01	1XH3	QIPFAMQMAY	pep73	0.2719	1.2149	1.6030
HLA-B*35:01	1XH3	LPPFSNVTWF	pep74	0.3944	0.6567	0.6794
HLA-B*35:01	1XH3	FPNITNLCPF	pep75	0.4307	1.3964	2.4222
HLA-B*44:03	4JQX	SETKCTLKSF	pep76	0.1588	0.6433	0.3948
HLA-B*14:02	3BVN	IVRFPNITNL	pep77	0.2910	0.5548	3.1800
HLA-B*44:02	1M6O	SETKCTLKSF	pep78	0.1215	0.6433	1.2068
HLA-B*44:02	1M6O	TESNKKFLPF	pep79	0.4851	1.0405	1.4687
HLA-C*07:02	5VGE	IVRFPNITNL	pep80	0.1895	0.5548	2.2266

HLA-A*23:01	swissmodel	TYVPAQEKNF	pep81	0.0366	0.7276	2.5229
HLA-A*23:01	swissmodel	GYLQPRTFLL	pep82	0.2811	0.7535	1.3508
HLA-A*23:01	swissmodel	CYFPLQSYGF	pep83	0.3803	0.7776	2.8308
HLA-A*23:01	swissmodel	IYSKHTPINL	pep84	0.3931	1.2064	0.5184
HLA-A*26:01	swissmodel	EILDITPCSF	pep85	0.1991	1.2698	1.7413
HLA-A*26:01	swissmodel	DSKVGGNYYN	pep86	0.2352	1.1165	1.6759
HLA-A*26:01	swissmodel	GWTAGAAAYY	pep87	0.2372	0.5358	1.9260
HLA-A*26:01	swissmodel	QIPFAMQMAY	pep88	0.4428	1.2149	NA
HLA-A*30:02	swissmodel	KVGGNYNYLY	pep89	0.1005	0.5338	1.3099
HLA-A*30:02	swissmodel	GWTAGAAAYY	pep90	0.1282	0.5358	1.8117
HLA-A*30:02	swissmodel	GFQPTNGVGY	pep91	0.2566	0.5547	1.7471
HLA-A*30:02	swissmodel	IGAEHVNSY	pep92	0.4353	1.2671	1.5989
HLA-A*31:01	swissmodel	STGSNVFQTR	pep93	0.3125	0.5411	1.6854
HLA-A*31:01	swissmodel	ASVYAWNRKR	pep94	0.3300	0.6453	2.3548
HLA-A*31:01	swissmodel	AYYVGYLQPR	pep95	0.4215	1.3309	4.4794
HLA-A*31:01	swissmodel	RKSNLKPFER	pep96	0.4348	0.8187	2.4331
HLA-B*35:03	swissmodel	LPIGINTRF	pep97	0.1519	1.3027	2.0459
HLA-B*35:03	swissmodel	LPFFSNVTWF	pep98	0.4127	0.6567	0.4809
HLA-B*38:01	swissmodel	HSAWVSHYPQF	pep99	0.2475	0.7170	1.6149
HLA-B*38:01	swissmodel	VRDPQTLEIL	pep100	0.2967	0.5446	4.0586
HLA-B*38:01	swissmodel	YVRKDGEWVL	pep101	0.3421	0.7238	1.3576
HLA-C*05:01	swissmodel	AVRDPQTLEI	pep102	0.1321	0.7083	3.4736
HLA-C*05:01	swissmodel	LVDLPIGINI	pep103	0.1770	1.3499	0.2044
HLA-C*05:01	swissmodel	TLDSKTQSLI	pep104	0.4872	0.8490	1.0923
HLA-C*07:01	swissmodel	IVRFPNITNL	pep105	0.1311	0.5548	4.0092
HLA-C*07:01	swissmodel	YVRKDGEWVL	pep106	0.2665	0.7238	2.4440
HLA-C*07:01	swissmodel	VRKDGEWVLL	pep107	0.4792	0.7326	0.7123
HLA-C*08:02	swissmodel	AVRDPQTLEI	pep108	0.4053	0.7083	1.3442
HLA-C*15:02	swissmodel	AVRDPQTLEI	pep109	0.4849	0.7083	2.5140
HLA-C*17:01	swissmodel	LVDLPIGINI	pep110	0.4774	1.3499	1.3017
HLA-A*24:02	2BCK	IYSKHTPINL	pep111	0.2880	1.2064	NA