Design of novel multi-epitope vaccines against Severe Acute respiratory syndrome validated through multistage molecular interaction and dynamics

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Supplementary table S1. Protein sequence retrieval, tertiary structures retrieval and homology modeling of chosen SARS-CoV proteins. SARS-CoV protein sequences were retrieved from NCBI. Available structure files (pdb) for SARS-CoV proteins were retrieved from RCSB PDB. SARS-CoV proteins with no tertiary structure available were subjected to homology modeling by Swissmodel.

S.No	SARS-CoV Protein	Number of sequence retrieved from NCBI/PDB	PDB ID of Available Structure	Template used for modeling	QMEAN
1	3a	47	-	5t77	- 2.29
2	3b	46	-	3qaz	- 0.09
3	7a	51	-	1xak	- 0.20
4	7b	57	-	5xtc	- 4.43
5	8a	45	-	3j2w	- 1.85
6	8b	45	-	5vz4	- 1.30
7	9b	46	2cme	-	-
8	Envelope	212	5x29	-	-
9	Membrane	170	-	4nv4	- 3.61
10	Nucleocapsid	194	2gib	4ud1	0.58
11	Spike	269	5xlr	-	-

Supplementary table S2. Shortlisted high scoring CTL epitopes. Selected high scoring CTL epitopes and their respective HLA alleles binders are listed above. *In-silico* analysis have shown all the selected epitopes to be non-toxic (Non-Toxin) as well as they show significant conservancy.

S.No	SARS-CoV Proteins	Epitope	IEDB epitope ID	Position	Length	HLA Class I Alleles	Percent of protein sequence matches at 100% identity (Conservancy)	ToxinPred Study
1	3a	MEAQFLYLY	41300	101-109	9	B*44:03, B*44:02	100.00% (4/4)	Non-Toxin
2	3a	YLYALIYFL	75003	107-115	9	A*02:01, A*02:06	100.00% (4/4)	Non-Toxin
3	3b	SLYMAISPKF	-	61-70	10	A*23:01, B*15:01, A*24:02	100.00% (3/3)	Non-Toxin
4	3b	LYMAISPKF	40855	62-70	9	A*23:01, A*24:02	100.00% (3/3)	Non-Toxin
5	7a	ALTCTSTHF	-	55-63	9	B*15:01	62.50% (5/8)	Non-Toxin
6	7b	TLIDFYLCFL	64842	5-14.	10	A*02:01	60.00% (3/5)	Non-Toxin
7	8a	SLCSCICTV	59033	11-19.	9	A*02:03	100.00% (1/1)	Non-Toxin
8	8b	ALIARCWYL	2618	55-63	9	A*02:01	100.00% (1/1)	Non-Toxin
9	9b	KVYPIILRL	-	41-49	9	A*32:01	100.00% (2/2)	Non-Toxin
10	Envelope	SLVKPTVYVY	-	50-59	10	B*15:01	92.86% (13/14)	Non-Toxin
11	Membrane	MWLSYFVASF	43014	90-99	10	A*23:01	86.67% (13/15)	Non-Toxin
12	Membrane	SYFVASFRLF	62549	93-102	10	A*23:01, A*24:02	86.67% (13/15)	Non-Toxin
13	Nucleocapsid	AQFAPSASAF	-	306-315	10	B*15:01	100.00% (17/17)	Non-Toxin
14	Nucleocapsid	TPSGTWLTY	65763	326-334	9	B*35:01	94.12% (16/17)	Non-Toxin
15	Spike	LTQDLFLPFY	40134	54-63	10	A*01:01	98.88% (88/89)	Non-Toxin
16	Spike	IPFKDGIYF	-	81-89	9	B*35:01	98.88% (88/89)	Non-Toxin
17	Spike	NAFNCTFEY	43144	155-163	9	B*35:01	97.75% (87/89)	Non-Toxin
18	Spike	LYNSTFFSTF	40884	355-364	10	A*23:01, A*24:02	70.79% (63/89)	Non-Toxin
19	Spike	STFFSTFKCY	-	358-367	10	A*11:01, A*30:02	70.79% (63/89)	Non-Toxin
20	Spike	CYWPLNDYGF	7451	474-483	10	A*23:01	60.67% (54/89)	Non-Toxin
21	Spike	WPLNDYGFY	-	476-484	9	B*35:01	60.67% (54/89)	Non-Toxin
22	Spike	RIYSTGNNVF	-	620-629	10	B*15:01	97.75% (87/89)	Non-Toxin
23	Spike	LGADSSIAY	36050	681-689	9	B*35:01	98.88% (88/89)	Non-Toxin
24	Spike	RSFIEDLLF	-	797-805	9	B*58:01	97.75% (87/89)	Non-Toxin
25	Spike	LLTDDMIAAY	-	846-855	10	A*01:01	93.26% (83/89)	Non-Toxin
26	Spike	LTDDMIAAY	39837	847-855	9	A*01:01	93.26% (83/89)	Non-Toxin
27	Spike	QIPFAMQMAY	-	877-886	10	B*35:01	100.00% (89/89)	Non-Toxin
28	Spike	IPFAMQMAY	-	878-886	9	B*35:01	100.00% (89/89)	Non-Toxin
29	Spike	FAMQMAYRF	-	880-888	9	B*35:01	100.00% (89/89)	Non-Toxin
30	Spike	AYFPREGVFVF	-	1069-1079	11	A*23:01	98.88% (88/89)	Non-Toxin
31	Spike	FPREGVFVF	17382	1071-1079	9	B*35:01	98.88% (88/89)	Non-Toxin
32	Spike	KWPWYVWLGF	-	1193-1202	10	A*23:01, A*24:02	100.00% (89/89)	Non-Toxin

Supplementary table S3. Shortlisted high scoring HTL epitopes. Selected high scoring HTL epitopes and their respective HLA alleles binders are listed above. *In-silico* analysis have shown all the selected epitopes to be non-toxic (Non-Toxin) as well as they show significant conservancy.

S.No	SARS Protein	Epitope	IEDB epitope ID	Position	Length	HLA Class II Alleles	Percent of protein sequence matches at 100% identity (Conservancy)	ToxinPred Study
1	3a	AQFLYLYALIYFLQC	-	103-117	15	DPA1*01:03 DPB1*02:01 DPA1*01 DPB1*04:01	100.00% (4/4)	Non-Toxin
2	3a	QFLYLYALIYFLQCI	50803	104-118	15	DPA1*01:03 DPB1*02:01 DPA1*01 DPB1*04:01	100.00% (4/4)	Non-Toxin
3	3b	TMSLYMAISPKFTTS	65259	59-73	15	DRB1*09:01	100.00% (3/3)	Non-Toxin
4	7a	SPLFLIVAALVFLIL	60111	99-113	15	DPA1*01:03 DPB1*02:01 DPA1*01 DPB1*04:01	25.00% (2/8)	Non-Toxin
5	7a	PLFLIVAALVFLILC	48324	100-114	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	25.00% (2/8)	Non-Toxin
6	7a	LFLIVAALVFLILCF	-	101-115	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	25.00% (2/8)	Non-Toxin
7	7a	FLIVAALVFLILCFT	-	102-116	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	25.00% (2/8)	Non-Toxin
8	7a	LIVAALVFLILCFTI	-	103-117	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	25.00% (2/8)	Non-Toxin
9	7b	TLIDFYLCFLAFLLF	-	5-19.	15	DPA1*01:03 DPB1*02:01 DPA1*01 DPB1*04:01	60.00% (3/5)	Non-Toxin
10	7b	LIDFYLCFLAFLLFL	-	6-20.	15	DPA1*01:03 DPB1*02:01 DPA1*01 DPB1*04:01	80.00% (4/5)	Non-Toxin
11	7b	IDFYLCFLAFLLFLV	-	7-21.	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	80.00% (4/5)	Non-Toxin

12	7b	DFYLCFLAFLLFLVL	-	8-22.	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	80.00% (4/5)	Non-Toxin
13	7b	FYLCFLAFLLFLVLI	-	9-23.	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	80.00% (4/5)	Non-Toxin
14	7b	YLCFLAFLLFLVLIM	74578	10-24.	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	80.00% (4/5)	Non-Toxin
15	7b	LCFLAFLLFLVLIML	-	11-25.	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPA1*01 DPB1*04:01	80.00% (4/5)	Non-Toxin
16	7b	CFLAFLLFLVLIMLI	-	12-26.	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	60.00% (3/5)	Non-Toxin
17	7b	FLAFLLFLVLIMLII	16500	13-27	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	60.00% (3/5)	Non-Toxin
18	8a	MKLLIVLTCISLCSC	41859	1-15.	15	DRB1*11:01	100.00% (1/1)	Non-Toxin
19	8b	ALGKVLPFHRWHTMV	-	23-37	15	DRB5*01:01	100.00% (1/1)	Non-Toxin
20	9b	VVPPALHLVDPQIQL	-	8-22.	15	DRB3*01:01	100.00% (2/2)	Non-Toxin
21	Envelope	NSVLLFLAFVVFLLV	-	15-29	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	71.43% (10/14)	Non-Toxin
22	Envelope	SVLLFLAFVVFLLVT	62216	16-30	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	64.29% (9/14)	Non-Toxin
23	Envelope	VLLFLAFVVFLLVTL	69592	17-31	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	64.29% (9/14)	Non-Toxin
24	Envelope	LLFLAFVVFLLVTLA	-	18-32	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	64.29% (9/14)	Non-Toxin

25	Envelope	LFLAFVVFLLVTLAI	-	19-33	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	64.29% (9/14)	Non-Toxin
26	Envelope	FLAFVVFLLVTLAIL	16503	20-34	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	71.43% (10/14)	Non-Toxin
27	Envelope	LAFVVFLLVTLAILT	34768	21-35	15	DPA1*01:03 DPB1*02:01 DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	71.43% (10/14)	Non-Toxin
28	Membrane	WNLVIGFLFLAWIML	-	19-33	15	DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	73.33% (11/15)	Non-Toxin
29	Membrane	NLVIGFLFLAWIMLL	-	20-34	15	DPA1*03:01 DPB1*04:02 DPA1*01 DPB1*04:01	73.33% (11/15)	Non-Toxin
30	Nucleocapsid	GTRNPNNNAATVLQL	-	148-162	15	DQA1*01:02 DQB1*06:02	94.12% (16/17)	Non-Toxin
31	Spike	MFIFLLFLTLTSGSD	41503	1-15.	15	DPA1*01:03 DPB1*02:01 DPA1*01 DPB1*04:01	85.39% (76/89)	Non-Toxin
32	Spike	GYQPYRVVVLSFELL	-	490-504	15	DPA1*01:03 DPB1*02:01	97.75% (87/89)	Non-Toxin
33	Spike	YQPYRVVVLSFELLN	-	491-505	15	DPA1*01:03 DPB1*02:01	97.75% (87/89)	Non-Toxin
34	Spike	QPYRVVVLSFELLNA	-	492-506	15	DPA1*01:03 DPB1*02:01	98.88% (88/89)	Non-Toxin
35	Spike	PYRVVVLSFELLNAP	-	493-507	15	DPA1*01:03 DPB1*02:01	98.88% (88/89)	Non-Toxin
36	Spike	YRVVVLSFELLNAPA	-	494-508	15	DPA1*01:03 DPB1*02:01	98.88% (88/89)	Non-Toxin

Supplementary table S4. World population coverage by the shortlisted CTL and HTL epitopes combined. With a standard deviation of 25.88 on an average 85.21 % of world population could be covered by the joint administration of selected CTL and HTL epitopes as vaccine candidate.

a projected population coverage
b average number of epitope hits / HLA combinations recognized by the population
c minimum number of epitope hits / HLA combinations recognized by 90% of the population

Population/Area	Class I & II combined		
	coverage[a]	average_hit[b]	pc90[c]
Austria	99.33%	35.03	17.04
Belarus	27.09%	0.27	0.14
Belgium	99.03%	31.56	5.81
Borneo	39.34%	10.08	2.42
Bulgaria	94.35%	5.38	1.48
Canada	2.25%	0.02	0.1
Central Africa	99.71%	51.05	23.36
Central America	94.41%	19.21	19.05
China	98.82%	35.92	4.8
Croatia	96.04%	6.47	1.94
Czech Republic	99.5%	36.59	22.03
Denmark	58.23%	0.71	0.24
East Africa	99.45%	42.6	20.66
East Asia	98.29%	26.13	4.04
England	99.7%	33.75	9.22
Europe	99.97%	60.33	34.2
Finland	99.44%	35.48	13.76
France	99.99%	62.23	36.8
Georgia	98.87%	31.98	5.81
Germany	99.72%	34.89	11.61
Greece	96.82%	32.64	19.53
Hong Kong	90.27%	3.25	1.01
India	99.42%	53.26	29.48
Indonesia	92.27%	14.27	1.16
Iran	90.26%	4.22	1.01
Ireland Northern	99.71%	34.79	23.07
Ireland South	99.65%	33.5	19.52
Israel	84.02%	3.91	0.63
Italy	98.31%	29.45	4.19
Japan	99.23%	41.01	7.09
Jordan	81.67%	2.89	0.55
Korea; South	97.49%	16.89	2.36
Lebanon	95.11%	32.27	19.27
Macedonia	72.67%	1.05	0.37
Malaysia	91.03%	16.96	1.09
Mexico	100.0%	59.0	49.08
Mongolia	98.81%	32.82	8.37
Netherlands	94.02%	28.61	1.81
North Africa	97.75%	30.28	4.12
North America	99.99%	58.12	34.32
Northeast Asia	98.88%	35.93	4.83
Norway	96.4%	29.37	19.13
Oceania	99.43%	43.58	7.88
Oman	90.69%	4.44	1.04
Pakistan	79.95%	2.42	0.5
Philippines	93.71%	4.57	1.56
Poland	96.53%	6.06	2.01
Portugal	93.57%	5.58	1.36
Romania	92.88%	5.98	1.36
Russia	99.99%	67.31	49.97
Saudi Arabia	97.9%	30.73	8.03
Scotland	68.25%	0.96	0.31
Serbia	35.2%	1.91	0.15

Singapore	93.6%	14.3	1.24
Slovakia	59.71%	23.23	-7.18
Slovenia	99.9%	58.54	31.82
South Africa	0.31%	3.35	-714.81
South America	98.69%	46.09	21.66
South Asia	99.56%	53.48	29.68
Southeast Asia	95.96%	12.57	1.52
Southwest Asia	98.24%	33.66	19.22
Spain	99.78%	53.13	30.56
Sri Lanka	52.39%	1.2	0.21
Sweden	99.99%	65.24	48.66
Taiwan	97.73%	14.35	1.94
Thailand	95.05%	12.36	1.3
Turkey	73.09%	1.97	0.37
Ukraine	33.58%	0.34	0.15
United Arab Emirates	2.19%	0.11	0.51
United Kingdom	68.78%	21.39	-9.36
United States	100.0%	58.13	33.93
Vietnam	88.6%	3.16	0.88
Wales	1.0%	0.01	0.1
West Africa	97.41%	30.85	3.1
West Indies	95.45%	6.25	1.57
World	99.39%	45.44	20.76
Average	85.21	24.83	1.03
Standard deviation	25.88	20.07	83.75

Supplementary table S5. Shortlisted B Cell epitopes. BepiPred Linear B Cell epitopes showing sequence overlap with CTL and HTL epitopes are shortlisted above. *In-silico* analysis have shown all the selected epitopes to be non-toxic (Non-Toxin) as well as they show significant amino acid sequence conservancy.

S.No.	SARS-CoV Protein	B Cell Epitope	Position	Length	Percent of protein sequence matches at 100% identity (Conservancy)	ToxinPred Study
1	3b	AISPKFTTSL	65-74	10	100.00% (3/3)	Non-Toxin
2	7b	MNELTLI	1-7.	7	80.00% (4/5)	Non-Toxin
3	8b	VQTCTPNVTINCQDPAGGAL	37-56	20	100.00% (1/1)	Non-Toxin
4	9b	MDPNQTNVVP	1-10.	10	100.00% (2/2)	Non-Toxin
5	9b	DAMGQGQNSADPKV	29-42	14	100.00% (2/2)	Non-Toxin
6	Nucleocapsid	DHIGTRNPNNN	145-155	11	100.00% (17/17)	Non-Toxin
7	Spike	HTFGNPVIPFK	74-84	11	60.67% (54/89)	Non-Toxin
8	Spike	YFAATEKSNV	88-97	10	98.88% (88/89)	Non-Toxin
9	Spike	YGFYTTTGIGYQ	481-492	12	66.29% (59/89)	Non-Toxin
10	Spike	ATVCGPKLSTD	508-518	11	98.88% (88/89)	Non-Toxin
11	Spike	RIYSTGNNVFQT	620-631	12	97.75% (87/89)	Non-Toxin
12	Spike	SLGADSSIAYSNNTIAIP	680-697	18	98.88% (88/89)	Non-Toxin
13	Spike	ILPDPLKPTKRS	787-798	12	93.26% (83/89)	Non-Toxin
14	Spike	KAYFP	1068-1072	5	98.88% (88/89)	Non-Toxin

Supplementary table S6. CTL epitope prediction. Detailed scoring of all screened CTL epitopes and their respective HLA class I allele binders. CTL epitopes were chosen on the basis of high "Total score" and higher number of HLA allele binders. Total score is a combined score of TAP score, MHC score, Proteasome score and Processing score.

S.No.	SARS-CoV Protein	Epitope	HLA Class I Alleles	Proteasome Score	TAP Score	MHC Score	Processing Score	Total Score	MHC IC50[nM]	Immunogenicity-Score
1	3a	MEAQFLYLY	B*44:03	1.43	1.23	-0.78	2.66	1.88	6	-0.0099
			B*44:02	1.43	1.23	-1.00	2.66	1.66	10.1	-0.0099
2	3a	YLYALIYFL	A*02:01	1.47	0.52	-0.40	1.99	1.59	2.5	0.21793
			A*02:06	1.47	0.52	-0.60	1.99	1.39	4	0.21793
3	3b	SLYMAISPKF	A*23:01	1.35	1.23	-0.96	2.57	1.61	9.2	-0.30129
			B*15:01	1.35	1.23	-1.10	2.57	1.47	12.6	-0.30129
			A*24:02	1.35	1.23	-1.12	2.57	1.45	13.2	-0.30129
4	3b	LYMAISPKF	A*23:01	1.35	1.27	-0.70	2.61	1.92	5	-0.17912
			A*24:02	1.35	1.27	-0.91	2.61	1.70	8.2	-0.17912
5	7a	ALTCTSTHF	B*15:01	1.48	1.11	-1.37	2.59	1.21	23.7	-0.10792
6	7b	TLIDFYLCFL	A*02:01	1.70	0.47	-0.93	2.17	1.24	8.6	0.18838
7	8a	SLCSCICTV	A*02:03	1.09	0.17	-0.89	1.27	0.37	7.8	-0.13401
8	8b	ALIARCWYL	A*02:01	1.39	0.50	-0.76	1.89	1.13	5.8	0.267
9	9b	KVYPIILRL	A*32:01	1.51	0.54	-1.13	2.05	0.92	13.5	0.2634
10	Envelope	SLVKPTVYVY	B*15:01	1.51	1.36	-1.50	2.87	1.37	31.5	-0.11674
11	Membrane	MWLSYFVASF	A*23:01	1.38	1.26	-0.90	2.63	1.73	8	-0.08445
12	Membrane	SYFVASFRLF	A*23:01	1.25	1.31	-0.56	2.56	2.00	3.6	0.10394
			A*24:02	1.25	1.31	-0.79	2.56	1.78	6.1	0.10394
13	Nucleocapsid	AQFAPSASAF	B*15:01	1.23	1.25	-0.70	2.48	1.78	5	-0.17446
14	Nucleocapsid	TPSGTWLTY	B*35:01	1.53	1.15	-0.84	2.67	1.83	6.9	0.24003
15	Spike	LTQDLFLPFY	A*01:01	1.52	1.23	-1.05	2.74	1.70	11.2	0.13652
16	Spike	IPFKDGIYF	B*35:01	1.39	1.05	-0.82	2.44	1.62	6.6	-0.01534
17	Spike	NAFNCTFEY	B*35:01	1.11	1.30	-0.59	2.41	1.82	3.9	0.17283
18	Spike	LYNSTFFSTF	A*23:01	1.38	1.20	-0.75	2.57	1.82	5.6	-0.02351
			A*24:02	1.38	1.20	-0.88	2.57	1.70	7.5	-0.02351
19	Spike	STFFSTFKCY	A*11:01	1.48	1.39	-1.34	2.87	1.53	22	-0.0708
			A*30:02	1.48	1.39	-1.46	2.87	1.41	28.7	-0.0708
20	Spike	CYWPLNDYGF	A*23:01	1.44	1.33	-1.10	2.78	1.68	12.5	0.0812
21	Spike	WPLNDYGFY	B*35:01	1.34	1.11	-0.85	2.45	1.60	7	0.10501
22	Spike	RIYSTGNNVF	B*15:01	1.53	1.32	-1.21	2.85	1.64	16.3	-0.0843
23	Spike	LGADSSIAY	B*35:01	1.60	1.19	-1.20	2.79	1.59	15.9	-0.14663
24	Spike	RSFIEDLLF	B*58:01	1.23	1.32	-0.72	2.54	1.82	5.3	0.27446
25	Spike	LLTDDMIAAY	A*01:01	1.38	1.20	-0.94	2.58	1.64	8.7	0.06668
26	Spike	LTDDMIAAY	A*01:01	1.38	1.21	-0.63	2.59	1.95	4.3	0.03968
27	Spike	QIPFAMQMAY	B*35:01	1.42	1.35	-1.16	2.77	1.61	14.5	-0.25308
28	Spike	IPFAMQMAY	B*35:01	1.42	1.17	-0.36	2.60	2.24	2.3	-0.32801
29	Spike	FAMQMAYRF	B*35:01	1.45	1.05	-0.80	2.50	1.70	6.3	-0.28061
30	Spike	AYFPREGVFVF	A*23:01	1.44	1.37	-1.17	2.81	1.64	14.8	0.36952
31	Spike	FPREGVFVF	B*35:01	1.44	0.93	-0.51	2.37	1.86	3.2	0.31233
32	Spike	KWPWYVWLGF	A*23:01	1.26	1.25	-1.03	2.51	1.48	10.8	0.47484
			A*24:02	1.26	1.25	-1.13	2.51	1.39	13.4	0.47484

Supplementary table S7. HTL epitope prediction. Percentile rank of HTL epitopes and their respective HLA class II allele binders. HTL epitopes were screened on the basis of percentile rank (lower the percentile number, higher the rank) and larger number of HLA allele binders. Last column show the method used for epitope screening.

S.No	SARS-CoV Protein	Epitope	HLA Class II Alleles	Percentile rank	Method used
1	3a	AQFLYLYALIYFLQC	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
2	3a	QFLYLYALIYFLQCI	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
3	3b	TMSLYMAISPKFTTS	DRB1*09:01	0.01	Consensus (comb.lib./smm/nn)
4	7a	SPLFLIVAALVFLIL	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
5	7a	PLFLIVAALVFLILC	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
6	7a	LFLIVAALVFLILCF	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
7	7a	FLIVAALVFLILCFT	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
8	7a	LIVAALVFLILCFTI	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
9	7b	TLIDFYLCFLAFLLF	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
10	7b	LIDFYLCFLAFLLFL	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
11	7b	IDFYLCFLAFLLFLV	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
12	7b	DFYLCFLAFLLFLVL	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
13	7b	FYLCFLAFLLFLVLI	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
14	7b	YLCFLAFLLFLVLIM	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
15	7b	LCFLAFLLFLVLIML	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
16	7b	CFLAFLLFLVLIMLI	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
17	7b	FLAFLLFLVLIMLII	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
18	8a	MKLLIVLTCISLCSC	DRB1*11:01	0.75	Consensus (smm/nn/sturniolo)
19	8b	ALGKVLPFHRWHTMV	DRB5*01:01	0.79	Consensus (smm/nn/sturniolo)
20	9b	VVPPALHLVDPQIQL	DRB3*01:01	0.03	Consensus (comb.lib./smm/nn)
21	Envelope	NSVLLFLAFVVFLLV	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
22	Envelope	SVLLFLAFVVFLLVT	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
23	Envelope	VLLFLAFVVFLLVTL	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)

24	Envelope	LLFLAFVVFLLVTLA	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
25	Envelope	LFLAFVVFLLVTLAI	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
26	Envelope	FLAFVVFLLVTLAIL	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
27	Envelope	LAFVVFLLVTLAILT	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
28	Membrane	WNLVIGFLFLAWIML	DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
29	Membrane	NLVIGFLFLAWIMLL	DPA1*03:01/DPB1*04:02	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
30	Nucleocapsid	GTRNPNNNAATVLQL	DQA1*01:02/DQB1*06:02	0.01	Consensus (comb.lib./smm/nn)
31	Spike	MFIFLLFLTLTSGSD	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
			DPA1*01/DPB1*04:01	0.01	Consensus (comb.lib./smm/nn)
32	Spike	GYQPYRVVVLSFELL	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
33	Spike	YQPYRVVVLSFELLN	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
34	Spike	QPYRVVVLSFELLNA	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
35	Spike	PYRVVVLSFELLNAP	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)
36	Spike	YRVVVLSFELLNAPA	DPA1*01:03/DPB1*02:01	0.01	Consensus (comb.lib./smm/nn)

Supplementary table S8. Homology modeling for HLA alleles. Tertiary structure of HLA alleles were modeled by homology modeling using SwissModel server. Templates were chosen with highest sequence identity. Generated models with acceptable QMEAN value were chosen for further studies.

S.No	HLA Class I Allele	Template used for modeling	% sequence identity	QMEAN
1	A0201	2vlj.1.A	100%	-1.03
2	A0203	3ox8.1.A	100%	-0.59
3	A2301	2bck.1.A	98.91%	-0.01
4	A2402	2bck.1.A	100%	-0.02
5	B1501	5txs.1.A	100%	0.14
6	B3501	1a9b.1.A	100%	-0.60
7	A0206	4l3c.11.A	99.64%	0.02
8	B4402	1m6o.1.A	100%	0.75
9	B4403	4jqx.1.A	100%	0.64
S.No	HLA Class II Allele	Template used for modeling	% sequence identity	QMEAN
1	DPA-101	4p5m.3.A	100%	(-)1.45
2	DPA1-0103	4p4r.1.A	100%	(-)0.73
3	DPA1-0201	3wex.1.A	99.45%	(-)0.01
4	DPB1-0401	4p57.1.B	9684%	(-)0.88
5	DRB1-0901	3pgd.1.B	91.41%	(-)0.44
6	DPB1-0201	4p5m.1.B	98.42%	(-)0.37
7	DRB1-1101	6atf.1.B	96.32%	0.65

Supplementary table S9. INF-γ epitopes from CTL and HTL MEVs. INF-γ inducing (POSITIVE) epitopes from CTL and HTL MEVs were screened by using "Motif and SVM hybrid" (MERCI & SVM) approaches.

CLT Epitopes also predicted to be IFN-gamma epitopes					
S.No	**Start-END**	**Sequence**	**Method**	**Result**	**Score**
1	68-82	RWANQCIFGHSPRQQ	MERCI	POSITIVE	2
2	69-83	WANQCIFGHSPRQQR	MERCI	POSITIVE	2
3	70-84	ANQCIFGHSPRQQRE	MERCI	POSITIVE	2
4	71-85	NQCIFGHSPRQQREG	MERCI	POSITIVE	2
5	72-86	QCIFGHSPRQQREGV	MERCI	POSITIVE	2
6	84-98	EGVGENVYAYWSSVS	MERCI	POSITIVE	1
7	85-99	GVGENVYAYWSSVSV	MERCI	POSITIVE	2
8	121-135	LYENNPSNNMTWKVA	MERCI	POSITIVE	1
9	122-136	YENNPSNNMTWKVAG	MERCI	POSITIVE	1
10	123-137	ENNPSNNMTWKVAGQ	MERCI	POSITIVE	2
11	124-138	NNPSNNMTWKVAGQG	MERCI	POSITIVE	2
12	125-139	NPSNNMTWKVAGQGV	MERCI	POSITIVE	1
13	126-140	PSNNMTWKVAGQGVL	MERCI	POSITIVE	1
14	127-141	SNNMTWKVAGQGVLH	MERCI	POSITIVE	1
15	206-220	SALTCTSTHFGGGGS	MERCI	POSITIVE	3
16	290-304	GGSMWLSYFVASFGG	MERCI	POSITIVE	1
17	291-305	GSMWLSYFVASFGGG	MERCI	POSITIVE	1
18	292-306	SMWLSYFVASFGGGG	MERCI	POSITIVE	1
19	317-331	FGGGGSAQFAPSASA	SVM	POSITIVE	1.4
20	318-332	GGGGSAQFAPSASAF	SVM	POSITIVE	1.3
21	319-333	GGGSAQFAPSASAFG	SVM	POSITIVE	1.2
22	320-334	GGSAQFAPSASAFGG	SVM	POSITIVE	1.2
23	321-335	GSAQFAPSASAFGGG	SVM	POSITIVE	1.2
24	322-336	SAQFAPSASAFGGGG	SVM	POSITIVE	1.3
25	338-352	TPSGTWLTYGGGGSL	SVM	POSITIVE	1
26	339-353	PSGTWLTYGGGGSLT	SVM	POSITIVE	1.1
27	391-405	GGGSLYNSTFFSTFG	MERCI	POSITIVE	1
28	392-406	GGSLYNSTFFSTFGG	MERCI	POSITIVE	1
29	403-417	TFGGGGSSTFFSTFK	MERCI	POSITIVE	1
30	404-418	FGGGGSSTFFSTFKC	MERCI	POSITIVE	1
31	405-419	GGGGSSTFFSTFKCY	MERCI	POSITIVE	1
32	406-420	GGGSSTFFSTFKCYG	MERCI	POSITIVE	1
33	407-421	GGSSTFFSTFKCYGG	MERCI	POSITIVE	1
34	408-421	GSSTFFSTFKCYGGG	MERCI	POSITIVE	1
35	409-423	SSTFFSTFKCYGGGG	MERCI	POSITIVE	1
36	410-424	STFFSTFKCYGGGGS	MERCI	POSITIVE	1
37	461-475	NVFGGGGSLGADSSI	SVM	POSITIVE	1.1
38	462-476	VFGGGGSLGADSSIA	SVM	POSITIVE	1.2
39	464-478	GGGGSLGADSSIAYG	SVM	POSITIVE	1.1
40	465-479	GGGSLGADSSIAYGG	SVM	POSITIVE	1.1
41	466-480	GGSLGADSSIAYGGG	SVM	POSITIVE	1.1
42	467-481	GSLGADSSIAYGGGG	SVM	POSITIVE	1.1
43	468-482	SLGADSSIAYGGGGS	SVM	POSITIVE	1.1
44	542-556	PFAMQMAYGGGGSFA	SVM	POSITIVE	1.2
45	543-557	FAMQMAYGGGGSFAM	SVM	POSITIVE	1.2
46	544-558	AMQMAYGGGGSFAMQ	SVM	POSITIVE	1.1
47	545-559	MQMAYGGGGSFAMQM	SVM	POSITIVE	1
48	546-560	QMAYGGGGSFAMQMA	SVM	POSITIVE	1.1
49	647-661	MAYGGGGSFAMQMAY	SVM	POSITIVE	1
50	548-562	AYGGGGSFAMQMAYR	SVM	POSITIVE	1.1
51	570-584	YFPREGVFVFGGGGS	SVM	POSITIVE	1
52	571-585	FPREGVFVFGGGGSF	SVM	POSITIVE	1
53	572-586	PREGVFVFGGGGSFP	SVM	POSITIVE	1
54	573-587	REGVFVFGGGGSFPR	SVM	POSITIVE	1
55	574-588	EGVFVFGGGGSFPRE	SVM	POSITIVE	1
56	575-589	GVFVFGGGGSFPREG	SVM	POSITIVE	1
57	576-590	VFVFGGGGSFPREGV	SVM	POSITIVE	1
58	577-591	FVFGGGGSFPREGVF	SVM	POSITIVE	1

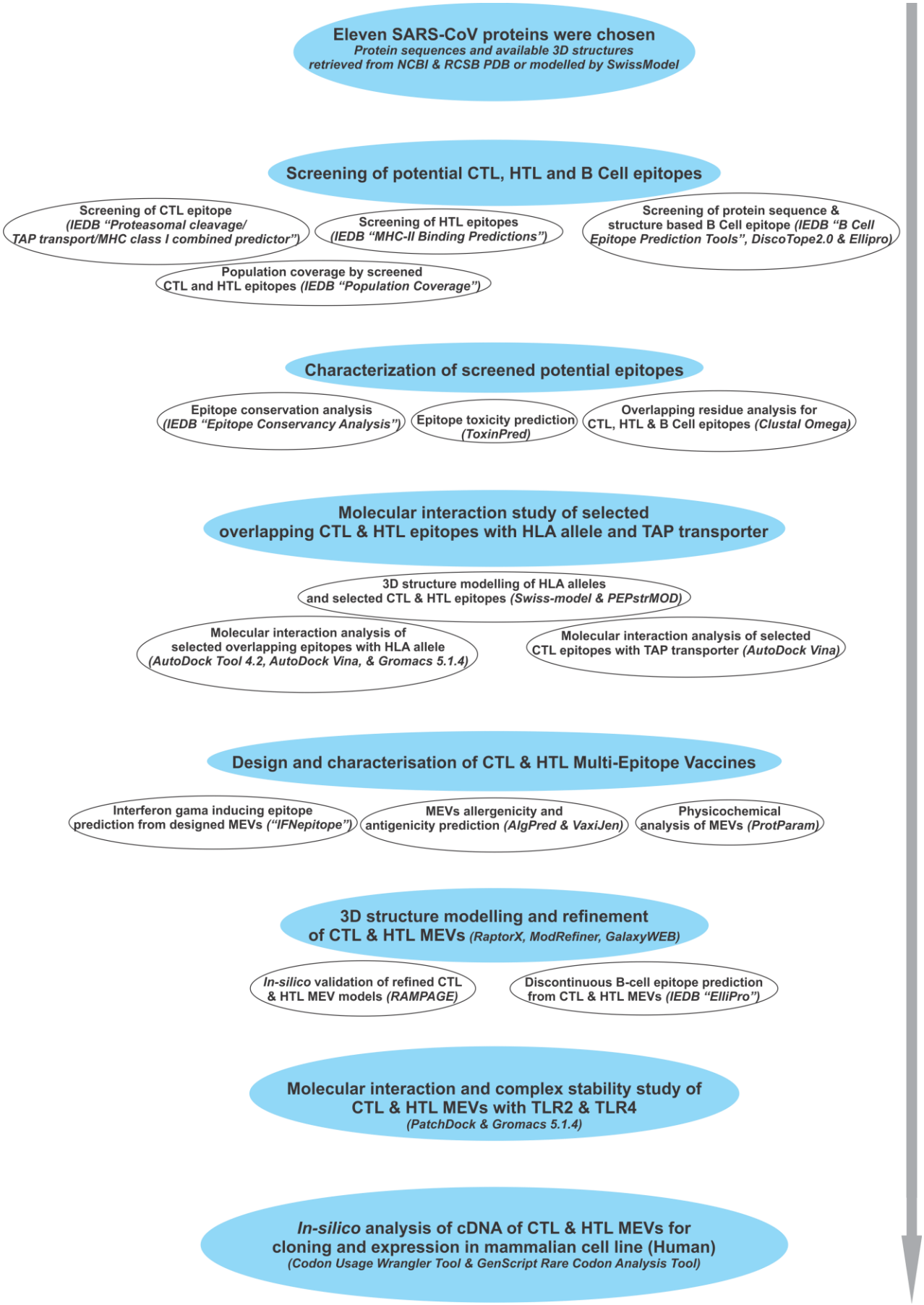
59	578-592	VFGGGGSFPREGVFV	SVM	POSITIVE	1
60	579-593	FGGGGSFPREGVFVF	SVM	POSITIVE	1
61	580-594	GGGGSFPREGVFVFG	SVM	POSITIVE	1
62	581-595	GGGSFPREGVFVFGG	SVM	POSITIVE	1
63	582-596	GGSFPREGVFVFGGG	SVM	POSITIVE	1
64	583-597	GSFPREGVFVFGGGG	SVM	POSITIVE	1
65	584-598	SFPREGVFVFGGGGS	SVM	POSITIVE	1
66	585-599	FPREGVFVFGGGGSK	SVM	POSITIVE	1
67	587-601	REGVFVFGGGGSKWP	SVM	POSITIVE	1
68	588-602	EGVFVFGGGGSKWPW	SVM	POSITIVE	1.1
HLT Epitopes also predicted to be IFN-gamma epitopes					
S.No	**Start-END**	**Sequence**	**Method**	**Result**	**Score**
1	68-82	RWANQCIFGHSPRQQ	MERCI	POSITIVE	2
2	69-83	WANQCIFGHSPRQQR	MERCI	POSITIVE	2
3	70-84	ANQCIFGHSPRQQRE	MERCI	POSITIVE	2
4	71-85	NQCIFGHSPRQQREG	MERCI	POSITIVE	2
5	72-86	QCIFGHSPRQQREGV	MERCI	POSITIVE	2
6	83-98	EGVGENVYAYWSSVS	MERCI	POSITIVE	1
7	84-99	GVGENVYAYWSSVSV	MERCI	POSITIVE	2
8	121-135	LYENNPSNNMTWKVA	MERCI	POSITIVE	1
9	122-136	YENNPSNNMTWKVAG	MERCI	POSITIVE	1
10	123-137	ENNPSNNMTWKVAGQ	MERCI	POSITIVE	2
11	124-138	NNPSNNMTWKVAGQG	MERCI	POSITIVE	2
12	125-139	NPSNNMTWKVAGQGV	MERCI	POSITIVE	1
13	126-140	PSNNMTWKVAGQGVL	MERCI	POSITIVE	1
14	127-141	SNNMTWKVAGQGVLH	MERCI	POSITIVE	1
15	239-253	VFLILCGGGGSLFLI	SVM	POSITIVE	1
16	541-549	QIQLGGGGS	SVM	POSITIVE	1.1
17	553-567	LLFLAFVVFLLVGGG	SVM	POSITIVE	1
18	554-568	LFLAFVVFLLVGGGG	SVM	POSITIVE	1
19	555-569	FLAFVVFLLVGGGGS	SVM	POSITIVE	1.1
20	556-570	LAFVVFLLVGGGGSS	SVM	POSITIVE	1.1
21	573-587	LFLAFVVFLLVTGGG	MERCI	POSITIVE	1
22	596-610	FVVFLLVTLGGGGSL	SVM	POSITIVE	1
23	597-611	VVFLLVTLGGGGSLL	SVM	POSITIVE	1.2
24	604-618	LGGGGSLLFLAFVVF	SVM	POSITIVE	1
25	605-619	GGGGSLLFLAFVVFL	SVM	POSITIVE	1.1
26	606-620	GGGSLLFLAFVVFLL	SVM	POSITIVE	1
27	625-639	GGGGSLFLAFVVFLL	SVM	POSITIVE	1
28	643-657	AIGGGGSFLAFVVFL	SVM	POSITIVE	1
29	644-658	IGGGGSFLAFVVFLL	SVM	POSITIVE	1.1
30	645-659	GGGGSFLAFVVFLLV	SVM	POSITIVE	1.1
31	662-676	AILGGGGSLAFVVFL	SVM	POSITIVE	1

Supplementary table S10. Refinement models of CTL and HTL MEVs. CTL and HTL MEVs models were refined by GalaxyWEB server and used for further studies. After refinement in particular Rama favored residues increased significantly.

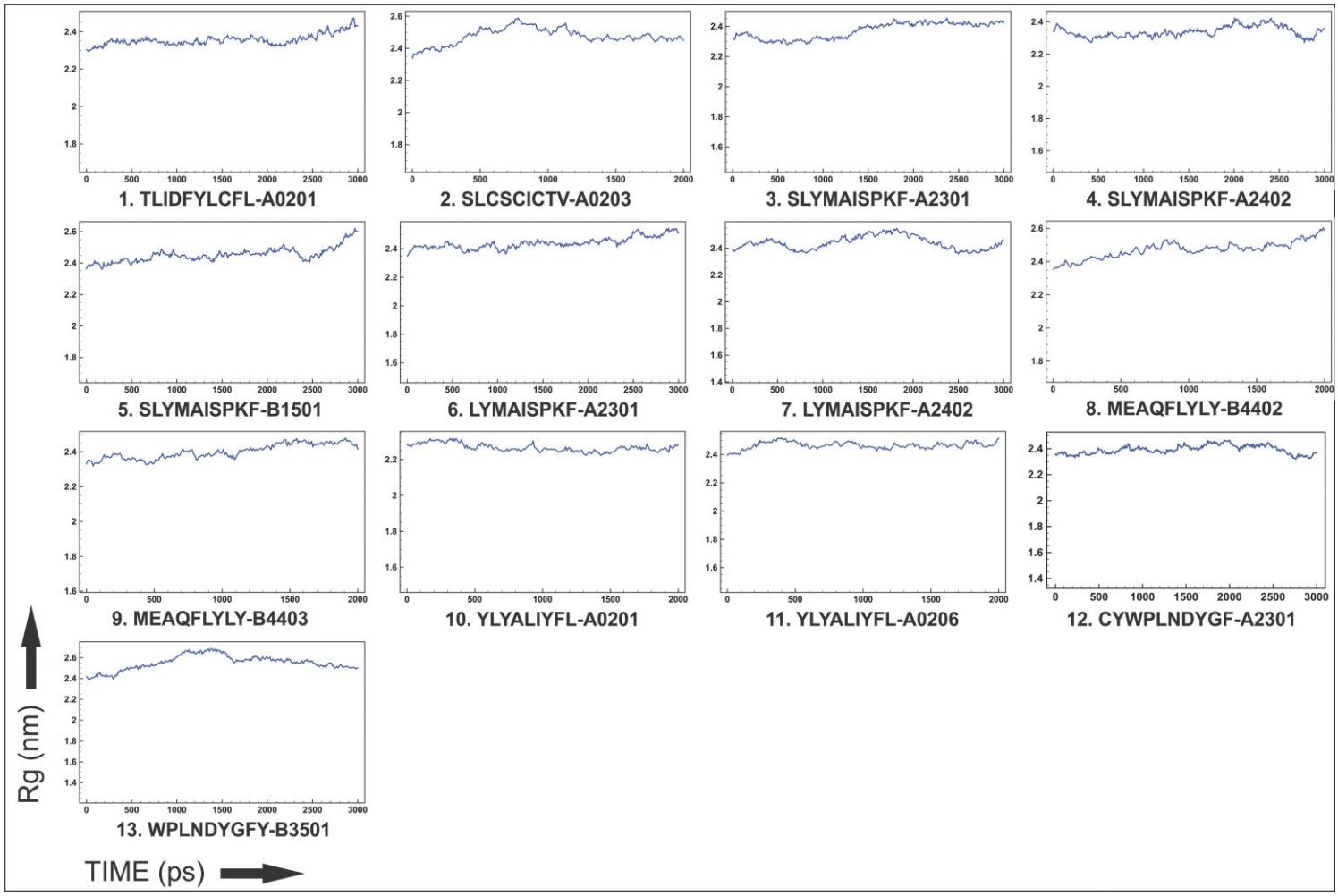
Galaxy Refinment for CTL MEV						
Model	**GDT-HA**	**RMSD**	**MolProbity**	**Clash score**	**Poor rotaSARS-CoV**	**Rama favored**
Initial	1.00	0.00	3.051	103.4	1.2	91.1
MODEL 1	0.9457	0.425	2.326	26.5	0.9	93.7
Galaxy Refinment for HTL MEV						
Initial	1.00	0.00	3.216	120.6	1.9	92.5
MODEL 1	0.9447	0.430	2.377	27.3	1.4	95.0

Supplementary table S11. B Cell discontineous epitopes of CTL & HTL MEVs. Discontinuous B Cell epitopes predicted by ElliPro (IEDB) from CTL & HTL MEVs.

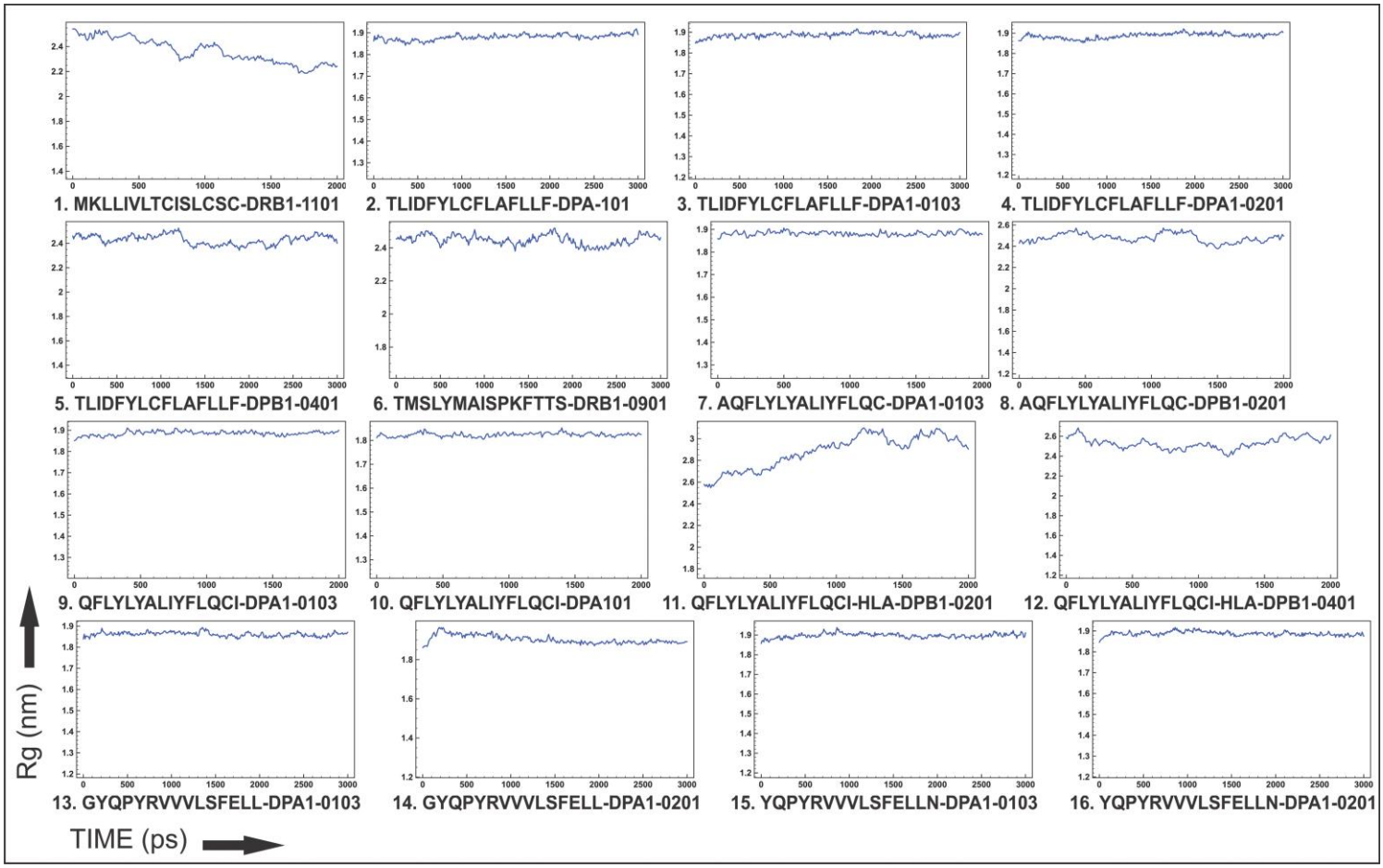
CTL MEV Discontinuous epitopes residues			
S.No	Residues	Number of residues	Score
1	G449, G450, G451, G452, S453, R454, I455, Y456	8	0.861
2	G464, G465, G466, G467, S468, L469, G470, A471, D472, S473, S474, I475, A476, Y477, G478, G479, G480, G481, S482, R483, S484, F485, I486, E487, D488, L489, L490, F491, G492, G493, G494, G495, S496, L497, L498, T499, D500, D501, M502, I503, A504, A505, Y506, G507, G508, G509, G510, S511, L512, T513, D514, D515, M516, I517, A518, A519, Y520, G521, G522, G523, G524, S525, Q526, I527, P528, F529, A530, M531, Q532, M533, A534, Y535, G536, G537, G538, G539, S540, I541, P542, F543, A544, M545, Q546, M547, A548, Y549, G550, G551, G552, G553, S554, F555, A556, M557, Q558, M559, A560, Y561, R562, F563, G564, G565, G566, G567, S568, A569, Y570, F571, P572, R573, E574, G575, V576, F577, V578, F579, G580, G581, G582, G583, S584, F585, P586, E588, G589, V590, F591, V592, F593, G594, G595, G596, G597, S598, K599, W600, P601, W602, Y603, V604, W605, L606	142	0.799
3	S457, T458, G459, N460, N461, V462, F463	7	0.782
4	I1, V2, V3, A4, V5, T6, G7, Y8, N9, C10, P11, G12, G13, K14, L15, T16, A17, L18, E19, R20, K21, K22, W58, D59, C60, K61, E63, S64, S65, A66, Q67, R68, W69, A70, N71, Q72, C73, I74, F75, G76, H77, S78, P79, R80, Q82, R83, E88, N89, V90, Y91, A92, Y93, W94, S95, S96, V97, S98, V99, E100, G101, L102, K103, K104, T105, A106, L155	66	0.684
5	D33, N36, G37, K38, L39, K40, N41, R42, N43, G44, T45, Y46, M47, P48, R49, G50, K51, M53, S116, K117, L118, P119, K120, L121, Y122, E123, N124, N125, P126, S127, N128, N129, M130, T131, W132, K133, V134, A135, G136, Q137, G138, V139, L140, S163, L165, Y166, A167, L168, I169, Y170, F171, L172, G173, G174, G175, G176, S177, S178, L179, S184, P185, K186, F187, G188, G189, G190	66	0.624
6	G405, G406, G407, G408, G433, F434, G435, G436, G437, G438, S439, W440, P441, L442, N443, D444, Y445, G446, F447, Y448	20	0.62
7	G218, G219, S220, T221, L222, I223, D224, F225	8	0.527
HTL MEV Discontinuous epitopes residues			
S.No	Residues	Number of residues	Score
1	I1, V2, V3, A4, V5, T6, G7, Y8, N9, C10, P11, G12, G13, K14, L15, T16, A17, L18, E19, R20, L56, T57, W58, D59, C60, K61, L62, E63, S64, S65, A66, Q67, R68, W69, A70, N71, Q72, C73, I74, F75, G76, H77, S78, P79, Q81, Q82, R83, E84, G85, V86, G87, E88, N89, V90, Y91, A92, Y93, W94, S95, S96, V97, S98, V99, E100, G101, L102, K103, K104, T105, A106, G107, T108, D109, A110, K112, S113, W114, S116, K117, L118, P119, K120, L121, Y122, E123, N124, N125, P126, S127, N128, N129, M130, T131, W132, K133, V134, A135, G136, Q137, G138, V139, L140, H141, Q144, A147, Y154, L155, Y156, A157, L158, I159, Y160, F161, L162, Q163, C164, G165, G166, G167, G168, S169, Q170, F171, L172, Y173, L174, Y175, A176, L177, I178, Y179, F180, C183, I184, G185, G186, G187, G188, S189, T190, M191, S192, K200, F201, T202, T203, S204, G205, G730, T731, R732, N733, L759, T760, S761, G762, S763, D764, G765, G766, G767, G768, S769, G770, Y771, Q772, P773, Y774, L803, N804, G805, G806, G807, G808, S809, Q810, P811, Y812, R813, L841, N842, A843, P844, G845, G846, G847, G848, S849, Y850	189	0.76
2	L300, F302, T303, I304, G305, V383, L384, G385, G386, G387, G388, S389, F390, L444, G445, G446, G447, G448, S449, C450, F451, L452, A453, F454, L456, F457, L460, I464, G465, G466, G467, G468, S469, F470, L471, A472, F473, L474, L475, F476, L477, V478, L479, I480, M481, L482, I483, I484, G485, G486, G487, G488, S489, M490, K491, L492, L493, I494, V495, L496, T497, C498, I499, S500, L501, C502, S503, C504, G505, G506, G507, G508, S509, A510, P540, Q541, I542, Q543, L544, G545, G546, G547, G548, S549, V552, L553, F555, L556, A557, V559, V560, F561, L562, L563, V564, G565, G566, G567, G568	99	0.698
3	L241, I242, L243, C244, G245, G246, G247, G248, S249, L250, F251, L252, I253, V254, A255, A256, L257, V258, F259, L262, C263, F264, G265, G266, G267, G268, S269, F270, L271, I272, V273, G327, G328, S329, L330, I331, D332, F333, Y334, L335, C336, F337, L338, A339, F340, L341, L342, F343, L344, G345, G346, G347, G348, S349, I350, F352, A358, L360, L361, F362, L363, V364, G365, G366, G367, Y410, L411, C412, H521, T522, M523, V524, G525, G526, G527, G528, S529, V530, V531, P532, P533, A534, L535, H536, L537, L591, L594, A595, F596, V597, V598, F599, L600, L601, V602, T603, L604, G605, G606, G607, G608, S609, L610, L611, L613, L664, G665, G666, G667, G668, S669, F672, V673, V674, F675, L676, L677, V678, T679, L680, A681, I682, L683, T684, G685, G686, G687, G688, S689, W690, N691, L692, V693, I694, G695, F696, L697, F698, L699, A700, W701, I702, G705, G706, G708	145	0.682
4	G405, G406, G407, G408, S409, F413, L414, F416, F517	9	0.668
5	G747, G748, S789, Y790, Q791, P792, Y793, L822, N823, A824, G827, G828, S829, P830, Y831, S856, F857, E858, L859, L860, N861, A862, P863, A864	24	0.536
6	N41, R42, N43, G44, T45	5	0.533



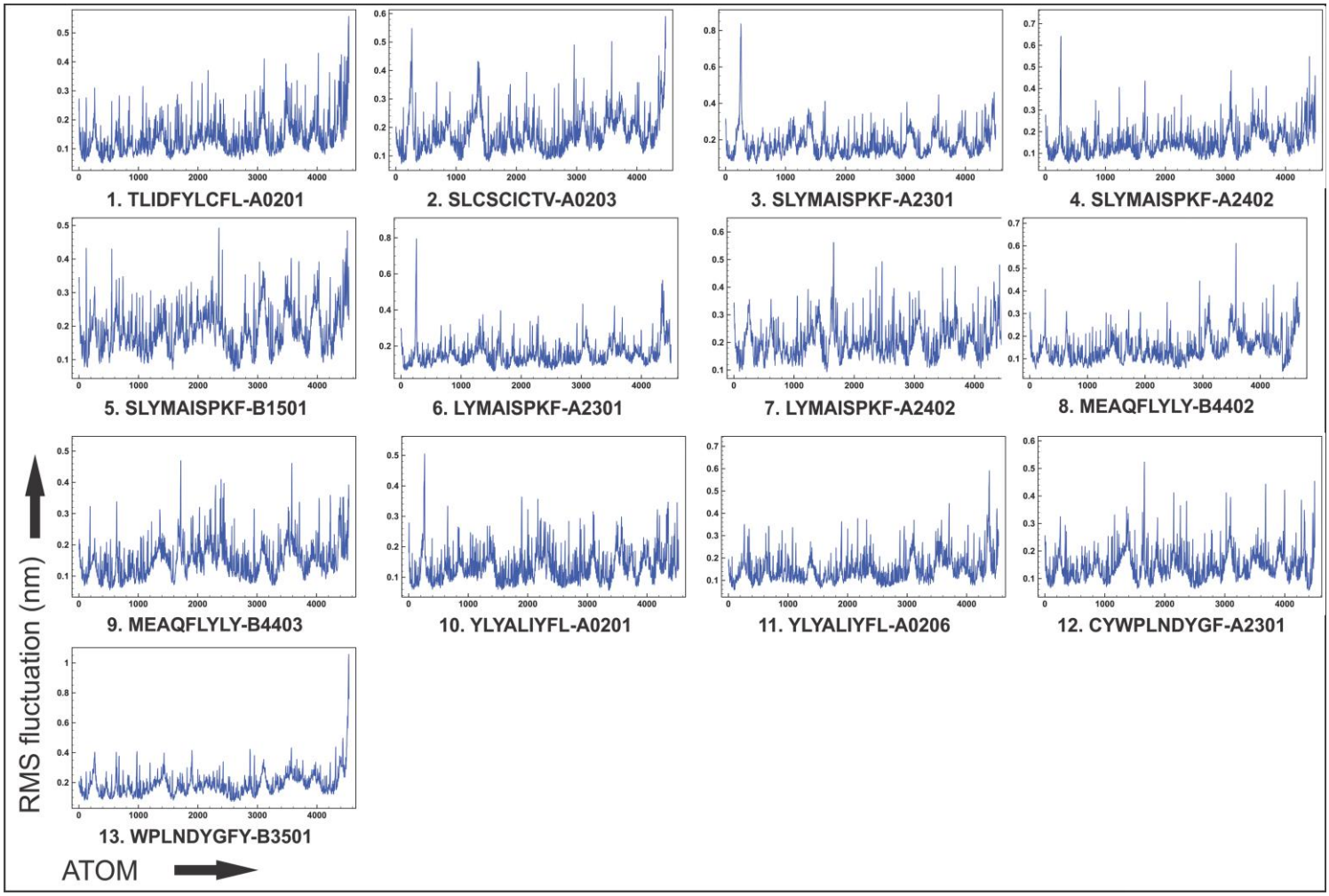
Supplementary figure S1. Workflow chart.



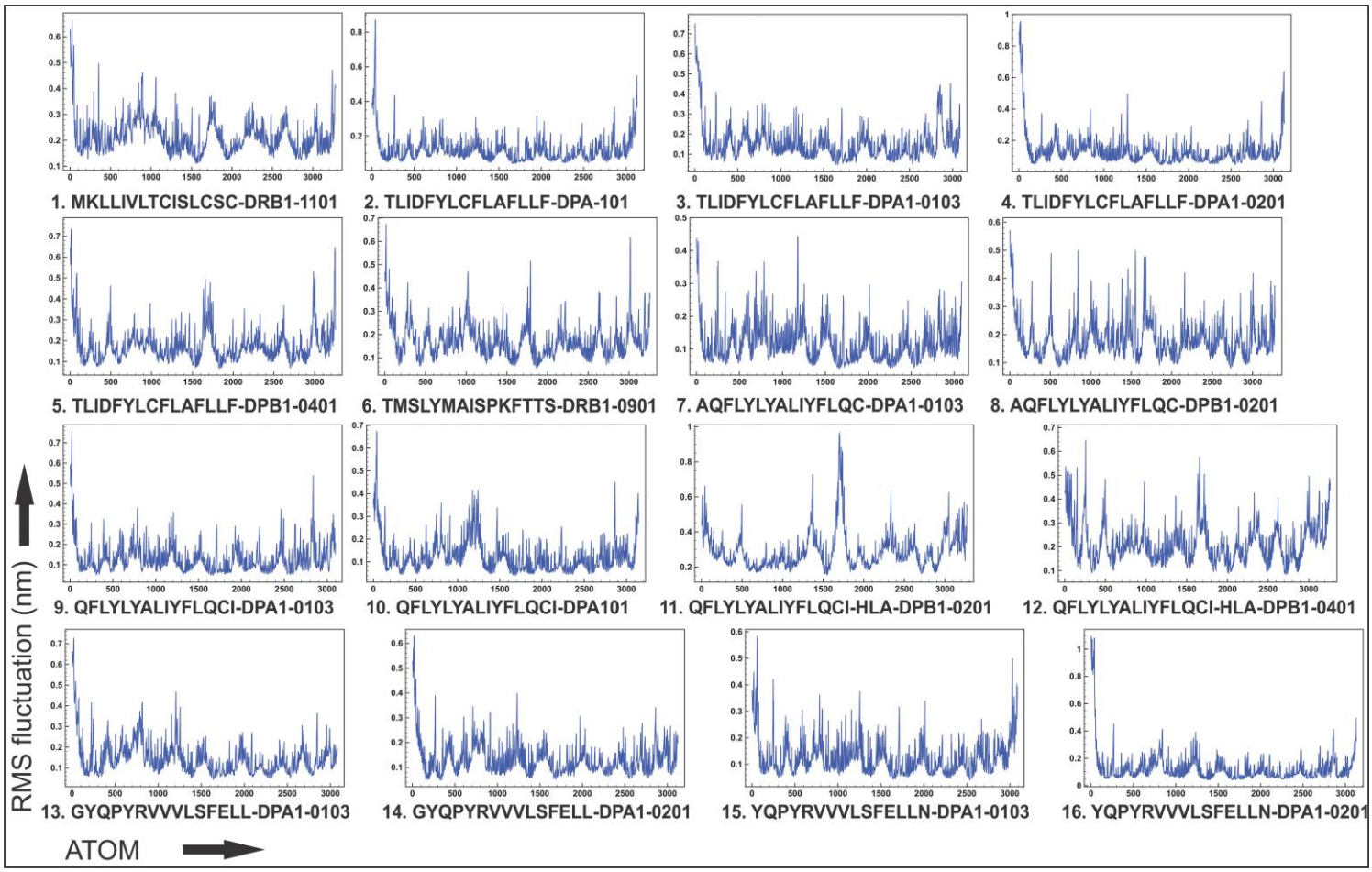
Supplementary figure S2 (A). The radius of gyration (Rg) across the time window of 3 ns for CTL epitope & HLA class I allele complexes.



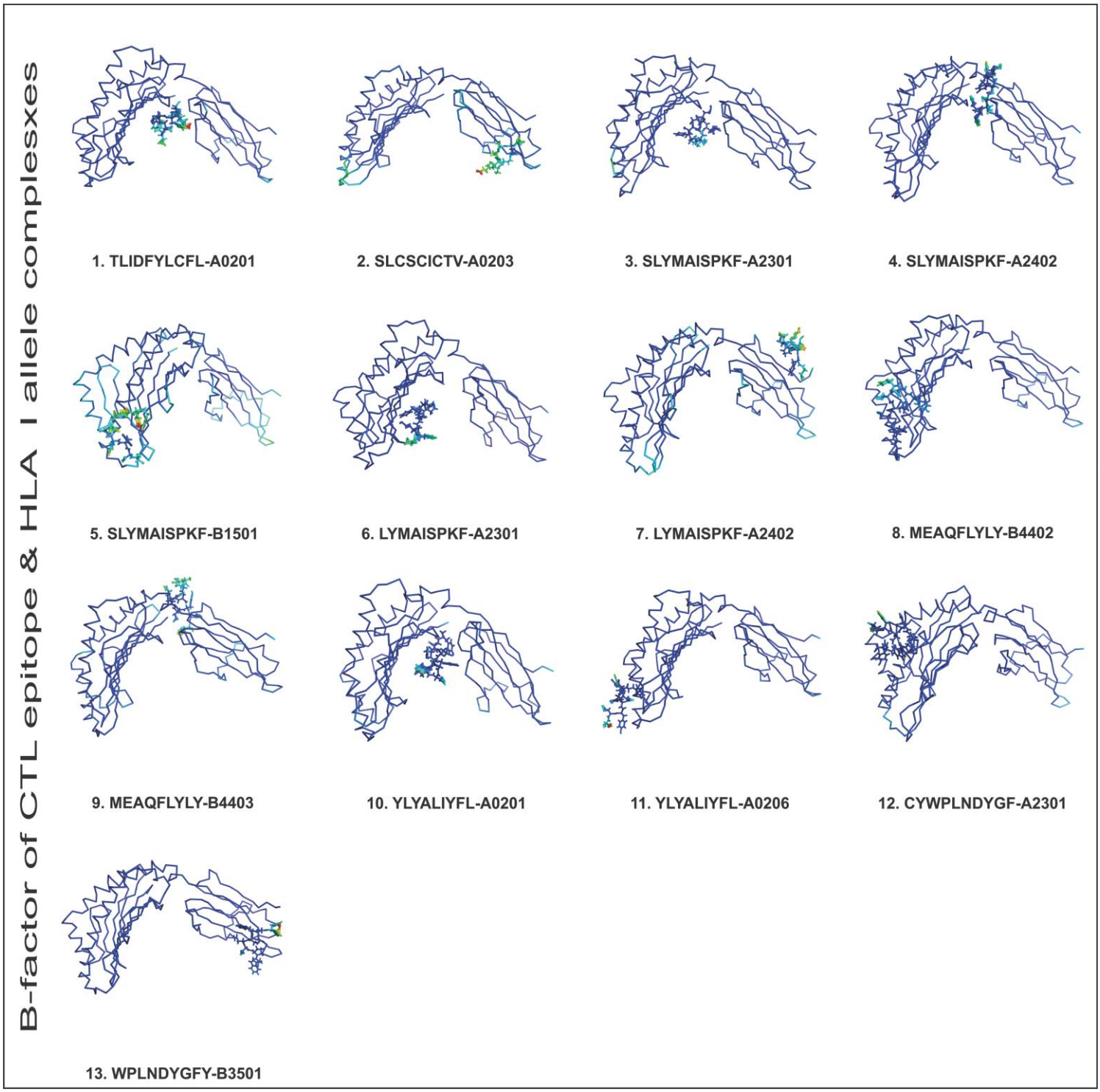
Supplementary figure S2 (B). The radius of gyration (Rg) across the time window of 3 ns for HTL epitope & HLA class II allele complexes.



Supplementary figure S3 (A). RMS fluctuation (nanometers) for all the atoms of CTL epitope & HLA class I allele complexes.

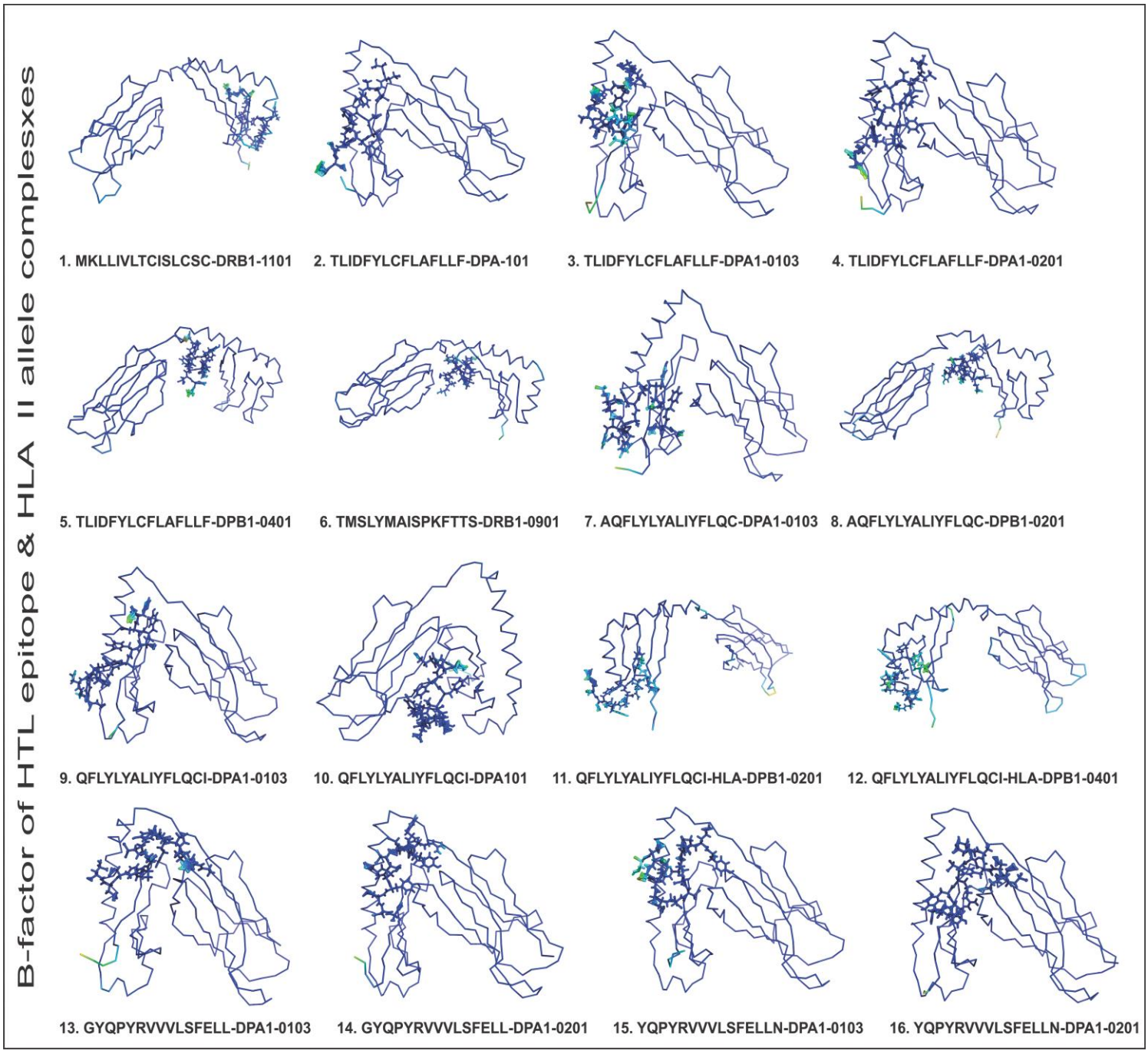


Supplementary figure S3 (B). RMS fluctuation (nanometers) for all the atoms of HTL epitope & HLA class II allele complexes.



Supplementary figure S4 (A). B-Factor of CTL epitope & HLA class I allele complexes. Epitopes are shown in sticks and HLA Class I alleles are shown in cartoons. The regions of complexes are shown in rainbow (VIBGYOR), the regions in blue being very stable and the

region towards red being relatively unstable. In the complexes shown above, most of the regions are in blue indicating the complexes to be highly stable.



Supplementary figure S4 (B). B-Factor of HTL epitope & HLA class II allele complexes. Epitopes are shown in sticks and HLA alleles are shown in cartoons. The regions of complexes are shown in rainbow (VIBGYOR), the regions in blue being very stable and the

region towards red being relatively unstable. In the complexes shown above, most of the regions are in blue indicating the complexes to be highly stable.