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Supplementary materials for-

A conserved subunit vaccine designed against SARS-CoV-2 variants showed evidence in neutralizing the virus.

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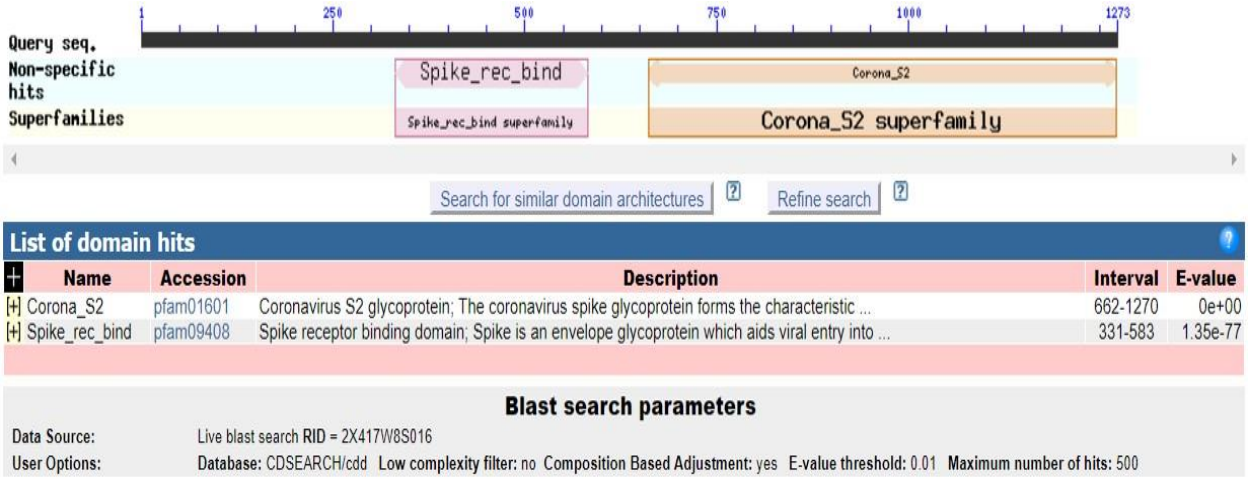

Fig S1: CDD search to find the major domains of Spike surface glycoprotein. Two distinct domains are observed in this protein e.g. S2 glycoprotein and Spike receptor binding domain (S1).

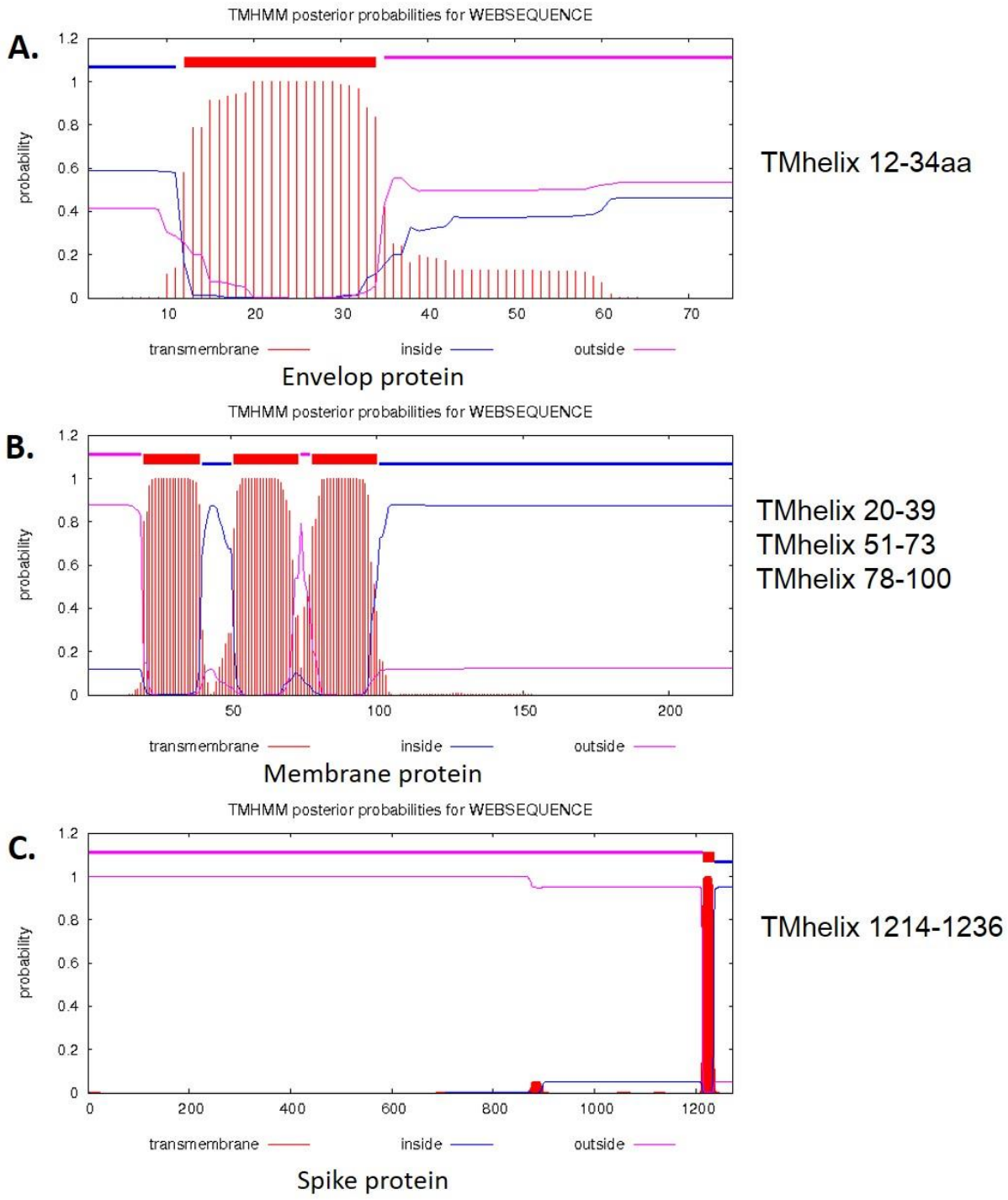

Fig S2: The transmembrane region prediction of selected (A) Envelope protein, (B) Membrane glycoprotein and (C) Spike surface glycoprotein by TMHMM.

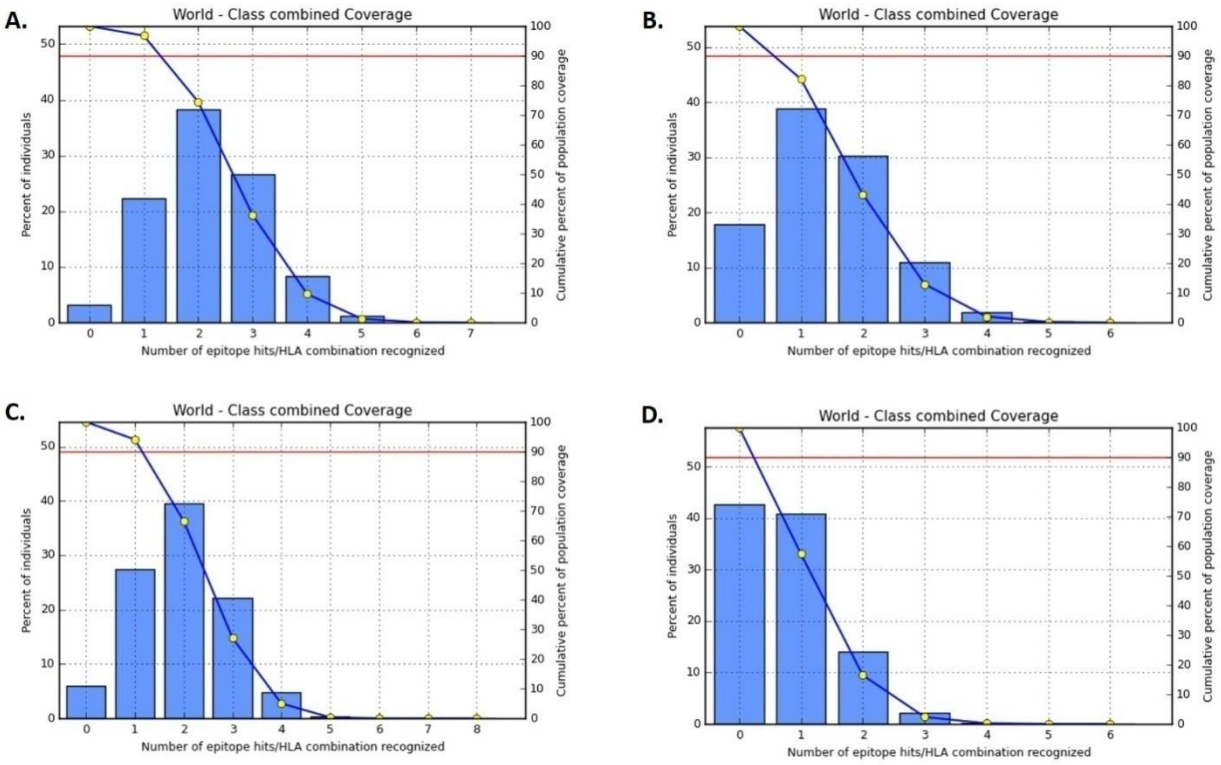

Fig S3: Population coverage analysis for four prominent epitopes on the basis of HLA interaction in the whole world. **(A)** The population coverage for epitope CVEnvA2 (96.77%), (B) The population coverage for epitope CVMemB2 (82.11%), **(C)** The population coverage for epitope CVS1A2 (94.07%), **(D)** The population coverage for epitope CVS2B2 (57.36%). The figures were prepared depending on the combined score of both MHC class I and MHC class II interaction. Notes: the line (-o-) in the graphs, points out the cumulative percentage of population coverage of the epitopes; the bars indicate the population coverage for each epitope.

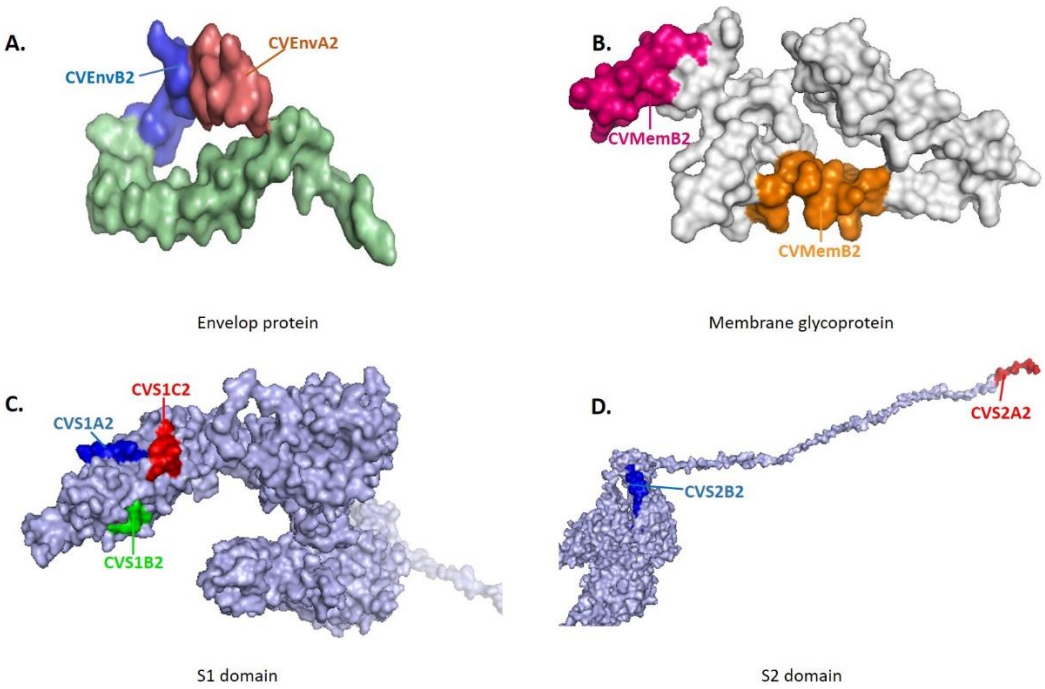

Fig S4: The 3D models of the Envelope protein (A), Membrane glycoprotein (B) and Surface glycoprotein (C and D). The surface location of the T-cell epitopes on the protein, A. CVEnvA2 (light red) and CVEnvB2 (Light Blue), B. CVMemA2 (Orange) and CVMemB2 (Pink), C. CVS1A2 (Blue), CVS1B2 (Green) and CVS1C2 (Red) and D. CVS2A2 (Red) and CVS2B2 (Blue).

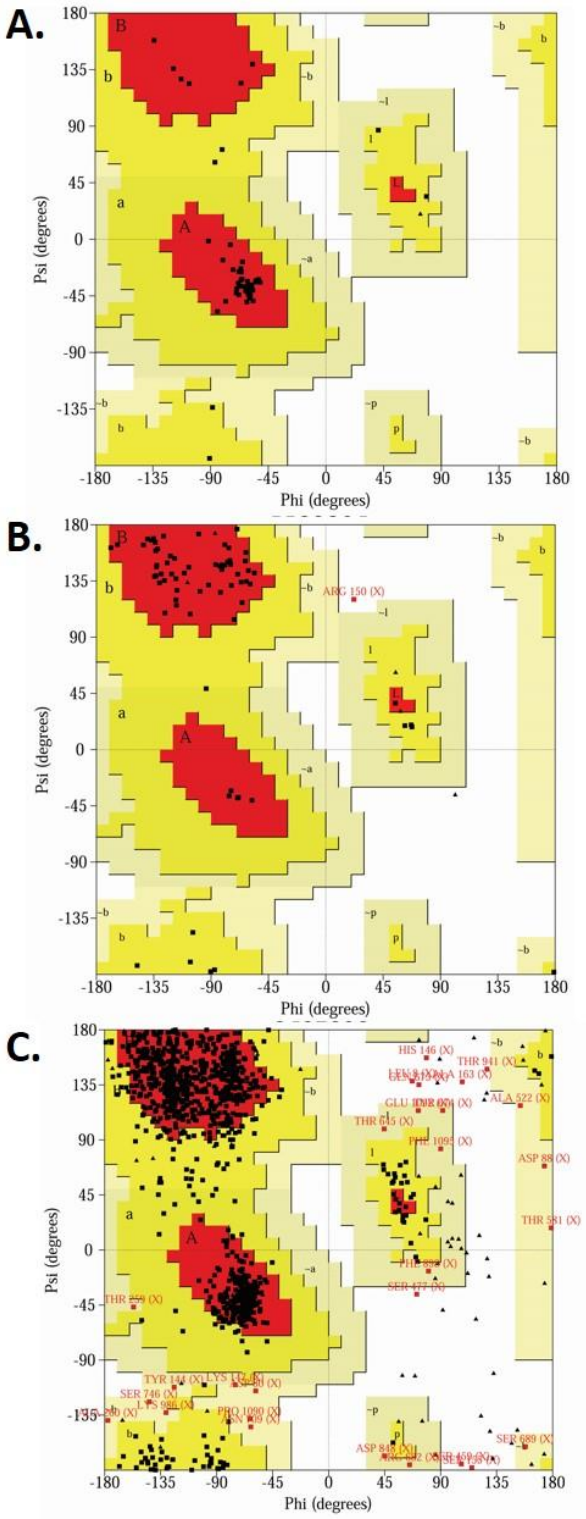

Fig S5: Ramachandran plot of the predicted model by PROCHECK, A. Envelope protein, B. Membrane glycoprotein and C. Spike surface glycoprotein, which shows that most of the residues are in the allowed region of the plot, proving the validity of the model.

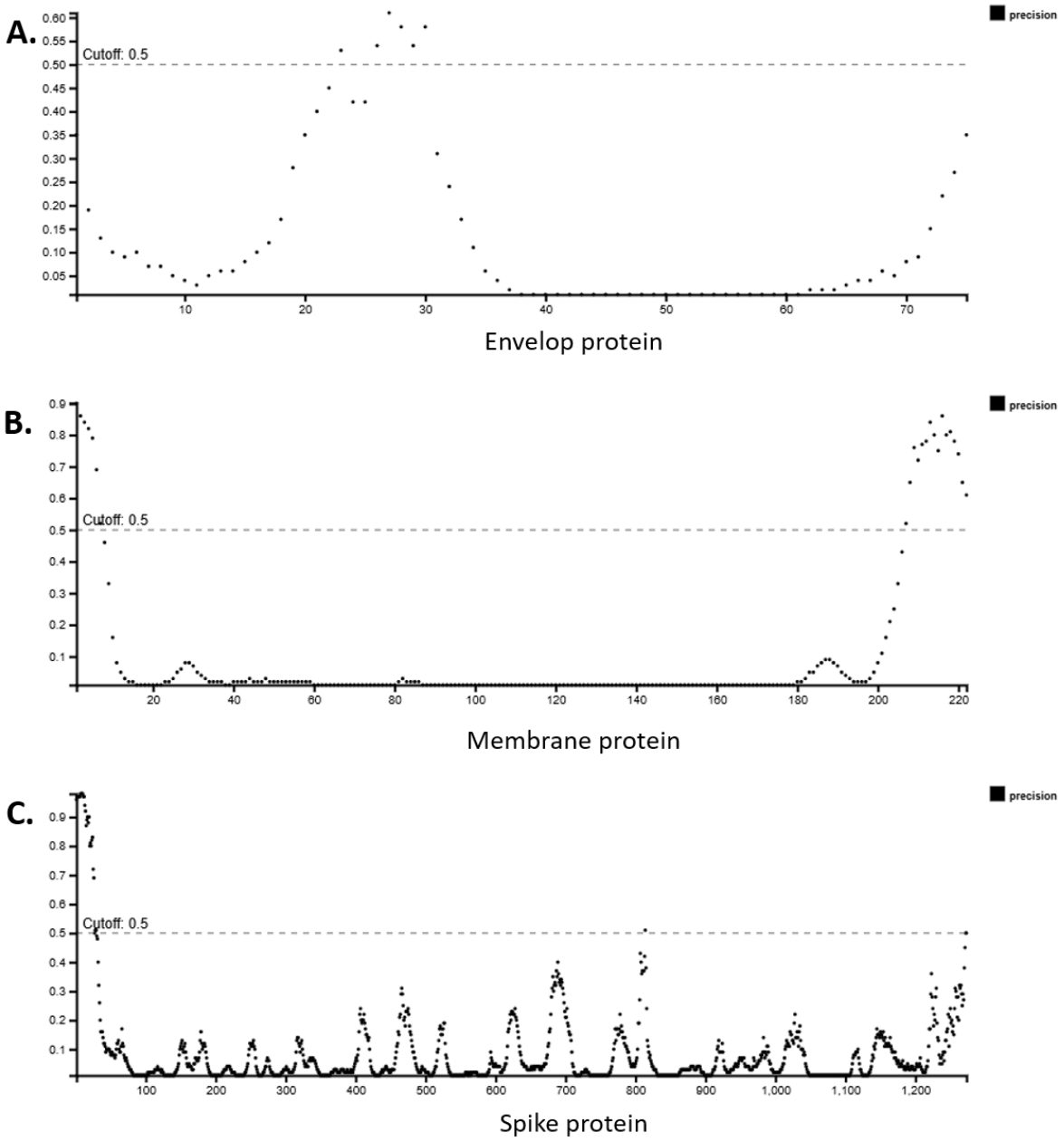

Fig S6: Disorder prediction of the amino acid sequences of A. Envelope protein, B. Membrane glycoprotein and C. Spike surface glycoprotein of Novel Corona Virus-2. Here, the potential epitopes localized outside of the disordered regions and securing their potentiality for being an effective vaccine candidate. Notes: Amino acids in the input sequence are considered disordered when the dotted line is above the gray dashed line, that is, when the confidence score is 0.5.

Receptor residue	Peptide residue
CYS D 164	VAL A 2
TRP D 156	ASN A 8
GLN D 155	ARG A 5
GLU D 152	LYS A 7
TRP D 147	ASN A 8
TRP D 133	ASN A 8
HIS D 114	ASN A 8
TYR D 99	VAL A 2
ARG D 97	SER A 4
THR D 73	ASN A 8
ALA D 69	VAL A 6
GLU D 63	TYR A 1
ILE D 52	TYR A 1
TYR D 7	VAL A 2
MET D 5	TYR A 1

Receptor residue	Peptide residue
TRP D 167	TYR A 1
TYR D 159	TYR A 3
TRP D 156	SER A 4
GLU D 152	ASN A 8
TRP D 147	LEU A 9
THR D 143	LEU A 9
ILE D 124	ASN A 8
TYR D 99	TYR A 3
ARG D 97	ARG A 5
ASP D 77	LEU A 9
HIS D 70	SER A 4
LYS D 66	TYR A 1
GLU D 55	TYR A 1
PHE D 33	TYR A 1
MET D 5	VAL A 2

Receptor residue	Peptide residue
TYR D 159	ARG A 5
TRP D 156	ARG A 5
GLU D 152	LEU A 9
GLU D 152	ARG A 5
LYS D 146	LEU A 9
ILE D 124	LEU A 9
TYR D 99	SER A 4
ARG D 97	ASN A 8
THR D 80	LEU A 9
THR D 73	VAL A 6
LYS D 66	TYR A 3
TYR D 59	TYR A 1
TRP D 51	TYR A 1
TYR D 7	TYR A 1

Fig S7: Contact maps between the 9-mer peptide of Envelope protein (YVYSRVKNL) with HLA-A*02:03. Here, the distances between two amino acids closer than 4.5 A° were shown. Polar contacts between the peptide-protein interactions shown by the red font.

Receptor residue	Peptide residue
THR A 163	ILE B 3
TYR A 159	ILE B 3
GLN A 155	GLY B 6
TRP A 147	LEU B 8
ILE A 124	ARG B 9
ASP A 116	LEU B 8
ARG A 114	GLY B 6
TYR A 99	ILE B 3
MET A 97	ARG B 9
LEU A 81	ARG B 9
ASP A 74	ARG B 9
GLN A 70	HIS B 7
VAL A 67	LEU B 4
ASN A 66	VAL B 2
ASN A 63	ALA B 1
ILE A 52	ALA B 1
PHE A 33	ALA B 1
TYR A 9	LEU B 4

Receptor residue	Peptide residue
TRP A 167	ILE B 3
TYR A 159	ARG B 5
ALA A 158	ARG B 5
GLN A 155	ARG B 5
THR A 143	ARG B 9
ILE A 124	LEU B 8
ARG A 114	LEU B 8
TYR A 99	ARG B 5
TYR A 99	VAL B 2
MET A 97	HIS B 7
ASP A 77	ARG B 9
THR A 73	ARG B 9
GLN A 70	ARG B 5
ASN A 66	LEU B 4
ASN A 63	LEU B 4
ARG A 62	ILE B 3
MET A 45	ALA B 1
TYR A 9	ARG B 9
TYR A 7	LEU B 4

Receptor residue	Peptide residue
TRP A 167	ALA B 1
TYR A 159	LEU B 4
TRP A 156	ARG B 5
TRP A 147	ARG B 9
LEU A 126	LEU B 8
ASP A 116	ARG B 9
ARG A 114	HIS B 7
TYR A 99	LEU B 4
TYR A 99	ALA B 1
ILE A 95	ARG B 9
ASP A 77	LEU B 8
GLN A 70	ARG B 9
GLN A 70	LEU B 4
ASN A 66	ILE B 3
ASN A 63	VAL B 2
GLU A 55	ALA B 1
VAL A 34	ALA B 1
TYR A 9	HIS B 7
TYR A 7	VAL B 2

Fig S8: Contact maps between the 9-mer peptide of Membrane glycoprotein (AVILRGHLR) with HLA-A*68:01. Here, the distances between two amino acids closer than 4.5 A° were shown. Polar contacts between the peptide-protein interactions shown by the red font.

Receptor residue	Peptide residue
CYS A 164	TRP B 9
TYR A 159	ALA B 8
ALA A 152	ALA B 4
LEU A 147	PHE B 3
LYS A 146	ARG B 2
THR A 143	THR B 1
ALA A 117	PHE B 3
ASP A 114	VAL B 6
SER A 99	TYR B 7
ARG A 97	PHE B 3
LEU A 81	PHE B 3
SER A 77	ARG B 2
ALA A 73	SER B 5
GLN A 70	SER B 5
GLU A 63	TRP B 9
VAL A 34	TYR B 7
TYR A 7	TRP B 9

Receptor residue	Peptide residue
CYS A 164	ALA B 8
LEU A 156	VAL B 6
ALA A 150	ARG B 2
LEU A 147	ARG B 2
LYS A 146	THR B 1
ILE A 124	PHE B 3
SER A 116	ALA B 4
ASP A 114	SER B 5
SER A 99	VAL B 6
ARG A 97	ARG B 2
ASN A 80	THR B 1
SER A 77	THR B 1
GLN A 70	TYR B 7
LYS A 66	TYR B 7
GLU A 63	TYR B 7
SER A 24	TYR B 7
TYR A 7	TYR B 7

Receptor residue	Peptide residue
TRP A 167	TRP B 9
THR A 163	TRP B 9
LEU A 156	ALA B 4
LEU A 147	ALA B 4
LEU A 147	THR B 1
THR A 143	PHE B 3
TYR A 123	PHE B 3
SER A 116	PHE B 3
ASP A 114	ALA B 4
ARG A 97	SER B 5
LEU A 95	PHE B 3
SER A 77	PHE B 3
VAL A 76	THR B 1
GLN A 70	VAL B 6
LYS A 66	VAL B 6
TYR A 59	TRP B 9
ASP A 9	TYR B 7
MET A 5	TRP B 9

Fig S9: Contact maps between the 9-mer peptide of S1 domain of Spike surface glycoprotein (TRFASVYAW) with HLA-C*07:02. Here, the distances between two amino acids closer than 4.5 A° were shown. Polar contacts between the peptide-protein interactions shown by the red font.

Receptor residue	Peptide residue
GLN A 156	VAL B 4
TRP A 147	PRO B 5
THR A 143	GLU B 8
TRP A 133	ALA B 6
ALA A 125	PRO B 5
TYR A 123	GLU B 8
ASP A 116	TYR B 3
ARG A 114	PRO B 5
ARG A 114	THR B 2
TYR A 99	THR B 2
ILE A 97	TYR B 3
TYR A 84	GLU B 8
THR A 80	GLU B 8
ASP A 77	ALA B 6
ASP A 74	TYR B 3

Receptor residue	Peptide residue
GLN A 155	VAL B 1
TRP A 147	VAL B 4
THR A 143	GLN B 7
TRP A 133	PRO B 5
ILE A 124	ALA B 6
ASP A 116	ALA B 6
GLN A 115	PRO B 5
ARG A 114	VAL B 4
ARG A 114	VAL B 1
MET A 98	VAL B 4
ILE A 97	THR B 2
LEU A 81	GLU B 8
ASP A 77	GLU B 8
ASP A 77	TYR B 3
THR A 73	TYR B 3

Receptor residue	Peptide residue
GLN A 156	PRO B 5
TRP A 147	GLN B 7
TRP A 147	VAL B 1
THR A 143	ALA B 6
LEU A 126	PRO B 5
ILE A 124	PRO B 5
ASP A 116	PRO B 5
GLN A 115	VAL B 4
ARG A 114	TYR B 3
TYR A 99	VAL B 4
ILE A 97	VAL B 4
ILE A 95	TYR B 3
THR A 80	LYS B 9
ASP A 77	GLN B 7
VAL A 76	LYS B 9
GLN A 70	THR B 2

Fig S10: Contact maps between the 9-mer peptide of S2 domain of Spike surface glycoprotein (VTYVPAQEK) with HLA-A*11:01. Here, the distances between two amino acids closer than 4.5 A° were shown. Polar contacts between the peptide-protein interactions shown by the red font.

Receptor residue	Peptide residue
TYR B 78	LEU C 13
THR B 77	LYS C 11
GLN B 70	ARG C 9
TRP B 61	TYR C 7
ASP B 57	TYR C 5
LEU B 53	PHE C 4
PHE B 40	ARG C 9
ARG B 29	TYR C 7
LEU B 11	SER C 8
TRP B 9	TYR C 5
ILE A 72	PHE C 4
ASN A 69	VAL C 6
VAL A 65	TYR C 7
ASN A 62	ARG C 9
ALA A 59	ASN C 12
GLU A 55	SER C 15
PHE A 54	LEU C 13
PHE A 32	LEU C 13
PHE A 22	VAL C 10

Receptor residue	Peptide residue
HIS B 81	ASN C 14
TYR B 78	VAL C 10
ARG B 71	ARG C 9
TRP B 61	SER C 8
ASP B 57	TYR C 7
PRO B 56	PHE C 4
TYR B 47	TYR C 7
CYS B 30	TYR C 5
GLU B 28	TYR C 7
LEU B 11	TYR C 5
ILE A 72	TYR C 5
ILE A 72	PRO C 2
VAL A 65	SER C 8
ASN A 62	VAL C 10
ALA A 61	VAL C 10
GLY A 58	VAL C 10
PHE A 54	SER C 15
SER A 53	LEU C 13
PHE A 22	ASN C 12

Receptor residue	Peptide residue
ASN B 82	LEU C 13
TYR B 78	LYS C 11
ALA B 74	ARG C 9
LEU B 67	ARG C 9
TRP B 61	VAL C 6
PRO B 56	TYR C 5
TYR B 47	ARG C 9
CYS B 30	TYR C 7
GLU B 28	ARG C 9
LEU B 11	TYR C 7
ARG A 76	PHE C 4
ILE A 72	SER C 3
ASN A 69	TYR C 5
VAL A 65	VAL C 6
ASN A 62	SER C 8
GLY A 58	ASN C 12
GLU A 55	ASN C 12
PHE A 54	ASN C 12
PHE A 32	ASN C 12

Fig S11: Contact maps between the 15-mer peptide of Envelope protein (KPSFYVYSRVKNLNS) with HLA-DRB1*01:01. Here, the distances between two amino acids closer than 4.5 A° were shown. Polar contacts between the peptide-protein interactions shown by the red font.

Receptor residue	Peptide residue
GLY B 86	GLY C 15
VAL B 85	ILE C 13
ASN B 82	ILE C 13
HIS B 81	ARG C 12
TYR B 78	HIS C 10
LEU B 67	LEU C 7
TRP B 61	ARG C 8
TYR B 60	ILE C 6
ASP B 57	VAL C 5
CYS B 30	LEU C 7
GLU B 28	LEU C 7
ILE A 72	VAL C 5
ALA A 68	ILE C 2
ALA A 61	HIS C 10
GLU A 55	LEU C 11
SER A 53	ILE C 13
PHE A 32	ALA C 14
ILE A 31	ALA C 14
PHE A 24	ALA C 14
PHE A 22	ARG C 12
GLN A 9	ARG C 12
ILE A 7	GLY C 15

Receptor residue	Peptide residue
THR B 90	GLY C 15
VAL B 85	ALA C 14
ASN B 82	ALA C 14
HIS B 81	ILE C 13
TYR B 78	LEU C 11
LEU B 67	ARG C 8
GLN B 64	ILE C 6
TRP B 61	ILE C 6
ASP B 57	ILE C 6
VAL B 38	LEU C 7
GLU B 28	ARG C 8
PHE B 13	GLY C 9
ASN A 69	VAL C 5
ASN A 62	HIS C 10
GLY A 58	HIS C 10
SER A 53	ALA C 14
PHE A 48	ALA C 14
ILE A 31	GLY C 15
PHE A 24	GLY C 15
MET A 23	ARG C 12
GLU A 11	HIS C 10
GLN A 9	HIS C 10

Receptor residue	Peptide residue
VAL B 85	GLY C 15
ASN B 82	GLY C 15
ASN B 82	ARG C 12
TYR B 78	ARG C 12
ARG B 71	GLY C 9
LEU B 67	ILE C 6
TRP B 61	LEU C 7
ASP B 57	LEU C 7
TYR B 47	LEU C 7
GLU B 28	GLY C 9
PHE B 13	HIS C 10
ASN A 69	LEU C 7
VAL A 65	ILE C 2
ALA A 59	HIS C 10
PHE A 54	ARG C 12
PHE A 48	GLY C 15
PHE A 32	ARG C 12
PHE A 26	GLY C 15
PHE A 24	ARG C 12
PHE A 22	HIS C 10
GLN A 9	LEU C 11

Fig S12: Contact maps between the 15-mer peptide of Membrane glycoprotein (VIGAVILRGHLRIAG) with HLA-DRB1*01:01. Here, the distances between two amino acids closer than 4.5 A° were shown. Polar contacts between the peptide-protein interactions shown by the red font.

Receptor residue	Peptide residue
ASN B 82	ARG C 5
THR B 71	VAL C 9
TRP B 61	VAL C 9
TYR B 37	TRP C 12
PHE B 11	SER C 8
HIS A 68	TRP C 12
LYS A 67	LYS C 15
THR A 61	TYR C 10
THR A 61	PHE C 6
GLN A 57	ALA C 7
GLN A 57	ASN C 2
PHE A 54	PHE C 1
ARG A 53	THR C 4
LEU A 47	ARG C 5
GLU A 25	ARG C 5
GLN A 21	PHE C 6
TYR A 9	SER C 8
TYR A 9	ARG C 5

Receptor residue	Peptide residue
LEU B 85	ARG C 5
GLU B 74	VAL C 9
ARG B 70	ASN C 2
TYR B 60	ASN C 13
PHE B 11	VAL C 9
ASN A 71	TRP C 12
HIS A 68	TYR C 10
ALA A 64	TYR C 10
THR A 61	ALA C 7
PHE A 58	PHE C 6
GLN A 57	THR C 4
PHE A 54	THR C 4
ARG A 53	ARG C 5
PHE A 51	THR C 4
GLU A 30	ARG C 5
TYR A 22	PHE C 6
GLY A 9	PHE C 6
TYR A 9	PHE C 6

Receptor residue	Peptide residue
THR B 77	ALA C 3
ARG B 70	VAL C 9
TYR B 60	ARG C 14
TYR B 30	TRP C 12
ILE A 72	TRP C 12
HIS A 68	ALA C 11
LYS A 67	TRP C 12
THR A 61	SER C 8
LEU A 60	TYR C 10
GLN A 57	PHE C 6
GLN A 57	PHE C 1
ARG A 53	PHE C 6
ARG A 52	THR C 4
GLU A 31	ARG C 5
SER A 23	ARG C 5
VAL A 10	PHE C 6
TYR A 9	ALA C 7

Fig S13: Contact maps between the 15-mer peptide of Spike surface glycoprotein, S1 (FNATRFASVYAWNRK) with DQA1/DQB1. Here, the distances between two amino acids closer than 4.5 A° were shown. Polar contacts between the peptide-protein interactions shown by the red font.

Receptor residue	Peptide residue
HIS B 81	ALA C 9
TYR B 78	TYR C 6
ARG B 71	GLU C 11
GLN B 70	GLU C 11
LEU B 67	LEU C 2
TRP B 61	PHE C 14
TRP B 61	HIS C 3
ASP B 57	HIS C 3
TYR B 47	VAL C 4
GLU B 28	VAL C 4
PHE B 13	VAL C 4
MET A 73	PHE C 1
ASN A 69	PHE C 1
VAL A 65	HIS C 3
ASN A 62	THR C 5
ALA A 59	VAL C 7
GLY A 58	VAL C 7
GLU A 55	GLN C 10
PHE A 22	PRO C 8
GLN A 9	PRO C 8
GLN A 9	THR C 5

Receptor residue	Peptide residue
TYR B 78	VAL C 7
ARG B 71	LYS C 12
GLN B 70	ASN C 13
LEU B 67	ASN C 13
GLN B 64	ASN C 13
TRP B 61	VAL C 4
TYR B 60	LEU C 2
ASP B 57	PHE C 1
CYS B 30	HIS C 3
PHE B 13	THR C 5
LEU B 11	VAL C 4
ASN A 69	HIS C 3
VAL A 65	THR C 15
ASN A 62	VAL C 7
ALA A 61	THR C 15
GLY A 58	GLN C 10
GLN A 57	GLN C 10
PHE A 54	VAL C 7
GLU A 11	THR C 5
GLN A 9	TYR C 6

Receptor residue	Peptide residue
TYR B 78	PRO C 8
THR B 77	GLU C 11
ARG B 71	TYR C 6
LEU B 67	PHE C 14
ASP B 66	ASN C 13
TRP B 61	LYS C 12
TRP B 61	LEU C 2
ASP B 57	LEU C 2
CYS B 30	VAL C 4
PHE B 13	TYR C 6
LEU B 11	THR C 5
ILE A 72	PHE C 1
ASP A 66	HIS C 3
ASN A 62	THR C 15
ASN A 62	HIS C 3
GLY A 58	THR C 15
GLY A 58	TYR C 6
PHE A 54	PRO C 8
PHE A 22	VAL C 7
GLN A 9	VAL C 7

Fig S14: Contact maps between the 15-mer peptide of S2 domain of Spike surface glycoprotein (FLHVTYVPAQEKNFT) with HLA-DRB1*01:01. Here, the distances between two amino acids closer than 4.5 A° were shown. Polar contacts between the peptide-protein interactions shown by the red font.

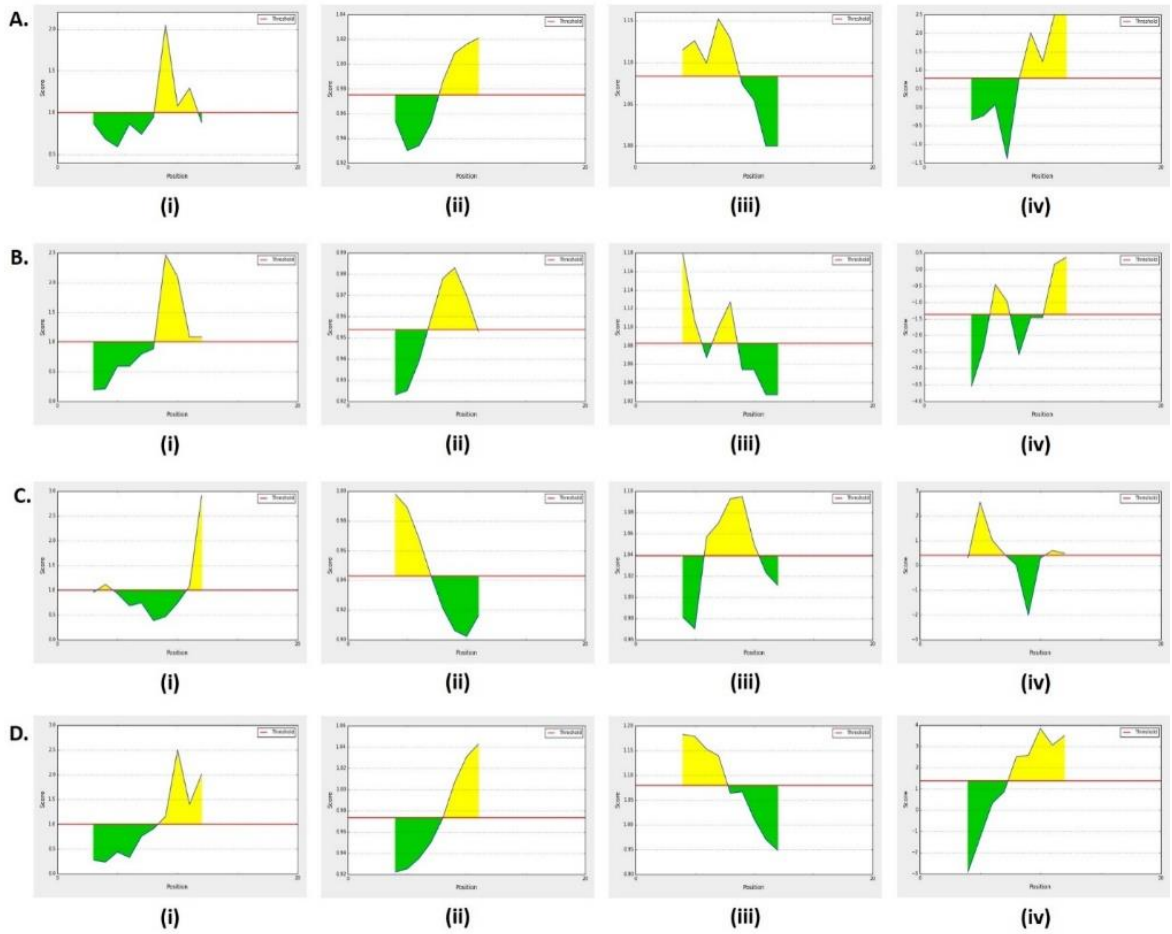

Fig S15: Prediction of B-cell epitope for epitope (A) CVEnvA2, (B) CVMemB2, (C) CVS1A2 and (D) CVS2B2. The column showed the analyses of the respective peptides with i. Emini surface accessibility prediction, ii. Karplus & Schulz Flexibility Prediction, iii. Kolaskar and Tongaonkar antigenicity prediction and, iv. Parker hydrophilicity prediction. Notes: the x-axis and y-axis of the plot reflects the sequence location and antigenic propensity, respectively. The areas over the threshold line are antigenic that are labeled as yellow.

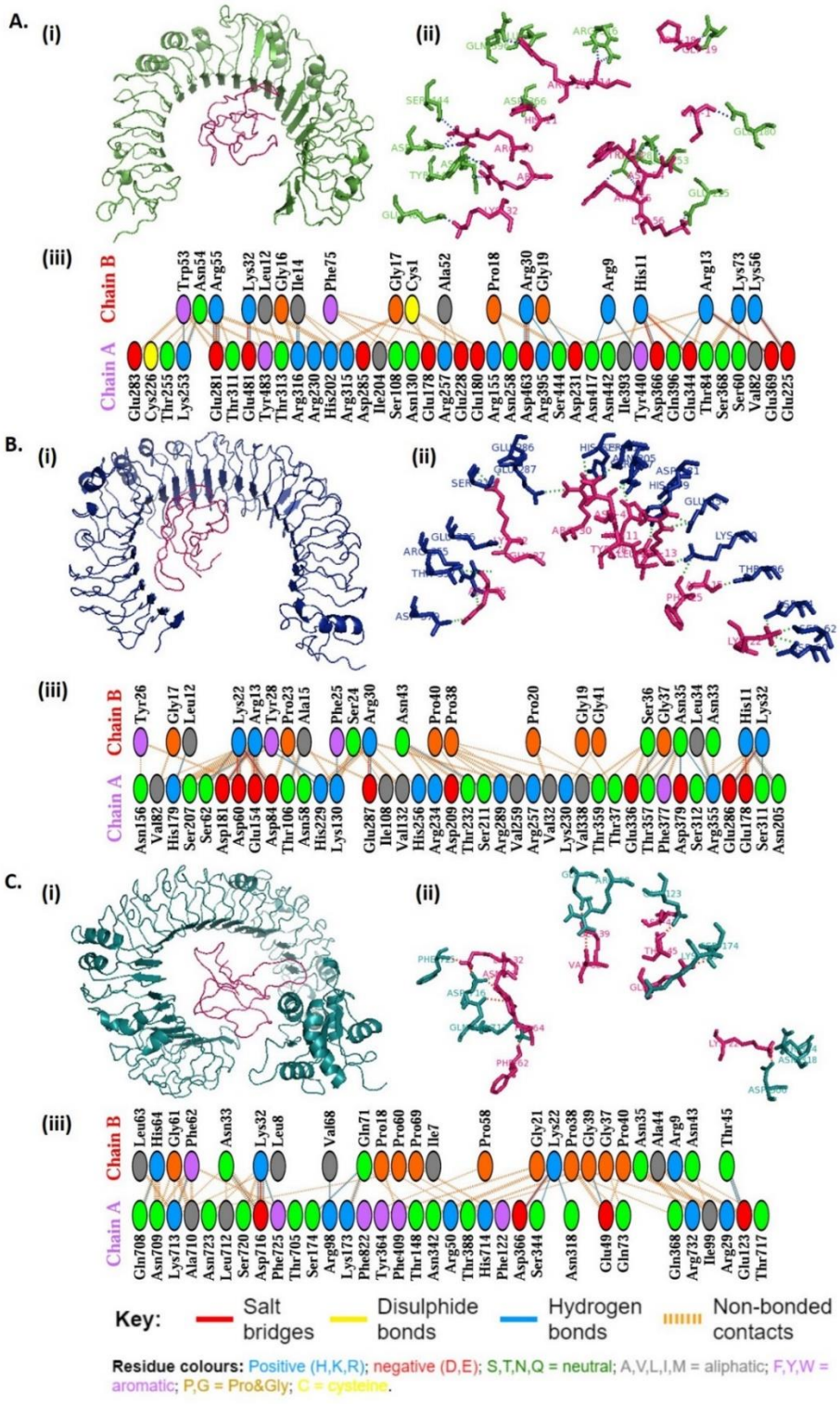

Fig S16: Docking of MEV with the Toll like receptors. A. (i) Cartoon representation of the docked complex with TLR2, (ii) The prominent residues of TLR2 and MEV involved in polar interaction, (iii) The different interacting residues extracted by PDBsum server. B. (i) Cartoon representation of the docked complex with TLR4, (ii) The prominent residues of TLR4 and MEV involved in polar interaction, (iii) The different interacting residues extracted by PDBsum server, and C. (i) Cartoon representation of the docked complex with TLR5, (ii) The prominent residues of TLR5 and MEV involved in polar interaction, (iii) The different interacting residues extracted by PDBsum server.

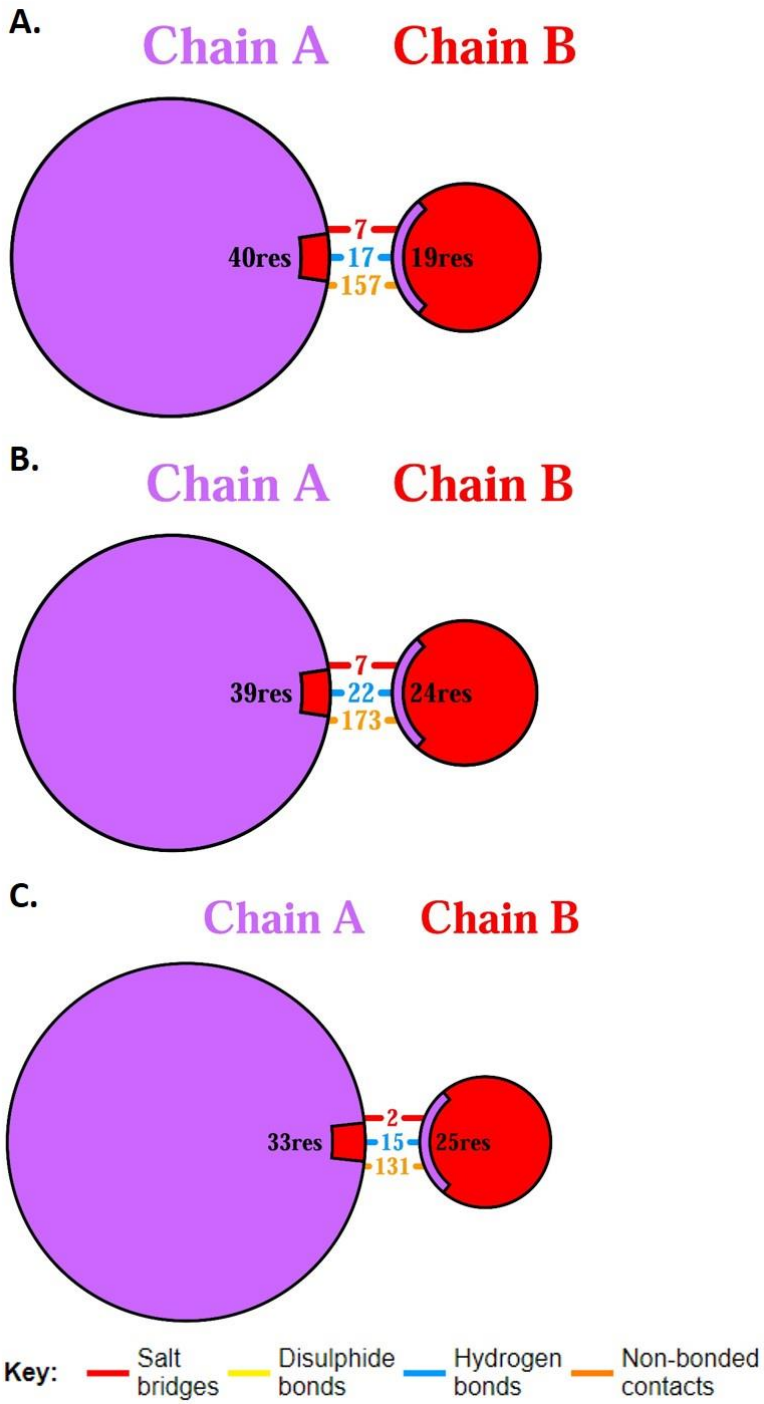

Fig S17: The Schematic diagram of the interactions between the multi-epitope vaccine and the TLR2 (A), TLR4 (B), and TLR5 (C). Different types of interactions are designated by different colors mentioned in the keys. The number of interacting residues in Chain A (TLR2, TLR4, or TLR5) and Chain B (CVMW) are shown inside the circle, and the number of possible bonds is shown in between the circle.

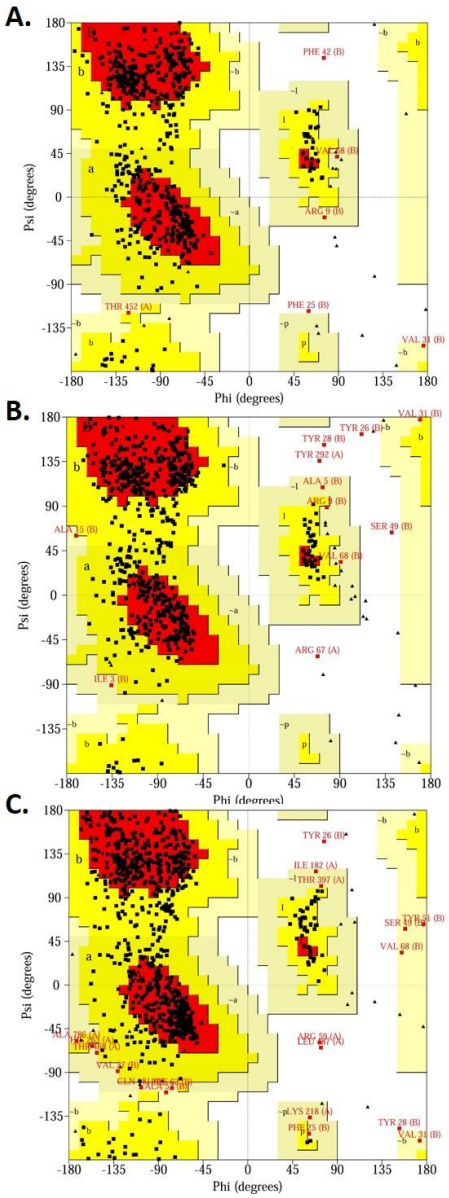

Fig S18: Ramachandran plot analysis of the docked complex of CVMW with Toll Like Receptors by PROCHECK. A. TLR2 complexed with CVMW vaccine construct. The 70.3% residues were in the most favoured region, 28.6% were in additional allowed region, 0.7% were in generously allowed regions, and 0.4% were in disallowed region. B. TLR4 complexed with CVMW vaccine construct. The 71.2% residues were in the most favoured region, 27.0% were in additional allowed region, 1.0% were in generously allowed regions, and 0.8% were in disallowed region. C. TLR5 complexed with CVMW vaccine construct. The 70.8% residues were in the most favoured region, 26.8% were in additional allowed region, 1.9% were in generously allowed regions, and 0.5% were in disallowed region.

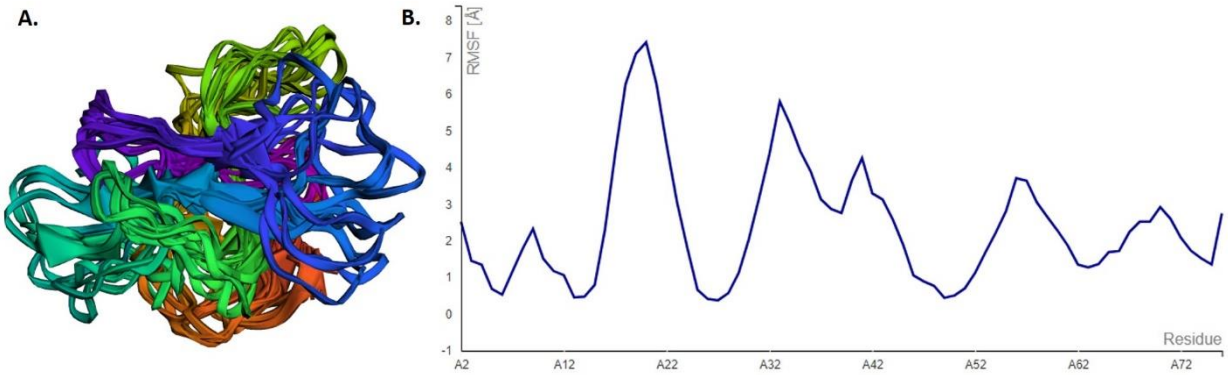

Fig S19: The Root Mean Square Fluctuation (RMSF) analyses of the multi-epitope vaccine, CVMW by CABS-flex v 2.0. A. The cartoon representation of the top ten models showing fluctuations in several regions of the vaccine. B. RMSF plot of the multi-epitope vaccine representing the obvious fluctuation on the residues during simulation.

Table S1: The predicted T-cell epitopes of Envelope protein, Membrane glycoprotein, and S1 and S2 domain of spike surface glycoprotein by the NetCTL server based on the combined score. Here, epitopes for the 10 different HLA supertypes of Envelope protein, 12 HLA supertypes of Membrane glycoprotein, S1 and S2 domain have been represented.

Super types	Predicted epitopes for Envelope protein (start position)	Combined score	Predicted epitopes for Membrane glycoprotein (start position)	Combined score	Predicted epitopes for S1 protein (start position)	Combined score	Predicted epitopes for S2 protein (start position)	Combined score
a1	LTALRLCAY (34)	2.3303	ATSRTLSYY (171)	3.7695	CVADYSVLY (361)	2.3459	LTDEMIAQY (865)	5.2958
a2	SLVKPSFYV (50)	1.4461	GLMWLSYFI (89)	1.5462	KIADYNYKL (417)	1.116	FIAGLIAIV (1220)	1.4022
a3	SFYVYSRVK (55)	1.3954	AVILRGHLR (142)	1.4462	SVYAWNRKR (349)	1.431	VTYVPAQEK (1065)	1.7543
a24	VFLLVTLAI (25)	1.2004	RYRIGNYKL (198)	1.3445	PYRVVVLSF (507)	1.6823	VYDPLQPEL (1137)	1.2944
a26	LTALRLCAY (34)	1.5975	ATSRTLSYY (171)	1.385	RISNCVADY (357)	1.4543	GTITSGWTF (880)	1.4942
b4					GEVFNATRF (339)	1.6183	AEIRASANL (1016)	1.6389
b7	FVSEETGTL (4)	1.1281	FAAYSRYRI (193)	1.2196	APATVCGPK (520)	0.8604	SPRRARSVA (680)	1.8685
b8	YVYSRVKNL (57)	1.1002	ELKKLLEQW (12)	1.2715	PYRVVVLSF (507)	1.6219	QDKNTQEVF (774)	1.4769
b27			SRYRIGNYK (197)	2.8527	TRFASVYAW (345)	0.8532	GRLQSLQTY (999)	2.6259
b39	FVSEETGTL (4)	0.9372	SFNPETNIL (111)	1.5475	IRGDEVRQI (402)	1.9243	AHFPREGVF (1087)	2.2944
b44			KEITVATSR (166)	1.1148				
b58	VSLVKPSFY (49)	1.2216	KLIFLWLLW (50)	1.8977				
b59					ASFSTFKCY (372)	1.139	QSAPHGVVF (1054)	1.9203
b62	LVKPSFYVY (51)	1.6543	WLSYFIASF (92)	1.6198	GQTGKIADY (413)	2.962	LGAENSVAY (699)	1.4998

Table S2: The potential CD8+ T-cell epitopes of Envelope protein and their respective MHC class I alleles with IC50 < 250 nM.

Peptides	Alleles	Number of Alleles
LTALRLCAY	HLA-A*01:01 (108.78), HLA-A*30:02 (241.8), HLA-B*15:01 (141.91)	3
SLVKPSFYV	HLA-A*02:06 (19.26), HLA-A*02:01 (21.43), HLA-A*02:03 (33.65), HLA-A*68:02 (141.45)	4
SFYVYSRVK	HLA-A*30:01 (96.15), HLA-A*11:01 (247.34)	2
VFLLVTLAI	HLA-A*23:01 (113.61)	1
FVSEETGTL	HLA-A*02:03 (87.29), HLA-A*02:06 (92.59), HLA-B*35:01 (193.9), HLA-A*68:02 (239.11)	4
YVYSRVKNL	HLA-A*02:03 (102.32)	1
VSLVKPSFY	HLA-A*30:02 (105.55)	1
LVKPSFYVY	HLA-B*15:01 (25.06), HLA-A*30:02 (171.58), HLA-A*30:01 (233.87), HLA-B*35:01 (157.97)	4

Table S3: The potential CD4+ T-cell epitopes of Envelope protein and their respective MHC class II alleles with IC50 < 200 nM.

Peptide	Alleles	Number of Alleles (Predivac Score)
LAI**LTALRLCAY**CCN	HLA-DRB1*01:04 (63.2), HLA-DRB1*10:02 (79.54), HLA-DQA1*01:02/ DQB1*05:01 (87.54), HLA-DQA1*01:06/DQB1*05:01 (87.54), HLA-DQA1*01:08/DQB1*05:01 (87.54), HLA-DQA1*01:09/DQB1*05:01 (87.54)	06 (80.46)
MYS**FVSEETGTL**IVN	HLA-DRB1*01:11 (53.85), HLA-DRB1*10:01 (76.67), HLA-DRB1*10:03 (76.67), HLA-DRB1*01:14 (75.37), HLA-DRB1*01:10 (87.76), HLA-DRB1*01:05 (64.93), HLA-DRB1*01:07 (64.93), HLA-DRB1*01:08 (64.93), HLA-DRB1*01:01 (64.93), HLA-DRB1*01:12 (64.93), HLA-DRB1*01:25 (64.93), HLA-DRB1*01:22 (64.93), HLA-DRB1*01:19 (64.93), HLA-DRB1*01:13 (40.9), HLA-DRB1*01:18 (60.17)	15 (82.49)
KPSF**YVYSRVKNL**NS	HLA-DRB1*07:06 (66.98), HLA-DRB1*16:14 (92.4), HLA-DRB1*16:12 (84.38), HLA-DRB1*07:01 (51.78), HLA-DRB1*07:05 (51.78), HLA-DRB1*07:03 (51.78), HLA-DRB1*07:07 (51.78), HLA-DRB1*07:13 (51.78), HLA-DRB1*07:08 (51.78), HLA-DRB1*07:16 (51.78), HLA-DRB1*07:15 (51.78), HLA-DRB1*07:19 (51.78), HLA-DRB1*07:14 (51.78), HLA-DRB1*11:11 (66.09), HLA-DRB1*16:16 (88.72), HLA-DRB1*16:02 (88.72), HLA-DRB1*16:11 (88.72), HLA-DRB1*07:12 (51.58), HLA-DRB1*07:11 (56.19), HLA-DRB1*07:09 (73.06), HLA-	127 (82.69)

	DRB1*16:10 (73.64), HLA-DRB1*07:04 (79.04), HLA-DRB5*01:02 (68.71), HLA-DRB5*01:08 (68.71), HLA-DRB1*01:09 (78.99), HLA-DRB1*01:13 (16.54), HLA-DRB5*01:01 (66.46), HLA-DRB5*01:14 (66.46), HLA-DRB5*01:13 (66.46), HLA-DRB5*01:05 (66.46), HLA-DRB1*10:01 (44.65), HLA-DRB1*10:03 (44.65), HLA-DRB1*01:10 (47.97), HLA-DRB1*01:21 (74.02), HLA-DRB1*01:11 (50.28), HLA-DRB1*01:14 (51.99), HLA-DRB1*01:05 (39.91), HLA-DRB1*01:07 (39.91), HLA-DRB1*01:08 (39.91), HLA-DRB1*01:01 (39.91), HLA-DRB1*01:12 (39.91), HLA-DRB1*01:25 (39.91), HLA-DRB1*01:22 (39.91), HLA-DRB1*01:19 (39.91), HLA-DRB1*01:18 (35.98), HLA-DRB1*01:04 (98.06), HLA-DRB3*03:01 (95.02), HLA-DRB1*09:05 (105.21), HLA-DRB1*09:07 (108.47), HLA-DRB1*09:01 (108.86), HLA-DRB1*09:09 (108.86), HLA-DRB1*01:20 (109.52), HLA-DRB1*01:24 (111.98), HLA-DRB5*01:04 (112.29), HLA-DRB1*01:17 (112.58), HLA-DRB5*01:03 (113.34), HLA-DRB1*10:02 (115.4), HLA-DRB1*09:02 (116.28), HLA-DRB5*01:12 (118.58), HLA-DRB1*14:16 (123.14), HLA-DRB1*11:13 (129.09), HLA-DRB1*11:08 (132.41), HLA-DRB3*02:09 (136.08), HLA-DRB3*02:21 (136.08), HLA-DRB1*08:08 (136.59), HLA-DRB1*08:11 (136.59), HLA-DRB1*15:06 (143.73), HLA-DRB1*15:13 (143.73), HLA-DRB1*15:01 (143.73), HLA-DRB1*15:09 (143.73), HLA-DRB1*15:20 (143.73), HLA-DRB1*15:16 (143.73), HLA-DRB1*15:24 (143.73), HLA-DRB1*15:22 (143.73), HLA-DRB3*02:17 (153.65), HLA-DRB1*15:07 (162.17), HLA-DRB3*02:16 (167.81), HLA-DRB3*02:15 (170.66), HLA-DRB3*02:14 (171.62), HLA-DRB1*09:08 (175.22), HLA-DRB1*01:06 (175.38), HLA-DRB1*13:08 (175.62), HLA-DRB1*14:09 (186.54), HLA-DRB1*08:07 (188.13), HLA-DRB1*09:03 (198.75), HLA-DPA1*01:03/DPB1*08:01 (194.99), HLA-DPA1*01:04/DPB1*08:01 (194.99), HLA-DPA1*01:05/DPB1*08:01 (194.99), HLA-DPA1*01:07/DPB1*08:01 (194.99), HLA-DPA1*01:08/DPB1*08:01 (194.99), HLA-DPA1*01:09/DPB1*08:01 (194.99), HLA-DPA1*01:10/DPB1*08:01 (194.99), HLA-DPA1*02:02/DPB1*08:01 (122.65), HLA-DPA1*02:03/DPB1*08:01 (194.99), HLA-DPA1*02:04/DPB1*08:01 (122.65), HLA-DPA1*02:02/DPB1*19:01 (126.81), HLA-DPA1*02:04/DPB1*19:01 (126.81), HLA-DPA1*03:02/DPB1*08:01 (128.12), HLA-DPA1*03:02/DPB1*19:01 (141.14), HLA-DPA1*03:02/DPB1*04:01 (148.56), HLA-DPA1*03:02/DPB1*23:01 (148.56), HLA-DPA1*03:02/DPB1*22:01 (175.54), HLA-DPA1*02:02/DPB1*01:01 (149.32), HLA-DPA1*02:04/DPB1*01:01 (149.32), HLA-DPA1*03:02/DPB1*16:01 (180.01), HLA-DPA1*03:02/DPB1*02:02 (111.88), HLA-DPA1*04:01/DPB1*02:01 (178.07), HLA-DPA1*04:01/DPB1*08:01 (176.96), HLA-DQA1*05:01/DQB1*04:01 (194), HLA-DQA1*05:01/DQB1*04:06 (194), HLA-DQA1*05:03/DQB1*04:06 (194), HLA-DQA1*05:03/DQB1*04:01 (194), HLA-DQA1*05:04/DQB1*04:01 (194), HLA-DQA1*05:04/DQB1*04:06 (194), HLA-DQA1*05:05/DQB1*04:06 (194), HLA-DQA1*05:05/ DQB1*04:01 (194), HLA-DQA1*05:06/DQB1*04:06 (194), HLA-DQA1*05:06/DQB1*04:01 (194), HLA-DQA1*05:07/DQB1*04:01 (194), HLA-DQA1*05:07/DQB1*04:06 (194), HLA-DQA1*05:08/DQB1*04:01 (194), HLA-DQA1*05:09/DQB1*04:06 (194), HLA-DQA1*05:09/ DQB1*04:01 (194), HLA-DQA1*05:08/DQB1*04:06 (194), HLA-DQA1*05:10/DQB1*04:06 (194), HLA-DQA1*05:10/DQB1*04:01 (194),	

	HLA-DQA1*05:11/DQB1*04:01 (194), HLA-DQA1*05:11/DQB1*04:06 (194)	
NIVN**VSLVKPSF Y**VY	HLA-DRB1*12:05 (181.5), HLA-DRB1*12:01 (181.5), HLA-DRB1*12:06 (181.53), HLA-DRB1*12:07 (181.53), HLA-DRB1*12:14 (181.53), HLA-DRB1*12:10 (181.53), HLA-DRB1*12:17 (181.53), HLA-DRB1*12:11 (165.49), HLA-DRB1*12:12 (142.3), HLA-DRB1*12:03 (111.95), HLA-DRB5*02:05 (88.26), HLA-DRB1*08:07 (137.52), HLA-DRB1*07:11 (65.78), HLA-DRB1*14:17 (56.76), HLA-DRB1*07:04 (93.31), HLA-DRB1*11:13 (63.92), HLA-DRB1*13:17 (85.45), HLA-DRB1*13:09 (133.61), HLA-DRB3*03:01 (44.46), HLA-DRB1*07:01 (94.61), HLA-DRB1*07:05 (94.61), HLA-DRB1*07:03 (94.61), HLA-DRB1*07:07 (94.61), HLA-DRB1*07:12 (86.51), HLA-DRB1*07:13 (94.61), HLA-DRB1*07:08 (94.61), HLA-DRB1*07:16 (94.61), HLA-DRB1*07:15 (94.61), HLA-DRB1*07:19 (94.61), HLA-DRB1*07:14 (94.61), HLA-DRB1*15:06 (129.68), HLA-DRB1*15:13 (129.68), HLA-DRB1*15:01 (129.68), HLA-DRB1*15:09 (129.68), HLA-DRB1*15:20 (129.68), HLA-DRB1*15:16 (129.68), HLA-DRB1*15:24 (129.68), HLA-DRB1*15:22 (129.68), HLA-DRB1*11:02 (65.44), HLA-DRB1*11:16 (65.44), HLA-DRB1*13:01 (65.44), HLA-DRB1*13:22 (65.44), HLA-DRB1*14:06 (170.5), HLA-DRB1*14:21 (55.77), HLA-DRB1*14:20 (170.5), HLA-DRB1*11:18 (126), HLA-DRB1*13:06 (126), HLA-DRB1*14:16 (93.18), HLA-DRB1*15:10 (181.64), HLA-DRB1*13:15 (139.32), HLA-DRB1*07:09 (121.98), HLA-DRB1*15:05 (87.7), HLA-DRB5*01:04 (130.33), HLA-DRB1*09:05 (119.96), HLA-DRB1*13:08 (139.41), HLA-DRB1*11:08 (156.48), HLA-DRB1*13:04 (111.9), HLA-DRB1*13:20 (47.69), HLA-DRB4*01:07 (185.07), HLA-DRB4*01:06 (185.07), HLA-DRB4*01:01 (185.07), HLA-DRB4*01:08 (185.07), HLA-DRB4*01:03 (185.07), HLA-DRB1*11:20 (159.19), HLA-DRB1*11:14 (159.19), HLA-DRB1*13:02 (159.19), HLA-DRB1*13:23 (159.19), HLA-DRB1*01:04 (84.48), HLA-DRB1*09:07 (154), HLA-DRB1*09:01 (168.8), HLA-DRB1*09:09 (168.8), HLA-DRB1*01:13 (29.72), HLA-DRB1*01:14 (66.92), HLA-DRB1*01:18 (40.32), HLA-DRB1*16:10 (174.38), HLA-DRB1*01:11 (77.71), HLA-DRB1*01:20 (117.69), HLA-DRB1*01:24 (146.8), HLA-DRB1*10:02 (122.79) HLA-DRB5*01:01 (187.57), HLA-DRB5*01:14 (187.57), HLA-DRB5*01:13 (187.57), HLA-DRB5*01:05 (187.57), HLA-DRB1*01:05 (67.51), HLA-DRB1*01:07 (67.51), HLA-DRB1*01:08 (67.51), HLA-DRB1*01:01 (67.51), HLA-DRB1*01:12 (67.51), HLA-DRB1*01:10 (100.15), HLA-DRB1*01:25 (67.51), HLA-DRB1*01:22 (67.51), HLA-DRB1*01:19 (67.51), HLA-DRB1*01:21 (175.09), HLA-DRB1*10:01 (113.81), HLA-DRB1*10:03 (113.81), HLA-DPA1*04:01/DPB1*08:01 (199.75), HLA-DQA1*01:03/DQB1*05:12 (166.52), HLA-DQA1*01:03/DQB1*05:01 (154.97)	98 (66.39)

Table S4: The potential CD8+ T-cell epitopes of Membrane glycoprotein and their respective MHC class I alleles with IC50 < 250 nM.

Peptide	allele	Allele no
ATSRTLSYY	HLA-C*12:03 (31.57), HLA-C*03:03 (32.18), HLA-A*30:02 (72.69), HLA-A*11:01 (141.35), HLA-A*29:02 (145.47), HLA-A*01:01 (177.64), HLA-C*14:02 (197.52), HLA-B*15:02 (220.92)	8
GLMWLSYFI	HLA-A*02:01 (5.15), HLA-A*02:06 (35.61), HLA-C*12:03 (43.27), HLA-A*32:01 (44.15), HLA-C*14:02 (157.26)	5
AVILRGHLR	HLA-A*31:01 (27.45), HLA-C*12:03 (41.04), HLA-C*03:03 (41.75), HLA-A*68:01 (95.17), HLA-C*07:01 (152.11), HLA-A*11:01 (157.87)	6
RYRIGNYKL	HLA-C*14:02 (36.03), HLA-C*12:03 (65.04), HLA-A*30:01 (70.46), HLA-C*07:02 (78.37), HLA-B*15:02 (78.75), HLA-A*23:01 (180.89)	6
FAAYSRYRI	HLA-C*03:03 (4.33), HLA-C*12:03 (32.59), HLA-A*68:02 (41.08), HLA-B*15:02 (47.99)	4
ELKKLLEQW	HLA-C*12:03 (9.89), HLA-C*14:02 (162.04),	2
SRYRIGNYK	HLA-C*14:02 (20.64), HLA-C*12:03 (33.05), HLA-C*03:03 (38.51), HLA-C*07:01 (39.46), HLA-B*27:05 (108.54), HLA-C*07:02 (187.57)	6
SFNPETNIL	HLA-C*07:02 (51.66), HLA-C*14:02 (85.83), HLA-C*12:03 (103.56), HLA-B*15:02 (165.66), HLA-C*03:03 (219.08)	5
KEITVATSR	HLA-C*12:03 (28.99), HLA-C*03:03 (166.19)	2
KLIFLWLLW	HLA-B*58:01 (11.46), HLA-A*32:01 (22.54), HLA-C*12:03 (43.17), HLA-B*57:01 (56.47)	4
WLSYFIASF	HLA-C*03:03 (16.28), HLA-B*15:01 (57.28), HLA-C*12:03 (85.55), HLA-B*15:02 (134.66), HLA-A*32:01 (181.53)	5

Table S5: The potential CD4+ T-cell epitopes of Membrane glycoprotein and their respective MHC class II alleles with IC50 < 200 nM.

Peptide	Alleles	Number of Alleles (Predivac Score)
VIG**AVILRG HLR**IAG	HLA-DRB1*13:20 (13.15), HLA-DRB1*11:02 (19.69), HLA-DRB1*11:16 (19.69), HLA-DRB1*13:01 (19.69), HLA-DRB1*13:22 (19.69), HLA-DRB1*13:04 (24.22), HLA-DRB1*14:21 (28.03), HLA-DRB1*01:04 (28.08), HLA-DRB1*01:20 (28.89), HLA-DRB1*11:03 (29.02), HLA-DRB1*13:24 (29.02), HLA-DRB1*01:18 (30.69), HLA-DRB1*01:13 (34.65), HLA-DRB1*14:16 (35.12), HLA-DRB1*11:18 (37.03), HLA-DRB1*13:06 (37.03), HLA-DRB1*11:25 (37.76), HLA-DRB1*13:18 (37.76), HLA-DRB1*13:08 (41.6), HLA-DRB1*11:04 (43.45), HLA-DRB1*13:11 (43.45), HLA-DRB1*15:05 (44.96), HLA-DRB5*01:01 (48.64), HLA-DRB5*01:14 (48.64),	119 (63.42)

	HLA-DRB5*01:13 (48.64), HLA-DRB5*01:05 (48.64), HLA-DRB1*01:06 (50.47), HLA-DRB1*11:11 (50.69), HLA-DRB1*01:12 (51.1), HLA-DRB1*01:07 (51.1), HLA-DRB1*01:08 (51.1), HLA-DRB1*01:01 (51.1), HLA-DRB1*01:05 (51.1), HLA-DRB1*01:25 (51.1), HLA-DRB1*01:22 (51.1), HLA-DRB1*01:19 (51.1), HLA-DRB1*11:01 (53.85), HLA-DRB1*11:12 (53.85), HLA-DRB1*11:09 (53.85), HLA-DRB1*11:10 (53.85), HLA-DRB1*11:15 (53.85), HLA-DRB1*11:24 (53.85), HLA-DRB1*11:29 (53.85), HLA-DRB1*11:28 (53.85), HLA-DRB1*13:05 (53.85), HLA-DRB1*13:14 (53.85), HLA-DRB1*10:02 (54.24), HLA-DRB1*08:20 (59.28), HLA-DRB1*15:10 (61.63), HLA-DRB1*11:21 (63.33), HLA-DRB1*01:10 (65.7), HLA-DRB5*01:02 (66.33), HLA-DRB5*01:08N (66.33), HLA-DRB1*01:14 (67.58), HLA-DRB5*01:04 (67.97), HLA-DRB1*08:04 (69.82), HLA-DRB1*14:15 (69.82), HLA-DRB1*13:21 (71.34), HLA-DRB1*13:19 (71.92), HLA-DRB4*01:07 (77.62), HLA-DRB4*01:06 (77.62), HLA-DRB4*01:01 (77.62), HLA-DRB4*01:08 (77.62), HLA-DRB4*01:03 (77.62), HLA-DRB1*15:06 (78.36), HLA-DRB1*15:13 (78.36), HLA-DRB1*15:01 (78.36), HLA-DRB1*15:09 (78.36), HLA-DRB1*15:20 (78.36), HLA-DRB1*15:16 (78.36), HLA-DRB1*15:24 (78.36), HLA-DRB1*15:22 (78.36), HLA-DRB1*08:06 (81.87), HLA-DRB1*15:04 (82.42), HLA-DRB1*01:11 (82.68), HLA-DRB1*11:05 (82.76), HLA-DRB1*11:27 (85.69), HLA-DRB1*14:06 (96.9), HLA-DRB1*14:20 (96.9), HLA-DRB1*01:02 (98.37), HLA-DRB1*15:18 (101.24), HLA-DRB1*14:25 (102.79), HLA-DRB1*14:22 (102.79), HLA-DRB1*12:03 (104.46), HLA-DRB1*01:09 (106.07), HLA-DRB1*12:19 (109.08), HLA-DRB5*02:05 (110.12), HLA-DRB1*14:12 (114.81), HLA-DRB1*15:21 (116.75), HLA-DRB5*02:04 (123.66), HLA-DRB5*01:03 (125.49), HLA-DRB1*11:06 (126.39), HLA-DRB1*07:11 (131.45), HLA-DRB1*16:09 (132.86), HLA-DRB1*01:24 (133.62), HLA-DRB1*08:01 (138.02), HLA-DRB1*08:16 (138.02), HLA-DRB1*13:07 (138.04), HLA-DRB1*08:05 (139.04), HLA-DRB1*11:08 (141.65), HLA-DRB1*15:07 (150.89), HLA-DRB1*16:10 (150.99), HLA-DRB1*08:08 (151.97), HLA-DRB1*08:11 (151.97), HLA-DRB1*15:23 (155.3), HLA-DRB1*10:01 (155.53), HLA-DRB1*10:03 (155.53), HLA-DRB1*12:12 (155.78), HLA-DRB1*15:15 (158.6), HLA-DRB1*08:10 (159.98), HLA-DRB1*01:21 (167.42), HLA-DRB1*08:24 (171.52), HLA-DRB1*15:12 (176.98), HLA-DRB1*04:13 (184.89), HLA-DRB1*01:17 (190.31), HLA-DRB1*04:02 (194.82), HLA-DRB1*14:01 (195.88) HLA-DPA1*03:02/DPB1*08:01 (187), HLA-DPA1*03:02/DPB1*19:01 (187.58)	
FAAYS**RYRI GNYKL**N	HLA-DRB1*01:13 (53.23), HLA-DRB1*15:05 (84.77), HLA-DRB5*01:01 (113.18), HLA-DRB5*01:14 (113.18), HLA-DRB5*01:13 (113.18), HLA-DRB5*01:05 (113.18), HLA-DRB1*01:18 (125.24), HLA-DRB5*01:02 (133.32), HLA-DRB5*01:08N (133.32), HLA-DRB1*13:04 (150.91), HLA-DRB1*11:11 (152.29), HLA-DRB1*01:10 (156.63), HLA-DRB1*01:12 (162), HLA-DRB1*01:07 (162), HLA-DRB1*01:08 (162), HLA-DRB1*01:01 (162), HLA-DRB1*01:05 (162), HLA-DRB1*01:25 (162), HLA-DRB1*01:22 (162), HLA-DRB1*01:19 (162), HLA-DRB1*15:06 (164.54), HLA-DRB1*15:13 (164.54), HLA-DRB1*15:01 (164.54), HLA-DRB1*15:09 (164.54), HLA-DRB1*15:20 (164.54), HLA-DRB1*15:16 (164.54), HLA-DRB1*15:24 (164.54), HLA-DRB1*15:22 (164.54), HLA-DRB1*07:11 (164.89), HLA-DRB1*01:14 (167.87), HLA-DRB1*14:16 (175.04), HLA-DRB1*14:21 (178.2), HLA-DRB1*14:25 (181.64), HLA-DRB1*14:22 (181.64), HLA-DRB5*01:03 (187.46), HLA-DRB1*11:01 (188.98), HLA-DRB1*11:12 (188.98), HLA-DRB1*11:09 (188.98), HLA-DRB1*11:10 (188.98), HLA-DRB1*11:15 (188.98), HLA-DRB1*11:24 (188.98), HLA-DRB1*11:29 (188.98), HLA-DRB1*11:28 (188.98), HLA-DRB1*13:05 (188.98), HLA-DRB1*13:14 (188.98), HLA-DRB1*11:02 (191.3), HLA-DRB1*11:16 (191.3), HLA-DRB1*13:01 (191.3), HLA-DRB1*13:22 (191.3), HLA-DRB1*01:04 (191.59), HLA-DRB1*10:02 (198.03), HLA-DRB1*09:05 (199.52)	52 (63.31)
G**FAAYSRYR I**GNYKL	HLA-DRB1*01:13 (59.31), HLA-DRB1*15:05 (65.8), HLA-DRB1*15:04 (73.83), HLA-DRB1*15:15 (74.54), HLA-DRB1*13:20 (75.17), HLA-DRB5*01:01 (95.36), HLA-DRB5*01:14 (95.36), HLA-DRB5*01:13 (95.36), HLA-DRB5*01:05 (95.36),	64 (63.31)

	HLA-DRB1*11:03 (101.03), HLA-DRB1*13:24 (101.03), HLA-DRB1*13:21 (102.94), HLA-DRB5*01:02 (105.89), HLA-DRB5*01:08N (105.89), HLA-DRB1*11:11 (113.84), HLA-DRB1*13:04 (117.84), HLA-DRB1*15:06 (127.61), HLA-DRB1*15:13 (127.61), HLA-DRB1*15:01 (127.61), HLA-DRB1*15:09 (127.61), HLA-DRB1*15:20 (127.61), HLA-DRB1*15:16 (127.61), HLA-DRB1*15:24 (127.61), HLA-DRB1*15:22 (127.61), HLA-DRB1*16:09 (127.66), HLA-DRB1*14:25 (129.22), HLA-DRB1*14:22 (129.22), HLA-DRB5*01:03 (130.37), HLA-DRB1*11:01 (130.44), HLA-DRB1*11:12 (130.44), HLA-DRB1*11:09 (130.44), HLA-DRB1*11:10 (130.44), HLA-DRB1*11:15 (130.44), HLA-DRB1*11:24 (130.44), HLA-DRB1*11:29 (130.44), HLA-DRB1*11:28 (130.44), HLA-DRB1*13:05 (130.44), HLA-DRB1*13:14 (130.44), HLA-DRB1*15:23 (131.1), HLA-DRB1*07:11 (139.2), HLA-DRB1*14:16 (140.73), HLA-DRB1*14:21 (155.86), HLA-DRB1*11:02 (161.76), HLA-DRB1*11:16 (161.76), HLA-DRB1*13:01 (161.76), HLA-DRB1*13:22 (161.76), HLA-DRB1*15:12 (161.94), HLA-DRB1*11:04 (166.51), HLA-DRB1*13:11 (166.51), HLA-DRB1*10:02 (168.26), HLA-DRB1*15:07 (169.81), HLA-DRB1*15:18 (174.61), HLA-DRB1*16:01 (175.13), HLA-DRB1*16:03 (175.13), HLA-DRB1*16:08 (175.13), HLA-DRB1*01:20 (176.67), HLA-DRB5*02:04 (177.53), HLA-DRB5*01:04 (177.89), HLA-DRB1*09:05 (185.83), HLA-DRB1*01:04 (186.97), HLA-DRB1*16:10 (187.8), HLA-DRB1*15:10 (192.03), HLA-DRB1*08:05 (193.87), HLA-DRB1*01:06 (199.73)	
FAAY**SRYRI GNYK**LN	HLA-DRB1*13:20 (90.82)	1 (63.31)
VGLM**WLSY FIASF**RL	HLA-DRB1*01:13 (27.47), HLA-DRB1*01:18 (39.16), HLA-DRB1*15:05 (39.94), HLA-DRB1*01:14 (42.04), HLA-DRB1*07:11 (52.03), HLA-DRB1*10:01 (54.28), HLA-DRB1*10:03 (54.28), HLA-DRB1*15:12 (54.59), HLA-DRB1*15:06 (54.82), HLA-DRB1*15:13 (54.82), HLA-DRB1*15:01 (54.82), HLA-DRB1*15:09 (54.82), HLA-DRB1*15:20 (54.82), HLA-DRB1*15:16 (54.82), HLA-DRB1*15:24 (54.82), HLA-DRB1*15:22 (54.82), HLA-DRB1*10:02 (56.13), HLA-DRB1*01:12 (59.75), HLA-DRB1*01:07 (59.75), HLA-DRB1*01:08 (59.75), HLA-DRB1*01:01 (59.75), HLA-DRB1*01:05 (59.75), HLA-DRB1*01:25 (59.75), HLA-DRB1*01:22 (59.75), HLA-DRB1*01:19 (59.75), HLA-DRB1*07:12 (64.62), HLA-DRB1*07:01 (66.14), HLA-DRB1*07:05 (66.14), HLA-DRB1*07:03 (66.14), HLA-DRB1*07:07 (66.14), HLA-DRB1*07:13 (66.14), HLA-DRB1*07:08 (66.14), HLA-DRB1*07:16 (66.14), HLA-DRB1*07:15 (66.14), HLA-DRB1*07:19 (66.14), HLA-DRB1*07:14 (66.14), HLA-DRB1*01:20 (69.78), HLA-DRB1*16:10 (73.01), HLA-DRB1*15:15 (76.16), HLA-DRB1*15:10 (76.34), HLA-DRB1*01:04 (76.68), HLA-DRB1*07:09 (80.7), HLA-DRB1*07:04 (85.42), HLA-DRB1*15:18 (85.68), HLA-DRB1*15:07 (85.91), HLA-DRB1*09:05 (89.58), HLA-DRB1*15:23 (90.11), HLA-DRB1*15:04 (96.12), HLA-DRB1*01:11 (98.28), HLA-DRB1*09:07 (101.43), HLA-DRB1*01:10 (107.37), HLA-DRB1*13:20 (108.14), HLA-DRB5*01:01 (109.43), HLA-DRB5*01:14 (109.43), HLA-DRB5*01:13 (109.43), HLA-DRB5*01:05 (109.43), HLA-DRB1*14:16 (111.84), HLA-DRB1*07:06 (113.27), HLA-DRB1*16:16 (113.39), HLA-DRB1*16:02 (113.39), HLA-DRB1*16:11 (113.39), HLA-DRB1*09:01 (114.82), HLA-DRB1*09:09 (114.82), HLA-DRB1*01:21 (115.4), HLA-DRB1*16:09 (116.69), HLA-DRB1*13:04 (119.75), HLA-DRB1*01:24 (126.29), HLA-DRB1*16:12 (126.82), HLA-DRB1*11:13 (126.83), HLA-DRB1*04:10 (127.6), HLA-DRB1*15:03 (128.74), HLA-DRB1*16:14 (130.34), HLA-DRB1*14:17 (134.9), HLA-DRB5*01:04 (136.65), HLA-DRB5*01:02 (146.5), HLA-DRB5*01:08N (146.5), HLA-DRB1*14:21 (149.84), HLA-DRB1*01:06 (152.36), HLA-DRB5*02:05 (154.56), HLA-DRB1*15:21 (156.02), HLA-DRB1*01:09 (158.89), HLA-DRB1*16:04 (165.91), HLA-DRB1*11:02 (167), HLA-DRB1*11:16 (167), HLA-DRB1*13:01 (167), HLA-DRB1*13:22 (167), HLA-DRB1*15:02 (181.32), HLA-DRB1*15:08 (181.32), HLA-DRB1*15:19 (181.32), HLA-DRB1*15:26	164 (66.37)

	(181.32), HLA-DRB1*15:14 (181.32), HLA-DRB1*12:03 (188.18), HLA-DRB1*16:01 (191.34), HLA-DRB1*16:03 (191.34), HLA-DRB1*16:08 (191.34), HLA-DPA1*03:02/DPB1*15:01 (28.97), HLA-DPA1*02:02/DPB1*15:01 (33.4), HLA-DPA1*02:04/DPB1*15:01 (33.4), HLA-DPA1*02:04/DPB1*02:01 (34.25), HLA-DPA1*04:01/DPB1*15:01 (40.39), HLA-DPA1*03:03/DPB1*02:01 (44.19), HLA-DPA1*03:02 DPB1*04:01 (44.84), HLA-DPA1*03:02/DPB1*23:01 (44.84), HLA-DPA1*01:03/DPB1*15:01 (45.16), HLA-DPA1*01:04/DPB1*15:01 (45.16), HLA-DPA1*01:05/DPB1*15:01 (45.16), HLA-DPA1*01:07/DPB1*15:01 (45.16), HLA-DPA1*01:08/DPB1*15:01 (45.16), HLA-DPA1*01:09/DPB1*15:01 (45.16), HLA-DPA1*01:10/DPB1*15:01 (45.16), HLA-DPA1*02:03/DPB1*15:01 (45.16), HLA-DPA1*02:02/DPB1*23:01 (45.96), HLA-DPA1*02:04/DPB1*23:01 (45.96), HLA-DPA1*04:01/DPB1*02:01 (46.83), HLA-DPA1*03:01/DPB1*15:01 (48.75), HLA-DPA1*03:03/DPB1*15:01 (48.75), HLA-DPA1*01:03/DPB1*02:01 (48.8), HLA-DPA1*01:07/DPB1*02:01 (48.8), HLA-DPA1*01:08/DPB1*02:01 (48.8), HLA-DPA1*01:09/DPB1*02:01 (48.8), HLA-DPA1*01:10/DPB1*02:01 (48.8), HLA-DPA1*02:03/DPB1*02:01 (48.8), HLA-DPA1*01:06/DPB1*15:01 (49.93), HLA-DPA1*02:01/DPB1*15:01 (49.93), HLA-DPA1*01:06/DPB1*02:01 (55.01), HLA-DPA1*02:01/DPB1*02:01 (55.01), HLA-DPA1*04:01/DPB1*04:01 (64.32), HLA-DPA1*04:01/DPB1*23:01 (64.32), HLA-DPA1*03:01/DPB1*04:01 (74.24), HLA-DPA1*03:01/DPB1*23:01 (74.24), HLA-DPA1*03:03/DPB1*04:01 (74.24), HLA-DPA1*03:03/DPB1*23:01 (74.24), HLA-DPA1*01:03/DPB1*04:01 (74.24), HLA-DPA1*01:04/DPB1*04:01 (74.24), HLA-DPA1*01:05/DPB1*04:01 (74.24), HLA-DPA1*01:08/DPB1*04:01 (74.24), HLA-DPA1*01:10/DPB1*23:01 (74.24), HLA-DPA1*02:03/DPB1*23:01 (74.24), HLA-DPA1*02:01/DPB1*04:01 (75.37), HLA-DPA1*02:01/DPB1*23:01 (75.37), HLA-DPA1*02:02/DPB1*04:02 (101.17), HLA-DPA1*02:04/DPB1*04:02 (101.17), HLA-DPA1*01:06/DPB1*04:02 (157.61), HLA-DPA1*01:07/DPB1*04:02 (183.21), HLA-DPA1*01:09/DPB1*04:02 (183.21), HLA-DPA1*01:10/DPB1*04:02 (183.21), HLA-DPA1*02:03/DPB1*04:02 (183.21), HLA-DQA1*05:01/DQB1*05:01 (86.13), HLA-DQA1*05:03/DQB1*05:01 (86.13), HLA-DQA1*05:04/DQB1*05:01 (86.13), HLA-DQA1*05:05/DQB1*05:01 (86.13), HLA-DQA1*05:06/DQB1*05:01 (86.13), HLA-DQA1*05:07/DQB1*05:01 (86.13), HLA-DQA1*05:08/DQB1*05:01 (86.13), HLA-DQA1*05:10/DQB1*05:01 (86.13), HLA-DQA1*05:09/DQB1*05:01 (86.13), HLA-DQA1*05:11/DQB1*05:01 (86.13), HLA-DQA1*01:01/DQB1*05:07 (144.01), HLA-DQA1*01:01/DQB1*05:01 (144.01), HLA-DQA1*01:04/DQB1*05:01 (144.01), HLA-DQA1*01:05/DQB1*05:01 (144.01), HLA-DQA1*01:07/DQB1*05:01 (144.01), HLA-DQA1*06:01/DQB1*05:01 (196.08), HLA-DQA1*06:02/DQB1*05:01 (196.08)	

Table S6: The potential CD8+ T-cell epitopes of S1 domain of Spike surface glycoprotein and their respective MHC class I alleles with IC50 < 250 nM.

Peptide	Allele	Allele no
CVADYSVLY	HLA-A*29:02 (19.22), HLA-B*35:01 (45.04), HLA-C*12:03 (54.23), HLA-C*03:03 (57.62), HLA-C*07:01 (138.73), HLA-A*68:01 (217.52), HLA-A*30:02 (224.63), HLA-A*26:01 (225.74), HLA-B*15:02 (245.04)	09
KIADYNYKL	HLA-A*02:01 (38.82), HLA-A*32:01 (53.20), HLA-A*02:06 (101.99), HLA-C*12:03 (108.95), HLA-B*15:02 (134.97), HLA-C*15:02 (193.38), HLA-C*03:03 (202.12)	07
SVYAWNRKR	HLA-C*12:03 (26.25), HLA-A*31:01 (29.96), HLA-C*03:03 (36.61), HLA-A*68:01 (67.53), HLA-C*07:01 (104.75), HLA-C*14:02 (120.68), HLA-A*11:01 (185.05)	07
PYRVVVLSF	HLA-C*14:02 (9.45), HLA-A*23:01 (46.71), HLA-C*12:03 (61.97), HLA-C*07:02 (66.86), HLA-B*15:02 (173.87), HLA-A*24:02 (193.92)	06
RISNCVADY	HLA-C*12:03 (23.62), HLA-C*03:03 (30.95), HLA-A*30:02 (54.89), HLA-C*05:01 (182.25), HLA-A*29:02 (231.61)	05
GEVFNATRF	HLA-C*03:03 (49.27), HLA-C*12:03 (92.09), HLA-B*40:01 (93.30), HLA-B*15:02 (217.39)	04
APATVCGPK	HLA-C*03:03 (22.32), HLA-C*12:03 (59.46), HLA-A*11:01 (163.04)	03
TRFASVYAW	HLA-C*12:03 (14.46), HLA-C*07:01 (33.13), HLA-C*03:03 (56.57), HLA-C*14:02 (64.36), HLA-B*39:01 (71.02), HLA-C*06:02 (137.03), HLA-B*58:01 (197.38), HLA-C*07:02 (204.72)	08
IRGDEVRQI	HLA-C*07:01 (16.64), HLA-C*12:03 (36.41), HLA-C*03:03 (54.90), HLA-C*07:02 (58.23), HLA-C*06:02 (70.93)	05
ASFSTFKCY	HLA-C*12:03 (9.75), HLA-C*03:03 (49.05), HLA-A*30:02 (111.29), HLA-B*15:01 (124.17), HLA-C*07:01 (183.30), HLA-C*14:02 (205.88), HLA-B*15:02 (228.68)	07
GQTGKIADY	HLA-C*03:03 (15.69), HLA-C*12:03 (36.08), HLA-A*30:02 (157.93)	03

Table S7: The potential CD4+ T-cell epitopes of S1 domain of Spike surface glycoprotein and their respective MHC class II alleles with IC50 < 200 nM.

Peptide	Alleles	Number of Alleles (Prediva c Score)
ISN**CVADYS VLY**NSA	HLA-DRB3*01:14 (91.14), HLA-DRB3*01:05 (82.26), HLA-DRB3*01:12 (71.47), HLA-DRB3*01:11 (71.47), HLA-DRB3*01:08 (71.47), HLA-DRB3*01:04 (71.47), HLA-DRB3*01:01 (71.47), HLA-DRB1*03:14 (185.26), HLA-DRB1*03:10 (126.96), HLA-DRB1*03:01 (180.92), HLA-DRB1*03:04 (180.92), HLA-DRB1*03:18 (180.92), HLA-DRB1*03:13 (180.92), HLA-DRB1*03:08 (180.92), HLA-DRB1*03:23 (180.92), HLA-DRB1*03:25 (180.92), HLA-DRB1*03:22 (180.92), HLA-DRB1*03:11 (86.53), HLA-DRB1*07:04 (186.08), HLA-DRB3*03:01 (197.16), HLA-DRB1*01:13 (166.15), HLA-DQA1*01:02/DQB1*05:01	25 (72.88)

	(141.24), HLA-DQA1*01:06/DQB1*05:01 (141.24), HLA-DQA1*01:08/DQB1*05:01 (141.24), HLA-DQA1*01:09/DQB1*05:01 (141.24)	
FA**SVYAWN RKR**ISNC	HLA-DRB5*01:03 (89.00), HLA-DRB5*01:01 (43.04), HLA-DRB5*01:14 (43.04), HLA-DRB5*01:13 (43.04), HLA-DRB5*01:05 (43.04), HLA-DRB5*01:02 (56.92), HLA-DRB5*01:08 (56.92), HLA-DRB5*01:04 (91.49), HLA-DRB5*02:05 (198.19), HLA-DRB1*01:20 (140.43), HLA-DRB1*01:04 (126.64)	11 (81.51)
NRK**RISNCV ADY**SVL	HLA-DRB1*11:20 (192.31), HLA-DRB1*11:14 (192.31), HLA-DRB1*13:02 (192.31), HLA-DRB1*13:23 (192.31), HLA-DRB3*03:01 (69.9)	5 (72.88)
FNA**TRFASV YAW**NRK	HLA-DPA1*04:01/DPB1*06:01 (196.22), HLA-DPA1*03:02/DPB1*13:01 (199.34), HLA-DQA1*01:03/DQB1*04:01 (182.97), HLA-DQA1*02:01/DQB1*04:01 (162.82), HLA-DQA1*02:01/DQB1*04:06 (162.82), HLA-DQA1*02:01/DQB1*03:01 (85.57), HLA-DQA1*05:01/DQB1*04:01 (100.98), HLA-DQA1*05:01/ DQB1*04:06 (100.98), HLA-DQA1*05:03/DQB1*04:06 (100.98), HLA-DQA1*05:03/DQB1*04:01 (100.98), HLA-DQA1*05:04/ DQB1*04:01 (100.98), HLA-DQA1*05:04/DQB1*04:06 (100.98), HLA-DQA1*05:05/DQB1*04:06 (100.98), HLA-DQA1*05:05/ DQB1*04:01 (100.98), HLA-DQA1*05:06/DQB1*04:06 (100.98), HLA-DQA1*05:06/DQB1*04:01 (100.98), HLA-DQA1*05:07/ DQB1*04:01 (100.98), HLA-DQA1*05:07/DQB1*04:06 (100.98), HLA-DQA1*05:08/DQB1*04:01 (100.98), HLA-DQA1*05:09/ DQB1*04:06 (100.98), HLA-DQA1*05:09/DQB1*04:01 (100.98), HLA-DQA1*05:08/DQB1*04:06 (100.98), HLA-DQA1*05:10/ DQB1*04:06 (100.98), HLA-DQA1*05:10/DQB1*04:01 (100.98), HLA-DQA1*05:11/DQB1*04:01 (100.98), HLA-DQA1*05:11/ DQB1*04:06 (100.98), HLA-DQA1*01:03/DQB1*06:01 (197.72), HLA-DQA1*02:01/DQB1*06:01 (152.09), HLA-DQA1*01:03/ DQB1*03:01 (114.98), HLA-DQA1*05:01/DQB1*03:01 (177.79), HLA-DQA1*05:03/DQB1*03:01 (177.79), HLA-DQA1*05:04/ DQB1*03:01 (177.79), HLA-DQA1*05:05/ DQB1*03:01 (177.79), HLA-DQA1*05:06/DQB1*03:01 (177.79), HLA-DQA1*05:07/ DQB1*03:01 (177.79), HLA-DQA1*05:08/DQB1*03:01 (177.79), HLA-DQA1*05:09/DQB1*03:01 (177.79), HLA-DQA1*05:10/ DQB1*03:01 (177.79), HLA-DQA1*05:11/DQB1*03:01 (177.79), HLA-DQA1*01:02/ DQB1*05:01 (173.73), HLA-DQA1*01:06/ DQB1*05:01 (173.73), HLA-DQA1*01:08/DQB1*05:01 (173.73), HLA-DQA1*01:09/DQB1*05:01 (173.73)	43 (81.51)
ADSFV**IRGD EVRQI**A	HLA-DRB1*01:11 (153.51), HLA-DRB1*01:13 (124.48), HLA-DRB1*01:18 (178.8), HLA-DRB1*03:01 (51.75), HLA-DRB1*03:04 (51.75), HLA-DRB1*03:05 (155.24), HLA-DRB1*03:06 (117.43), HLA-DRB1*03:07 (134.41), HLA-DRB1*03:08 (51.75), HLA-DRB1*03:10 (45.78), HLA-DRB1*03:11 (25.08), HLA-DRB1*03:13 (51.75), HLA-DRB1*03:14 (114.28), HLA-DRB1*03:15 (75.52), HLA-DRB1*03:17 (156.61), HLA-DRB1*03:18 (51.75), HLA-DRB1*03:19 (72.02), HLA-	50 (64.85)

	DRB1*03:20 (135.26), HLA-DRB1*03:21 (134.41), HLA-DRB1*03:22 (51.75), HLA-DRB1*03:23 (51.75), HLA-DRB1*03:24 (57.18), HLA-DRB1*03:25 (51.75), HLA-DRB1*03:26 (117.43), HLA-DRB1*07:04 (142.56), HLA-DRB1*11:07 (134.41), HLA-DRB1*11:13 (147.3), HLA-DRB1*11:14 (115.74), HLA-DRB1*11:20 (115.74), HLA-DRB1*13:02 (115.74), HLA-DRB1*13:16 (149.89), HLA-DRB1*13:20 (179.83), HLA-DRB1*13:23 (115.74), HLA-DRB1*14:09 (184.47), HLA-DRB1*14:17 (105.14), HLA-DRB1*14:21 (71.86), HLA-DRB3*01:01 (70.36), HLA-DRB3*01:04 (70.36), HLA-DRB3*01:05 (73.96), HLA-DRB3*01:08 (70.36), HLA-DRB3*01:11 (70.36), HLA-DRB3*01:12 (70.36), HLA-DRB3*01:14 (81.82), HLA-DRB3*03:01 (60.24), HLA-DRB4*01:04 (152.6), HLA-DRB5*02:05 (157), HLA-DQA1*01:02/ DQB1*05:01 (179.51), HLA-DQA1*01:06/DQB1*05:01 (179.51), HLA-DQA1*01:08/DQB1*05:01 (179.51), HLA-DQA1*01:09/ DQB1*05:01 (179.51)	

Table S8: The potential CD8+ T-cell epitopes of S2 domain of Spike surface glycoprotein and their respective MHC class I alleles with IC50 < 250 nM.

Peptides	HLA	No. of Alleles
LTDEMIAQY	HLA-C*12:03 (6.50), HLA-C*05:01 (10.51), HLA-A*01:01 (67.07), HLA-C*14:02 (178.08)	4
FIAGLIAIV	HLA-A*02:06 (12.46), HLA-A*68:02 (17.48), HLA-A*02:01 (20.19), HLA-C*12:03 (33.82), HLA-C*03:03 (58.83)	5
VTYVPAQEK	HLA-C*03:03 (9.41), HLA-C*15:02 (19.34), HLA-C*12:03 (26.25), HLA-C*14:02 (29.21), HLA-A*11:01 (53), HLA-A*03:01 (107.1), HLA-A*30:01 (223.34)	7
VYDPLQPEL	HLA-C*14:02 (4.79), HLA-C*07:02 (8.04), HLA-C*12:03 (16.68), HLA-C*08:02 (65.34), HLA-B*15:02 (150.39), HLA-C*06:02 (220.19)	6
GTITSGWTF	HLA-C*03:03 (45.46), HLA-C*12:03 (70.50), HLA-B*58:01 (91.47), HLA-B*15:02 (145.29)	4
AEIRASANL	HLA-C*03:03 (11.98), HLA-B*40:01 (25.87), HLA-B*15:02 (55.88), HLA-C*12:03 (70.02), HLA-B*40:02 (93.51)	5
SPRRARSVA	HLA-B*07:02 (5.65), HLA-C*12:03 (18.42), HLA-B*15:02 (195.08)	3
QDKNTQEVF	HLA-C*12:03 (14.39), HLA-C*14:02 (133.54), HLA-B*15:02 (134.66)	3
GRLQSLQTY	HLA-C*12:03 (41.42), HLA-C*03:03 (88.43), HLA-C*07:01 (98.67), HLA-C*14:02 (121.79), HLA-C*07:02 (126.23), HLA-B*15:02 (128.59), HLA-C*06:02 (159.52)	7
AHFPREGVF	HLA-C*12:03 (31.2), HLA-C*03:03 (73.89), HLA-C*07:02 (144.6), HLA-B*15:02 (148.33), HLA-C*14:02 (216.58)	5
QSAPHGVVF	HLA-C*03:03 (35.53), HLA-B*15:01 (60.53), HLA-B*15:02 (76.25), HLA-B*58:01 (106.73), HLA-C*12:03 (122.8), HLA-A*32:01 (185.75), HLA-C*15:02 (201.57)	7
LGAENSVAY	HLA-B*35:01 (8.58), HLA-C*03:03 (20.92), HLA-C*12:03 (45.94), HLA-B*15:01 (122.18), HLA-B*15:02 (148.67)	5

Table S9: The potential CD4+ T-cell epitopes of S2 domain of Spike surface glycoprotein and their respective MHC class II alleles with IC50 < 200 nM.

Peptide	Alleles	Number of Alleles (Prediva c Score)
IWLG**FIA GLIAIV**M V	HLA-DRB1*01:24 (96.15), HLA-DRB1*01:14 (56.71), HLA-DRB1*01:21 (111.68), HLA-DRB1*07:09 (177.7), HLA-DRB1*01:18 (46.42), HLA-DRB1*07:04 (176.93), HLA-DRB1*07:12 (178.63), HLA-DRB1*07:11 (143.95), HLA-DRB1*10:01 (92.81), HLA-DRB1*10:03 (92.81), HLA-DRB1*01:13 (37.12), HLA-DRB1*01:11 (95.77), HLA-DRB3*03:01 (92.89), HLA-DRB1*01:05 (73.8), HLA-DRB1*01:07 (73.8), HLA-DRB1*01:08 (73.8), HLA-DRB1*01:01 (73.8), HLA-DRB1*01:12 (73.8), HLA-DRB1*01:25 (73.8), HLA-DRB1*01:22 (73.8), HLA-DRB1*01:19 (73.8),	38 (81.88)

	HLA-DRB1*01:10 (188.68), HLA-DPA1*04:01/ DPB1*15:01 (123.14), HLA-DPA1*03:01/ DPB1*15:01 (196.43), HLA-DPA1*03:03/DPB1*15:01 (196.43), HLA-DPA1*03:02/DPB1*15:01 (134.35), HLA-DPA1*02:02/ DPB1*15:01 (172.46), HLA-DPA1*02:04/DPB1*15:01 (172.46), HLA-DQA1*05:01/ DQB1*05:01 (175.42), HLA-DQA1*05:03/ DQB1*05:01 (175.42), HLA-DQA1*05:04/DQB1*05:01 (175.42), HLA-DQA1*05:05/ DQB1*05:01 (175.42), HLA-DQA1*05:06/ DQB1*05:01 (175.42), HLA-DQA1*05:07/ DQB1*05:01 (175.42), HLA- DQA1*05:08/ DQB1*05:01 (175.42), HLA-DQA1*05:10/ DQB1*05:01 (175.42), HLA-DQA1*05:09/DQB1*05:01 (175.42), HLA-DQA1*05:11/DQB1*05:01 (175.42),	
FLH**VTYV PAQEK**NF T	HLA-DRB5*01:04 (133.52), HLA-DRB5*02:05 (154.35), HLA-DRB5*01:01 (109.6), HLA-DRB5*01:14 (109.6), HLA-DRB5*01:13 (109.6), HLA-DRB5*01:05 (109.6), HLA-DRB5*01:02 (152.81), HLA-DRB5*01:08 (152.81), HLA-DRB1*10:01 (82.23), HLA-DRB1*10:03 (82.23), HLA-DRB1*01:13 (38.81), HLA-DRB1*10:02 (142.52), HLA-DRB1*01:14 (103.66), HLA-DRB1*01:10 (141.26), HLA-DRB1*01:04 (184.43), HLA-DRB1*14:21 (147.21), HLA-DRB1*01:05 (120.64), HLA-DRB1*01:07 (120.64), HLA-DRB1*01:08 (120.64), HLA-DRB1*01:01 (120.64), HLA-DRB1*01:12 (120.64), HLA-DRB1*01:11 (120.64), HLA-DRB1*01:25 (120.64), HLA-DRB1*01:22 (120.64), HLA-DRB1*01:19 (120.64), HLA-DRB1*01:18 (95.22), HLA-DRB1*14:17 (196.31), HLA-DRB1*13:20 (175.07)	28 (70.02)
YTMS**LGA ENSVAY**S N	HLA-DRB1*01:11 (85.65), HLA-DRB3*03:01 (178.72)	2 (77.51)

Table S10: EPISOPT analyses for the affinity of the potential 9-mer epitopes with MHC class I alleles.

Peptide Name	Sequence	HLA I binding profile
CVS2A1	FIAGLIAIV	A0201, A0202, A0203 A0204 A0205 A0206 A0207 A0209 A0214 A6802 B3801
CVS2B1	VTYVPAQEK	A0301 A1101 A3301 A6801
CVS1C1	CVADYSVLY	A1101 A6801 B1508 B1517 C0702
CVS1B1	IRGDEVRQI	B1510 B2706 B39011 C0702
CVEnvA1	YVYSRVKNL	A0202 A0203 A0206 A0214 B0801 B1517 B4402
CVS1A1	TRFASVYAW	B2701 B2702 B2704 B2705 B2709 B3909 C0702
CVMemB1	AVILRGHLR	A1101 A3101 A3301 A6601 A6801
CVMemA1	WLSYFIASF	A0203 A6802
CVEnvB1	VSLVKPSFY	

Table S11: Predivac analyses for the potential 15-mer peptides depending on the interaction with DRB1 alleles eg. 01:01, 03:01, 04:01, 07:01, 08:01, 10:01, 11:01, 12:01, 13:02, 14:01, and 15:01. The antigenicity of the peptides were assessed by Vaxijen v2.0.

Name	PEPTIDE	DRB1*01:01	DRB1*03:01	DRB1*04:01	DRB1*07:01	DRB1*08:03	DRB1*10:01	DRB1*11:01	DRB1*12:01	DRB1*13:02	DRB1*14:01	DRB1*15:01	Vaxijen score[a]
CVEnvA2	KPSF**YVYS RVKNL**NS	82.69	59.05	86.50	78.55	80.46	85.87	81.03	59.83	86.88	71.90	84.43	0.8229
CVEnvB2	NIVN**VSLV KPSFY**VY	66.39	63.18	66.41	71.73	59.79	69.75	63.76	85.74	69.79	64.03	60.92	0.7680
CVMemA2	VGLM**WLS YFIASF**RL	66.37	61.72	68.58	68.70	59.46	68.18	61.27	62.12	71.85	62.50	84.42	0.6658
CVMemB2	VIG**AVILR GHLR**IAG	63.42	73.02	59.81	72.98	74.41	63.36	69.18	72.32	64.47	73.79	70.96	0.4903
CVS1A2	FNA**TRFAS VYAW**NRK	81.51	51.56	71.88	80.83	64.03	81.42	70.10	61.28	75.76	55.32	79.41	0.4491
CVS1B2	ADSFV**IRG DEVRQI**A	64.85	75.58	70.30	71.06	68.11	63.75	64.33	65.27	75.63	71.01	74.20	-0.0663
CVS1C2	ISN**CVADY SVLY**NSA	72.88	75.54	71.13	76.27	79.86	77.17	63.19	67.49	67.26	71.83	89.75	-0.3853
CVS2A2	IWLG**FIAG LIAIV**MV	81.88	57.86	78.00	82.18	69.93	82.88	72.24	74.67	75.30	62.15	86.80	0.6150
CVS2B2	FLH**VTYVP AQEK**NFT	70.02	71.79	73.43	83.14	69.54	71.69	71.63	74.21	79.13	65.08	72.82	1.1908

[a] The threshold value was set at 4.0. The probable antigen has score more than 4.

Table S12: Population coverage of the potential peptides of Envelope protein. Here the combined population coverage of MHC class I and MHC class II presented for the World population and different regions of the world.

population/area	Coverage[a] for the peptide CVEnvA2	Coverage[a] for the peptide CVEnvB2
Central Africa	90.25%	73.86%
Central America	80.89%	34.47%
East Africa	91.12%	70.87%
East Asia	79.96%	73.04%
Europe	99.79%	74.36%
North Africa	74.18%	66.36%
North America	99.95%	74.86%
Northeast Asia	99.57%	60.97%
Oceania	99.87%	50.2%
South Africa	3.15%	40.9%
South America	92.17%	50.08%
South Asia	98.83%	79.92%
Southeast Asia	60.18%	46.07%
Southwest Asia	76.01%	60.17%
West Africa	93.67%	86.58%
West Indies	64.07%	77.03%
World	96.77%	71.88%
Average	**82.38**	**64.21**
Standard deviation	**23.36**	**14.52**

[a] projected population coverage

Table S13: Population coverage of the potential peptides of membrane glycoprotein**. Here the combined population coverage of MHC class I and MHC class II presented for the World population and different regions of the world.**

population/area	Coverage[a] for the peptide CVMemA2	Coverage[a] for the peptide CVMemB2
Central Africa	100.0%	74.36%
Central America	82.23%	24.06%
East Africa	100.0%	80.22%
East Asia	95.57%	73.82%
Europe	100.0%	87.14%
North Africa	91.2%	80.3%
North America	100.0%	82.32%
Northeast Asia	100.0%	78.44%
Oceania	100.0%	71.3%
South Africa	37.52%	61.01%
South America	99.39%	68.58%
South Asia	100.0%	84.64%
Southeast Asia	90.41%	70.09%
Southwest Asia	92.96%	70.68%
West Africa	100.0%	89.08%
West Indies	86.73%	66.84%
World	99.82%	82.11%
Average	**92.7**	**73.23**
Standard deviation	**14.81**	**14.38**

[a] projected population coverage

Table S14: Population coverage of the potential peptides of S1 domain of Spike surface glycoprotein**. Here the combined population coverage of MHC class I and MHC class II presented for the World population and different regions of the world.**

population/area	Coverage[a] for the peptide CVS1A2	Coverage[a] for the peptide CVS1B2	Coverage[a] for the peptide CVS1C2
Central Africa	94.36%	87.59%	82.11%
Central America	81.77%	6.46%	4.99%
East Africa	95.35%	84.51%	80.04%
East Asia	87.15%	69.05%	64.51%
Europe	97.28%	85.09%	76.46%
North Africa	96.69%	83.35%	77.67%
North America	91.42%	72.4%	67.41%
Northeast Asia	91.21%	68.11%	56.89%
Oceania	88.75%	62.02%	52.28%
South Africa	74.29%	83.21%	76.78%
South America	83.37%	60.83%	52.35%
South Asia	93.98%	70.06%	64.37%
Southeast Asia	86.88%	69.54%	57.74%
Southwest Asia	94.04%	86.81%	83.63%
West Africa	95.16%	71.02%	76.71%
West Indies	91.33%	56.9%	68.95%
World	94.07%	79.01%	70.77%
Average	**90.42**	**70.35**	**65.51**
Standard deviation	**5.95**	**18.52**	**18.03**

[a] projected population coverage

Table S15: Population coverage of the potential peptides of S2 domain of Spike surface glycoprotein**. Here the combined population coverage of MHC class I and MHC class II presented for the World population and different regions of the world.**

population/area	Coverage[a] for the peptide CVS2A2	Coverage[a] for the peptide CVS2B2
Central Africa	81.28%	32.61%
Central America	72.66%	4.04%
East Africa	88.56%	33.4%
East Asia	79.83%	53.92%
Europe	88.33%	62.45%
North Africa	75.07%	43.02%
North America	84.9%	51.88%
Northeast Asia	86.62%	64.37%
Oceania	89.1%	57.88%
South Africa	27.5%	51.92%
South America	77.42%	29.65%
South Asia	71.37%	64.12%
Southeast Asia	46.68%	51.64%
Southwest Asia	80.4%	45.35%
West Africa	90.88%	45.56%
West Indies	64.02%	32.57%
World	87.5%	57.36%
Average	**76.01**	**45.98**
Standard deviation	**16.23**	**15.2**

[a] projected population coverage

Table S16: The properties of the final multi-epitope vaccines.

	Vaccine for world (except South Africa) (CVMW)	Vaccine for the South Africa (CVMS)
Arrangement	C- CVMemB2-**L***-CVEnvA2-**L***- CVS1A2-**L***-CVS2B2	C- CVMemB2-**L***- CVS1A2-**L***- CVS2B2-**L***-CVEnvB2
Sequence	CVIGAVILRGHLRIAGGPGPGKPSFYVYSRVKNLNSGPGPGFNATRFASVYAWNRKGPGPGFLHVTYVPAQEKNFT	CVIGAVILRGHLRIAGGPGPGFNATRFASVYAWNRKGPGPGFLHVTYVPAQEKNFTGPGPGNIVNVSLVKPSFYVY
Antigenicity	Vaxigen Score: **0.6839**	Vaxigen Score: **0.5563**
Allergenicity	PROBABLE NON-ALLERGEN	PROBABLE NON-ALLERGEN
Solubility	Protein-Sol score: **0.698**	Protein-Sol score: **0.620**
Secondary structure prediction	SOPMA : Alpha helix (Hh) : 11 is 14.47% 3_{10} helix (Gg) : 0 is 0.00% Pi helix (Ii) : 0 is 0.00% Beta bridge (Bb) : 0 is 0.00% Extended strand(Ee): 17 is 22.37% Beta turn (Tt) : 9 is 11.84% Bend region (Ss) : 0 is 0.00% Random coil (Cc) : 39 is 51.32% Ambiguous states (?): 0 is 0.00% Other states : 0 is 0.00%	SOPMA : Alpha helix (Hh) : 3 is 3.95% 3_{10} helix (Gg) : 0 is 0.00% Pi helix (Ii) : 0 is 0.00% Beta bridge (Bb) : 0 is 0.00% Extended strand(Ee): 29 is 38.16% Beta turn (Tt) : 9 is 11.84% Bend region (Ss) : 0 is 0.00% Random coil (Cc) : 35 is 46.05% Ambiguous states (?): 0 is 0.00% Other states : 0 is 0.00%
ProtParam	**Molecular weight:** 8117.34 **Theoretical pI:** 10.45 **Estimated half-life:** The N-terminal of the sequence considered is C (Cys). The estimated half-life is: 1.2 hours (mammalian reticulocytes, in vitro). >20 hours (yeast, in vivo). >10 hours (Escherichia coli, in vivo). **Instability index:** The instability index (II) is computed to be 28.88 This classifies the protein as stable. **Aliphatic index:** 70.53 **Grand average of hydropathicity (GRAVY):** -0.166	**Molecular weight:** 8057.32 **Theoretical pI:** 10.13 **Estimated half-life:** The N-terminal of the sequence considered is C (Cys). The estimated half-life is: 1.2 hours (mammalian reticulocytes, in vitro). >20 hours (yeast, in vivo). >10 hours (Escherichia coli, in vivo). **Instability index:** The instability index (II) is computed to be 29.90 This classifies the protein as stable. **Aliphatic index:** 83.29 **Grand average of hydropathicity (GRAVY):** 0.125

***L**= GPGPG Linker

Table S17: Linear B-cell epitopes in the multi epitope vaccine.

CVMW			
Rank	Sequence	Start position	Score
1	HLRIAGAAYFNATRFA	29	0.89
2	KAAYFLHVTYVPAQEK	52	0.83
3	CKPSFYVYSRVKNLNS	1	0.76
4	NATRFASVYAWNRKAA	39	0.75
CVMS			
Rank	Sequence	Start position	Score
1	HLRIAGAAYFNATRFA	29	0.89
2	KAAYFLHVTYVPAQEK	52	0.83
3	SFYVYAAYVIGAVILR	12	0.80
4	NATRFASVYAWNRKAA	39	0.75
5	NVSLVKPSFYVYAAYV	5	0.58

Table S18: Conformational B-cell epitope in the multi epitope vaccine.

CVMW			
No.	Peptide	Number of residues	Score
1	WNRKA	5	0.744
2	VPAQEKNFT	9	0.653
3	NATR	4	0.609
CVMS			
No.	Peptide	Number of residues	Score
1	YAWNRKA	7	0.683
2	CNIVNVSLVKPS	12	0.673
3	YVPAQEKNFT	10	0.618

Table S19: The epitopes interacted with different HLAs shown in different supplementary tables. Candidate HLA selected depending upon strong interaction and availability of crystal structure in RCSB. The respective crystal structures downloaded and docking studies performed.

No.	epitope	HLA	Crystal structures	Reference Tables
1.	CVEnvA1	HLA-A*02:03	3ox8	Table S1
2.	CVEnvA2	HLA-DRB1*01:01	2FSE	Table S2
3.	CVMemB1	HLA-A*68:01	6PBH	Table S3
4.	CVMemB2	HLA-DRB1*01:01	2FSE	Table S4
5.	CVS1A1	HLA-C*07:02	5VGE	Table S5
6.	CVS1A2	DQA1/DQB1 (candidate of DQ allele)	1JK8	Table S6
7.	CVS2B1	HLA-A*11:01	6JP3	Table S7
8.	CVS2B2	HLA-DRB1*01:01	2FSE	Table S8

Table S20: Conservancy of the multi-epitopes construct among the new UK variants.

Countries included	Number of protein in analysis	Conservancy of epitope construct 1	Conservancy of epitope construct 2
England	4,199	100%	100%
Scotland	50	100%	100%
Wales	62	100%	100%
Italy	13	100%	100%
Portugal	19	100%	100%
Denmark	9	100%	100%
Ireland	7	100%	100%
Netherland	3	100%	100%
Finland	2	100%	100%
Norway	2	100%	100%
Sweden	1	100%	100%
Spain	1	100%	100%
France	1	100%	100%
Canada	2	100%	100%
Israel	4	100%	100%
South Korea	3	100%	100%
Japan	5	100%	100%
Hong Kong	1	100%	100%
Singapore	1	100%	100%
Australia	4	100%	100%
Gibraltar	1	100%	100%
Total	4,390		

Table S21: Conservancy analyses of the selected 15-mer peptides for CVMW and CVMS using the sequences downloaded from NCBI consisting of mixed strains.

Name	Peptide	Percent of protein sequence matches at identity <= 100%
CVEnvA2	KPSFYVYSRVKNLNS	96.30% (78/81)
CVEnvB2	NIVNVSLVKPSFYVY	96.30% (78/81)
CVMemB2	VIGAVILRGHLRIAG	97.96% (240/245)
CVS1A2	FNATRFASVYAWNRK	99.30% (993/1000)
CVS2B2	FLHVTYVPAQEKNFT	99.20% (992/1000)

Table S22: The statistics of the refined docked model of CVMW and TLRs are shown in the table. A lower HADDOCK score represents the strong binding between the Protein and the peptide. The Gibbs free energy in the interactions between CVMW and TLRs calculated by PRODIGY is also shown.

Parameters	TLR2	TLR4	TLR5
HADDOCK score	-199.5 +/- 2.3	-210.6 +/- 6.7	-214.3 +/- 3.2
Cluster size	20	20	20
RMSD from the overall lowest-energy structure	0.6 +/- 0.4	0.6 +/- 0.3	0.7 +/- 0.4
Van der Waals energy	-88.3 +/- 6.8	-90.3 +/- 7.3	-100.9 +/- 4.8
Electrostatic energy	-568.6 +/- 42.5	-675.5 +/- 18.8	-483.6 +/- 9.7
Desolvation energy	2.5 +/- 4.2	14.8 +/- 2.0	-16.7 +/- 1.1
Restraints violation energy	0.0 +/- 0.0	0.0 +/- 0.0	0.0 +/- 0.0
Buried Surface Area	3000.1 +/- 116.6	2777.2 +/- 15.5	3158.8 +/- 63.2
PRODIGY ΔG (kcal mol^{-1})	-16.2	-16.4	-12.9

Supplementary Material SM1: The amino acids involved in the interaction between The TLR2 (Atom 1) and Multi-epitope vaccine, CVMW (Atom 2). The Hydrogen Bonds, Salt bridges and non-bonded interactions are mentioned with their distances.

Hydrogen bonds

	<----- A T O M 1 ----->					<----- A T O M 2 ----->				
	Atom no.	Atom name	Res name	Res no.	Chain		Atom no.	Atom name	Res name	Res no.	Chain	Distance
1.	1894	OE1	GLU	225	A	<-->	5879	NZ	LYS	56	B	2.60
2.	1956	OD1	ASP	231	A	<-->	5512	N	GLY	19	B	2.73
3.	2166	NZ	LYS	253	A	<-->	5843	O	TRP	53	B	2.96
4.	2166	NZ	LYS	253	A	<-->	5849	OD1	ASN	54	B	2.72
5.	2449	OE1	GLU	281	A	<-->	5855	N	ARG	55	B	3.29
6.	2450	OE2	GLU	281	A	<-->	5864	NH1	ARG	55	B	2.66
7.	2788	NH1	ARG	316	A	<-->	5488	O	ILE	14	B	2.74
8.	2791	NH2	ARG	316	A	<-->	5488	O	ILE	14	B	2.90
9.	3306	OD1	ASP	366	A	<-->	5450	NE2	HIS	11	B	2.69
10.	3333	OE1	GLU	369	A	<-->	5472	NH1	ARG	13	B	2.65
11.	3598	OE1	GLN	396	A	<-->	5472	NH1	ARG	13	B	3.01
12.	3798	OD1	ASN	417	A	<-->	5431	NH2	ARG	9	B	2.93
13.	4035	OH	TYR	440	A	<-->	5428	NH1	ARG	9	B	3.10
14.	4072	OG	SER	444	A	<-->	5625	NH2	ARG	30	B	3.08
15.	4249	OD2	ASP	463	A	<-->	5622	NH1	ARG	30	B	2.77
16.	4249	OD2	ASP	463	A	<-->	5625	NH2	ARG	30	B	2.82
17.	4426	OE1	GLU	481	A	<-->	5645	NZ	LYS	32	B	2.69

Non-bonded contacts

	<----- A T O M 1 ----->					<----- A T O M 2 ----->				
	Atom no.	Atom name	Res name	Res no.	Chain		Atom no.	Atom name	Res name	Res no.	Chain	Distance
1.	288	CB	SER	60	A	<-->	6028	CE	LYS	73	B	3.72
2.	289	OG	SER	60	A	<-->	6028	CE	LYS	73	B	3.44
3.	515	CG2	VAL	82	A	<-->	6029	NZ	LYS	73	B	3.74
4.	530	CB	THR	84	A	<-->	6027	CD	LYS	73	B	3.79
5.	530	CB	THR	84	A	<-->	6028	CE	LYS	73	B	3.56
6.	531	OG1	THR	84	A	<-->	6027	CD	LYS	73	B	3.78
7.	531	OG1	THR	84	A	<-->	6028	CE	LYS	73	B	3.30
8.	531	OG1	THR	84	A	<-->	6029	NZ	LYS	73	B	3.88
9.	533	CG2	THR	84	A	<-->	6027	CD	LYS	73	B	3.75
10.	747	OG	SER	108	A	<-->	6055	CZ	PHE	75	B	3.67
11.	969	ND2	ASN	130	A	<-->	6053	CE1	PHE	75	B	3.50
12.	969	ND2	ASN	130	A	<-->	6055	CZ	PHE	75	B	3.35
13.	1208	CD	ARG	155	A	<-->	6051	CD1	PHE	75	B	3.85
14.	1208	CD	ARG	155	A	<-->	6053	CE1	PHE	75	B	3.64
15.	1212	NH1	ARG	155	A	<-->	5360	CB	CYS	1	B	3.43
16.	1212	NH1	ARG	155	A	<-->	5361	SG	CYS	1	B	3.13
17.	1444	OE2	GLU	178	A	<-->	5361	SG	CYS	1	B	3.41
18.	1461	CD	GLU	180	A	<-->	5357	N	CYS	1	B	3.50
19.	1462	OE1	GLU	180	A	<-->	5357	N	CYS	1	B	3.31
20.	1463	OE2	GLU	180	A	<-->	5357	N	CYS	1	B	2.93
21.	1670	CG	HIS	202	A	<-->	5850	ND2	ASN	54	B	3.64
22.	1671	ND1	HIS	202	A	<-->	5850	ND2	ASN	54	B	3.49
23.	1673	CD2	HIS	202	A	<-->	5850	ND2	ASN	54	B	3.65
24.	1674	CE1	HIS	202	A	<-->	5850	ND2	ASN	54	B	3.43

25.	1675	NE2	HIS	202	A	<-->	5850	ND2	ASN	54	B	3.54
26.	1693	CD1	ILE	204	A	<-->	5361	SG	CYS	1	B	3.52
27.	1893	CD	GLU	225	A	<-->	5879	NZ	LYS	56	B	3.47
28.	1894	OE1	GLU	225	A	<-->	5876	CG	LYS	56	B	3.45
29.	1894	OE1	GLU	225	A	<-->	5877	CD	LYS	56	B	3.84
30.	1894	OE1	GLU	225	A	<-->	5878	CE	LYS	56	B	3.64
31.	1894	OE1	GLU	225	A	<-->	5879	NZ	LYS	56	B	2.60
32.	1895	OE2	GLU	225	A	<-->	5879	NZ	LYS	56	B	3.61
33.	1901	CB	CYS	226	A	<-->	5848	CG	ASN	54	B	3.74
34.	1902	SG	CYS	226	A	<-->	5847	CB	ASN	54	B	3.68
35.	1921	OE1	GLU	228	A	<-->	5825	CB	ALA	52	B	3.41
36.	1942	CZ	ARG	230	A	<-->	5357	N	CYS	1	B	3.69
37.	1943	NH1	ARG	230	A	<-->	5357	N	CYS	1	B	3.10
38.	1946	NH2	ARG	230	A	<-->	5357	N	CYS	1	B	3.53
39.	1946	NH2	ARG	230	A	<-->	5359	CA	CYS	1	B	3.77
40.	1946	NH2	ARG	230	A	<-->	5361	SG	CYS	1	B	3.37
41.	1955	CG	ASP	231	A	<-->	5507	CB	PRO	18	B	3.82
42.	1956	OD1	ASP	231	A	<-->	5506	CA	PRO	18	B	3.34
43.	1956	OD1	ASP	231	A	<-->	5510	C	PRO	18	B	3.50
44.	1956	OD1	ASP	231	A	<-->	5507	CB	PRO	18	B	3.23
45.	1956	OD1	ASP	231	A	<-->	5512	N	GLY	19	B	2.73
46.	1956	OD1	ASP	231	A	<-->	5514	CA	GLY	19	B	3.75
47.	1957	OD2	ASP	231	A	<-->	5507	CB	PRO	18	B	3.74
48.	2163	CG	LYS	253	A	<-->	5849	OD1	ASN	54	B	3.59
49.	2164	CD	LYS	253	A	<-->	5849	OD1	ASN	54	B	3.78
50.	2165	CE	LYS	253	A	<-->	5843	O	TRP	53	B	3.06
51.	2165	CE	LYS	253	A	<-->	5849	OD1	ASN	54	B	3.66
52.	2166	NZ	LYS	253	A	<-->	5842	C	TRP	53	B	3.58
53.	2166	NZ	LYS	253	A	<-->	5843	O	TRP	53	B	2.96
54.	2166	NZ	LYS	253	A	<-->	5848	CG	ASN	54	B	3.88
55.	2166	NZ	LYS	253	A	<-->	5849	OD1	ASN	54	B	2.72
56.	2188	OG1	THR	255	A	<-->	5849	OD1	ASN	54	B	3.89
57.	2208	CB	ARG	257	A	<-->	5504	O	GLY	17	B	3.17
58.	2209	CG	ARG	257	A	<-->	5504	O	GLY	17	B	3.80
59.	2210	CD	ARG	257	A	<-->	5504	O	GLY	17	B	3.25
60.	2217	NH2	ARG	257	A	<-->	5825	CB	ALA	52	B	3.74
61.	2225	CB	ASN	258	A	<-->	5507	CB	PRO	18	B	3.74
62.	2226	CG	ASN	258	A	<-->	5507	CB	PRO	18	B	3.89
63.	2228	ND2	ASN	258	A	<-->	5507	CB	PRO	18	B	3.64
64.	2447	CG	GLU	281	A	<-->	5840	CZ3	TRP	53	B	3.57
65.	2448	CD	GLU	281	A	<-->	5860	CD	ARG	55	B	3.61
66.	2448	CD	GLU	281	A	<-->	5864	NH1	ARG	55	B	3.76
67.	2449	OE1	GLU	281	A	<-->	5855	N	ARG	55	B	3.29
68.	2449	OE1	GLU	281	A	<-->	5857	CA	ARG	55	B	3.66
69.	2449	OE1	GLU	281	A	<-->	5871	O	ARG	55	B	3.75
70.	2449	OE1	GLU	281	A	<-->	5858	CB	ARG	55	B	3.14
71.	2449	OE1	GLU	281	A	<-->	5859	CG	ARG	55	B	3.48
72.	2449	OE1	GLU	281	A	<-->	5860	CD	ARG	55	B	3.38
73.	2450	OE2	GLU	281	A	<-->	5839	CZ2	TRP	53	B	3.89
74.	2450	OE2	GLU	281	A	<-->	5841	CH2	TRP	53	B	3.66
75.	2450	OE2	GLU	281	A	<-->	5860	CD	ARG	55	B	3.22
76.	2450	OE2	GLU	281	A	<-->	5861	NE	ARG	55	B	3.89
77.	2450	OE2	GLU	281	A	<-->	5863	CZ	ARG	55	B	3.69
78.	2450	OE2	GLU	281	A	<-->	5864	NH1	ARG	55	B	2.66
79.	2468	OE1	GLU	283	A	<-->	5828	N	TRP	53	B	3.51
80.	2468	OE1	GLU	283	A	<-->	5830	CA	TRP	53	B	3.83
81.	2468	OE1	GLU	283	A	<-->	5843	O	TRP	53	B	3.74
82.	2468	OE1	GLU	283	A	<-->	5831	CB	TRP	53	B	3.38
83.	2489	OD1	ASP	285	A	<-->	5502	CA	GLY	17	B	3.23
84.	2490	OD2	ASP	285	A	<-->	5485	CG2	ILE	14	B	3.36

85.	2729	CB	THR	311	A	<-->	5841	CH2	TRP	53	B	3.44
86.	2730	OG1	THR	311	A	<-->	5864	NH1	ARG	55	B	3.58
87.	2732	CG2	THR	311	A	<-->	5839	CZ2	TRP	53	B	3.83
88.	2732	CG2	THR	311	A	<-->	5841	CH2	TRP	53	B	3.61
89.	2732	CG2	THR	311	A	<-->	5864	NH1	ARG	55	B	3.60
90.	2748	OG1	THR	313	A	<-->	5838	CE3	TRP	53	B	3.77
91.	2748	OG1	THR	313	A	<-->	5840	CZ3	TRP	53	B	3.25
92.	2748	OG1	THR	313	A	<-->	5841	CH2	TRP	53	B	3.45
93.	2750	CG2	THR	313	A	<-->	5459	CD1	LEU	12	B	3.57
94.	2750	CG2	THR	313	A	<-->	5460	CD2	LEU	12	B	3.79
95.	2767	CD	ARG	315	A	<-->	5462	O	LEU	12	B	3.22
96.	2767	CD	ARG	315	A	<-->	5485	CG2	ILE	14	B	3.80
97.	2768	NE	ARG	315	A	<-->	5462	O	LEU	12	B	3.05
98.	2768	NE	ARG	315	A	<-->	5457	CB	LEU	12	B	3.79
99.	2768	NE	ARG	315	A	<-->	5459	CD1	LEU	12	B	3.43
100.	2770	CZ	ARG	315	A	<-->	5462	O	LEU	12	B	3.82
101.	2771	NH1	ARG	315	A	<-->	5485	CG2	ILE	14	B	3.65
102.	2774	NH2	ARG	315	A	<-->	5457	CB	LEU	12	B	3.71
103.	2774	NH2	ARG	315	A	<-->	5460	CD2	LEU	12	B	3.35
104.	2785	NE	ARG	316	A	<-->	5499	O	GLY	16	B	3.65
105.	2787	CZ	ARG	316	A	<-->	5488	O	ILE	14	B	3.23
106.	2787	CZ	ARG	316	A	<-->	5499	O	GLY	16	B	3.58
107.	2788	NH1	ARG	316	A	<-->	5488	O	ILE	14	B	2.74
108.	2791	NH2	ARG	316	A	<-->	5488	O	ILE	14	B	2.90
109.	2791	NH2	ARG	316	A	<-->	5485	CG2	ILE	14	B	3.76
110.	2791	NH2	ARG	316	A	<-->	5498	C	GLY	16	B	3.83
111.	2791	NH2	ARG	316	A	<-->	5499	O	GLY	16	B	3.59
112.	3091	CD	GLU	344	A	<-->	5448	CD2	HIS	11	B	3.38
113.	3092	OE1	GLU	344	A	<-->	5444	CB	HIS	11	B	3.88
114.	3092	OE1	GLU	344	A	<-->	5448	CD2	HIS	11	B	3.45
115.	3092	OE1	GLU	344	A	<-->	5463	N	ARG	13	B	3.84
116.	3092	OE1	GLU	344	A	<-->	5465	CA	ARG	13	B	3.89
117.	3092	OE1	GLU	344	A	<-->	5466	CB	ARG	13	B	3.73
118.	3093	OE2	GLU	344	A	<-->	5445	CG	HIS	11	B	3.83
119.	3093	OE2	GLU	344	A	<-->	5448	CD2	HIS	11	B	3.34
120.	3305	CG	ASP	366	A	<-->	5450	NE2	HIS	11	B	3.15
121.	3306	OD1	ASP	366	A	<-->	5448	CD2	HIS	11	B	3.58
122.	3306	OD1	ASP	366	A	<-->	5449	CE1	HIS	11	B	3.67
123.	3306	OD1	ASP	366	A	<-->	5450	NE2	HIS	11	B	2.69
124.	3307	OD2	ASP	366	A	<-->	5449	CE1	HIS	11	B	3.72
125.	3307	OD2	ASP	366	A	<-->	5450	NE2	HIS	11	B	2.98
126.	3323	OG	SER	368	A	<-->	5449	CE1	HIS	11	B	3.89
127.	3323	OG	SER	368	A	<-->	5450	NE2	HIS	11	B	3.45
128.	3332	CD	GLU	369	A	<-->	5472	NH1	ARG	13	B	3.50
129.	3333	OE1	GLU	369	A	<-->	5468	CD	ARG	13	B	3.09
130.	3333	OE1	GLU	369	A	<-->	5469	NE	ARG	13	B	3.80
131.	3333	OE1	GLU	369	A	<-->	5471	CZ	ARG	13	B	3.65
132.	3333	OE1	GLU	369	A	<-->	5472	NH1	ARG	13	B	2.65
133.	3334	OE2	GLU	369	A	<-->	5472	NH1	ARG	13	B	3.89
134.	3562	CG2	ILE	393	A	<-->	5449	CE1	HIS	11	B	3.35
135.	3562	CG2	ILE	393	A	<-->	5450	NE2	HIS	11	B	3.79
136.	3563	CD1	ILE	393	A	<-->	5449	CE1	HIS	11	B	3.62
137.	3584	NH1	ARG	395	A	<-->	5472	NH1	ARG	13	B	3.75
138.	3587	NH2	ARG	395	A	<-->	5468	CD	ARG	13	B	3.53
139.	3597	CD	GLN	396	A	<-->	5472	NH1	ARG	13	B	3.86
140.	3598	OE1	GLN	396	A	<-->	5472	NH1	ARG	13	B	3.01
141.	3798	OD1	ASN	417	A	<-->	5431	NH2	ARG	9	B	2.93
142.	4034	CZ	TYR	440	A	<-->	5428	NH1	ARG	9	B	3.66
143.	4034	CZ	TYR	440	A	<-->	5431	NH2	ARG	9	B	3.87
144.	4035	OH	TYR	440	A	<-->	5428	NH1	ARG	9	B	3.10

145.	4054	ND2	ASN	442	A	<-->	5622	NH1	ARG	30	B	3.23
146.	4072	OG	SER	444	A	<-->	5625	NH2	ARG	30	B	3.08
147.	4247	CG	ASP	463	A	<-->	5625	NH2	ARG	30	B	3.63
148.	4248	OD1	ASP	463	A	<-->	5625	NH2	ARG	30	B	3.74
149.	4249	OD2	ASP	463	A	<-->	5621	CZ	ARG	30	B	3.20
150.	4249	OD2	ASP	463	A	<-->	5622	NH1	ARG	30	B	2.77
151.	4249	OD2	ASP	463	A	<-->	5625	NH2	ARG	30	B	2.82
152.	4425	CD	GLU	481	A	<-->	5645	NZ	LYS	32	B	3.20
153.	4426	OE1	GLU	481	A	<-->	5643	CD	LYS	32	B	3.65
154.	4426	OE1	GLU	481	A	<-->	5644	CE	LYS	32	B	3.44
155.	4426	OE1	GLU	481	A	<-->	5645	NZ	LYS	32	B	2.69
156.	4427	OE2	GLU	481	A	<-->	5645	NZ	LYS	32	B	3.27
157.	4449	OH	TYR	483	A	<-->	5643	CD	LYS	32	B	3.67

Salt bridges

	<----- A T O M 1 ----->					<----- A T O M 2 ----->					
	Atom no.	Atom name	Res name	Res no.	Chain		Atom no.	Atom name	Res name	Res no.	Chain	Distance
1.	1895	OE2	GLU	225	A	<-->	5879	NZ	LYS	56	B	2.60
2.	2450	OE2	GLU	281	A	<-->	5864	NH1	ARG	55	B	2.66
3.	3092	OE1	GLU	344	A	<-->	5450	NE2	HIS	11	B	3.93
4.	3307	OD2	ASP	366	A	<-->	5450	NE2	HIS	11	B	2.69
5.	3334	OE2	GLU	369	A	<-->	5472	NH1	ARG	13	B	2.65
6.	4249	OD2	ASP	463	A	<-->	5622	NH1	ARG	30	B	2.77
7.	4426	OE1	GLU	481	A	<-->	5645	NZ	LYS	32	B	2.69

Number of salt bridges: 7

Number of hydrogen bonds: 17

Number of non-bonded contacts: 157

Supplementary Material SM2: The amino acids involved in the interaction between The TLR4 (Atom 1) and Multi-epitope vaccine, CVMW (Atom 2). The Hydrogen Bonds, Salt bridges and non-bonded interactions are mentioned with their distances.

Hydrogen bonds

	<----- A T O M 1 ----->					<----- A T O M 2 ----->				
	Atom no.	Atom name	Res name	Res no.	Chain		Atom no.	Atom name	Res name	Res no.	Chain	Distance
1.	326	OD2	ASP	60	A	<-->	6014	NZ	LYS	22	B	2.71
2.	342	OG	SER	62	A	<-->	6014	NZ	LYS	22	B	2.69
3.	563	OD2	ASP	84	A	<-->	6014	NZ	LYS	22	B	2.63
4.	771	OG1	THR	106	A	<-->	5972	O	ALA	15	B	2.70
5.	977	NZ	LYS	130	A	<-->	5957	O	ARG	13	B	2.89
6.	977	NZ	LYS	130	A	<-->	6046	O	PHE	25	B	2.95
7.	1202	OE2	GLU	154	A	<-->	5953	NH2	ARG	13	B	2.71
8.	1452	NE2	HIS	179	A	<-->	5940	O	LEU	12	B	3.03
9.	1471	OD2	ASP	181	A	<-->	5953	NH2	ARG	13	B	2.74
10.	1707	OD1	ASN	205	A	<-->	5924	ND1	HIS	11	B	2.99
11.	1726	OG	SER	207	A	<-->	6079	OH	TYR	28	B	2.71
12.	1761	OG	SER	211	A	<-->	6215	ND2	ASN	43	B	2.79
13.	1944	O	HIS	229	A	<-->	6103	NH2	ARG	30	B	2.85
14.	1938	ND1	HIS	229	A	<-->	6079	OH	TYR	28	B	3.24
15.	2493	OE1	GLU	286	A	<-->	6123	NZ	LYS	32	B	2.82
16.	2504	OE2	GLU	287	A	<-->	6100	NH1	ARG	30	B	3.02
17.	2745	OG	SER	311	A	<-->	6123	NZ	LYS	32	B	3.07
18.	3002	OE1	GLU	336	A	<-->	6168	N	GLY	37	B	2.69
19.	3195	NH1	ARG	355	A	<-->	6148	O	LEU	34	B	2.73
20.	3198	NH2	ARG	355	A	<-->	6154	OD1	ASN	35	B	3.12
21.	3216	OG1	THR	357	A	<-->	6159	O	ASN	35	B	3.21
22.	3418	OD2	ASP	379	A	<-->	6155	ND2	ASN	35	B	3.06

Non-bonded contacts

	<----- A T O M 1 ----->					<----- A T O M 2 ----->				
	Atom no.	Atom name	Res name	Res no.	Chain		Atom no.	Atom name	Res name	Res no.	Chain	Distance
1.	46	CB	VAL	32	A	<-->	6001	O	PRO	20	B	3.86
2.	47	CG1	VAL	32	A	<-->	6001	O	PRO	20	B	3.41
3.	48	CG2	VAL	32	A	<-->	6001	O	PRO	20	B	3.77
4.	90	OG1	THR	37	A	<-->	5994	O	GLY	19	B	3.83
5.	92	CG2	THR	37	A	<-->	6001	O	PRO	20	B	3.76
6.	304	CG	ASN	58	A	<-->	6023	CG	PRO	23	B	3.87
7.	305	OD1	ASN	58	A	<-->	6023	CG	PRO	23	B	3.07
8.	306	ND2	ASN	58	A	<-->	6023	CG	PRO	23	B	3.86
9.	324	CG	ASP	60	A	<-->	6014	NZ	LYS	22	B	3.18
10.	325	OD1	ASP	60	A	<-->	6014	NZ	LYS	22	B	2.93
11.	326	OD2	ASP	60	A	<-->	6007	N	LYS	22	B	3.71
12.	326	OD2	ASP	60	A	<-->	6009	CA	LYS	22	B	3.79
13.	326	OD2	ASP	60	A	<-->	6013	CE	LYS	22	B	3.75
14.	326	OD2	ASP	60	A	<-->	6014	NZ	LYS	22	B	2.71
15.	341	CB	SER	62	A	<-->	6014	NZ	LYS	22	B	3.76
16.	342	OG	SER	62	A	<-->	6013	CE	LYS	22	B	3.46
17.	342	OG	SER	62	A	<-->	6014	NZ	LYS	22	B	2.69
18.	544	CG1	VAL	82	A	<-->	6022	CB	PRO	23	B	3.46
19.	544	CG1	VAL	82	A	<-->	6023	CG	PRO	23	B	3.40

20.	545	CG2	VAL	82	A	<-->	5978	N	GLY	17	B	3.80
21.	545	CG2	VAL	82	A	<-->	5980	CA	GLY	17	B	3.48
22.	560	CB	ASP	84	A	<-->	6024	CD	PRO	23	B	3.84
23.	561	CG	ASP	84	A	<-->	6014	NZ	LYS	22	B	3.17
24.	562	OD1	ASP	84	A	<-->	6014	NZ	LYS	22	B	3.54
25.	563	OD2	ASP	84	A	<-->	6009	CA	LYS	22	B	3.38
26.	563	OD2	ASP	84	A	<-->	6018	C	LYS	22	B	3.24
27.	563	OD2	ASP	84	A	<-->	6019	O	LYS	22	B	3.75
28.	563	OD2	ASP	84	A	<-->	6012	CD	LYS	22	B	3.84
29.	563	OD2	ASP	84	A	<-->	6013	CE	LYS	22	B	3.67
30.	563	OD2	ASP	84	A	<-->	6014	NZ	LYS	22	B	2.63
31.	563	OD2	ASP	84	A	<-->	6020	N	PRO	23	B	3.32
32.	563	OD2	ASP	84	A	<-->	6024	CD	PRO	23	B	3.54
33.	770	CB	THR	106	A	<-->	5972	O	ALA	15	B	3.56
34.	771	OG1	THR	106	A	<-->	5971	C	ALA	15	B	3.60
35.	771	OG1	THR	106	A	<-->	5972	O	ALA	15	B	2.70
36.	773	CG2	THR	106	A	<-->	5972	O	ALA	15	B	3.34
37.	789	CG1	ILE	108	A	<-->	6031	OG	SER	24	B	3.65
38.	791	CD1	ILE	108	A	<-->	6021	CA	PRO	23	B	3.53
39.	791	CD1	ILE	108	A	<-->	6022	CB	PRO	23	B	3.85
40.	975	CD	LYS	130	A	<-->	5972	O	ALA	15	B	3.36
41.	975	CD	LYS	130	A	<-->	5970	CB	ALA	15	B	3.75
42.	975	CD	LYS	130	A	<-->	6034	O	SER	24	B	3.57
43.	976	CE	LYS	130	A	<-->	6034	O	SER	24	B	3.22
44.	976	CE	LYS	130	A	<-->	6046	O	PHE	25	B	3.29
45.	977	NZ	LYS	130	A	<-->	5957	O	ARG	13	B	2.89
46.	977	NZ	LYS	130	A	<-->	5945	CG	ARG	13	B	3.88
47.	977	NZ	LYS	130	A	<-->	6046	O	PHE	25	B	2.95
48.	995	CB	VAL	132	A	<-->	6031	OG	SER	24	B	3.88
49.	996	CG1	VAL	132	A	<-->	6031	OG	SER	24	B	3.69
50.	997	CG2	VAL	132	A	<-->	6030	CB	SER	24	B	3.85
51.	997	CG2	VAL	132	A	<-->	6031	OG	SER	24	B	3.41
52.	1200	CD	GLU	154	A	<-->	5947	NE	ARG	13	B	3.20
53.	1200	CD	GLU	154	A	<-->	5949	CZ	ARG	13	B	3.76
54.	1200	CD	GLU	154	A	<-->	5953	NH2	ARG	13	B	3.43
55.	1201	OE1	GLU	154	A	<-->	5945	CG	ARG	13	B	3.30
56.	1201	OE1	GLU	154	A	<-->	5946	CD	ARG	13	B	3.72
57.	1201	OE1	GLU	154	A	<-->	5947	NE	ARG	13	B	3.01
58.	1202	OE2	GLU	154	A	<-->	5947	NE	ARG	13	B	3.10
59.	1202	OE2	GLU	154	A	<-->	5949	CZ	ARG	13	B	3.33
60.	1202	OE2	GLU	154	A	<-->	5953	NH2	ARG	13	B	2.71
61.	1202	OE2	GLU	154	A	<-->	6052	CD1	TYR	26	B	3.70
62.	1202	OE2	GLU	154	A	<-->	6054	CE1	TYR	26	B	3.44
63.	1220	ND2	ASN	156	A	<-->	5953	NH2	ARG	13	B	3.49
64.	1220	ND2	ASN	156	A	<-->	6054	CE1	TYR	26	B	3.67
65.	1439	CD	GLU	178	A	<-->	5926	CD2	HIS	11	B	3.73
66.	1439	CD	GLU	178	A	<-->	5928	NE2	HIS	11	B	3.65
67.	1440	OE1	GLU	178	A	<-->	5923	CG	HIS	11	B	3.38
68.	1440	OE1	GLU	178	A	<-->	5924	ND1	HIS	11	B	3.81
69.	1440	OE1	GLU	178	A	<-->	5926	CD2	HIS	11	B	3.22
70.	1440	OE1	GLU	178	A	<-->	5928	NE2	HIS	11	B	3.59
71.	1441	OE2	GLU	178	A	<-->	5926	CD2	HIS	11	B	3.69
72.	1441	OE2	GLU	178	A	<-->	5928	NE2	HIS	11	B	3.34
73.	1449	ND1	HIS	179	A	<-->	5946	CD	ARG	13	B	3.70
74.	1450	CD2	HIS	179	A	<-->	5945	CG	ARG	13	B	3.77
75.	1451	CE1	HIS	179	A	<-->	5944	CB	ARG	13	B	3.79
76.	1451	CE1	HIS	179	A	<-->	5945	CG	ARG	13	B	3.73
77.	1451	CE1	HIS	179	A	<-->	5946	CD	ARG	13	B	3.80
78.	1451	CE1	HIS	179	A	<-->	6073	CG	TYR	28	B	3.61
79.	1451	CE1	HIS	179	A	<-->	6074	CD1	TYR	28	B	3.55

80.	1451	CE1	HIS	179	A	<-->	6075	CD2	TYR	28	B	3.86
81.	1451	CE1	HIS	179	A	<-->	6076	CE1	TYR	28	B	3.77
82.	1452	NE2	HIS	179	A	<-->	5939	C	LEU	12	B	3.87
83.	1452	NE2	HIS	179	A	<-->	5940	O	LEU	12	B	3.03
84.	1452	NE2	HIS	179	A	<-->	5943	CA	ARG	13	B	3.80
85.	1452	NE2	HIS	179	A	<-->	5944	CB	ARG	13	B	3.64
86.	1452	NE2	HIS	179	A	<-->	5945	CG	ARG	13	B	3.62
87.	1468	CB	ASP	181	A	<-->	5953	NH2	ARG	13	B	3.81
88.	1469	CG	ASP	181	A	<-->	5953	NH2	ARG	13	B	3.59
89.	1471	OD2	ASP	181	A	<-->	5949	CZ	ARG	13	B	3.58
90.	1471	OD2	ASP	181	A	<-->	5950	NH1	ARG	13	B	3.55
91.	1471	OD2	ASP	181	A	<-->	5953	NH2	ARG	13	B	2.74
92.	1706	CG	ASN	205	A	<-->	5924	ND1	HIS	11	B	3.41
93.	1706	CG	ASN	205	A	<-->	5927	CE1	HIS	11	B	3.68
94.	1707	OD1	ASN	205	A	<-->	5924	ND1	HIS	11	B	2.99
95.	1707	OD1	ASN	205	A	<-->	5927	CE1	HIS	11	B	3.33
96.	1708	ND2	ASN	205	A	<-->	5924	ND1	HIS	11	B	3.44
97.	1725	CB	SER	207	A	<-->	6079	OH	TYR	28	B	3.73
98.	1726	OG	SER	207	A	<-->	6076	CE1	TYR	28	B	3.67
99.	1726	OG	SER	207	A	<-->	6078	CZ	TYR	28	B	3.33
100.	1726	OG	SER	207	A	<-->	6079	OH	TYR	28	B	2.71
101.	1745	OD2	ASP	209	A	<-->	6212	CB	ASN	43	B	3.58
102.	1760	CB	SER	211	A	<-->	6215	ND2	ASN	43	B	3.79
103.	1761	OG	SER	211	A	<-->	6212	CB	ASN	43	B	3.45
104.	1761	OG	SER	211	A	<-->	6213	CG	ASN	43	B	3.59
105.	1761	OG	SER	211	A	<-->	6215	ND2	ASN	43	B	2.79
106.	1943	C	HIS	229	A	<-->	6103	NH2	ARG	30	B	3.44
107.	1944	O	HIS	229	A	<-->	6103	NH2	ARG	30	B	2.85
108.	1937	CG	HIS	229	A	<-->	6103	NH2	ARG	30	B	3.62
109.	1938	ND1	HIS	229	A	<-->	6079	OH	TYR	28	B	3.24
110.	1938	ND1	HIS	229	A	<-->	6097	NE	ARG	30	B	3.42
111.	1938	ND1	HIS	229	A	<-->	6099	CZ	ARG	30	B	3.64
112.	1938	ND1	HIS	229	A	<-->	6103	NH2	ARG	30	B	3.29
113.	1940	CE1	HIS	229	A	<-->	6097	NE	ARG	30	B	3.30
114.	1940	CE1	HIS	229	A	<-->	6099	CZ	ARG	30	B	3.74
115.	1940	CE1	HIS	229	A	<-->	6103	NH2	ARG	30	B	3.83
116.	1949	CG	LYS	230	A	<-->	6191	O	PRO	40	B	3.83
117.	1950	CD	LYS	230	A	<-->	6191	O	PRO	40	B	3.43
118.	1950	CD	LYS	230	A	<-->	6194	CA	GLY	41	B	3.59
119.	1970	CB	THR	232	A	<-->	6215	ND2	ASN	43	B	3.79
120.	1973	CG2	THR	232	A	<-->	6191	O	PRO	40	B	3.71
121.	1973	CG2	THR	232	A	<-->	6213	CG	ASN	43	B	3.88
122.	1973	CG2	THR	232	A	<-->	6215	ND2	ASN	43	B	3.74
123.	1990	CD	ARG	234	A	<-->	6215	ND2	ASN	43	B	3.88
124.	1994	NH1	ARG	234	A	<-->	6219	O	ASN	43	B	3.85
125.	2200	CD2	HIS	256	A	<-->	6100	NH1	ARG	30	B	3.30
126.	2208	CB	ARG	257	A	<-->	6100	NH1	ARG	30	B	3.60
127.	2208	CB	ARG	257	A	<-->	6103	NH2	ARG	30	B	3.83
128.	2209	CG	ARG	257	A	<-->	6191	O	PRO	40	B	3.78
129.	2211	NE	ARG	257	A	<-->	6186	CA	PRO	40	B	3.66
130.	2214	NH1	ARG	257	A	<-->	6177	CD	PRO	38	B	3.77
131.	2236	CG2	VAL	259	A	<-->	6191	O	PRO	40	B	3.51
132.	2236	CG2	VAL	259	A	<-->	6187	CB	PRO	40	B	3.89
133.	2492	CD	GLU	286	A	<-->	6123	NZ	LYS	32	B	3.40
134.	2493	OE1	GLU	286	A	<-->	6122	CE	LYS	32	B	3.73
135.	2493	OE1	GLU	286	A	<-->	6123	NZ	LYS	32	B	2.82
136.	2494	OE2	GLU	286	A	<-->	6123	NZ	LYS	32	B	3.86
137.	2502	CD	GLU	287	A	<-->	6100	NH1	ARG	30	B	3.83
138.	2504	OE2	GLU	287	A	<-->	6100	NH1	ARG	30	B	3.02
139.	2524	CD	ARG	289	A	<-->	6187	CB	PRO	40	B	3.82

140.	2745	OG	SER	311	A	<-->	6123	NZ	LYS	32	B	3.07
141.	2753	OG	SER	312	A	<-->	6122	CE	LYS	32	B	3.29
142.	2753	OG	SER	312	A	<-->	6123	NZ	LYS	32	B	3.24
143.	3000	CG	GLU	336	A	<-->	6159	O	ASN	35	B	3.67
144.	3001	CD	GLU	336	A	<-->	6162	CA	SER	36	B	3.74
145.	3001	CD	GLU	336	A	<-->	6168	N	GLY	37	B	3.32
146.	3002	OE1	GLU	336	A	<-->	6162	CA	SER	36	B	3.63
147.	3002	OE1	GLU	336	A	<-->	6166	C	SER	36	B	3.61
148.	3002	OE1	GLU	336	A	<-->	6168	N	GLY	37	B	2.69
149.	3002	OE1	GLU	336	A	<-->	6170	CA	GLY	37	B	3.53
150.	3002	OE1	GLU	336	A	<-->	6177	CD	PRO	38	B	3.30
151.	3003	OE2	GLU	336	A	<-->	6168	N	GLY	37	B	3.64
152.	3019	CG1	VAL	338	A	<-->	6163	CB	SER	36	B	3.87
153.	3019	CG1	VAL	338	A	<-->	6164	OG	SER	36	B	3.63
154.	3194	CZ	ARG	355	A	<-->	6148	O	LEU	34	B	3.70
155.	3195	NH1	ARG	355	A	<-->	6128	O	LYS	32	B	3.54
156.	3195	NH1	ARG	355	A	<-->	6147	C	LEU	34	B	3.50
157.	3195	NH1	ARG	355	A	<-->	6148	O	LEU	34	B	2.73
158.	3198	NH2	ARG	355	A	<-->	6138	C	ASN	33	B	3.77
159.	3198	NH2	ARG	355	A	<-->	6139	O	ASN	33	B	3.31
160.	3198	NH2	ARG	355	A	<-->	6147	C	LEU	34	B	3.90
161.	3198	NH2	ARG	355	A	<-->	6148	O	LEU	34	B	3.85
162.	3198	NH2	ARG	355	A	<-->	6154	OD1	ASN	35	B	3.12
163.	3215	CB	THR	357	A	<-->	6159	O	ASN	35	B	3.62
164.	3216	OG1	THR	357	A	<-->	6159	O	ASN	35	B	3.21
165.	3218	CG2	THR	357	A	<-->	6158	C	ASN	35	B	3.78
166.	3218	CG2	THR	357	A	<-->	6159	O	ASN	35	B	3.25
167.	3218	CG2	THR	357	A	<-->	6164	OG	SER	36	B	3.65
168.	3237	OG1	THR	359	A	<-->	6164	OG	SER	36	B	3.49
169.	3400	CZ	PHE	377	A	<-->	6153	CG	ASN	35	B	3.71
170.	3400	CZ	PHE	377	A	<-->	6154	OD1	ASN	35	B	3.57
171.	3400	CZ	PHE	377	A	<-->	6155	ND2	ASN	35	B	3.35
172.	3416	CG	ASP	379	A	<-->	6155	ND2	ASN	35	B	3.70
173.	3418	OD2	ASP	379	A	<-->	6155	ND2	ASN	35	B	3.06

Salt bridges

	<----- A T O M 1 ----->						<----- A T O M 2 ----->					
	Atom no.	Atom name	Res name	Res no.	Chain		Atom no.	Atom name	Res name	Res no.	Chain	Distance
1.	326	OD2	ASP	60	A	<-->	6014	NZ	LYS	22	B	2.71
2.	563	OD2	ASP	84	A	<-->	6014	NZ	LYS	22	B	2.63
3.	1202	OE2	GLU	154	A	<-->	5953	NH2	ARG	13	B	2.71
4.	1441	OE2	GLU	178	A	<-->	5928	NE2	HIS	11	B	3.34
5.	1471	OD2	ASP	181	A	<-->	5953	NH2	ARG	13	B	2.74
6.	2493	OE1	GLU	286	A	<-->	6123	NZ	LYS	32	B	2.82
7.	2503	OE1	GLU	287	A	<-->	6100	NH1	ARG	30	B	3.02

Number of salt bridges: 7

Number of hydrogen bonds: 22

Number of non-bonded contacts: 173

Supplementary Material SM3: The amino acids involved in the interaction between The TLR5 (Atom 1) and Multi-epitope vaccine, CVMW (Atom 2). The Hydrogen Bonds, Salt bridges and non-bonded interactions are mentioned with their distances.

Hydrogen bonds

	<----- A T O M 1 ----->					<----- A T O M 2 ----->				
	Atom no.	Atom name	Res name	Res no.	Chain	Atom no.	Atom name	Res name	Res no.	Chain	Distance
1.	266	OE1	GLU	49	A	8188	N	GLY	39	B	2.92
2.	758	NH1	ARG	98	A	8472	O	VAL	68	B	3.12
3.	1003	OE1	GLU	123	A	8234	N	THR	45	B	2.84
4.	1003	OE1	GLU	123	A	8238	OG1	THR	45	B	2.75
5.	1512	NZ	LYS	173	A	8497	O	GLN	71	B	2.80
6.	1522	OG	SER	174	A	8493	NE2	GLN	71	B	2.83
7.	2896	OD1	ASN	318	A	8022	NZ	LYS	22	B	2.83
8.	3150	OG	SER	344	A	8022	NZ	LYS	22	B	2.90
9.	3365	OD2	ASP	366	A	8022	NZ	LYS	22	B	2.67
10.	6412	OE1	GLN	708	A	8430	NE2	HIS	64	B	3.00
11.	6460	NZ	LYS	713	A	8411	O	PHE	62	B	2.85
12.	6495	O	ASP	716	A	8131	NZ	LYS	32	B	2.95
13.	6492	OD1	ASP	716	A	8131	NZ	LYS	32	B	2.61
14.	6493	OD2	ASP	716	A	8143	ND2	ASN	33	B	2.72
15.	6599	O	PHE	725	A	8131	NZ	LYS	32	B	2.80

Non-bonded contacts

	<----- A T O M 1 ----->					<----- A T O M 2 ----->				
	Atom no.	Atom name	Res name	Res no.	Chain	Atom no.	Atom name	Res name	Res no.	Chain	Distance
1.	56	CD	ARG	29	A	8196	CG	PRO	40	B	3.87
2.	57	NE	ARG	29	A	8196	CG	PRO	40	B	3.37
3.	57	NE	ARG	29	A	8197	CD	PRO	40	B	3.77
4.	59	CZ	ARG	29	A	8196	CG	PRO	40	B	3.58
5.	63	NH2	ARG	29	A	8183	CB	PRO	38	B	3.39
6.	63	NH2	ARG	29	A	8196	CG	PRO	40	B	3.86
7.	63	NH2	ARG	29	A	8197	CD	PRO	40	B	3.75
8.	266	OE1	GLU	49	A	8186	C	PRO	38	B	3.88
9.	266	OE1	GLU	49	A	8183	CB	PRO	38	B	3.29
10.	266	OE1	GLU	49	A	8184	CG	PRO	38	B	3.25
11.	266	OE1	GLU	49	A	8185	CD	PRO	38	B	3.20
12.	266	OE1	GLU	49	A	8188	N	GLY	39	B	2.92
13.	266	OE1	GLU	49	A	8190	CA	GLY	39	B	3.70
14.	266	OE1	GLU	49	A	8197	CD	PRO	40	B	3.81
15.	267	OE2	GLU	49	A	8197	CD	PRO	40	B	3.72
16.	276	NE	ARG	50	A	8197	CD	PRO	40	B	3.61
17.	282	NH2	ARG	50	A	8188	N	GLY	39	B	3.56
18.	282	NH2	ARG	50	A	8190	CA	GLY	39	B	3.40
19.	511	NE2	GLN	73	A	8178	CA	GLY	37	B	3.52
20.	511	NE2	GLN	73	A	8185	CD	PRO	38	B	3.68
21.	758	NH1	ARG	98	A	8472	O	VAL	68	B	3.12
22.	758	NH1	ARG	98	A	8469	CG1	VAL	68	B	3.45
23.	770	CG1	ILE	99	A	8231	CB	ALA	44	B	3.73
24.	771	CG2	ILE	99	A	8227	O	ASN	43	B	3.68
25.	772	CD1	ILE	99	A	8231	CB	ALA	44	B	3.77
26.	993	CE2	PHE	122	A	8478	C	PRO	69	B	3.64
27.	993	CE2	PHE	122	A	8479	O	PRO	69	B	3.50

28.	1002	CD	GLU	123	A	<-->	8234	N	THR	45	B	3.80
29.	1003	OE1	GLU	123	A	<-->	8230	CA	ALA	44	B	3.65
30.	1003	OE1	GLU	123	A	<-->	8232	C	ALA	44	B	3.47
31.	1003	OE1	GLU	123	A	<-->	8231	CB	ALA	44	B	3.85
32.	1003	OE1	GLU	123	A	<-->	8234	N	THR	45	B	2.84
33.	1003	OE1	GLU	123	A	<-->	8236	CA	THR	45	B	3.55
34.	1003	OE1	GLU	123	A	<-->	8237	CB	THR	45	B	3.57
35.	1003	OE1	GLU	123	A	<-->	8238	OG1	THR	45	B	2.75
36.	1004	OE2	GLU	123	A	<-->	8230	CA	ALA	44	B	3.87
37.	1254	CG2	THR	148	A	<-->	8490	CG	GLN	71	B	3.67
38.	1508	CB	LYS	173	A	<-->	8493	NE2	GLN	71	B	3.68
39.	1510	CD	LYS	173	A	<-->	8497	O	GLN	71	B	3.79
40.	1510	CD	LYS	173	A	<-->	8490	CG	GLN	71	B	3.89
41.	1511	CE	LYS	173	A	<-->	8497	O	GLN	71	B	3.65
42.	1512	NZ	LYS	173	A	<-->	8497	O	GLN	71	B	2.80
43.	1522	OG	SER	174	A	<-->	8491	CD	GLN	71	B	3.89
44.	1522	OG	SER	174	A	<-->	8493	NE2	GLN	71	B	2.83
45.	2896	OD1	ASN	318	A	<-->	8021	CE	LYS	22	B	3.62
46.	2896	OD1	ASN	318	A	<-->	8022	NZ	LYS	22	B	2.83
47.	3129	CB	ASN	342	A	<-->	8022	NZ	LYS	22	B	3.40
48.	3130	CG	ASN	342	A	<-->	8022	NZ	LYS	22	B	3.58
49.	3131	OD1	ASN	342	A	<-->	8021	CE	LYS	22	B	3.51
50.	3131	OD1	ASN	342	A	<-->	8022	NZ	LYS	22	B	3.24
51.	3150	OG	SER	344	A	<-->	8022	NZ	LYS	22	B	2.90
52.	3344	CE2	TYR	364	A	<-->	8012	CA	GLY	21	B	3.75
53.	3346	OH	TYR	364	A	<-->	8012	CA	GLY	21	B	3.78
54.	3363	CG	ASP	366	A	<-->	8022	NZ	LYS	22	B	3.61
55.	3365	OD2	ASP	366	A	<-->	8020	CD	LYS	22	B	3.71
56.	3365	OD2	ASP	366	A	<-->	8021	CE	LYS	22	B	3.44
57.	3365	OD2	ASP	366	A	<-->	8022	NZ	LYS	22	B	2.67
58.	3384	NE2	GLN	368	A	<-->	8019	CG	LYS	22	B	3.76
59.	3594	OG1	THR	388	A	<-->	7994	CG	PRO	18	B	3.48
60.	3794	CE1	PHE	409	A	<-->	7995	CD	PRO	18	B	3.65
61.	3796	CZ	PHE	409	A	<-->	7995	CD	PRO	18	B	3.70
62.	6381	O	THR	705	A	<-->	8406	CD2	PHE	62	B	3.54
63.	6381	O	THR	705	A	<-->	8408	CE2	PHE	62	B	3.24
64.	6417	O	GLN	708	A	<-->	8428	CD2	HIS	64	B	3.85
65.	6412	OE1	GLN	708	A	<-->	8428	CD2	HIS	64	B	3.67
66.	6412	OE1	GLN	708	A	<-->	8429	CE1	HIS	64	B	3.79
67.	6412	OE1	GLN	708	A	<-->	8430	NE2	HIS	64	B	3.00
68.	6427	C	ASN	709	A	<-->	8399	O	GLY	61	B	3.81
69.	6428	O	ASN	709	A	<-->	8399	O	GLY	61	B	3.46
70.	6421	CB	ASN	709	A	<-->	8402	CA	PHE	62	B	3.86
71.	6421	CB	ASN	709	A	<-->	8406	CD2	PHE	62	B	3.43
72.	6422	CG	ASN	709	A	<-->	8433	O	HIS	64	B	3.34
73.	6422	CG	ASN	709	A	<-->	8424	CB	HIS	64	B	3.73
74.	6423	OD1	ASN	709	A	<-->	8432	C	HIS	64	B	3.86
75.	6423	OD1	ASN	709	A	<-->	8433	O	HIS	64	B	2.93
76.	6423	OD1	ASN	709	A	<-->	8424	CB	HIS	64	B	3.26
77.	6423	OD1	ASN	709	A	<-->	8425	CG	HIS	64	B	3.48
78.	6423	OD1	ASN	709	A	<-->	8428	CD2	HIS	64	B	3.21
79.	6424	ND2	ASN	709	A	<-->	8406	CD2	PHE	62	B	3.73
80.	6424	ND2	ASN	709	A	<-->	8433	O	HIS	64	B	3.44
81.	6429	N	ALA	710	A	<-->	8399	O	GLY	61	B	3.74
82.	6429	N	ALA	710	A	<-->	8402	CA	PHE	62	B	3.81
83.	6431	CA	ALA	710	A	<-->	8398	C	GLY	61	B	3.61
84.	6431	CA	ALA	710	A	<-->	8399	O	GLY	61	B	3.18
85.	6433	C	ALA	710	A	<-->	8399	O	GLY	61	B	3.78
86.	6434	O	ALA	710	A	<-->	8395	N	GLY	61	B	3.79
87.	6434	O	ALA	710	A	<-->	8399	O	GLY	61	B	3.52

88.	6432	CB	ALA	710	A	<-->	8405	CD1	PHE	62	B	3.85
89.	6432	CB	ALA	710	A	<-->	8407	CE1	PHE	62	B	3.73
90.	6450	CD2	LEU	712	A	<-->	8140	CB	ASN	33	B	3.79
91.	6456	CB	LYS	713	A	<-->	8399	O	GLY	61	B	3.32
92.	6456	CB	LYS	713	A	<-->	8411	O	PHE	62	B	3.77
93.	6457	CG	LYS	713	A	<-->	8411	O	PHE	62	B	3.21
94.	6458	CD	LYS	713	A	<-->	8142	OD1	ASN	33	B	3.69
95.	6459	CE	LYS	713	A	<-->	7895	O	ILE	7	B	3.88
96.	6459	CE	LYS	713	A	<-->	7904	O	LEU	8	B	3.75
97.	6459	CE	LYS	713	A	<-->	8411	O	PHE	62	B	3.54
98.	6459	CE	LYS	713	A	<-->	8420	O	LEU	63	B	3.31
99.	6460	NZ	LYS	713	A	<-->	8411	O	PHE	62	B	2.85
100.	6460	NZ	LYS	713	A	<-->	8420	O	LEU	63	B	3.72
101.	6460	NZ	LYS	713	A	<-->	8415	CB	LEU	63	B	3.51
102.	6473	CE1	HIS	714	A	<-->	8388	N	PRO	60	B	3.89
103.	6494	C	ASP	716	A	<-->	8131	NZ	LYS	32	B	3.85
104.	6495	O	ASP	716	A	<-->	8131	NZ	LYS	32	B	2.95
105.	6490	CB	ASP	716	A	<-->	8143	ND2	ASN	33	B	3.83
106.	6491	CG	ASP	716	A	<-->	8131	NZ	LYS	32	B	3.15
107.	6491	CG	ASP	716	A	<-->	8140	CB	ASN	33	B	3.69
108.	6491	CG	ASP	716	A	<-->	8143	ND2	ASN	33	B	3.51
109.	6492	OD1	ASP	716	A	<-->	8128	CG	LYS	32	B	3.83
110.	6492	OD1	ASP	716	A	<-->	8130	CE	LYS	32	B	3.67
111.	6492	OD1	ASP	716	A	<-->	8131	NZ	LYS	32	B	2.61
112.	6493	OD2	ASP	716	A	<-->	8135	C	LYS	32	B	3.85
113.	6493	OD2	ASP	716	A	<-->	8127	CB	LYS	32	B	3.38
114.	6493	OD2	ASP	716	A	<-->	8128	CG	LYS	32	B	3.53
115.	6493	OD2	ASP	716	A	<-->	8131	NZ	LYS	32	B	3.52
116.	6493	OD2	ASP	716	A	<-->	8137	N	ASN	33	B	3.16
117.	6493	OD2	ASP	716	A	<-->	8139	CA	ASN	33	B	3.69
118.	6493	OD2	ASP	716	A	<-->	8140	CB	ASN	33	B	3.39
119.	6493	OD2	ASP	716	A	<-->	8141	CG	ASN	33	B	3.52
120.	6493	OD2	ASP	716	A	<-->	8143	ND2	ASN	33	B	2.72
121.	6502	CG2	THR	717	A	<-->	7910	CD	ARG	9	B	3.72
122.	6533	CA	SER	720	A	<-->	8129	CD	LYS	32	B	3.52
123.	6538	O	SER	720	A	<-->	8129	CD	LYS	32	B	3.61
124.	6534	CB	SER	720	A	<-->	8129	CD	LYS	32	B	3.72
125.	6565	OD1	ASN	723	A	<-->	8130	CE	LYS	32	B	3.88
126.	6599	O	PHE	725	A	<-->	8130	CE	LYS	32	B	3.37
127.	6599	O	PHE	725	A	<-->	8131	NZ	LYS	32	B	2.80
128.	6664	CG	ARG	732	A	<-->	8161	CG	ASN	35	B	3.69
129.	6664	CG	ARG	732	A	<-->	8162	OD1	ASN	35	B	3.59
130.	6664	CG	ARG	732	A	<-->	8163	ND2	ASN	35	B	3.63
131.	7583	CD1	PHE	822	A	<-->	8380	CD	PRO	58	B	3.86

Salt bridges

	<----- A T O M 1 ----->						<----- A T O M 2 ----->					
	Atom no.	Atom name	Res name	Res no.	Chain		Atom no.	Atom name	Res name	Res no.	Chain	Distance
1.	3364	OD1	ASP	366	A	<-->	8022	NZ	LYS	22	B	2.67
2.	6492	OD1	ASP	716	A	<-->	8131	NZ	LYS	32	B	2.61

Number of salt bridges: 2

Number of hydrogen bonds: 15

Number of non-bonded contacts: 131