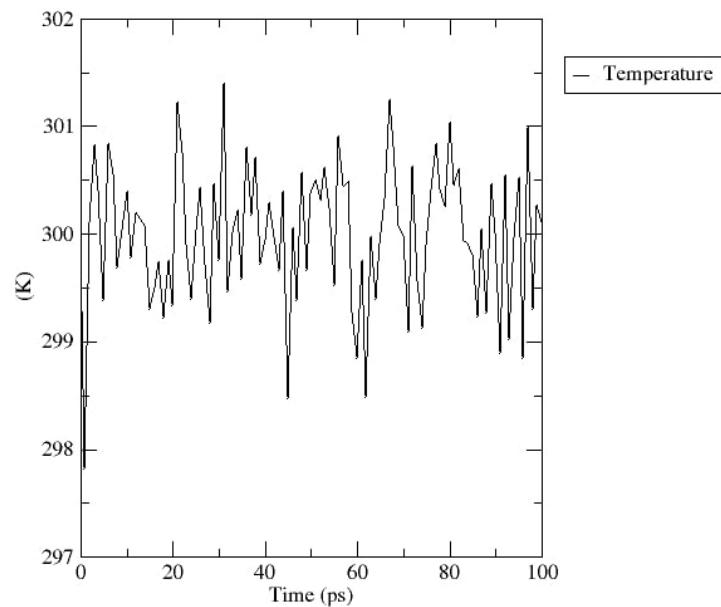
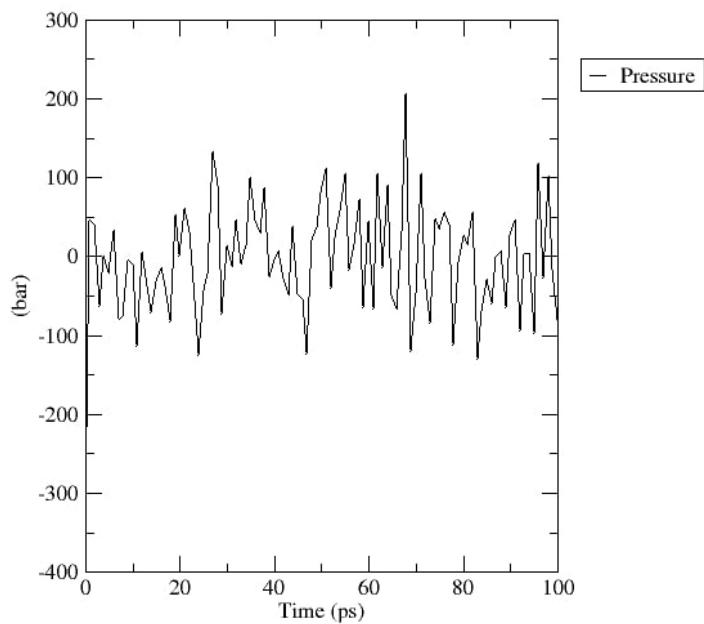


### GROMACS Energies



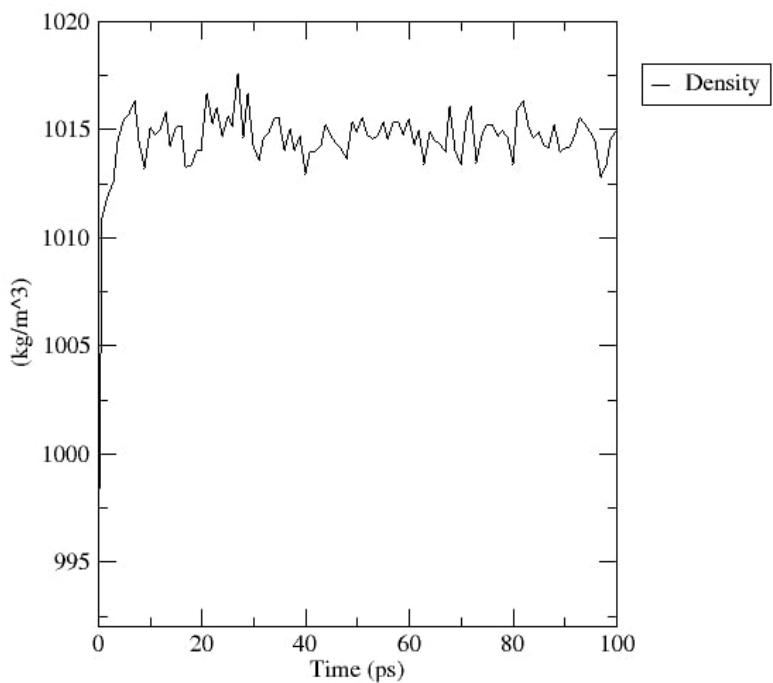
**Figure S1.** Graph showing minute fluctuations in the system's temperature during NVT equilibration steps.

### GROMACS Energies

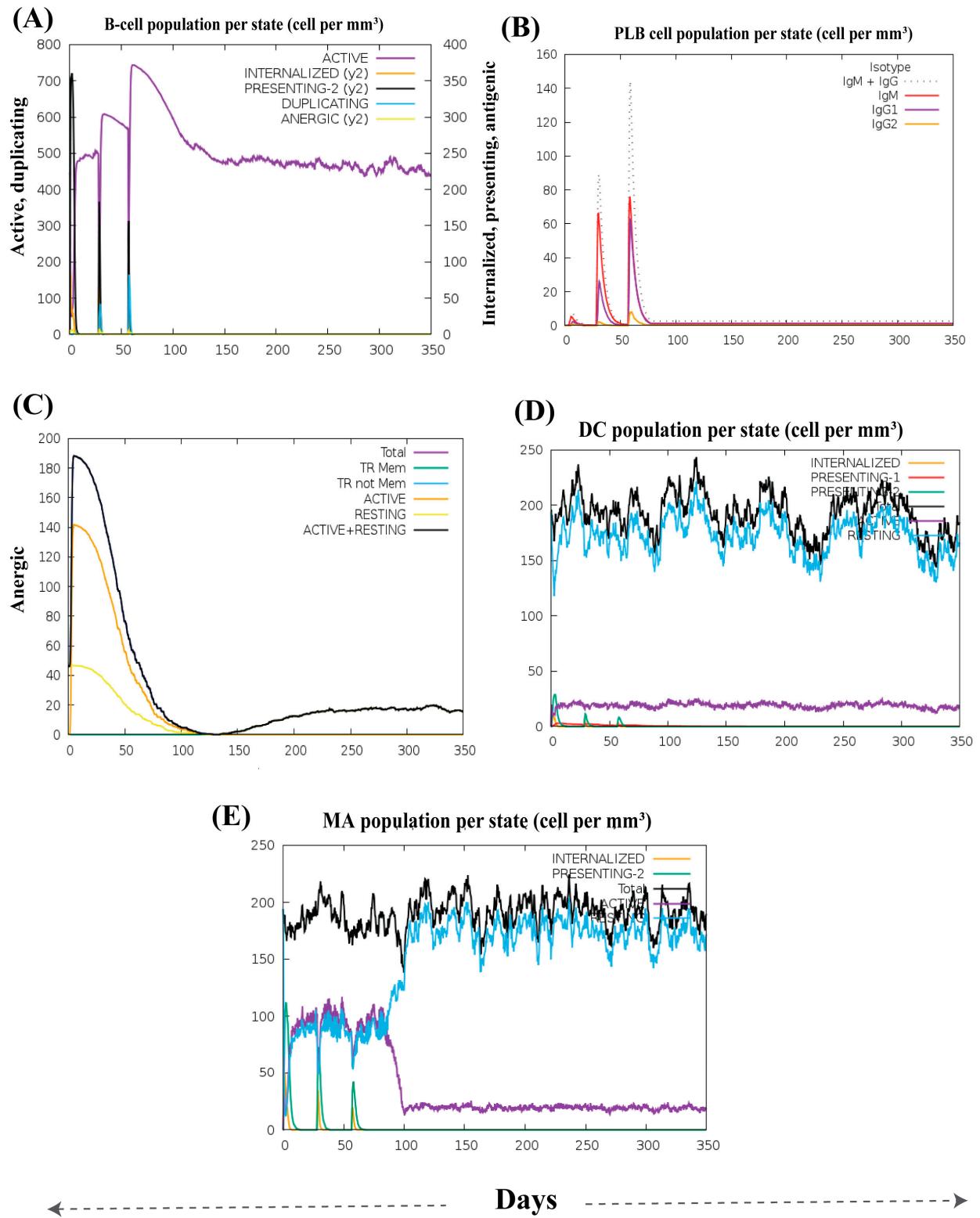


**Figure S2.** Graph showing minute fluctuations in the system's pressure during NPT equilibration steps.

### GROMACS Energies



**Figure S3.** Graph showing minute fluctuations in the system's density during NPT equilibration steps.



**Figure S4.** The immunostimulatory potential of the constructed vaccine. **(A)** population/state of active B-cell **(B)** population/state of plasma B-cell and their isotypes **(C)** decrease in the population of regulatory T-cell **(D)** population/state of dendritic cell **(E)** macrophage (MA) activity. All units are given in cells per mm<sup>3</sup> in three consecutive immunological responses.

**Table S1.** Table showing HADDOCK score of top epitope-protein docked cluster along with standard deviation.

HLA class	Finalized epitopes	HLA alleles	RSV protein	HADDOCK score	Standard Deviation (SD)
HLA class I epitopes	NIDIFNPKY	HLA-A*0101	Fusion	-97.1	5.6
	LIAVGLLY			-90.3	3.6
	IMITIIIV		Fusion	-85.4	2
	LLHNVNAGK		Fusion	-104.2	3.9
	KTKNTTTK		Glycoprotein	-113.8	2.4
	ITIELSNIK			-105.4	1.7
	KQLLPIVNK		Fusion	-107.7	3.7
	IASGIAVSK			-105	5.3
HLA class II epitopes	LGFLLGVGSAIASGI	DRB1*0101	Fusion	-93.2	3.3
	LLLYCKARSTPVTLS			-88.9	2.5
	AIFIASANHKVTLT		Glycoprotein	-117.4	3.3
	AIFIASANHKVTLT		Glycoprotein	-117.1	1.2

**Table S2.** Table showing the main HADDOCK results of multi-epitope with TLR4. It includes the docking score and all other properties along with their standard deviations.

Parameters	Vaccine-TLR4 cluster
HADDOCK score	-143.3 +/- 9.6
Size of Cluster	20
RMSD from the overall lowest-energy structure	0.3 +/- 0.2
Van der Waals energy	-89.5 +/- 3.9
Electrostatic energy	-371.2 +/- 4.1
Desolvation energy	20.4 +/- 10.0
Restraints violation energy	0.0 +/- 0.00
Total Buried Surface Area	2496.4 +/- 32.1
Z-Score	0

**Supplementary File S1:** The amino acid sequence of the RSV multi-epitope vaccine (in FASTA format). The adjuvant sequence has been italicized; underlined letters have been used to indicate T-cell epitopes whereas bold letters have been used to indicate the linkers (EAAAK and GPGPG).

```
>RSV_Vaccine
MTPQNITDLCAEYHNTQIHTLNDKIFSYTESLAGKREMAIITFKNGATFQVEVPGSQHID
SQKKAIERMKDTTLRIAYLTEAKVEKLCVWNNKTPHAIAAISMANEAAAKAIIFIASANHK
VTLTGPGPGKTNTTTKGPGPGITIELSNIGPGPGLGFLLGVGSAIASGIAVSKGPGPG
GKQLLPIVNKGPGPGNIDIFNPKYGPGPGGLLHNVNAGKGPGPGIMITIIIVGPGPGLIA
VGLLYCKARSTPVTLS
```

**Supplementary File S2:** The optimized codon sequence of the RSV vaccine (in FASTA format).

```
>Optimized_codon_sequence_RSV_vaccine
ATGACCCCGCAGAACATCACCGACCTGTGCCTGAATACCACAAACACCCAGATCCACACC
CTGAACGACAAAATCTTCTCTTACACCGAATCTCTGGCTGGTAAACGTGAAATGGCTATC
ATCACCTCAAAAACGGTGCTACCTTCAGGTTGAAGTTCCGGGTTCTCAGCACATCGAC
TCTCAGAAAAAGCTATCGAACGTATGAAAGACACCCCTCGGTATCGCTTACCTGACCGAA
GCTAAAGTTGAAAAACTGTGCGTTGGAACAACAAAACCCGCACGCTATCGCTGCTATC
TCTATGGCTAACGAAGCTGCTGCTAAAGCTATCATCTTCATCGCTTCTGCTAACACACAAA
GTTACCCCTGACCGGTCCGGTCAAACCAAAAACACCACCAACCAAGGTCCCG
GGTCCGGGTATCACCATCGAACTGTCTAACATCAAAGGTCCGGGTCCAGGGCTGGCTTC
CTGCTGGGTGTTGGTCTGCTATCGCTTCTGGTATCGCTGTTCTAAAGGTCCGGGTCCG
GGTAAACAGCTGCTGCCGATCGTTAACAAAGGTCCGGGTCCGGTAACATCGACATCTTC
AACCCGAAATAACGGTCCGGTCCGGTCTGCTGCACAACGTTAACGCTGGTAAAGGTCCG
GGTCCGGGTATCATGATCACCACCATCATCGTTGGTCCGGTCCGGTCTGATCGCT
GTTGGTCTGCTGCTACTGCAAAGCTCGTTACCCCGTTACCCCTGTCT
```