Prioritizing Promising Vaccine Models against Astrovirus MLB2 Using Integrated Vaccinomics and Immunoinformatics Approaches

Supplementary Material

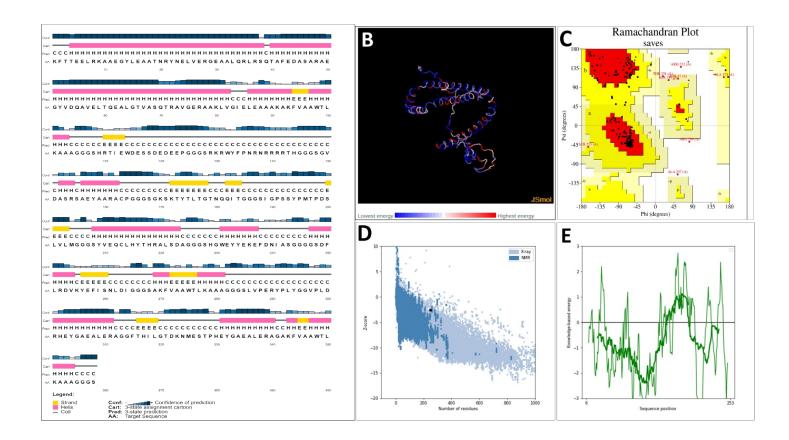


Figure S1: Predicted Secondary and tertiary structure, refinement and validation of MLB2-V1. (A). 2D structure of vaccine construct. (B) Refined 3D Structure (C) Ramachandran plot of the refined structure. (D) the overall model quality, reassuringly positioning the protein structure within favored boundaries (E) highlights the local model quality, demonstrating the strong alignment of most protein segments with knowledge-based energy principles.

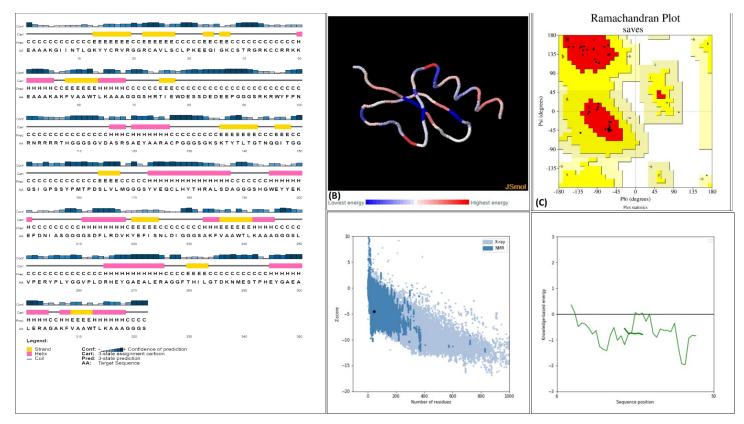


Figure S2: Predicted Secondary and tertiary structure, refinement and validation of MLB2-V2. (A). 2D structure of vaccine construct. (B) Refined 3D Structure. (c) Ramachandran plot of the refined structure. (D) the overall model quality, reassuringly positioning the protein structure within favored boundaries (E) highlights the local model quality, demonstrating the strong alignment of most protein segments with knowledge-based energy principles.

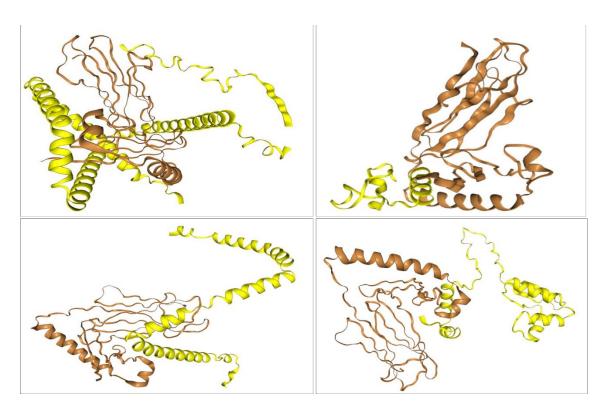


Figure S3: vaccine construct docked complex with HLA immune receptor.

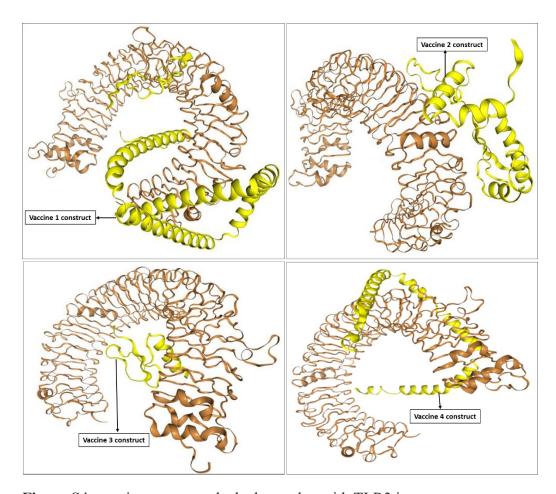


Figure S4: vaccine construct docked complex with TLR3 immune receptor.

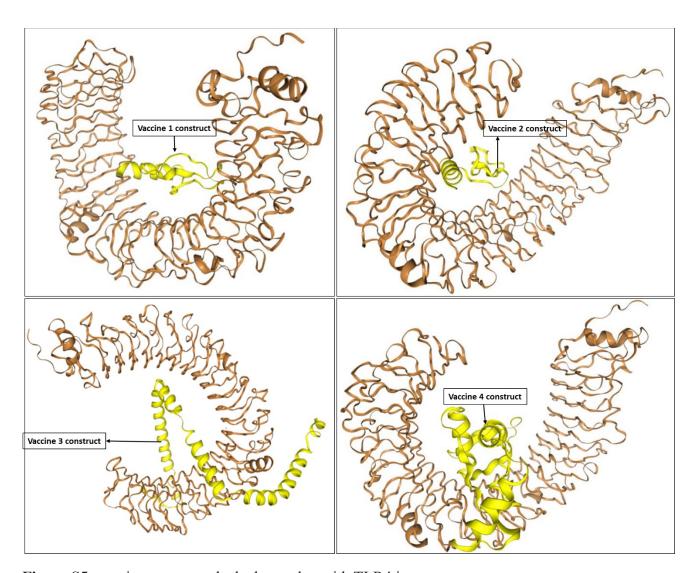


Figure S5: vaccine construct docked complex with TLR4 immune receptor.

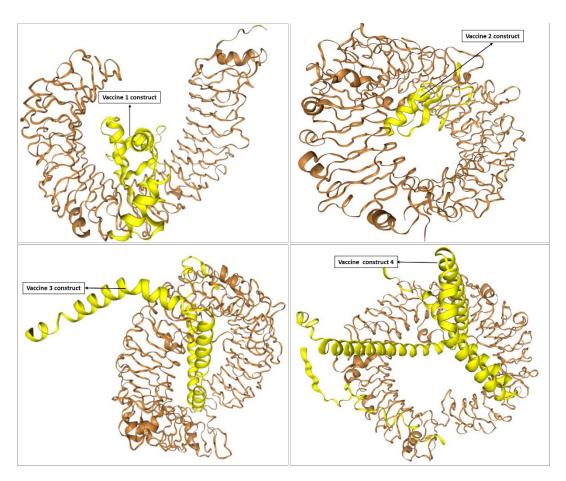


Figure S6: vaccine construct docked complex with TLR4 immune receptor.

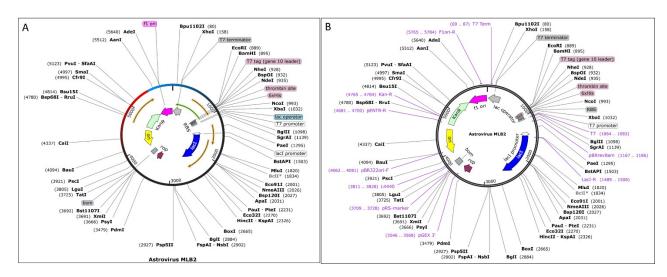


Figure S7: The *in-silico* cloning assessment of model vaccine constructs. Structure of MEVs is cloned in the pET-28a(+) expression vector, i.e. (A) MLB2-V1 (B) MLB2-V2.

Table S1: Population coverage of the top-ranked MHCs alleles across different ethnicities.

	WEU38090.1		APB03098.1	
Region	MHC-I	MHC-II	MHC-I	MHC-II
Central Africa	98.00%	62.84%	96.39%	62.84%
Central America	9.07%	53.91%	9.07%	53.91%
East Africa	98.38%	68.53%	97.40%	68.53%
East Asia	99.93%	82.41%	99.65%	82.41%
Europe	100.00%	87.47%	99.99%	87.47%
North Africa	99.59%	76.07%	99.11%	76.07%
North America	99.99%	90.03%	99.84%	90.03%
Northeast Asia	98.50%	60.80%	98.16%	60.80%
Oceania	99.13%	60.21%	98.59%	60.21%
South Africa	99.52%	32.10%	99.99%	54.03%
South America	99.34%	63.52%	99.40%	32.10%
South Asia	99.89%	76.44%	96.65%	63.52%
Southeast Asia	99.64%	58.83%	98.34%	76.44%
Southwest Asia	98.57%	45.29%	98.53%	58.83%
West Africa	99.05%	65.81%	97.67%	45.29%
West Indies	99.51%	70.02%	98.02%	65.81%
World	99.97%	83.81%	99.79%	83.81%
Average	94%	66.95%	93.66%	66.22 %