In silico modelling and characterization of Epstein–Barr virus LMP1 protein

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Supporting Information

Table S1 Ab initio docking results for LMP1 predicted structure.

Model No.	No. of Subunits	Interface Area (in Angstrom ^{2})	Docking Score
1	2-mer	2279.7	2350.543
2	2-mer	2173.8	2206.530
3	2-mer	1804.2	2103.901
4	5-mer	7891.9	1012.986
5	3-mer	3869.4	914.557

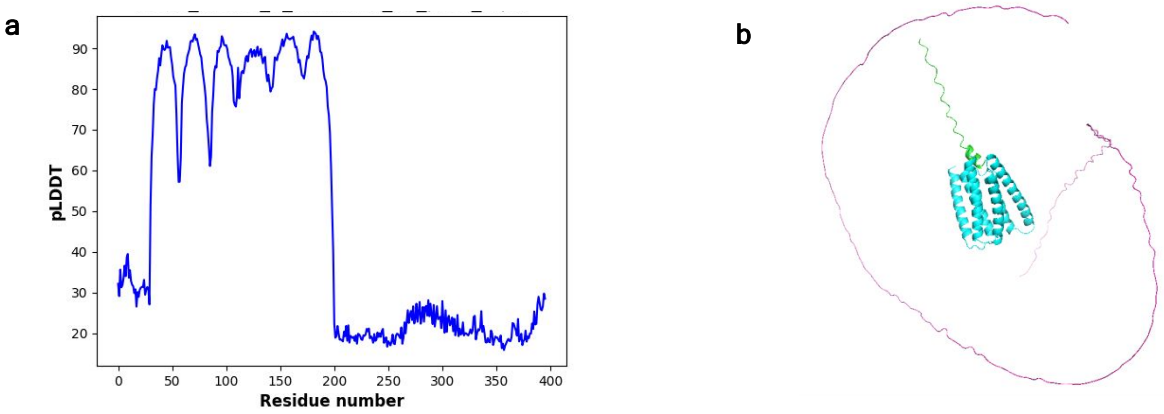

Figure S1 (a) Per-residue confidence score for LMP1 model 3 **(b)** AlphaFold2 LMP1 model 3 image

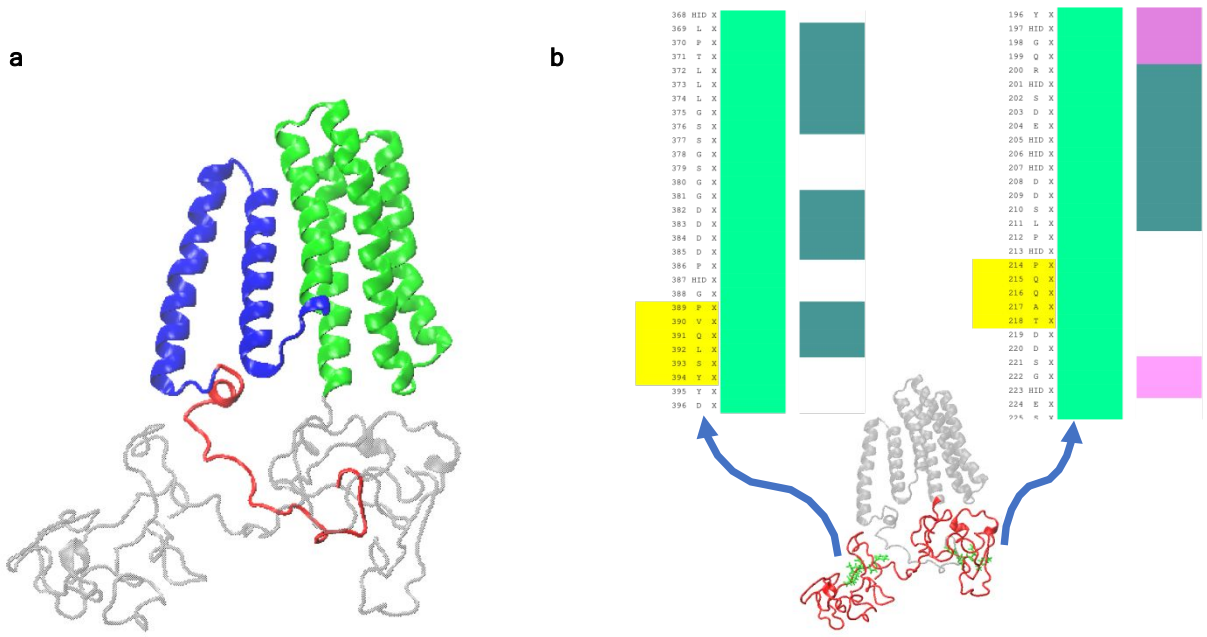

Figure S2 (a) The molecular image of TMD3-6 (green colour) and TMD1-2 (blue colour) responsible for the oligomerisation of the LMP1 protein. The red-colour chain represents the N-terminal domain of the LMP1 protein. **(b)** The CTAR1 and CTAR2 domains activate the cells.

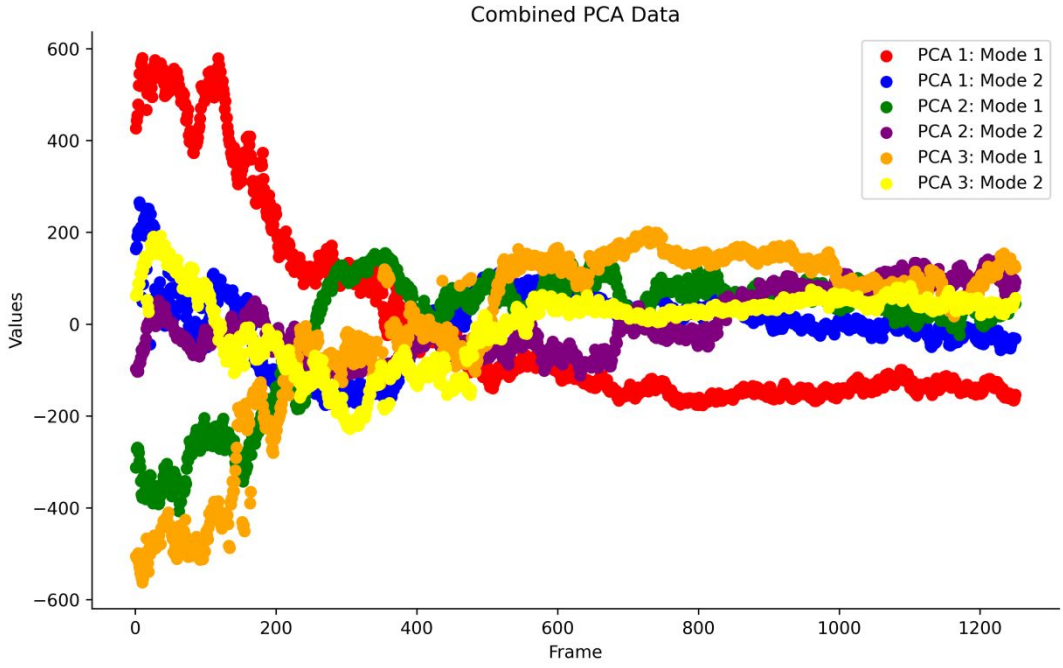

Figure S3 Graph shows combined PCA data for all the triplicate runs with the values on the y-axis and frame on the x-axis.