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## Non-active site mutations disturb loop dynamics, dimerization, viral budding and egress of

## **VP40 of the Ebola virus**

## **Supplementary Material**

Marissa Balmith<sup>a</sup> and Mahmoud E.S. Soliman<sup>a\*</sup>

<sup>a</sup>Molecular Modeling and Drug Design Research Group, School of Health Sciences, University

of KwaZulu-Natal, Westville Campus, Durban 4001, South Africa

\* Corresponding author: Mahmoud E.S. Soliman

 Dean and Head of School of Health Sciences, Full Professor: Pharmaceutical Sciences, University of KwaZulu-Natal, Westville Campus, Durban 4001, South Africa.
Department of Pharmaceutical Organic Chemistry, Faculty of Pharmacy, Zagazig University, Zagazig, Egypt.
College of Pharmacy and Pharmaceutical Sciences, Florida Agricultural and Mechanical University, FAMU, Tallahassee, Florida 32307, USA.

Email: soliman@ukzn.ac.za

Telephone: +27 031 260 7413, Fax: +27 031 260 779

**Table 1:**  $C\alpha$  residues involved in the loop region and dimerization of VP40 and their average distances from each other during simulation time.

Residues	Wildtype (WT)	K98A	T100A	N101A	K98/T100A/N101A
Distance (Å)					
G394-P399	5.07	4.86	4.95	5.02	4.98
K395-N398	6.09	5.93	6.29	6.13	5.87
K395-T397	5.00	5.59	5.57	5.50	5.73
A396-P399	6.46	6.70	6.48	6.57	6.72
G394-A396	6.46	6.59	6.57	6.59	6.56
G97-P102	5.00	4.91	5.08	5.00	4.78
K98-N101	6.16	6.05	6.43	6.08	5.98
K98-T100	5.43	5.45	5.58	5.51	5.35
G97-A99	6.62	6.55	6.91	6.61	6.08
A99-P102	6.53	6.78	6.43	6.69	7.66
D80-D377	5.52	5.46	5.47	5.60	5.55
A84-A381	6.23	6.49	6.51	6.30	6.49
M87-M384	8.30	8.24	8.38	8.57	8.52



**Figure 2:** PCA scatter plot projecting principal components (PC1, PC2 and PC3) in the space of **(A)** Mutation K98A, **(B)** Mutation T100A, **(C)** Mutation N101A of VP40 respectively.