Supporting Information for

Conformational Flexibility of the Protein-Protein Interfaces of the Ebola Virus VP40 Structural Matrix Filament

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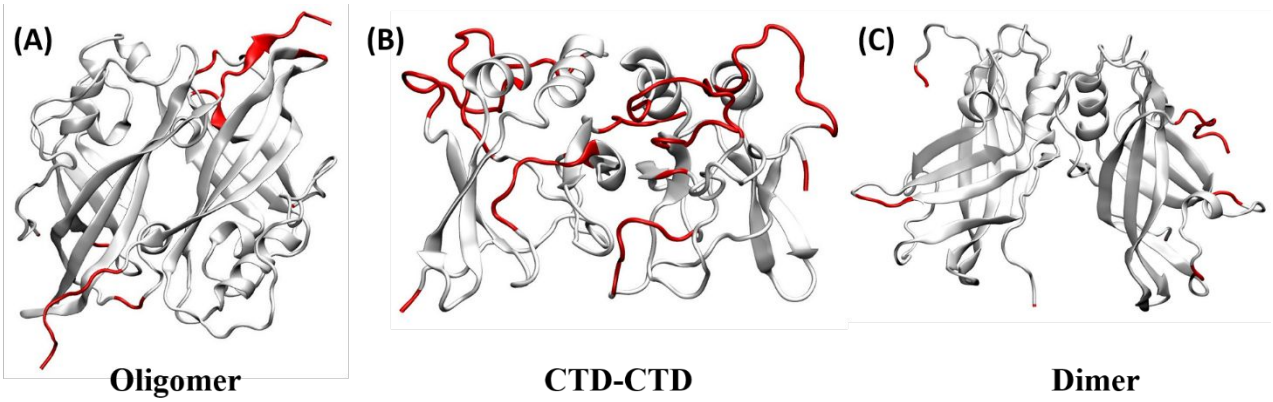

Figure S1. For each interface, residues that were missing from the PDB 3D crystal structure have been inserted using the Modeller 9.17 software package[19]. Residues highlighted in red are residues that were added using Modeller.

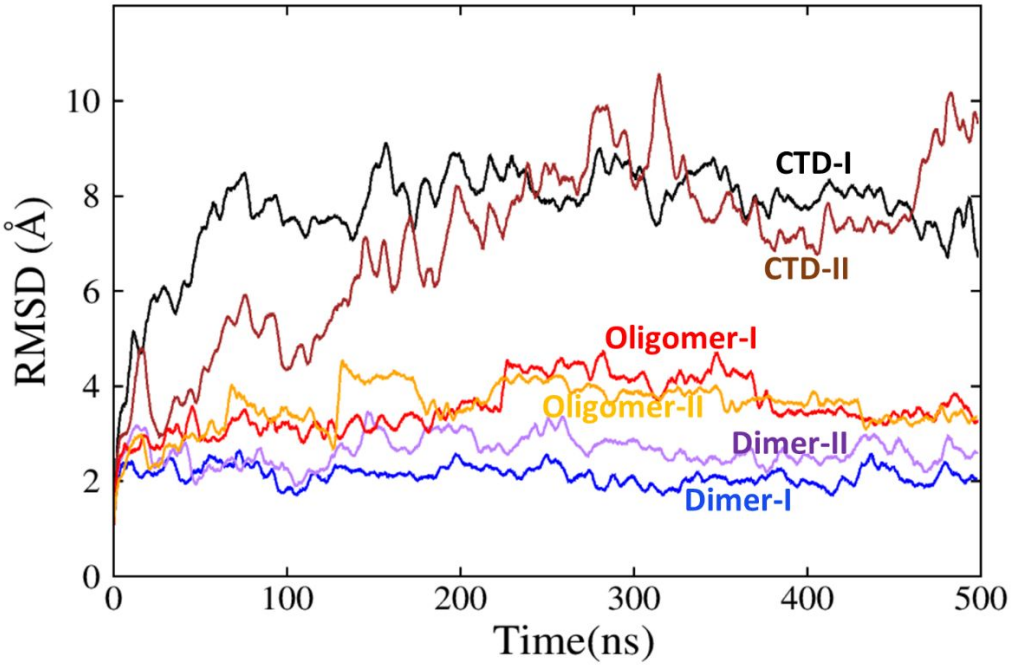

Figure S2. For each interface, the RMSD of each member is plotted separately. The results show that for each interface, both members exhibit similar flexibility.

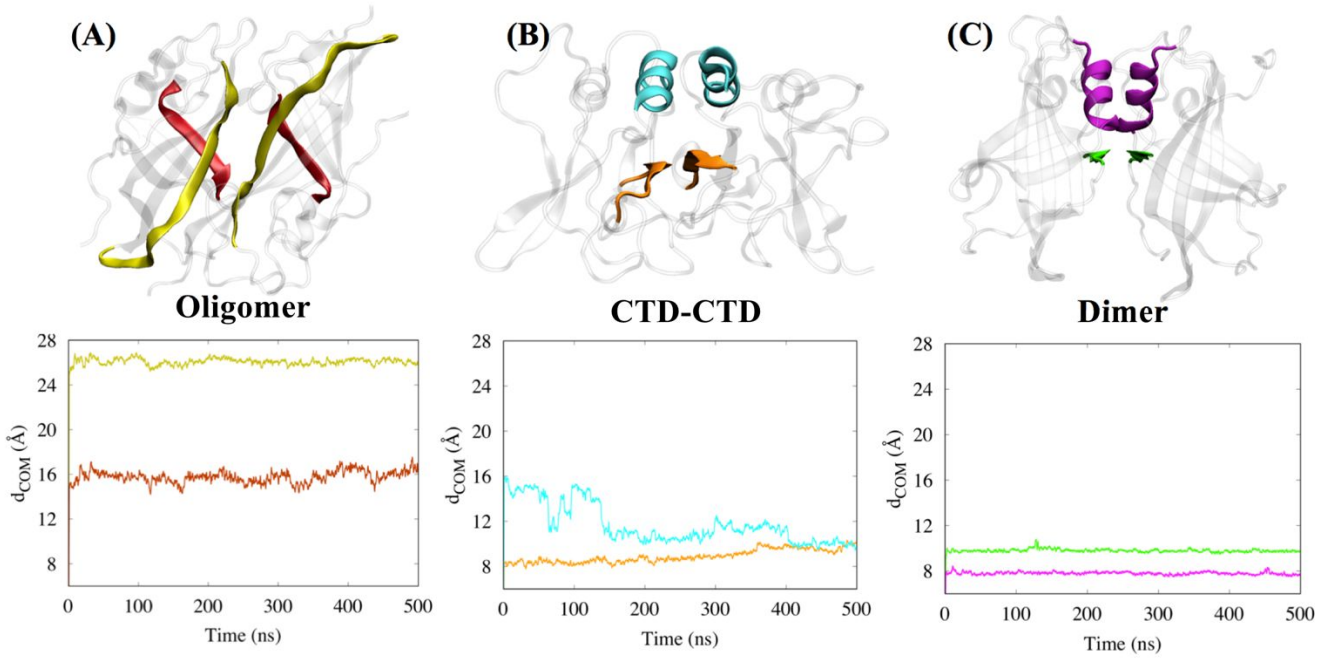

Figure S3. For the structural elements located at the three interfaces of Fig. 4, fluctuations in the distance between the structural elements of each group as a function of simulation time.

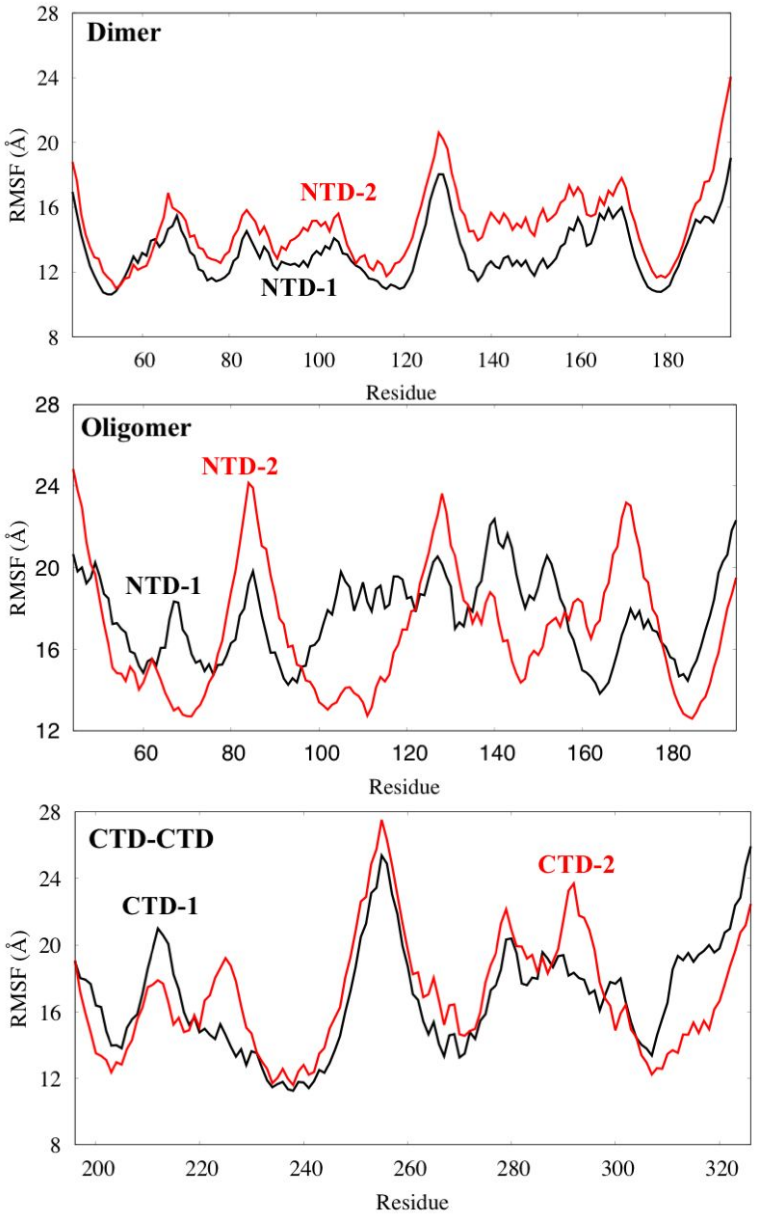

Figure S4. Root-mean-square fluctuations (RMSF) computed from the last 100 ns trajectory for the C_α atoms of the interface structural elements of Fig. 4.

Table S1. An expanded version of Table 2 with additional information about the interactions.

Community	Oligomer			Dimer			CTD-CTD		
	NTD1	NTD2	Interaction-type	NTD1	NTD-2	Interaction-type	CTD1	CTD-2	Interaction-type
Comm-1	P93	P187	hydrophobic	A113, L117	T112	hydrogen bond	V306, I304, T308	T304	hydrogen bond
	K90, I92	A189	hydrophobic , hydrogen bond	I54, A55	R52	hydrogen bond			
	M89, K90	T190	hydrogen bond	D56, D57	R52	salt-bridge			
	L88, M89	W191	hydrogen bond	A55, I59	L117	hydrophobic			
	L88, V87	T192	hydrogen bond	A55, M116	M116	hydrogen bond			
	Q91	A188, A189	hydrogen bond	T112	L117	hydrogen bond			
	I92	A189	Hydrophobic	R52, M116, L117	A55	hydrophobic , hydrogen bond			
				R52	D57	salt-bridge			
				L117	I59	hydrophobic			
				D109, S110, A113	D109	hydrophobic , hydrogen bond			
Comm-2	S70, V100	P164	hydrophobic , hydrogen bond				P234	Q238, T242	hydrogen bond
	V100	E160, F161,V162, L163	hydrophobic , hydrogen bond						
	A72, Q184	W95	hydrophobic , hydrogen bond						
	L186,P187	P93							
Comm-3	T190	M89, K90	hydrogen bond				L295	R214, S316	hydrogen bond
	W191	L88, M89	hydrogen bond				P297	K212, L213, P215,	hydrophobic, hydrogen bond
	W95, Q160, F161, L163	V100	hydrophobic , hydrogen bond						
Comm-4	P165	S70	hydrogen bond				H315	I293	hydrogen bond
	W95	L186	hydrophobic						
Comm-5	D102	P165	hydrogen bond						
Total Connections	33			19			11		

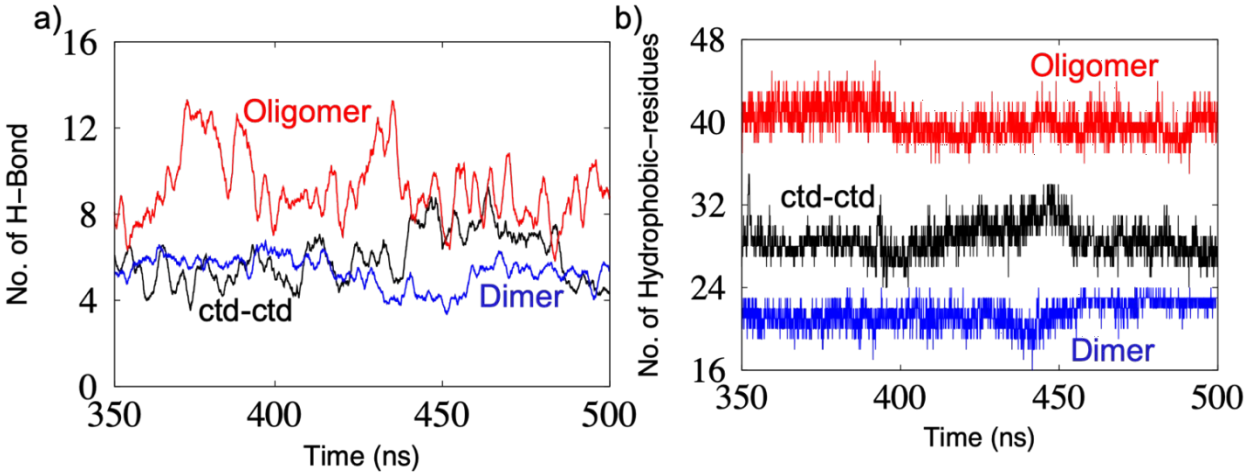

Figure S5. The time-evolution of the inter-domain contacts listed in Table 2 and Table S1. a) Evolution of the number of hydrogen bonds with respect to time for all three interfaces for the last 150 ns. b) Number of hydrophobic residues within 6.4 Å of the domain-domain interface during the last 150 ns of simulation.