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Supplementary Material

Investigating substitutions in antibody-antigen complexes using molecular dynamics: a case study with broad-spectrum, influenza A antibodies

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Table S2 – Changes in mean distance between the centres of gravity of selected pairs of residues in the CR6261 complex with the substitution HA2 D19N, compared to the WT complex. Distances were computed by *cpptraj* from the final 2ns of the initial production simulation.

Residue Pair		distance WT - distance D19N (Å)	binding energy in D19 relative to WT
K292	F74	-0.10	increased
L52	F74	0.52	increased
K292	D72	-0.77	decreased
D46	N31	1.52	increased
Q42	N31	1.54	increased
Q42	N97	0.52	increased
N19	Y100A	-0.35	decreased