

**Table S2. Essential node pairs detected in four Fel d 1 simulated systems.** Nodes that appear more than once are grouped by color. Interactions detected between pairs by PDBsum for the crystallographic structure are in parentheses.

	<b>Interface (Chain A - Chain B)</b>	<b>Chain A</b>	<b>Chain B</b>
Without Ca <sup>2+</sup>	Lys29-Asp82 (1HB, NBC) <b>Leu132</b> - <b>Leu94</b>	Cys44-Cys118 (DS) Ile64-Val102	Leu41-Tyr119 (NBC) <b>Phe85</b> -Met134 (NBC)
	Leu31- <b>Leu94</b> Asn91- <b>Leu129</b> (NBC) <b>Leu132</b> - <b>Phe85</b> (NBC)	<b>Cys3</b> -Ala74 Val10-Phe84	<b>Val6</b> -Tyr81 <b>Asn37</b> - <b>Arg127</b>
Minimal Glycosylation	<b>Phe85</b> -Asp130 (NBC) Val128- <b>Leu94</b>	<b>Val6</b> - <b>Phe80</b> Ile40-Asn122 (NBC)	<b>Val6</b> - <b>Phe80</b> <b>Asn37</b> - <b>Arg127</b>
	Ser139-Thr76 (NBC)		
	<b>Phe85</b> - <b>Leu132</b> (NBC) Asn89- <b>Leu129</b> (NBC) Thr135- <b>Phe85</b> (NBC)	Lys7-Phe80 <b>Asn37</b> - <b>Arg127</b> (2HB)	<b>Cys3</b> -Tyr65 <b>Asn37</b> -Val128

HB: hydrogen bond(s), NBC: non-bonded contacts, DS: disulfide bridge.

Note: There is a pair in the simulation with Ca<sup>2+</sup> (Leu129B-Arg127B) that connects the interface pair (Asn91-Leu129) to the 'hinge' pair (Arg127-Asn37).