

Figure 1  
Entry of anthrax toxin into cells.

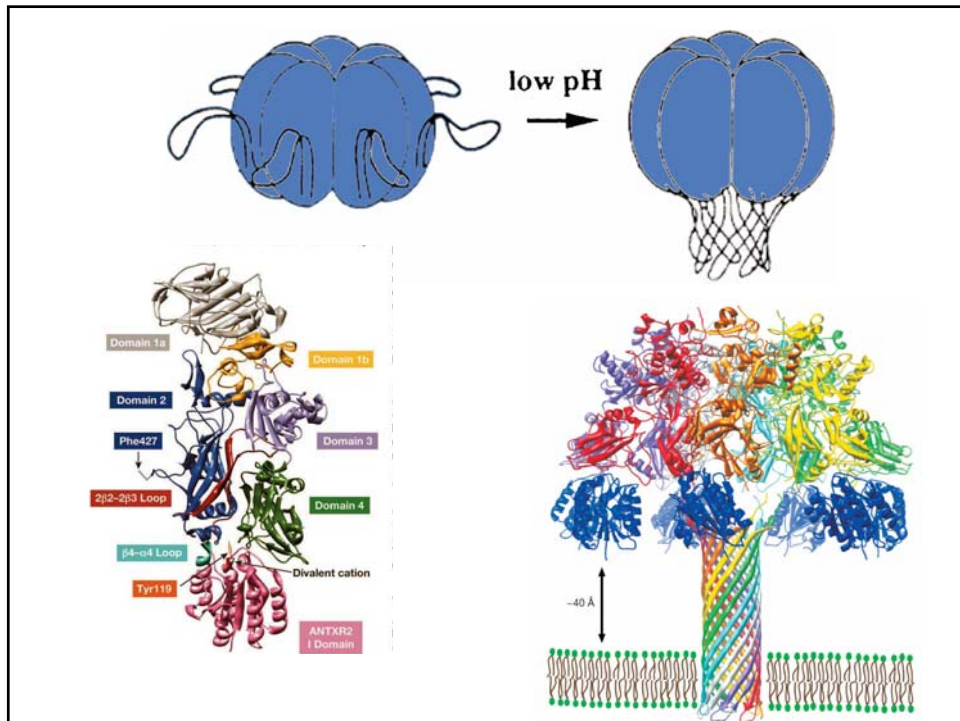
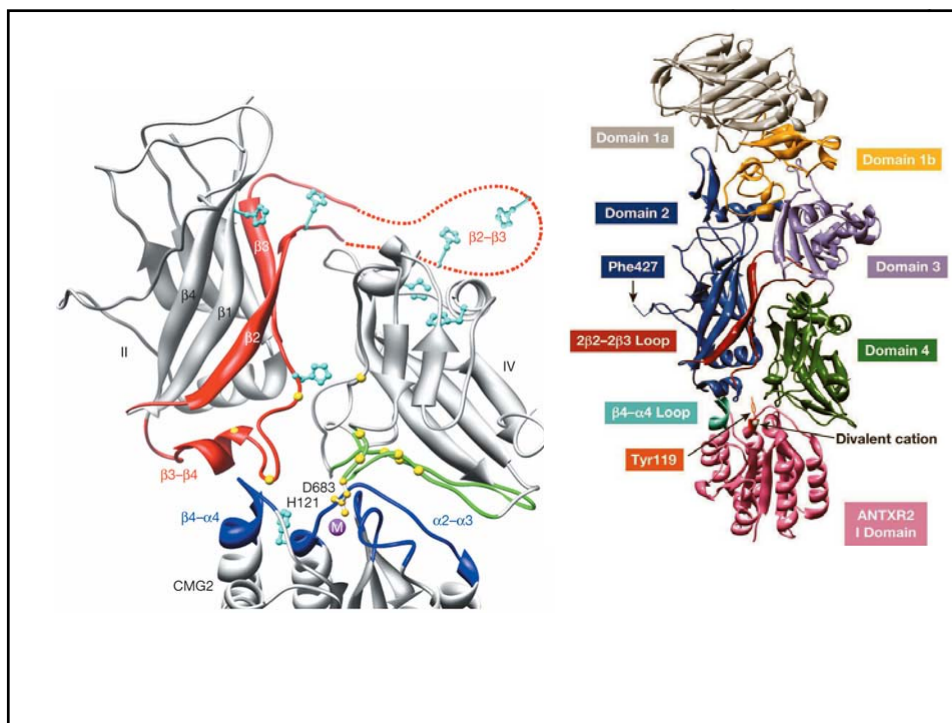
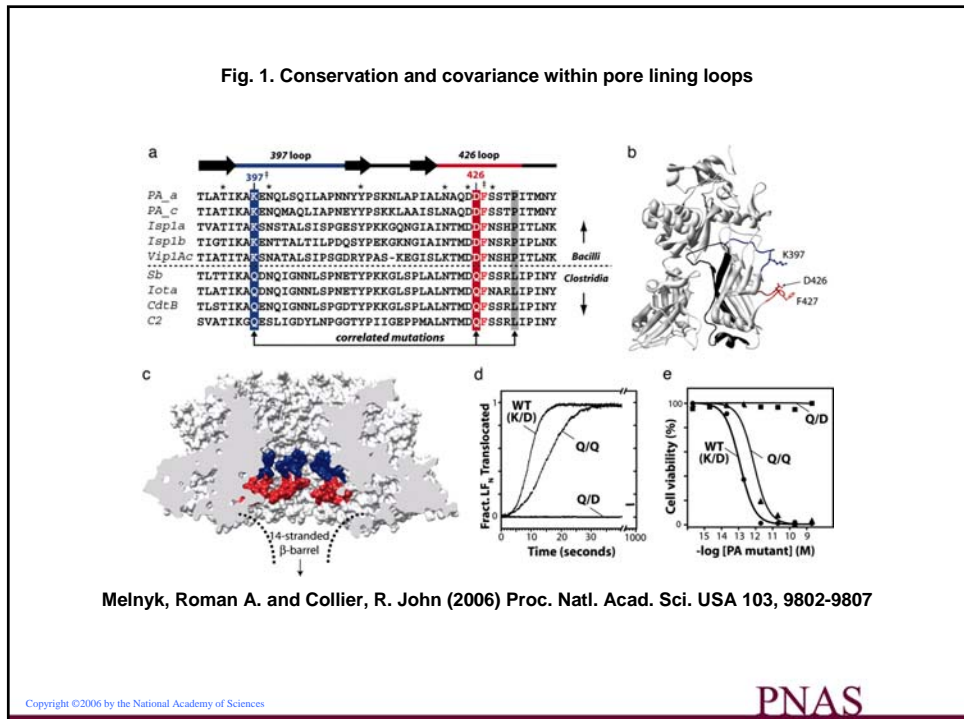
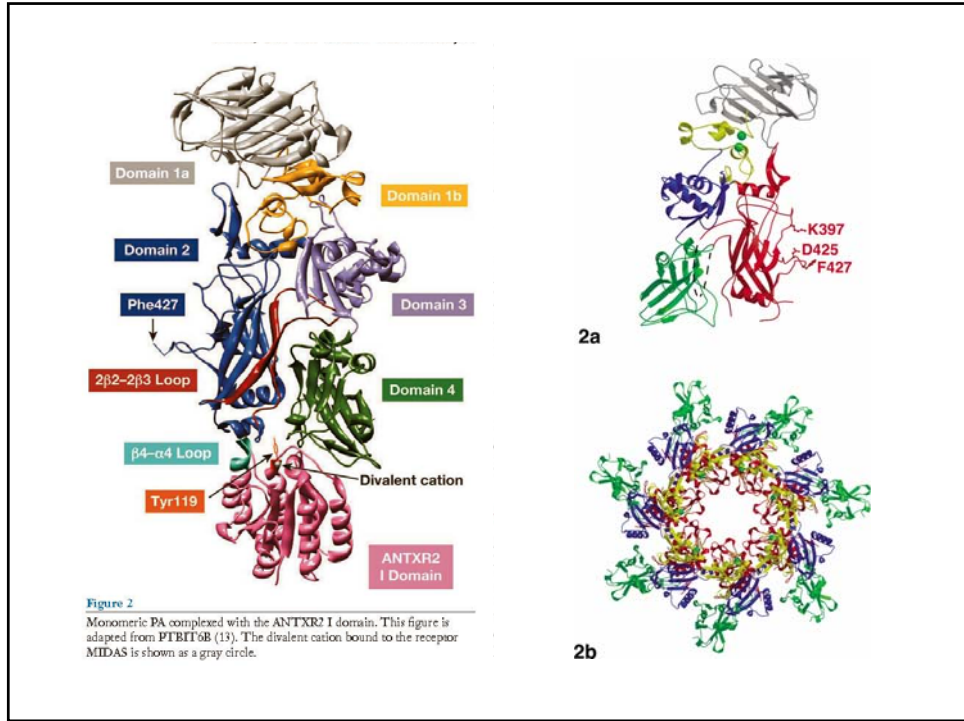


Table 1 **Data collection and refinement statistics**

Parameter	Value	
Space group	$P2_12_12_1$	
Unit cell (Å)	$a = 88.2, b = 94.1, c = 135.6$	
Resolution (Å)	30–2.5	
Wavelength (Å)	0.892	
$R_{\text{merge}}$ (%)	17.6 (99.1)	
$I/\sigma$	11.5 (2.4)	
$\sigma$ -cutoff	None	
Average redundancy	5.3 (5.2)	
Completeness (%)	99.9	
Mosaicity	0.4	
$R_{\text{work}}$ (last shell)	20.7 (27.5)	
$R_{\text{free}}$ (last shell)	26.6 (37.2)	
$\sigma$ -cutoff	None	
$B$ factors (Å <sup>2</sup> )*	32.9, 21.4, 23.3	
r.m.s.d. bond lengths (Å)	0.17	
r.m.s.d. bond angles (°)	1.65	
Ramachandran plot (residues, %)		
Most favoured	655	86.3%
Additionally allowed	101	13.3%
Generously allowed	3	0.4%
Disallowed	0	0%

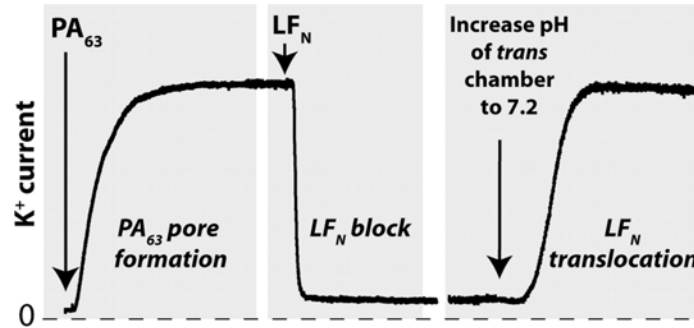
Values in parentheses refer to the highest resolution shell (2.59–2.50 Å).  
 \*The three values are for Wilson, main chain and side chain, respectively.





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Fig. 2. Typical record of a planar bilayer experiment showing changes in K<sup>+</sup> current in response to PA<sub>63</sub> pore formation, LF<sub>N</sub>-induced block, and pH-induced LF<sub>N</sub> translocation at a membrane potential of +10 mV (cis-positive)



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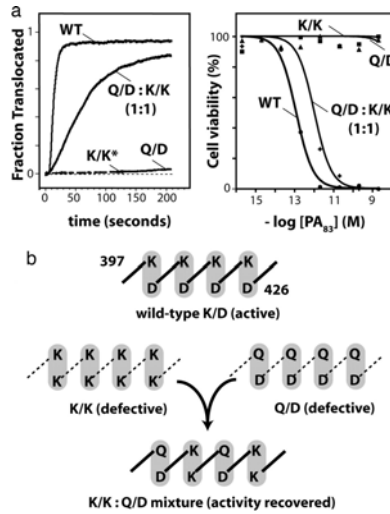
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Table 1. Pore formation, LF<sub>N</sub> block, and translocation across planar lipid bilayers and into cells for a panel of 397/426 mutant constructs

PA 397/426	Pore formation	LF <sub>N</sub> block, %	Translocation $\tau_{1/2}$ sec	Toxicity EC <sub>50</sub> , fold decrease
K/D	+	95	13	—
Q/Q	+	95	16	6.0
Q/D	+	98	>1,000	>10,000
Q/E	+	98	>1,000	>10,000
K/K	+	—	—	>10,000
Q/K	+	35	48	85
K/N	+	30	27	2.7
Q/N	+	90	38	17
K/E	+	93	12	3.1
K/Q	+	57	17	3.4
N/N	+	—	—	>10,000
E/E	+	—	—	>10,000

Positive (+) pore formation was determined by the ability of a particular mutant to form both SDS-resistant heptamers on SDS/PAGE and K<sup>+</sup>-conducting channels in planar lipid bilayers. The degree of LF<sub>N</sub> block was quantitated after perfusing the 1-ml cis chamber twice with 3 ml of pH 5.5 buffer. Translocation across planar lipid bilayers was initiated by increasing the pH of the trans compartment to 7–7.2 with a fixed amount of KOH with a holding potential,  $\Delta\psi = 10$  mV. The fold decrease in toxicity to cells was calculated by taking the ratio of the mutant EC<sub>50</sub> to the WT EC<sub>50</sub> ( $1.3 \times 10^{-13}$  M). Mutants that did not result in an decreases in cell viability within the concentrations used for these assays were deemed as >10,000-fold defective.

Fig. 3. Complementation indicates an intersubunit interaction model

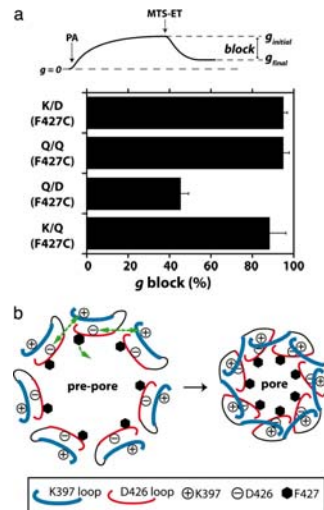


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Fig. 4. The 397-426 interaction determines prominence of F427 within lumen



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