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SUPPLEMENTARY INFORMATION

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Tc toxin activation requires unfolding and refolding of a β-propeller

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Supplementary Table 1. Cryo-EM data collection, refinement and validation statistics

	#1 ABC_{wt} (EMDB-0149) (PDB 6H6E)	#2 ABC_{D651A} (EMDB-0150) (PDB 6H6F)
Data collection and processing		
Magnification	X 122,870	X 122,270
Voltage (kV)	300	300
Electron exposure (e–/Å^2)	20	15.7
Defocus range (μm)		
Pixel size (Å)	1.14	1.10
Symmetry imposed	C1	C1
Initial particle images (no.)	205,336	137,733
Final particle images (no.)	89,148	132,033
Map resolution (Å)	3.95	3.72
FSC threshold	0.143	0.143
Map resolution range (Å)	3.2-10	3.2-10
Refinement		
Initial model used (PDB code)	1VW1, 4O9X	6H6E
Model resolution (Å)	3.95	3.72
FSC threshold		
Model resolution range (Å)	3.2-10	3.2-10
Map sharpening *B* factor (Å^2)	-68.03	-49.43
Model composition		
Non-hydrogen atoms	112,922	114,303
Protein residues	14,231	14,388
Ligands		
B factors (Å^2)	107.7	111.1
Protein		
R.m.s. deviations	0.0207	0.0202
Bond lengths (Å)	1.68	1.64
Bond angles (°)		
Validation		
MolProbity score	0.89	0.78
Clashscore	1.32	0.95
EMRinger Score	1.83	2.09
Rosetta FSCwork/FSCFree	0.5802/0.5434	0.5781/0.5472
Poor rotamers (%)	0.01	0
Ramachandran plot		
Favored (%)	97.86	98.13
Allowed (%)	99.58	99.67
Disallowed (%)	0.26	0.22

Supplementary Table 2. **Data collection and refinement statistics (molecular replacement)**

	empty TcdB2-TccC3
Data collection	
Space group	$P3_221$
Cell dimensions	
a, *b*, *c* (Å)	231.33, 231.33, 141.97
α, β, γ (°)	90, 90, 120
Resolution (Å)	48.64 - 3.004 (3.111 - 3.004)*
R_{merge}	0.5751 (5.172)
$I / \sigma I$	7.34 (0.68)
Completeness (%)	99.88 (99.80)
Redundancy	20.64 (20,79)
Refinement	
Resolution (Å)	48.64 - 3.004 (3.111 - 3.004)
No. reflections	87102 (8634)
R_{work} / R_{free}	21.56 (37.28)/ 25.31 (39.09)
No. atoms	17193
Protein	17058
Ligand/ion	0
Water	135
B-factors	
Protein	80.22
Ligand/ion	0
Water	56.64
R.m.s. deviations	
Bond lengths (Å)	0.003
Bond angles (°)	0.58

*Values in parentheses are for highest-resolution shell.