Supporting information

Pruitt, *et. al.*

Figure Legends

References

Figure S1

Figure S2

Figure S3

Figure S4

Figure S1

The TcdA (*green*) and VcRTx (*blue*) CPDs are shown as overlayed ribbon diagrams with InsP6 shown as sticks. Lysine residues 577, 766, 777, and 794 from TcdA CPD are shown as *orange* sticks. Secondary structure elements that are present in the TcdA CPD but not the VcRTx CPD are labeled.

Figure S2

Comparison of the TcdA and VcRTx CPD structures and sequences. *A-B,* The structures of the TcdA (*A*) and VcRTx (*B*) CPDs are shown in the same orientation with the secondary structural elements annotated and color coded (α-helices in *green*; β-strands in *blue*). We have labeled the secondary structural elements to maintain consistency with the VcRTx CPD and caspase-7 literature. *C,* The TcdA and VcRTx CPD sequences were aligned based on their structures (1) and displayed in ESPript (2). Strictly conserved residues are shown in *white* letters with a *red* background. Residues that are similar are boxed in *red* letters with *white* backgrounds. The secondary structural elements are marked above and below the sequences and the numbering corresponds to that of TcdA.

Figure S3

Effect of InsP6 on the structural stability to the TcdA CPD. TcdA CPD (at 1 mg/mL in 50 mM NaCl, 20 mM Tris, pH 8.0) was incubated with chymotrypsin for 1 hour at room temperature. The presence of 1 mM InsP6 provides significant protection from proteolysis. Similar results were obtained with trypsin (data not shown).

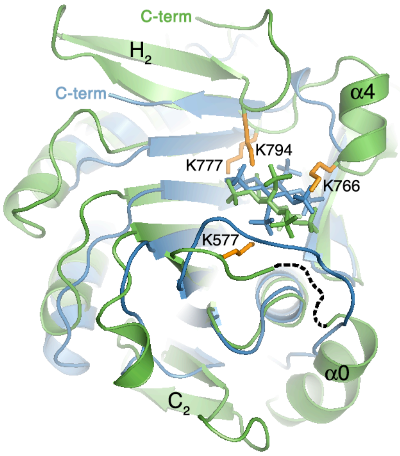
Figure S4

Conserved residues of the CPD. *A,* The TcdA CPD sequence (YP001087137) was aligned to sequences from four LCTs (TcdB (CAC19891), TcsL (CAA57959), TpeL (ACF49258), TcnA (CAA88565)) and five diverse homologs found in gram-negative bacteria (VcRTx (ZP01975348), VsRTx (ZP00989505), Plu3217 (NP930444), PmHI4320 (YP002151764), AhRTx (YP855898)) using ClustalW (3). There are 14 strictly conserved residues shown in *white* letters with a *red* background.

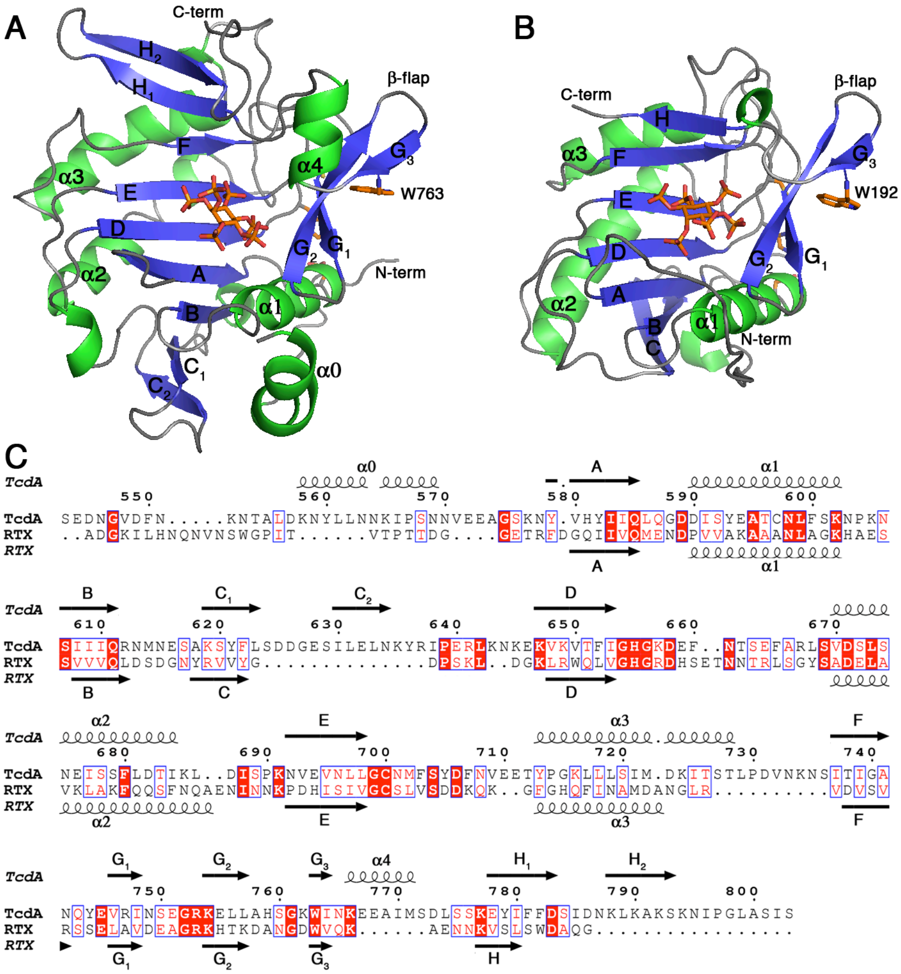
References

1. Holm, L., and Park, J. (2000) *Bioinformatics* **16**, 566-567
2. Gouet, P., Courcelle, E., Stuart, D. I., and Metoz, F. (1999) *Bioinformatics* **15**, 305-308
3. Thompson, J. D., Higgins, D. G., and Gibson, T. J. (1994) *Nucleic Acids Res* **22**, 4673-4680

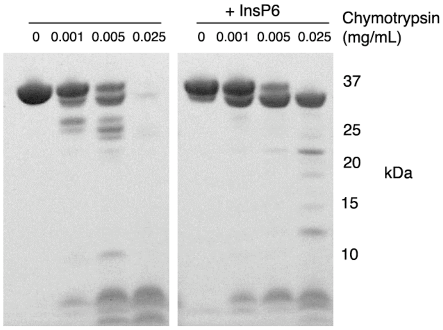
Supplemental Figure 1:



Supplemental Figure 2:



Supplemental Figure 3:



Supplemental Figure 4: