BIOLOGICAL CRYSTALLOGRAPHY

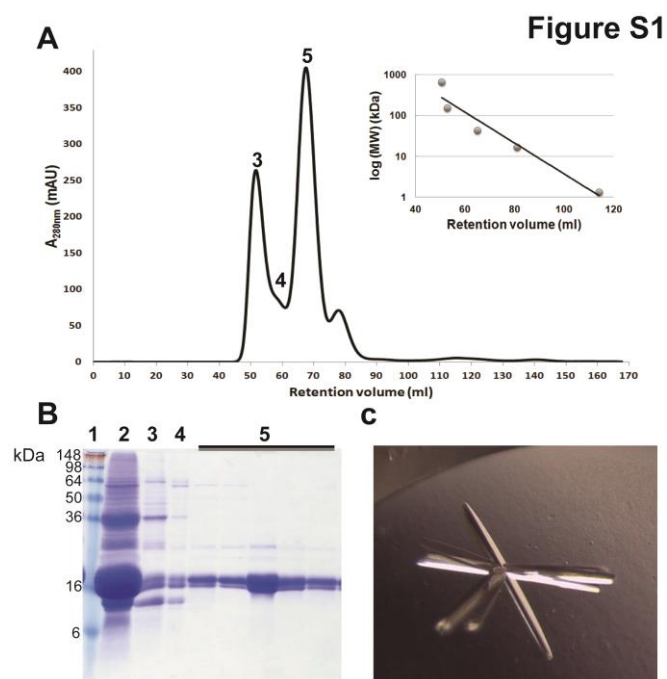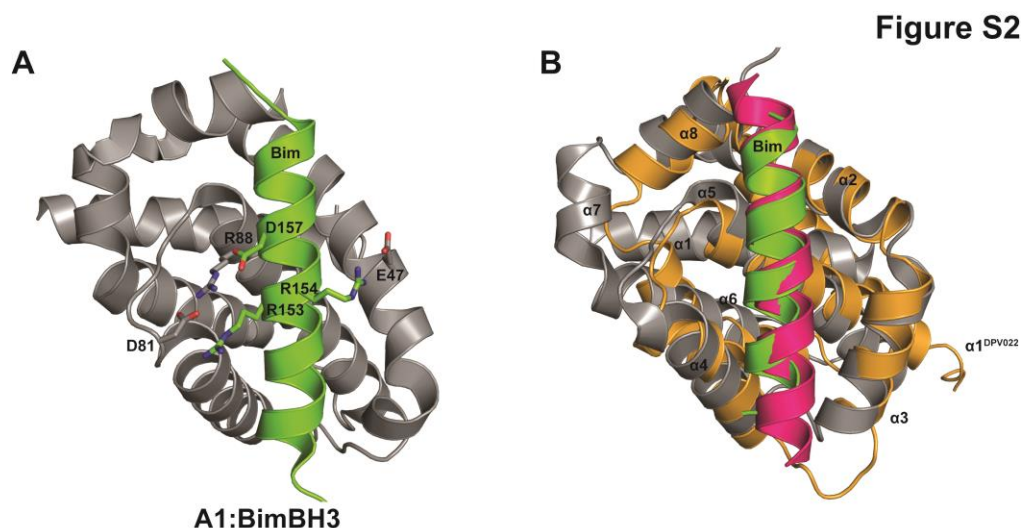Acta Cryst

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Supporting information for article:

Structural basis of *Deerpox virus*-mediated inhibition of apoptosis
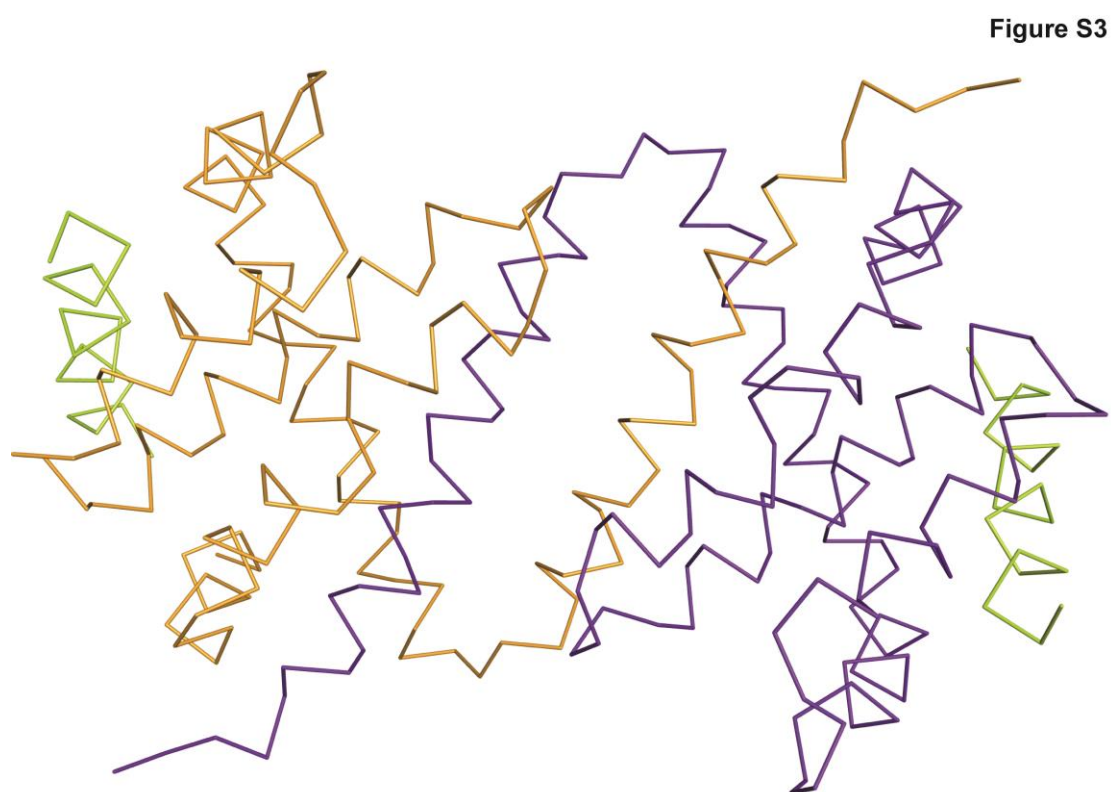
Denis R. Burton, Sofia Caria, Bevan Marshall, Michele Barry and Marc Kvansakul
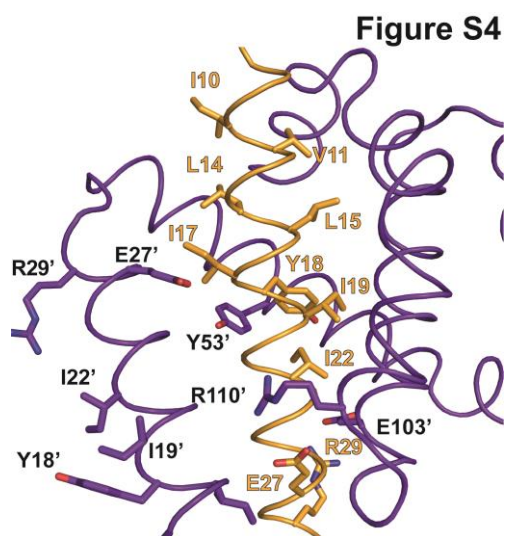
Figure S1   Purification and crystallization of DPV022. **A)** Gel Filtration trace of DPV022.
Calibration of the Superdex 75 16/60 column is shown in the box. Molecular weight
standards used were bovine thyroglobulin (670kDa), bovine γ-globulin (158kDa), chicken
ovalbumin (44kDa), horse myoglobin (17kDa), vitamin B12 (1.35kDa). The labels are
consistent with the following gel **B)** SDS-PAGE analysis of DPV022. Lanes are 1) Marker, 2)
the crude sample, 3) the void of the column, 4) the first peak and 5) fractions from the second
peak, the peak of interest. **C)** Crystals of DPV022ΔC24 in complex with Bim BH3.
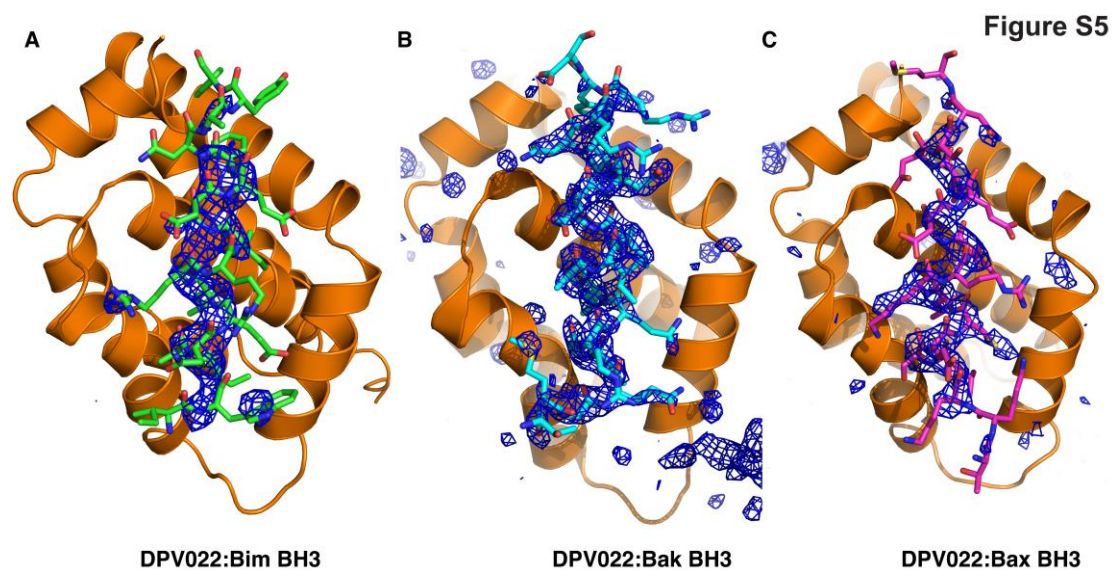
Figure S2 DPV022 is a hybrid of the cellular Bcl-2 proteins A1/Bfl1 and Mcl-1. **A)** A1/Bfl1 binds the BimBH3 domain peptide in a manner where two out of three salt-bridges are in near identical configurations to DPV022 **B)** Superimposition of DPV022 (gold) and Mcl-1 (grey) bound to Bim BH3 reveals a similar topology in the binding grove (α2-5). Matched α-helices between Mcl-1 and DPV022 are labeled only once, with the diverging α1 helices marked individually.
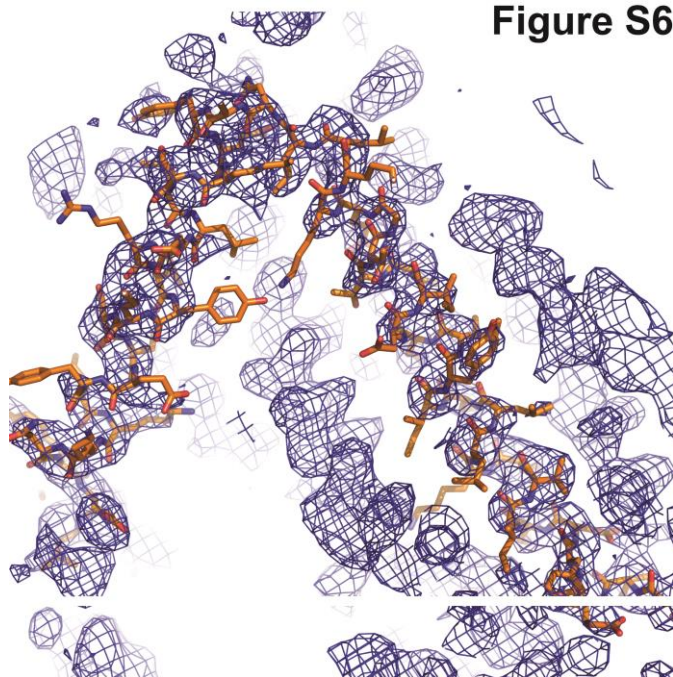

Figure S3 Cα trace of DPV022 in complex with Bim BH3. DPV022 is shown in gold and purple, Bim BH3 peptides are shown in lime green.
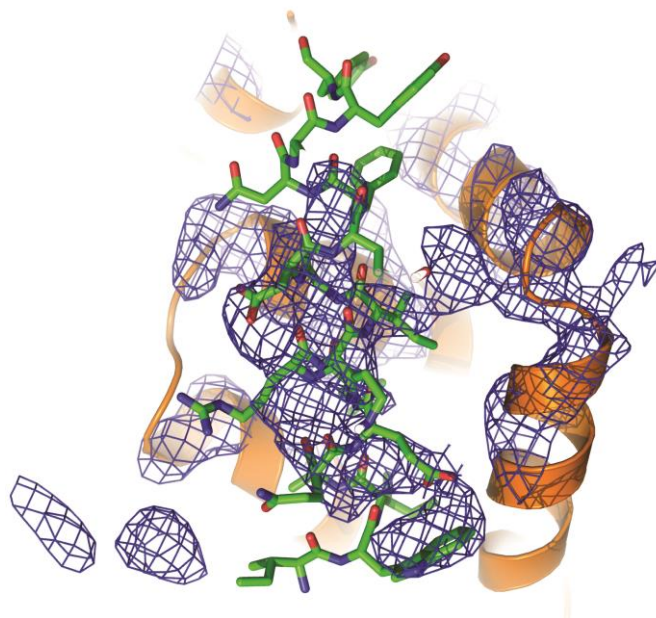
Figure S4 Dimer interface of DPV022. Individual DPV022 protein chains are coloured in gold and purple. Residues that are part of the interface are shown as sticks.

Figure S5 Unbiased Fo-Fc difference map of DPV022:BH3 domain complexes. Maps are contoured at 3σ. A) The model shown is the final refined model of DPV022:Bim BH3. B) The model shown is the final refined model of DPV022:Bak BH3. C) The model shown is the final refined model of DPV022:Bax BH3.

Figure S6

Figure S6 SIRAS phased map after solvent flattening of DPV022:Bim BH3 complex. Map is contoured at 1σ. The view shows the α1 and α2 helices of the final refined model of DPV022:Bim BH3.

Figure S7

Figure S7 SIRAS phased map after solvent flattening of DPV022:Bim BH3 complex. Map is contoured at 1σ. The view shows the Bim BH3 domain of the final refined model of DPV022:Bim BH3.