SUPPLAMENTARY TABLE & FIGURE LEGENDS

Supplementary Table 1. Metal binding affinities of $_{ba}$MntA as determined by isothermal titration calorimetry (ITC). Also shown are the standard errors of the fit to the data.

Supplementary Figure 1. Overexpression and purification of $_{ba}$MntA. (A) The soluble fraction of cells transformed with plasmid p-*mntA* was isolated before or after addition of IPTG, as indicated. 50 μg total protein were separated by SDS-PAGE and visualized by coomassie staining. A prominent band of ~35 kDa (corresponding to the expected molecular weight of baMntA) is observed only in of extracts prepared from induced cells. (B) The soluble fraction of cells overexpressing $_{ba}$MntA was loaded onto an ion-exchange column and the column-UNBOUND fraction was collected and concentrated (not shown). This fraction was then injected onto a 120 mL preparative gel filtration column (HiLoad 16/600 Superdex 200). Shown is a coomassie staining of SDS-PAGE of the gel filtration elution fractions. The boxed fractions were pooled, and re-concentrated to 25-30 mg/mL and the 3 μg of the final product is shown in the leftmost lane. (C) 5 μL of purified $_{ba}$MntA at 30 mg/mL were injected onto a 24 mL 10/300 Superdex 200 gel filtration column. (D) 150 μg each from vitamin B12, carbonic anhydrase, ovalbumin, and conalbumin were injected onto the same column as in C and their elution volumes were used to generate a standard curve (see methods). The molecular weights of the markers (in kDa) are given in parenthesis, the $_{ba}$MntA data point is shown in red. Also shown is the goodness of the fit, R^2.

Supplementary Figure 2. Quality assessment of the baMntA model. (A) Ramachandran plots for the template (MtsA, PDB ID 3HH8) and the model, as indicated. Red, brown, yellow, and off-white areas represent most to least favorable phi-psi combinations, respectively. Each blue dot is one residue. Almost all of the residues of the model are within the highly favorable areas with a very similar distribution to that of the template. (B) ProSA results: The Z-score indicates overall model quality. Its value is displayed in a plot that contains the Z -scores of all experimentally determined protein chains currently in the PDB. In this plot, groups of structures from different sources are distinguished by different colors (X-ray in pale blue, NMR in blue). The score of the structure of interest (template and model) is highlighted in black. The model was assigned a slightly better score than the template (Z-scores of -8.99 and -8.38, respectively), and both reside in the allowed score area. (C) ConSurf analysis of the distribution of conserved and variable residues in the modeled structure of baMntA. For comparison the same analysis was performed on the homologous PsaA (PDB I.D 1PSZ) that was not used as a template for modeling of baMntA. The proteins' backbone is shown in a cartoon representation, colored according to the ConSurf scale. The distribution of conserved and variable residues is very similar in PsaA and baMntA with a highly conserved core and a variable surface.

Supplementary Figure 3. Amino acid sequence alignment of *Bacillus anthracis* MntA, Streptococcus *pneumonia* PsaA, *Treponema pallidum* TroA, *Escherichia coli* ZnuA, *Synechocystis sp.* MntC, and *Streptococcus pyogenes* MtsA. Metal coordinating residues are highlighted in yellow and green.