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Supporting information for article:

Cap-domain closure enables diverse substrate recognition by a C2-type haloacid dehalogenase-like sugar phosphatase PfHAD1

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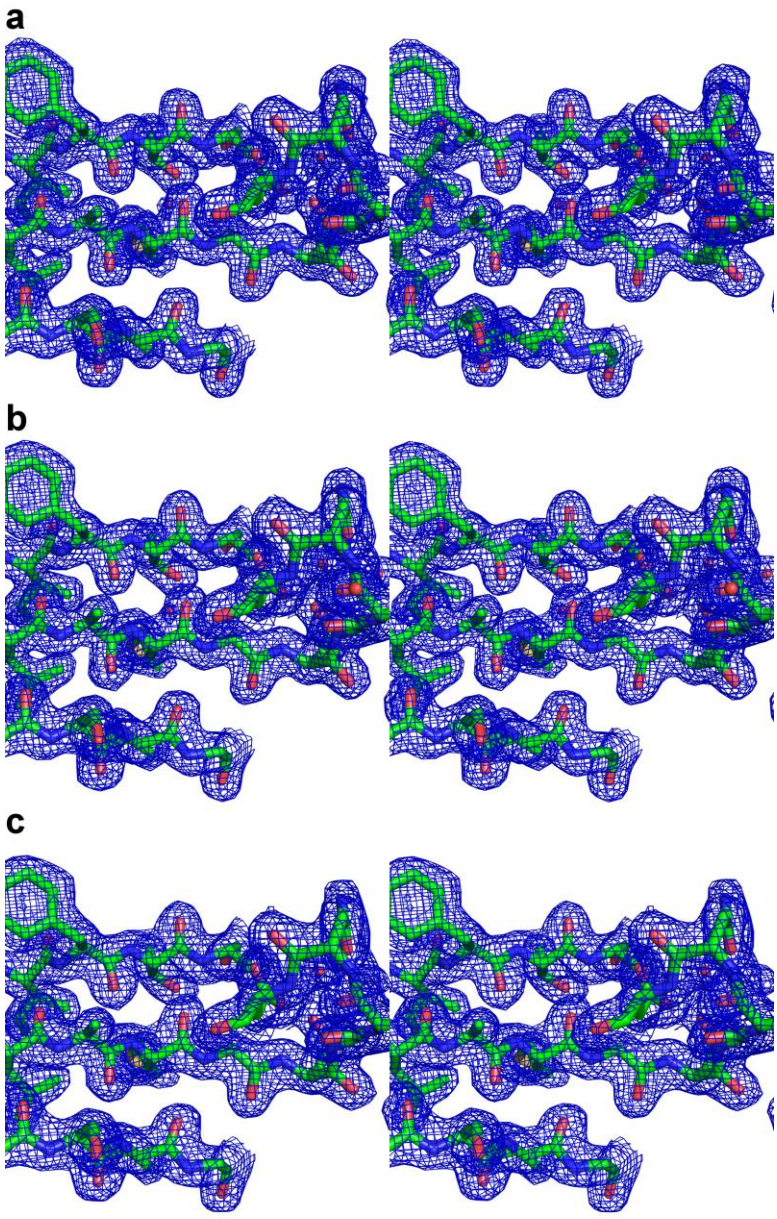

Figure S1 Stereo image of the electron density maps for representative regions of the substrate-bound PfHAD1-D27A structures. The 2fo-fc electron density map contoured at 1.0 σ is colored blue for (*a*) man6p, (*b*) glu6p, and (*c*) gly3p.

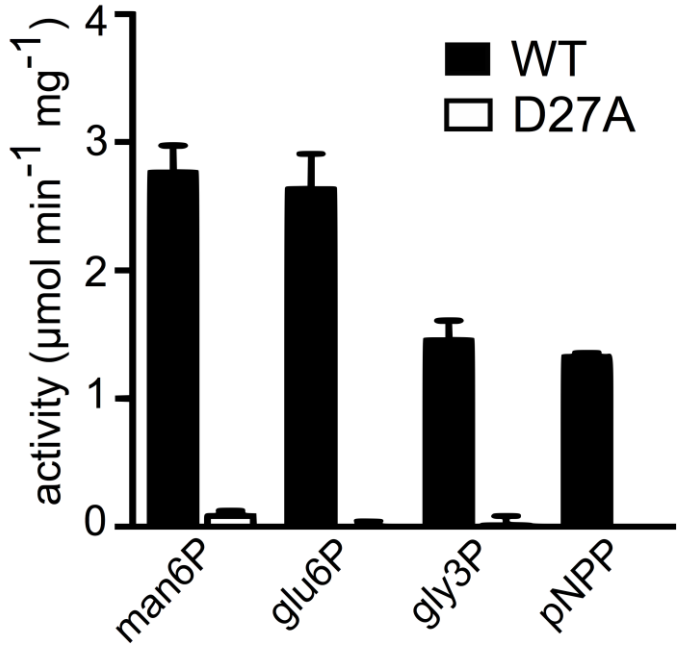

Figure S2 PfHAD1-D27A is inactive. Mutation of the Asp-27 nucleophile to an alanine residue renders recombinant PfHAD1 enzyme inactive against all substrates tested: mannose-6-phosphate (man6P), glucose-6-phosphate (glu6P), glyceraldehyde 3-phosphate (gly3P), and *para*-nitrophenylphosphate (*p*NPP).

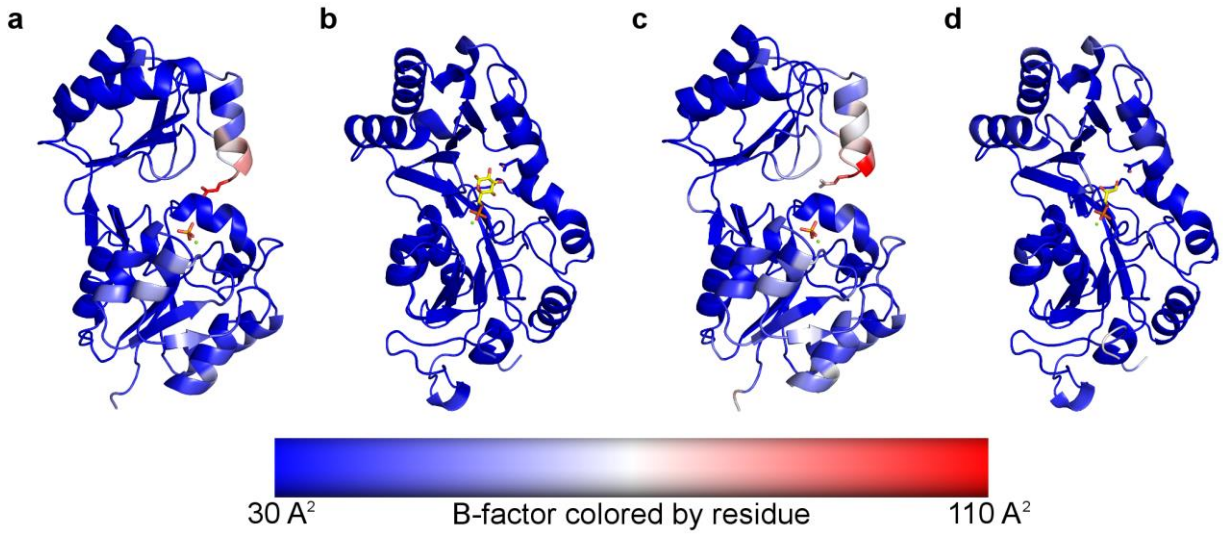

Figure S3 The cap domain contains a flexible substrate recognition element that is ordered upon substrate binding and cap closure. (*a*) glu6p open conformation. (*b*) glu6p closed conformation. (*c*) gly3p open conformation. (*d*) gly3p closed conformation. In the open conformations (*a*,*c*), the region of the cap domain that is important for substrate recognition has high B-factor values, indicating disorder and flexibility in this region. In the closed conformations(*b*,*d*), this region becomes ordered, as reflected by the low B-factor values.

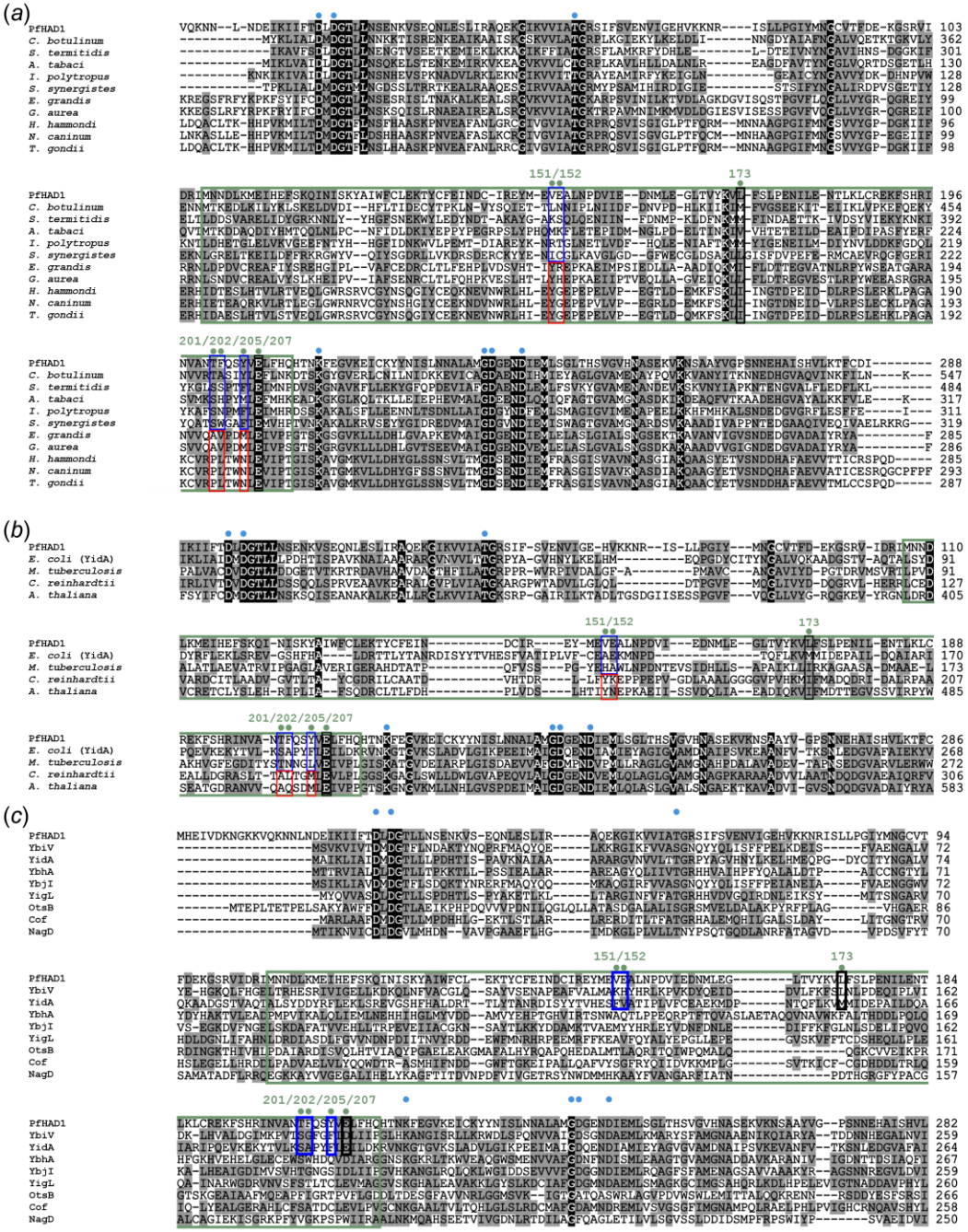

Figure S4 Sequence alignment of PfHAD1 homologs from other organisms. Sequence alignments are shown for (*a*) an unbiased sampling of the ten closest PfHAD1 homologs, (*b*) PfHAD1 homolog sequences from selected model organisms, (*c*) sequences of PfHAD1 homologs from *E. coli* with known substrate preferences. The cap domain is boxed in green, and substrate-binding core and cap residues in PfHAD1 are annotated with blue and green dots, respectively. The blue and red boxes denote two subdivisions of PfHAD1 homologs.