



**Supplementary Figure S8. Unique structural features of BOS.**

**a,b.** BOS loops (green) comprising residues 76-93 and 199-210 (green) adopt a different conformation from that of the corresponding loops in other HCT homologs. **c,d.** The active site tunnel of HCTs is typically straight, as shown here for *Sorghum bicolor* HCT (PDB ID: 4KE4, gold). **e,f.** By contrast, the tunnel in BOS (gray) is bent at about 15 degrees at its middle. Oxalyl-CoA (magenta) and L-DAPA (cyan) were docked into the active site (see text for details). The figure was generated using PyMol (Molecular Graphics System, version 2.4, Schrödinger, LLC).