Supplemental Information (Moore and Jia, 2010)

Supplemental Figure Legends

Supplemental Figure S1. Solvent-flattened experimentally phased map from Solve/Resolve to 3.0 Å resolution. Showing the initial traced model as a green C_{α} representation, the Selenium positions as pink crosses and the map, contoured at 3 σ , in purple. Displayed using Coot (41).

Supplemental Figure S2. Representative Sigmaa-weighted $2|F|_{obs}$ - $|F|_{calc}$ electron density map at 2.4 Å resolution, contoured at 1.0 σ in the vicinity of the cavity at juncture of the four domains. The polypeptide chain is depicted as a stick model, waters are drawn as red crosses. Map calculated within the CCP4 package (45) and displayed with Coot (41).

Supplemental Figure S3. Ramachandran Plot of the refined FlhA_C model. Calculated with Procheck (53) in CCP4 (45).

Supplemental Figure S4. Superposition of FlhA_C domains with Dali hits (46). Overlaid structural fragments depicted as C-alpha traces of the similar polypeptide segments. Superpositions calculated using lsqkab in the CCP4 package (45). Drawn with Molscript/Raster3D (49,50). (A) Thioredoxin-like domain (blue) overlaid onto thioredoxin, pdb entry 2P0G (in magenta). Equivalences are (FlhA residues first) 397-404 = 5-12; 438-446 = 36-44; 453-464 = 48-59; 524-536 = 69-81. (B) Helical domain (green) overlaid onto ribonucleotide reductase pdb entry 2R1R (in magenta). Equivalences are (FlhA residues first): 543-552 = 101-110; 555-562 = 116-123; 567-574 = 128-135; 605-614 = 190-199. (C) C-terminal domain (gold) overlaid onto 3G5J (putative sulfurase, in magenta). Residue Equivalences are (FlhA residues first): 620-625 = 5-10; 632-637 = 16-21; 669-681 = 73-85; 685-691 = 88-94; 692-712 = 97-117.

Supplemental Figure S5. Ribbon diagram of the FlhA_C dimer observed in the crystal lattice. Colored as Figure 1 of the main text. View approximately looking down the crystallographic twofold axis. Drawn with Molscript/Raster3D (49,50). Residue Q437, which corresponds to the *Salmonella flhA* V404M mutation, a pseudorevertant of a nonmotile *ΔfliIΔfliH* null, is shown as a yellow stick model.