

cryocooled by plunging into liquid nitrogen. All data were collected at 100 K using a Rigaku R-AXIS IV image plate detector mounted on a rotating anode source. Data were integrated and scaled using the programs DENZO and SCALEPACK (*S3*). The crystals belonged to space group $P2_12_12_1$ and contained two molecules in the asymmetric unit.

Multiple Isomorphous replacement, model building and refinement

Isomorphous heavy atom derivatives were prepared by soaking crystals at room temperature in well solutions containing either 0.5 mM thimerosal ($C_9H_9HgO_2SNa$) or 0.5 mM mercury acetate ($Hg[C_2H_3O_2]_2$) for 1 hour, or 20 mM sodium tungstate (Na_2WO_4) for 3 hours. Data were collected and processed as above, and scaled against the native data set. Heavy atom sites were located by inspection of Patterson functions. Most crystallographic computing used programs from the CCP4 suite (*S4*). Phases from the thimerosal and mercury acetate derivatives were calculated using SOLVE (*S5*), and used to locate two tungstate clusters (each containing the same arrangement of twelve tungsten atoms) in a difference Fourier map (Figure S2). MIR phases from the three derivatives were calculated using SOLVE (figure of merit 0.75) and generated an easily interpretable electron density map after density modification by solvent flattening (42% solvent) using the program RESOLVE (*S6*). An initial model was built by RESOLVE (*S6*), and manually completed using the XFIT program in the XTALVIEW software package (*S7*). The model was refined using REFMAC5 (*S8*), using refinement parameters for the IP_6 ligand that were generated using the SKETCHER program in CCP4 (*S4*). It is possible that some of the solvent molecules currently assigned as water are other species, such as sodium ions, although this is not apparent from the electron density or inspection