

**Table S1. Crystallographic Data**

	Native	Thimerosal	Mercury Acetate	Sodium Tungstate
a (Å)	52.2	52.3	52.6	52.1
b (Å)	121.4	121.7	121.8	120.8
c (Å)	127.5	127.6	127.8	127.4
Resolution (Å)	20-1.7 (1.76-1.7)	20-2.7 (2.8-2.7)	20-2.7 (2.8-2.7)	20-2.6 (2.69-2.6)
# total reflections	388,243	228,747	54,141	120,441
# unique reflections	82,849	22,696	20,785	25,089
Completeness (%)	92.3 (62.5)	100 (100)	89.7 (87.9)	99.5 (99.8)
Mosaicity (°)	0.5	0.6	0.7	0.7
I/σ(I)	35.2 (5.0)	21.2 (9.3)	10.9 (4.6)	8.7 (2.9)
R <sub>merge</sub> <sup>a</sup>	3.9 (25.9)	13.4 (26.9)	9.2 (19.4)	11.2 (26.8)

Numbers in parenthesis are for the high-resolution bin

$$^a R_{\text{merge}} = 100 \times \frac{\sum |I - \langle I \rangle|}{\sum I}$$

**Table S2. Refinement statistics**

R <sub>cryst</sub> (%) <sup>a</sup>	17.4
R <sub>free</sub> (%) <sup>b</sup>	20.7
# Protein residues modeled	741
# Solvent molecules	670
RMSD bonds (Å)	0.015
RMSD angles (°)	1.554
φ, ψ Most favored (%)	92.7
φ, ψ Additional Allowed (%)	6.4
<B> Overall (Å <sup>2</sup> )	19.9
<B> Main Chain (Å <sup>2</sup> )	17.8
<B> Side Chains (Å <sup>2</sup> )	20.2
<B> Water (Å <sup>2</sup> )	28.0
<B> IP <sub>6</sub> (Å <sup>2</sup> )	14.6

$$^a R_{\text{cryst}} = 100 \times \frac{\sum ||F_{\text{obs}}| - k|F_{\text{calc}}||}{\sum |F_{\text{obs}}|}$$

<sup>b</sup>R<sub>free</sub> = The R<sub>factor</sub> against 5% of the data removed prior to refinement  
Stereochemistry was analyzed using PROCHECK (S17)