Table I. Crystallographic data and refinement statistics

	Native data set	Thiomersal derivative data set[g]
Space group	$P2_1$ (No. 4)	$P2_1$ (No. 4)
Cell axes *a*, *b*, *c and* β	31.9Å, 37.3Å, 56.4Å and 105.4°	31.8Å, 37.4Å, 56.5Å and 105.2°
Resolution range (outer shell)	50.0 (1.60-1.54 Å)	25.0 (1.7-1.66 Å)
No. of observed reflections	53616	90244
No. of unique reflections	18705	28522
R_{sym} overall(outer shell) [a]	4.0 %(18.8%)	4.1% (14.7%)
$I/\sigma(I)$ overall(outer shell)	14.8 (5.4)	16.2 (7.5)
Completeness overall(outer shell)	97.4% (90.1%)	95.9%(93.1%)
Phasing power (centric/acentric)[b]	0.90/1.14	
R_{Cullis} (centric/acentric)[c]	0.82/0.77	
Figure-of-merit (centric/acentric)[d]	0.16/0.27	
No. of refined atoms		
protein	1030	
water	119	
R-factor/free *R*-factor[e]	0.18/0.22	
R.m.s.d. bond lengths/bond angles[f]	0.011Å/1.2°	

[a] $R_{sym} = \sum_h \sum_i | I_i(h) - \langle I(h) \rangle | / \sum_h \sum_i I_i(h)$, where $I_i(h)$ and $\langle I(h) \rangle$ are the *i*th and mean measurement of the intensity of reflection *h*.

[b] Phasing power $= \sum F_H^{calc} / \sum | F_{PH}^{obs} - F_{PH}^{calc} |$, where F_H^{calc} is the calculated heavy atom amplitude and F_{PH}^{obs} and F_{PH}^{calc} are the observed and calculated heavy atom derivative structure factor amplitudes, respectively

[c] $R_{Cullis} = \sum | F_{PH}^{obs} \pm F_P^{obs} | - | F_H^{calc} | / \sum | F_{PH}^{obs} - F_P^{obs} |$, where F_{PH}^{obs} is the observed heavy atom derivative structure factor amplitude, F_P^{obs} is the observed native structure factor amplitude, and F_H^{calc} is the calculated heavy atom amplitude

[d] Figure-of-merit $= | \int_\alpha P(\alpha) \exp(i\alpha) d_\alpha / \int_\alpha P(\alpha) d_\alpha |$, with α ranging from 0 to 2π.

[e] $R = \sum | F_P^{obs} - F_P^{calc} | / \sum F_P^{obs}$, where F_P^{obs} and F_P^{calc} are the the observed and calculated structure factor amplitudes, respectively

[f] rmsd, root-mean-square-deviation from the parameter set for ideal stereochemistry (Engh and Huber, 1991)

[g] mercury-binding sites were at cysteine 228