Supplementary Table 1 Structure determination of PH1033.

	Native (condition I)	Hg-derivative		
Space group	$P3_121$		$P3_121$	
Unit-cell parameters (Å)	$a = b = 95.7$, $c = 44.2$		$a = b = 95.4$, $c = 42.1$	
		Peak	Inflection	Remote
Wavelength (Å)	1.0000	1.0079	1.0088	0.9900
Resolution range (Å)	40–2.2 (2.28–2.20)	40–2.9 (3.00–2.90)	40–2.9 (3.00–2.90)	40–2.9 (3.00–2.90)
No. of unique reflections	12147 (1172)	4816 (469)	4852 (460)	4860 (461)
Redundancy	6.3 (6.5)	6.0 (5.5)	5.8 (5.2)	5.7 (4.9)
Completeness (%)	99.9 (100)	97.6 (95.7)	96.9 (93.3)	96.8 (92.2)
R_{sym} [†] (%)	5.5 (36.1)	7.2 (34.7)	7.1 (35.7)	7.0 (38.0)
$\langle I/\sigma(I)\rangle$	12.3 (4.3)	11.9 (3.9)	11.5 (3.5)	13.4 (3.6)
Phasing				
Resolution (Å)			40–3.1	
Figure of merit (before solvent flattering)			0.50	
Refinement				
Resolution range (Å)	32.5–2.2			
R_{cryst}/R_{free} (%)	23.2/24.8			
r.m.s. deviation				
Bond lengths (Å)	0.007			
Bond angles (°)	1.3			

[†] $R_{sym} = \sum_{hkl} \sum_i |I_i(hkl) - \langle I(hkl)\rangle| / \sum_{hkl} \sum_i I_i(hkl)$, where $\langle I(hkl)\rangle$ is the mean intensity of multiple $I_i(hkl)$ observations of Bijvoet-equivalent indices. Values in parentheses are for the outermost shell.