Table 1. Data collection and MIR phasing statistics

	Native	PIP	PTN
Data collection			
Resolution (Å)	2.4(2.35,2.4)	3.0(3.11-3.0)	3.0(3.11-3.0)
Completeness[*](%)	99.4(100)	91.6(63.4)	95.7(80.2)
Multiplicity	18.6	6.5	5.6
$\langle I/\sigma(I)\rangle$ [*]	39.0(3.7)	15.4(2.2)	10.5(1.0)
R_{merge} [*]	0.11(0.57)	0.05(0.38)	0.13(0.58)
Wilson B ($Å^2$)	58.3	67.7	79.2
MIR phasing			
Resolution (Å)		50 – 4.0	50 – 4.0
Sites per molecule		3[†]	4
Total occupation		0.77	0.95
Phasing Power[‡‼]	1.4(1.7)[1.1]		1.1(1.3)[1.1]
R_{Cullis}[‡¶]	0.71(0.76)[0.93]		0.82(0.82)[0.92]

[*]Numbers in parentheses are values in the high resolution shell, where $R_{merge}=\Sigma(I_i-\langle I\rangle)/\Sigma I_i$ summed over all independent reflections.

[†]Each site was split into pairs. [‡]The three numbers represent summation over: centric(acentric)[acentric anomalous] reflections.

[‼]Root mean square (rms) f_h/residual=$\sqrt{(\Sigma(F_{deri}-F_{PH})^2)}$, where f_h and F_{PH} are the calculated heavy-atom and derivative structure factors, respectively.

[¶]$R_{cullis}=\Sigma||f_h|-(|F_{deri}|-|F_{nati}|)|/\Sigma||F_{deri}|-|F_{nati}||$, where F_{deri} and F_{nati} are the observed derivative and native structure factors, respectively.