

**Table 1. Data collection, structure solution, and refinement**

	Co, peak data	Pt, peak data
Data collection		
Wavelength, Å	1.6059	1.0723
Space group	P2 <sub>1</sub>	P2 <sub>1</sub>
Unit cell dimension		
a, Å	90.1	90.3
b, Å	67.3	66.8
c, Å	147.7	148.4
β, °	96.8	97.2
Resolution limit*	50–2.5 (2.6–2.5)	50–3.2 (3.3–3.2)
<i>I</i> /σ( <i>I</i> )	16.5 (2.2)	12 (5.3)
<i>R</i> <sub>merge</sub> , % <sup>†</sup>	7.0 (49.1)	7.7 (23.7)
Completeness, %	91.1 (54.7)	98.4 (99.8)
Redundancy	3.5	3.6
Structure solution		
No. of sites		26
Figure of merit <sup>‡</sup>		
Before DM		0.37
After DM		0.56
<i>R</i> <sub>Cullis</sub> (centric/acentric/anomalous, %) <sup>§</sup>		0.58/0.46/0.89
Phasing power (centric/acentric) <sup>¶</sup>		0.98/1.19
Refinement		
Resolution range, Å	50–2.6	
<i>R</i> factor <sup>  </sup>	21.3	
<i>R</i> <sub>free</sub> <sup>**</sup>	24.9	
No. of reflections ( <i>F</i> > 0)	50,885	
Model		
No. of aminoacids	1,290	
No. of water molecules	459	
No. of Cbl	2	
No. of sugars	4	
Residues in generously allowed regions	29	
Residues in disallowed regions	0	
Stereochemical ideality		
Bonds, Å	0.01	
Angles, °	1.874	
Dihedral angles, °	22.167	
Improper angles, °	1.127	

\*Values in parentheses refer to the highest-resolution shell.

<sup>†</sup> $R_{\text{merge}}(I) = \frac{\sum I_i - \langle I \rangle \sum I_i}{\sum I_i}$ , where  $I_i$  is the intensity of the *i*th observation,  $\langle I \rangle$  is the mean intensity of the reflection, and the summation extends over all data.

<sup>‡</sup>Figure of merit is defined as  $\cos(\sigma(\Delta\phi))$ .

<sup>§</sup> $R_{\text{Cullis}}(\text{iso})$  = ratio of lack of closure to isomorphous difference.  $R_{\text{Cullis}}(\text{ano})$  = ratio of lack of closure to anomalous difference.

<sup>¶</sup>Phasing power is the rms ( $|F_{\text{H}}|/E$ ), where  $F_{\text{H}}$  is the calculated structure factor amplitude due to scattering by the heavy atom, and  $E$  is the residual lack of closure error.

<sup>||</sup> $R$  factor =  $\frac{\sum ||F_{\text{O}}| - |F_{\text{C}}||}{\sum |F_{\text{O}}|}$ , where  $F_{\text{O}}$  is observed structure factor amplitude,  $|F_{\text{C}}|$  is calculated structure factor amplitude, and the summation extends over all data.

<sup>\*\*</sup> $R_{\text{free}}$  is the *R* factor obtained for a test set of reflections, consisting of a randomly selected 3% subset (1,529 reflections) of the diffraction data, not used during refinement.