Table 1 Data collection and processing

Values for the outer shell are given in parentheses.

Diffraction source	Rotating anode
Wavelength (Å)	1.5418
Temperature (K)	100
Detector	CCD Saturn
Crystal-detector distance (mm)	45 mm
Rotation range per image (°)	1
Total rotation range (°)	56
Exposure time per image (s)	5
Space group	$P4_32_12$
$a = b$, c (Å)	76.979, 38.089
Mosaicity (°)	0.8
Resolution range (Å)	50.0 – 1.80 (1.83 – 1.80)
Total No. of reflections	31609
No. of unique reflections	10554
Completeness (%)	94.7 (85.1)
Redundancy	3.0 (1.8)
$\langle I/\sigma(I) \rangle$	32.0 (2.7)
R_{merge}	4.8 (37.1)
Overall B-factor from Wilson plot (Å^2)	38.2

Table 2 Structure solution and refinement

Values for the outer shell are given in parentheses.

Resolution range (Å)	25.55-1.80
Completeness (%)	94.4
σ cutoff	0
No. of reflections, working set	9988
No. of reflections, test set	499
Final R_{cryst}	18.1
Final R_{free}	24.4
Cruickshank DPI	0.175
No. of non-H atoms	1235
Protein	1087
Ion	1
Ligand	39
R.m.s. deviations	
Bonds (Å)	0.017
Angles (°)	1.67
Average *B*-factors (Å^2)	
All atoms	31.2
Au+ Ion	44.9*
Ramachandran plot	
Most favoured (%)	95.4
Allowed (%)	4.6

*occupancy of Au+ ion 0.6, the occupancy factor has been evaluated on the basis of the observation of the residual positive and negative peaks in the Fo-Fc electron density maps