

Table S1. Data collection and refinement statistics (SAD)

	Se Derivative ns2 ¹⁻¹⁹⁹
Data collection	
Wave length	0.97917
Space group	P4 ₁ 22
Cell dimensions	
<i>a, b, c</i> (Å)	101.0, 101.0, 165.8
α, β, γ (°)	90.0, 90.0, 90.0
Resolution (Å)	50-3.05 (3.16-3.05) *
Unique reflections	31292
R_{merge} (%)	9.0 (73.5)
$l/\sigma l$	20.6 (3.8)
Completeness (%)	98.9 (96.3)
Redundancy	8.5 (8.6)
Structure determination	
Figure of merit (by SAD)	0.45
Figure of merit (after density modification)	0.81
Refinement	
Resolution (Å)	48.49-3.05
No. reflections	31252
$R_{\text{work}} / R_{\text{free}}$ (%)	23.1/27.1
No. atoms	
Protein	2511
Ligand/ion	0
R.m.s. deviations	
Bond lengths (Å)	0.01
Bond angles (°)	1.24
Average B-factor	
Mean	69
Ramachandran plot	
Most favored (%)	91
Outlier (%)	3

*Values in parentheses are for the highest-resolution shell.