

Supplementary Table S2: Pan3 crystallographic data collection and refinement statistics.

Data collection statistics

Wavelength (Å)	0.9795
Space group	<i>P1</i>
Unit cell parameters: a, b, c (Å); α , β , γ (°)	51.5, 146.0, 149.9; 89.8, 81.1, 82.8
Resolution range (outer shell in brackets; Å)	52.21 – 2.42 (2.48 – 2.42)
Unique reflections	160,956
Total observations	1,170,731
$\langle I / \sigma(I) \rangle$: all (outer shell)	14.3 (2.4)
$R_{p.i.m.}$: all (outer shell)	4.0 (35.9)
Completeness: all (outer shell) (%)	98.5 (98.0)
Multiplicity	7.3
Wilson B-factor	49.1

Refinement statistics

Non-hydrogen atoms	27,217
Metal ions	8 \times Mg ²⁺
Ligands	8 \times ATP
Number of water molecules	984
Bond length deviation from ideal values (Å)	0.004
Bond angle deviation from ideal values (°)	0.875
Ramachandran favoured/outliers (%)	99.1/0.0
All-atom clashscore	3.28
Reflections used in refinement	160,878
Random reflections assigned for cross-validation	8,073
R_{work}/R_{free} (%)	19.0/23.4
Estimate of the coordinate error (Å)	0.3