Table S1. Data collection and refinement statistics (Molecular Replacement)

Data collection Space group P61 Cell dimensions 413.5, 98.9 Resolution (Å) 50.00-3.16 (3.26-3.16) b R_{merge}^{c} 15.6 (78.7) $I/\sigma I$ 13.8 (2.0) Completeness (%) 100.0 (100.0) Redundancy 9.2 (8.3) Refinement Resolution (Å) Resolution (Å) 49.63-3.16 (3.24-3.16) No. reflections 157,861 R_{work} / R_{free}^{d} 22.4 / 24.9 (33.0 / 36.0) No. atoms Protein Ligand/ion 4 Water 0 B-factors (Ų) 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations 0		
Space group P61 Cell dimensions 413.5, 98.9 Resolution (Å) 50.00-3.16 (3.26-3.16) b R_{merge}^c 15.6 (78.7) $I/\sigma I$ 13.8 (2.0) Completeness (%) 100.0 (100.0) Redundancy 9.2 (8.3) Refinement 49.63-3.16 (3.24-3.16) No. reflections 157,861 R_{work}/R_{free}^d 22.4 / 24.9 (33.0 / 36.0) No. atoms 23,896 Ligand/ion 4 Water 0 B-factors (Ų) 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations 0		Mtd-P1•Prn-E ^a
Cell dimensions $a, c (Å)$ $413.5, 98.9$ Resolution (Å) $50.00-3.16 (3.26-3.16)^b$ R_{merg}^c $15.6 (78.7)$ $I/\sigma I$ $13.8 (2.0)$ Completeness (%) $100.0 (100.0)$ Redundancy $9.2 (8.3)$ Refinement Resolution (Å) $49.63-3.16 (3.24-3.16)$ No. reflections $157,861$ R_{work} / R_{free}^d $22.4 / 24.9 (33.0 / 36.0)$ No. atoms $23,896$ Ligand/ion 4 Water 0 B-factors (Ų) 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations	Data collection	
$a, c(Å)$ $413.5, 98.9$ Resolution (Å) $50.00-3.16 (3.26-3.16)^b$ R_{merge}^c $15.6 (78.7)$ $I/\sigma I$ $13.8 (2.0)$ Completeness (%) $100.0 (100.0)$ Redundancy $9.2 (8.3)$ Refinement Resolution (Å) $49.63-3.16 (3.24-3.16)$ No. reflections $157,861$ R_{work} / R_{free}^d $22.4 / 24.9 (33.0 / 36.0)$ No. atoms $23,896$ Ligand/ion 4 Water 0 B -factors (Ų) 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations	Space group	P6 ₁
Resolution (Å) $50.00-3.16 (3.26-3.16)^b$ R_{merge}^{c} $15.6 (78.7)$ $I/\sigma I$ $13.8 (2.0)$ Completeness (%) $100.0 (100.0)$ Redundancy $9.2 (8.3)$ Refinement Resolution (Å) $49.63-3.16 (3.24-3.16)$ No. reflections $157,861$ R_{work} / R_{free}^{d} $22.4 / 24.9 (33.0 / 36.0)$ No. atoms $23,896$ Ligand/ion 4 Water 0 B-factors (Ų) 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations	Cell dimensions	
Rmerge 15.6 (78.7) I/ ol 13.8 (2.0) Completeness (%) 100.0 (100.0) Redundancy 9.2 (8.3) Refinement 49.63-3.16 (3.24-3.16) Resolution (Å) 49.63-3.16 (3.24-3.16) No. reflections 157,861 Rwork / Rfree ^d 22.4 / 24.9 (33.0 / 36.0) No. atoms 23,896 Ligand/ion 4 Water 0 B-factors (Ų) 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations 0	a, c (Å)	413.5, 98.9
I / ol 13.8 (2.0) Completeness (%) 100.0 (100.0) Redundancy 9.2 (8.3) Refinement Resolution (Å) 49.63-3.16 (3.24-3.16) No. reflections 157,861 Rwork / Rfree ^d 22.4 / 24.9 (33.0 / 36.0) No. atoms 23,896 Ligand/ion 4 Water 0 B-factors (Ų) 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations 0	Resolution (Å)	50.00-3.16 (3.26-3.16) ^b
I / ol 13.8 (2.0) Completeness (%) 100.0 (100.0) Redundancy 9.2 (8.3) Refinement Resolution (Å) 49.63-3.16 (3.24-3.16) No. reflections 157,861 Rwork / Rfree ^d 22.4 / 24.9 (33.0 / 36.0) No. atoms 23,896 Ligand/ion 4 Water 0 B-factors (Ų) 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations 0	R _{merge} ^c	15.6 (78.7)
Refinement 9.2 (8.3) Resolution (Å) 49.63-3.16 (3.24-3.16) No. reflections 157,861 Rwork / Rfree d 22.4 / 24.9 (33.0 / 36.0) No. atoms 23,896 Ligand/ion 4 Water 0 B-factors (Ų) 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations 0		13.8 (2.0)
Refinement Resolution (Å) 49.63-3.16 (3.24-3.16) No. reflections 157,861 Rwork / Rfree d 22.4 / 24.9 (33.0 / 36.0) No. atoms 23,896 Ligand/ion 4 Water 0 B-factors (Ų) 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations	Completeness (%)	100.0 (100.0)
Resolution (Å) 49.63-3.16 (3.24-3.16) No. reflections 157,861 R_{work} / R_{free}^{d} 22.4 / 24.9 (33.0 / 36.0) No. atoms 23,896 Ligand/ion 4 Water 0 B-factors (Ų) 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations	Redundancy	9.2 (8.3)
Resolution (Å) 49.63-3.16 (3.24-3.16) No. reflections 157,861 R_{work} / R_{free}^{d} 22.4 / 24.9 (33.0 / 36.0) No. atoms 23,896 Ligand/ion 4 Water 0 B-factors (Ų) 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations		
No. reflections $157,861$ R_{work} / R_{free}^d $22.4 / 24.9 (33.0 / 36.0)$ No. atoms $23,896$ Ligand/ion 4 Water 0 B -factors (\mathring{A}^2) 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations	Refinement	
Rwork / Rfree d 22.4 / 24.9 (33.0 / 36.0) No. atoms 23,896 Ligand/ion Water 0 4 B-factors (Ų) 69.5 Ligand/ion 52.3 52.3 Water 0 0		49.63-3.16 (3.24-3.16)
No. atoms 23,896 Ligand/ion 4 Water 0 B-factors (Ų) 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations 52.3	No. reflections	
Protein 23,896 Ligand/ion 4 Water 0 B-factors (Ų) 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations 52.3	$R_{\text{work}} / R_{\text{free}}^{\text{a}}$	22.4 / 24.9 (33.0 / 36.0)
Ligand/ion 4 Water 0 B-factors (Ų) 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations	No. atoms	
Water 0 B-factors (Ų) 69.5 Protein 52.3 Water 0 R.m.s. deviations 69.5	Protein	23,896
B-factors (Ų) Protein 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations	Ligand/ion	4
Protein 69.5 Ligand/ion 52.3 Water 0 R.m.s. deviations	•	0
Ligand/ion 52.3 Water 0 R.m.s. deviations	<i>B</i> -factors (Å ²)	
Water 0 R.m.s. deviations	Protein	69.5
R.m.s. deviations	Ligand/ion	52.3
	Water	0
D I (l /Å) 0 000	R.m.s. deviations	
3 ()	Bond lengths (Å)	0.008
Bond angles (°) 1.141	Bond angles (°)	1.141
Estimated coordinate error (Å) ^e 0.312, 0.246	Estimated coordinate error (Å) ^e	0.312, 0.246

^aData collected from single crystal.

$${}^{\text{c}}\mathsf{R}_{\text{merge}} = 100 \text{ x } \frac{\sum_{h} \sum_{i} \left|I_{h,i} - I_{h}\right|}{\sum_{h} \sum_{i} I_{h,i}}, \text{ where } \mathsf{I}_{\text{h}} \text{ is the mean intensity of symmetry-related reflections, } \mathsf{I}_{\text{h,i}}.$$

$${}^{\text{d}}\mathsf{R} = 100 \text{ x } \frac{\sum_{hkl} \left|F_{obs} - F_{calc}\right|}{\sum_{hkl} F_{obs}}, \text{ where } \mathsf{R}_{\text{free}} \text{ is calculated for a randomly chosen 5 \% of reflections (F > 0)}$$

omitted from refinement, and R_{work} is calculated for the remaining 95 % of reflections (F > 0) included in refinement.

^bHighest resolution shell is shown in parenthesis.

 $^{^{\}mathrm{e}}$ First value based on R_{free} , and second on maximum likelihood.