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**DP1 H451A**

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**Data collection**

Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Wavelength (Å)	1.04
Cell dimensions	
a, b, c (Å)	85.7, 91.2, 143.9
α, β, γ (°)	90, 90, 90
Resolution (Å)	48.0-2.60 (2.72- 2.60) <sup>a</sup>
Rsym (%)	3.8 (64.7)
I/σ(I)	12.0 (1.1)
Completeness (%)	100 (100)
Redundancy	8.5 (8.8)
CC <sub>(1/2)</sub> <sup>b</sup> (%)	99.6 (61.7)

**Refinement**

Resolution (Å)	47.2-2.60
No. reflections	35447
<i>R</i> <sub>work</sub> / <i>R</i> <sub>free</sub>	22.9/25.5
No. atoms	
Protein	7036
Ions	23
Water	63
B-factors (Å <sup>2</sup> )	
Protein	81.2
Ligand	100.3
Water	74.4
R.m.s deviations	
Bond lengths (Å)	0.009
Bond angles (°)	1.10
Ramachandran	
Favored/outliers (%) <sup>c</sup>	96.0/0.35
Molprobit <sup>4</sup> score	1.60

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