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|  | **DP1 H451A** |
| **Data collection** |  |
| Space group | P212121 |
| 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)a |
| Rsym (%)  I/σ(I) | 3.8 (64.7)  12.0 (1.1) |
| Completeness (%) | 100 (100) |
| Redundancy  CC(1/2)b (%) | 8.5 (8.8)  99.6 (61.7) |
|  |  |
| **Refinement** |  |
| Resolution (Å) | 47.2-2.60 |
| No. reflections | 35447 |
| *Rwork/Rfree* | 22.9/25.5 |
| No. atoms |  |
| Protein | 7036 |
| Ions | 23 |
| Water | 63 |
| B-factors (Å2) |  |
| 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 (%)c | 96.0/0.35 |
| Molprobity4 score | 1.60 |
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