

Data collection and processing statistics

X-ray source	PROXIMA-1, Soleil
Wavelength [Å]	0.9786
Detector	EIGER-X 16M
Space group	P 2 ₁ 2 ₁ 2 ₁
Cell: a; b; c [Å]	66.93; 90.66; 95.86
α; β; γ [°]	90.00; 90.00; 90.00
Resolution [Å]	47.97–2.15 (2.22–2.15)
Unique reflections	32481 (2789)
Multiplicity	13.6 (13.3)
Completeness [%]	100.0 (99.9)
R _{merge} [%]	11.5 (51.2)
R _{pim} [%]	3.2 (14.5)
I/σI	17.5 (4.9)
CC1/2	0.999 (0.975)

Refinement statistics

Number of reflections	30800 (2398)
R _{cryst} [%]	16.5
R _{free} [%]	21.7
Total number of atoms	
Protein	4169
Ligand	111
Water	382
R.m.s.d. bonds [Å]	0.007
R.m.s.d. angles [°]	1.544
Ramachandran Plot statistics	
Most favoured [%]	97.9
Allowed [%]	1.9
Disallowed [%]	0.2

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