

Table 1. Data collection and refinement statistics.

Wavelength	0.9235
Resolution range	49.72 - 2.60 (2.697 - 2.60)
Space group	P 4 ₃ 2 ₁ 2
Unit cell	72.19 72.19 137.14 90 90 90
Total reflections	482755 (43140)
Unique reflections	11689 (1135)
Multiplicity	41.3 (38.0)
Completeness (%)	99.64 (99.56)
Mean I/sigma(I)	30.86 (2.53)
Wilson B-factor	63.30
R-merge	0.09956 (1.663)
R-meas	0.1008 (1.685)
R-pim	0.01561 (0.2697)
CC_{1/2}	1 (0.914)
CC*	1 (0.977)
Reflections used in refinement	11669 (1134)
Reflections used for R-free	598 (53)
R-work	0.2246 (0.3888)
R-free	0.2534 (0.4179)
CC(work)	0.927 (0.721)
CC(free)	0.937 (0.748)
Number of non-hydrogen atoms	2340
macromolecules	2144
ligands	196
Coordinate error (Maximum-likelihood based)	0.43
Phase error (°, Maximum-likelihood based)	33.42
RMS(bonds)	0.001
RMS(angles)	0.44
Correct sugar puckers (%)	99.0
Correct backbone conformations (%)	93.0
Clashscore	2.62
Average B-factor	62.95
macromolecules	59.43
ligands	101.50
Number of TLS groups	1

Statistics for the highest-resolution shell are shown in parentheses.