Resolution range	40.74 - 2.26 (2.341 - 2.26)
Space group	C 1 2 1
Unit cell	80.2 81.49 64.88 90 121.37 90
Total reflections	73970 (6634)
Unique reflections	16448 (1524)
Multiplicity	4.5 (4.4)
Completeness (%)	98.04 (91.75)
Mean I/sigma(I)	11.74 (1.77)
Wilson B-factor	43.77
R-merge	0.09554 (0.7352)
R-meas	0.1081 (0.8347)
R-pim	0.04968 (0.3885)
CC1/2	0.997 (0.658)
CC*	0.999 (0.891)
Reflections used in refinement	16441 (1523)
Reflections used for R-free	822 (76)
R-work	0.1908 (0.2857)
R-free	0.2258 (0.3070)
CC(work)	0.956 (0.728)
CC(free)	0.942 (0.637)
Number of non-hydrogen atoms	2754
macromolecules	2651
ligands	20
solvent	83
Protein residues	335
RMS(bonds)	0.014
RMS(angles)	1.66
Ramachandran favored (%)	97.86
Ramachandran allowed (%)	2.14
Ramachandran outliers (%)	0.00
Rotamer outliers (%)	5.86
Clashscore	2.27
Average B-factor	47.87
macromolecules	47.09
ligands	162.61
solvent	44.88

Suppl. Table 1. Data collection and refinement statistics.
Statistics for the highest-resolution shell are shown in parentheses.