Table 1. Summary of crystallographic data collection , reduction and refinement for inhibitor **21** with cdk2.

space group	$P2_12_12_1$
real space cell parameter	
a	53.72 Å
b	72.78 Å
c	72.54 Å
number of reflections collected	259,247
number of unique reflections	27,035
*R*symm (on *F*)	7.50 %
maximum observed resolution	1.8 Å
completeness	98.8 %
refinement program	CNX
resolution range used	20.0 – 1.8 Å
reflections used in the refinement:	26,859 ($F/\sigma > 0$)
crystallographic *R*-factor	25.9 %
crystallographic free *R*-factor	28.8 %
average *B*-factor (protein)	38.5 $Å^2$
average *B*-factor (ligand)	35.8 $Å^2$
residues in final model	298
total number of atoms	2,551 (2,398 protein, 25 ligand, 128 solvent)
rms. deviation bond distances	0.006 Å
rms. deviation bond angles	1.2°
rms. deviation dihedral angles	22.4°
rms. deviation improper angles	0.78°