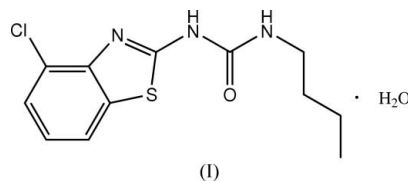


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## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.035  
 $wR$  factor = 0.096  
Data-to-parameter ratio = 14.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.1-Butyl-3-(4-chloro-1,3-benzothiazol-2-yl)urea  
monohydrateIn the crystal structure of the title compound,  $\text{C}_{12}\text{H}_{14}\text{ClN}_3\text{OS}\cdot\text{H}_2\text{O}$ , the butyl(chlorobenzo[*d*]thiazolyl)urea molecule, excluding butyl H atoms, displays a roughly planar structure. The water molecules link with the urea derivative molecules *via*  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonding.Received 24 May 2006  
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## Comment

1-Butyl-3-(4-chlorobenzo[*d*]thiazol-2-yl)urea is useful as an inhibitor of serine/threonine and tyrosine kinases (Cusack *et al.*, 2003). Recently we obtained single crystals of its monohydrate, (I), and determined the crystal structure of (I).The molecular structure of (I) is shown in Fig. 1. The butyl(chlorobenzo[*d*]thiazolyl)urea molecule, excluding butyl H atoms, displays a roughly planar structure. The  $\text{C}9-\text{C}10-\text{C}11-\text{C}12$  torsion angle of  $-178.95(19)^\circ$  shows the extended conformation of the butyl group. The  $\text{N}3-\text{C}9$  bond distance indicates a typical single bond, but the  $\text{N}2-\text{C}7$  bond is much shorter than the  $\text{N}3-\text{C}9$  bond (Table 1) and shows somewhat the character of a  $\text{C}=\text{N}$  double bond. This is presumably due to the overlap of the non-bonding orbital of the imino N2 atom with the  $\pi$  orbital of the thiazole ring.The water molecules link with the urea derivative molecules *via*  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonding (Table 2), which helps to stabilize the crystal structure.

## Experimental

Butan-1-amine (9 mmol) was mixed with a dry tetrahydrofuran solution (12 ml) of phenyl 4-chlorobenzo[*d*]thiazol-2-ylcarbamate (3 mmol). The mixture was heated for 20 min at 423 K in a microwave synthetic reactor. The solvent was then removed under reduced pressure. Colourless prismatic single crystals of (I) were obtained from an acetone–water (10:1) solution.

## Crystal data

 $\text{C}_{12}\text{H}_{14}\text{ClN}_3\text{OS}\cdot\text{H}_2\text{O}$   
 $M_r = 301.8$   
Triclinic,  $P\bar{1}$   
 $a = 7.0075(16)$  Å  
 $b = 7.6324(18)$  Å  
 $c = 14.826(3)$  Å  
 $\alpha = 96.568(4)^\circ$   
 $\beta = 91.451(4)^\circ$   
 $\gamma = 114.775(4)^\circ$  $V = 712.9(3)$  Å<sup>3</sup>  
 $Z = 2$   
 $D_x = 1.406$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
 $\mu = 0.42$  mm<sup>-1</sup>  
 $T = 293(2)$  K  
Prism, colourless  
 $0.30 \times 0.26 \times 0.20$  mm

Data collection

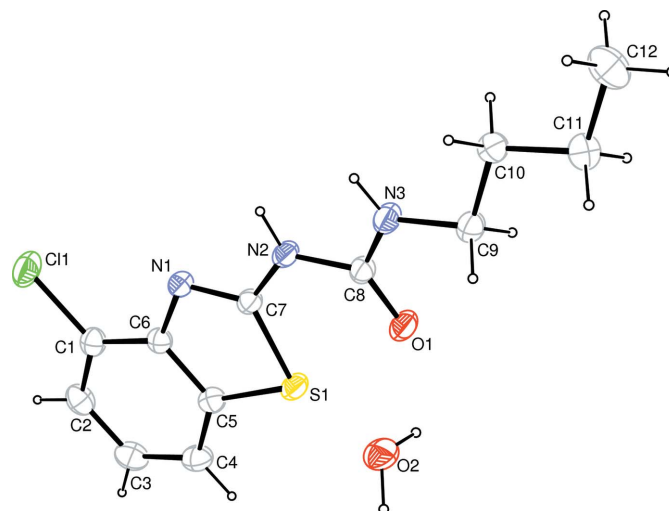
Bruker SMART 1000 CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 2002)  
 $T_{\min} = 0.885$ ,  $T_{\max} = 0.921$

3635 measured reflections  
 2507 independent reflections  
 1939 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$   
 $\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.035$   
 $wR(F^2) = 0.096$   
 $S = 1.02$   
 2507 reflections  
 173 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0458P)^2 + 0.1733P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.34 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.21 \text{ e } \text{Å}^{-3}$



**Figure 1**  
 The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

**Table 1**

Selected bond lengths (Å).

S1—C5	1.741 (2)	N2—C7	1.365 (3)
S1—C7	1.753 (2)	N2—C8	1.391 (3)
O1—C8	1.223 (2)	N3—C8	1.333 (3)
N1—C6	1.386 (2)	N3—C9	1.453 (3)
N1—C7	1.300 (3)		

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N2—H2 $\cdots$ O2 <sup>i</sup>	0.86	2.05	2.826 (2)	149
N3—H3 $\cdots$ O2 <sup>i</sup>	0.86	2.21	2.962 (2)	147
O2—H2B $\cdots$ N1 <sup>ii</sup>	0.85	2.13	2.939 (2)	158
O2—H2C $\cdots$ O1 <sup>iii</sup>	0.85	2.19	2.918 (2)	144

Symmetry codes: (i)  $-x + 2, -y + 1, -z$ ; (ii)  $x - 1, y - 1, z$ ; (iii)  $-x + 1, -y + 1, -z$ .

Water H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$ . Methyl H atoms were placed in calculated positions with  $C-H = 0.96 \text{ Å}$  and the torsion angle was refined to fit the electron density;  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ . Other H atoms were placed in calculated positions with  $N-H = 0.86 \text{ Å}$ , and  $C-H = 0.93$  (aromatic) or  $0.97 \text{ Å}$  (methylene), and refined in riding mode, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1999); software used to prepare material for publication: SHELXTL.

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