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1-(4-Chloro-1,3-benzothiazol-2-yl)-3-propylurea monohydrate

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Key indicators

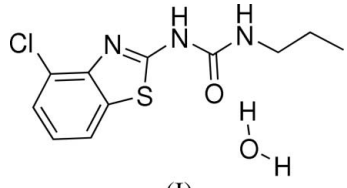
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.037
wR factor = 0.105
Data-to-parameter ratio = 17.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the crystal structure of the title compound, $C_{11}H_{12}ClN_3OS\cdot H_2O$, the urea derivative molecule, excluding propyl H atoms, displays a roughly planar structure. The water molecules link the urea derivative molecules *via* O—H···O, O—H···N and N—H···O hydrogen bonding, forming columns parallel to the *a* axis.

Comment

In recent years, considerable attention has been paid to the investigation of structures and properties of complexes containing 2-substituted benzimidazoles, benzothiazoles and benzoxazoles because they have been found to possess diverse applications in the fields of medicine, agriculture and industry. For example, 2-trifluoromethylbenzimidazoles are reported to be extremely active herbicides (Burton *et al.*, 1967). The title compound, (I), is useful as an inhibitor of serine/threonine and tyrosine kinases (Cusack *et al.*, 2003). We report here the crystal structure of (I).



(I)

The main molecule of (I) (Fig. 1) is almost planar. The dihedral angle between the Cl1/N1/S1/C1–C7 and O1/N2/N3/C8–C11 planes is 2.34 (5)°. The bond lengths and angles are comparable to those observed for a similar structure, 1-butyl-3-(4-chloro-1,3-benzothiazol-2-yl)urea monohydrate (Li *et al.*, 2006).

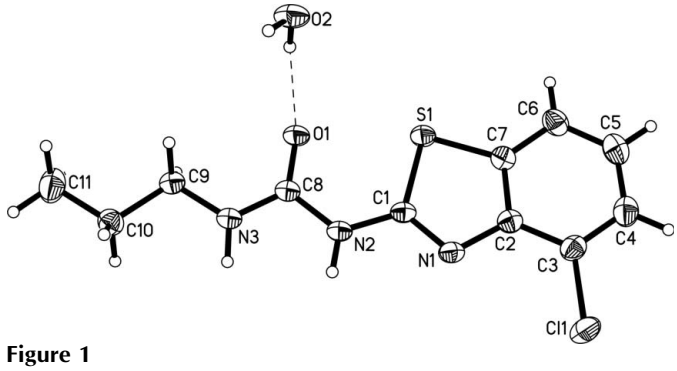


Figure 1
View of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. The dashed line indicates an O—H···O hydrogen bond.

O—H···O, N—H···O and N—H···N hydrogen bonds (Table 1) link the water molecules and the urea derivative molecules, forming columns parallel to the *a* axis.

Experimental

Propan-1-amine (9 mmol) was mixed with a dry tetrahydrofuran (12 ml) solution of phenyl 4-chloro-1,3-benzothiazol-2-ylcarbamate (3 mmol). The mixture was heated for 20 min at 423 K in a microwave synthetic reactor. After reaction, the solvent was removed under reduced pressure. Colourless single crystals of (I) were obtained from an acetone–water (10:1) solution after 10 d. Analysis calculated for $C_{11}H_{12}ClN_3OS$: C 48.98, H 4.48, N 15.58%; found: C 48.71, H 4.27, N 15.39%.

Crystal data

$C_{11}H_{12}ClN_3OS\cdot H_2O$
$M_r = 287.76$
Triclinic, $P\overline{1}$
$a = 6.8742\ (15)$ Å
$b = 7.2537\ (16)$ Å
$c = 14.729\ (2)$ Å
$\alpha = 97.509\ (5)^\circ$
$\beta = 94.600\ (8)^\circ$
$\gamma = 111.419\ (8)^\circ$
$V = 671.3\ (2)$ Å^3
$Z = 2$
$D_x = 1.424$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.44$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
0.24 × 0.20 × 0.10 mm

Data collection

Rigaku Saturn diffractometer
ω scans
Absorption correction: multi-scan (Jacobson, 1998)
$T_{min} = 0.893$, $T_{max} = 0.958$
6546 measured reflections
3134 independent reflections
2212 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.9^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.105$
$S = 1.01$
3134 reflections
180 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0605P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O1	0.83 (1)	2.09 (1)	2.891 (2)	162 (2)
O2—H2B···N1^{i}	0.85 (1)	2.09 (1)	2.8816 (19)	155 (2)
N2—H2···O2^{ii}	0.88 (1)	2.43 (1)	3.164 (2)	142 (2)
N3—H3···O2^{ii}	0.90 (1)	1.95 (1)	2.8358 (19)	167 (2)

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

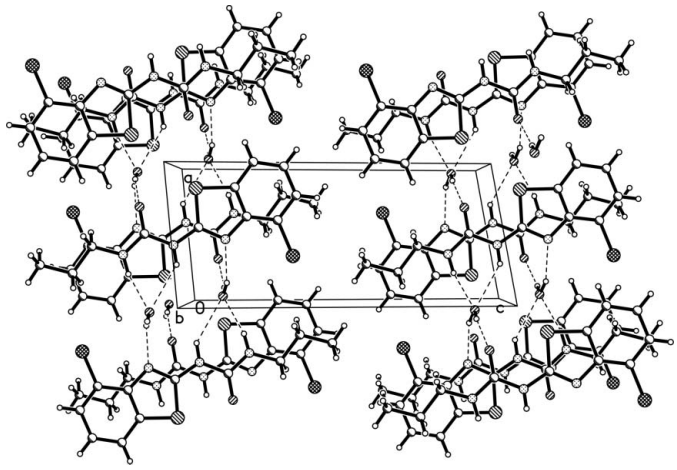


Figure 2
The crystal packing of (I), viewed down the *b* axis. Dashed lines indicate hydrogen bonds.

Water and imine H atoms were located in a difference Fourier map and refined with O—H and N—H distance restraints of 0.84 (1) and 0.90 (1) Å, respectively. C-bound H atoms were placed in calculated positions, with C—H = 0.93 (aromatic), 0.96 (methyl) or 0.97 Å (methylene), and refined using a riding model, with U_{iso}(H) = $1.2U_{eq}$(C) or $1.5U_{eq}$(methyl C).

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2005); software used to prepare material for publication: *CrystalStructure*.

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