

3-(2-Anilino-1,3-thiazol-4-yl)-2H-chromen-2-one. Corrigendum

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In the original report by Chopra, Venugopala, Jayashree & Guru Row [*Acta Cryst.* (2006), E62, o2663–o2665], the chemical name is given incorrectly in the title. The correct title is '6-Bromo-3-[2-(2-methylanilino)-1,3-thiazol-4-yl]-2H-chromen-2-one'.

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Key indicators

Single-crystal X-ray study
T = 290 K
Mean $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$
R factor = 0.037
wR factor = 0.091
Data-to-parameter ratio = 14.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

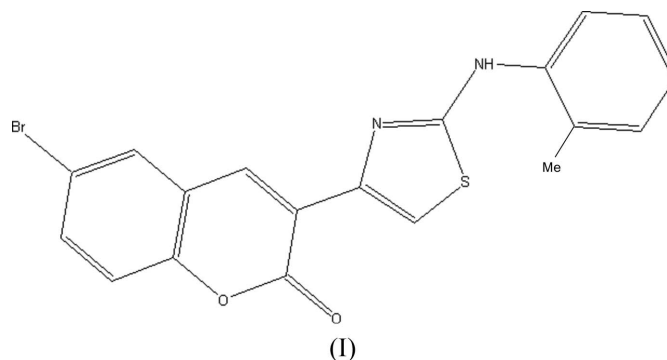
The crystal structure of the title compound, $\text{C}_{19}\text{H}_{13}\text{BrN}_2\text{O}_2\text{S}$, contains two molecules (*A* and *B*) in the asymmetric unit. The planar coumarin systems make dihedral angles of 5.47 (1) and 6.42 (1)° with the thiazole rings in the two unique molecules. The structure is stabilized by intermolecular $\text{N}-\text{H}\cdots\text{N}$, $\text{N}-\text{H}\cdots\text{O}$, $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\pi$ hydrogen bonds and aromatic stacking interactions; intramolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds also influence the molecular conformation.

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Comment

Coumarins are an important class of organic compounds with vast structural diversity and they find useful applications in synthetic chemistry, medicinal chemistry and photochemistry (Vishnumurthy *et al.*, 1996, 1997, 1999). The formation of [2 + 2]-cycloaddition products upon irradiation (Vishnumurthy *et al.*, 2001) of coumarin and its derivatives has demonstrated the importance of preorganization of molecules in the crystalline solid state.



In the title compound, (I) (Fig. 1 and Table 1), the coumarin systems are planar in each of the two unique molecules in the asymmetric unit, with maximum deviations of 0.035 (3) and 0.043 (3) Å for atoms C9 and C28, respectively. In both molecules the conformation is locked *via* intramolecular $\text{C}-\text{H}\cdots\text{O}$ interactions (involving H11 and H30). In the asymmetric unit, the two molecules, *A* and *B*, are linked by $\text{N}-\text{H}\cdots\text{N}$ and $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds (Fig. 1 and Table 2). The structure is further stabilized by intermolecular $\text{N}-\text{H}\cdots\text{O}$, $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{Br}$ and $\text{C}-\text{H}\cdots\pi$ interactions (Table 2, and Figs. 2 and 3). Furthermore, $\pi-\pi$ stacking interactions link $\text{Cg}1\cdots\text{Cg}2(-x, -y, -z)$, $\text{Cg}2\cdots\text{Cg}3(1-x, -y, -z)$ and $\text{Cg}6\cdots\text{Cg}6(1-x, -y, 1-z)$ with separations of 3.782 (3), 3.735 (3) and 3.992 (3) Å between the centroids (*Cg*1 is the thiazoyl ring S1, N2, C10–C12, *Cg*2 is the pyranone ring O2, C1–C9, *Cg*3 is the phenyl ring C1–C6 and *Cg*6 is the thiazoyl ring S2, N3, C29–C31.).

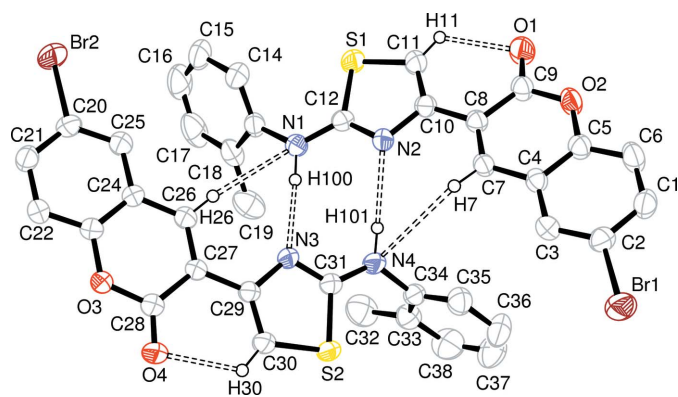


Figure 1
ORTEP-3 (Farrugia, 1997) view of the asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

Experimental

The compound was synthesized in accordance with the procedure reported in the literature (Venugopala *et al.*, 2004). Single crystals of the compound were grown from a solution in dichloromethane/hexane (2:1 *v/v*).

Crystal data

$C_{19}H_{13}BrN_2O_2S$
 $M_r = 413.28$
 Triclinic, $P\bar{1}$
 $a = 10.940$ (7) Å
 $b = 12.172$ (8) Å
 $c = 15.039$ (10) Å
 $\alpha = 93.025$ (10)°
 $\beta = 108.484$ (10)°
 $\gamma = 112.653$ (9)°

$V = 1717$ (2) Å³
 $Z = 4$
 $D_x = 1.598$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 2.53$ mm⁻¹
 $T = 290$ (2) K
 Needle, yellow
 0.36 × 0.06 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{min} = 0.463$, $T_{max} = 0.884$

17861 measured reflections
 6816 independent reflections
 5066 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.026$
 $\theta_{max} = 26.4^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.092$
 $S = 1.02$
 6816 reflections
 461 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.3557P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.018$
 $\Delta\rho_{max} = 0.72$ e Å⁻³
 $\Delta\rho_{min} = -0.53$ e Å⁻³

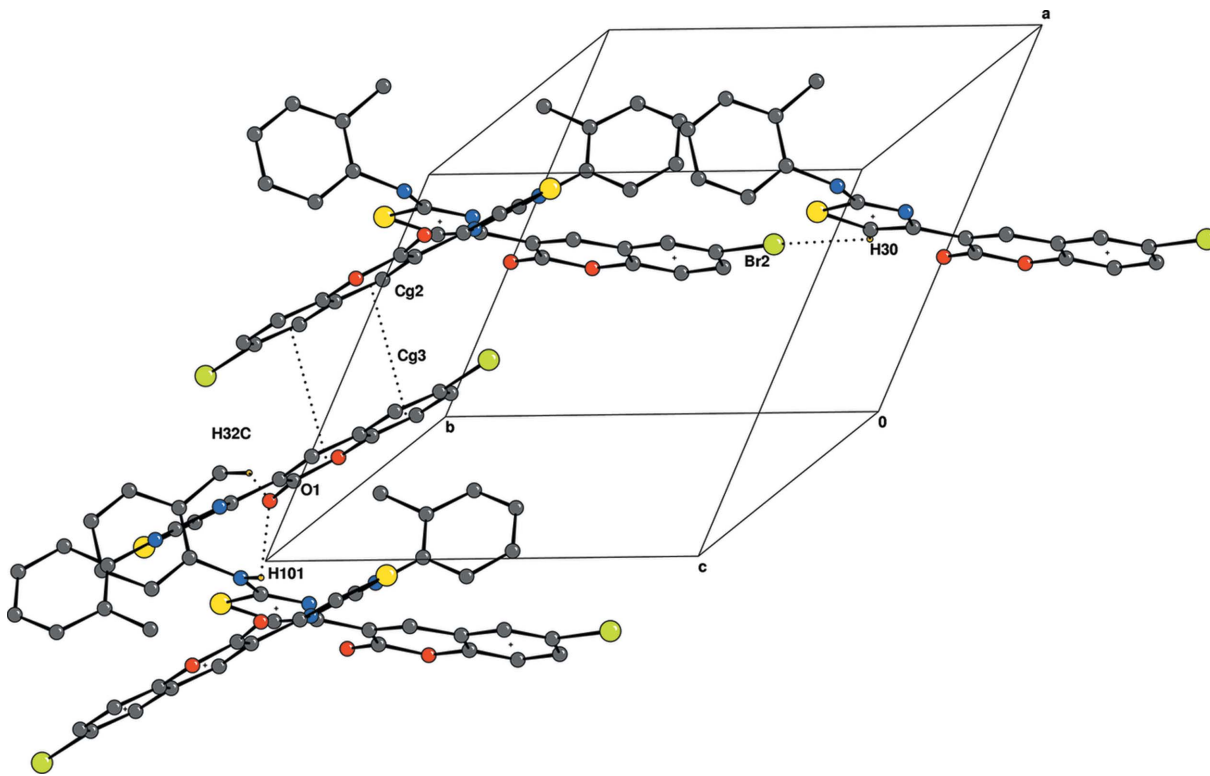


Figure 2
 Packing diagram of (I), highlighting the N–H···O and C–H···O interactions and one of the π – π contacts. Cg2 and Cg3 are the centroids of the pyranone O2–C9 and benzene C1–C6 rings. Hydrogen bonds are drawn as, and ring centroids are joined by, dotted lines. H atoms not involved in the interactions shown have been omitted.

Table 1
Selected geometric parameters (Å, °).

Br1—C2	1.901 (3)	S2—C30	1.725 (3)
Br2—C20	1.890 (3)	S1—C11	1.722 (3)
C31—N4—C34	122.1 (2)	C12—N1—C13	123.2 (2)
C12—N1—C13—C18	127.0 (3)	C13—N1—C12—N2	−178.5 (2)
C34—N4—C31—N3	−166.7 (3)	C31—N4—C34—C35	−102.6 (3)

Table 2
Hydrogen-bond geometry (Å, °).

Cg8 is the centroid of the C20—C25 benzene ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N4—H101...N2	0.81 (4)	2.48 (4)	3.245 (4)	156 (3)
N1—H100...N3	0.90 (3)	2.17 (3)	3.067 (4)	177 (3)
C7—H7...N2	0.93	2.55	2.873 (4)	101
C26—H26...N3	0.93	2.49	2.841 (4)	102
C30—H30...O4	0.93	2.25	2.825 (3)	120
C11—H11...O1	0.93	2.20	2.774 (4)	120
N4—H101...O1 ⁱ	0.81 (4)	2.45 (3)	2.970 (4)	123 (3)
C32—H32C...O1 ⁱ	0.96	2.49	3.262 (5)	138
C30—H30...Br2 ⁱⁱ	0.93	2.92	3.504 (3)	122
C14—H14...Cg8 ⁱⁱⁱ	0.93	2.83	3.677 (5)	152

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

The amino H atom was located in a difference Fourier map and refined isotropically. The remaining H atoms were placed in idealized positions ($C-H = 0.93$ and 0.96 Å) and constrained to ride on their parent atoms [$U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C)$].

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

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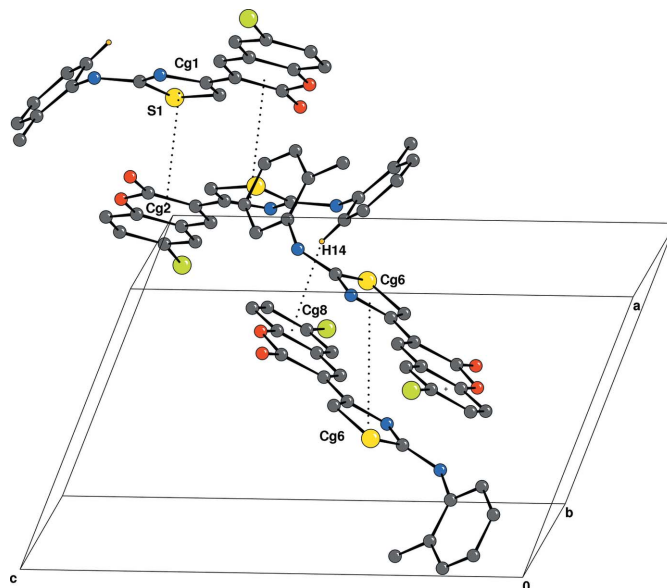


Figure 3

$C-H \cdots \pi$ and $\pi-\pi$ interactions in the title compound; Cg1 and Cg6 are the centroids of the thiazole rings from the two adjacent molecules in the asymmetric unit. The ring centroids are joined by dotted lines. Cg8 is the centroid of the C20—C25 benzene ring, which participates in a $C-H \cdots \pi$ interaction. H atoms not involved in the interactions shown have been omitted.

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