Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-[6-(4-Bromophenyl)imidazo[2,1-*b*]-thiazol-3-yl]-*N*′-(1-ethylpropylidene)-acetohydrazide

Mehmet Akkurt,[a]* Şerife Pınar Yalçın,[a] Elif Gürsoy,[b] Nuray Ulusoy Güzeldemirci[b] and Orhan Büyükgüngör[c]

[a]Department of Physics, Faculty of Arts and Sciences, Erciyes University, 38039 Kayseri, Turkey, [b]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Istanbul University, 34116 Istanbul, Turkey, and [c]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey
Correspondence e-mail: akkurt@erciyes.edu.tr

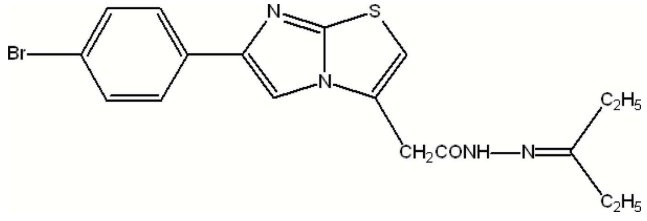
Received 29 May 2007; accepted 31 May 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.007 Å; R factor = 0.060; wR factor = 0.156; data-to-parameter ratio = 20.0.

In the title compound, $C_{18}H_{19}BrN_4OS$, the thiazole and imidazole rings make a dihedral angle of 0.7 (2)° with each other. The dihedral angle between the benzene ring and the mean plane of the fused rings is 2.99 (15)°. The crystal structure is stabilized by intermolecular N—H···O hydrogen bonds and possible C—H···O interactions.

Related literature

For related literature, see: Akkurt *et al.* (2005); Amarouch *et al.* (1987); Andreani *et al.* (1993); Hanson *et al.* (1991); Allen *et al.* (1987) Öztürk Yıldırım, Akkurt, Ur, Cesur, Cesur & Büyükgüngör (2005); Öztürk Yıldırım, Akkurt, Ur, Cesur, Cesur & Heinemann (2005); Ulusoy (2002).



Experimental

Crystal data

$C_{18}H_{19}BrN_4OS$
M_r = 419.34
Triclinic, $P\overline{1}$
a = 6.9591 (6) Å
b = 11.8636 (10) Å
c = 13.1247 (11) Å
α = 65.411 (6)°
β = 78.892 (7)°
γ = 75.193 (6)°
V = 947.99 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.29 mm^{-1}
T = 296 K
0.73 × 0.55 × 0.45 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.285, T_{max} = 0.425
17037 measured reflections
4441 independent reflections
3359 reflections with $I > 2\sigma(I)$
R_{int} = 0.082

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.157
S = 1.02
4441 reflections
222 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—HN3···O1^{i}	0.83 (5)	2.03 (5)	2.844 (4)	169 (4)
C17—H17B···O1^{i}	0.97	2.56	3.326 (9)	136

Symmetry code: (i) $-x+1, -y, -z$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for use of the Stoe IPDS II diffractometer (purchased under grant F.279 of the University Research Fund).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2439).

References

Akkurt, M., Yıldırım, S. Ö., Ur, F., Cesur, Z., Cesur, N. & Büyükgüngör, O. (2005). *Acta Cryst.* E**61**, o718–o720.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Amarouch, H., Loiseau, P. R., Bacha, C., Caujolle, R., Payard, M., Loiseau, P. M., Bories, C. & Gayral, P. (1987). *Eur. J. Med. Chem.* **22**, 463–466.
Andreani, A., Rambaldi, M., Locatelli, A., Bossa, R., Fraccari, A. & Galatulas, I. (1993). *Pharm. Acta Helv.* **68**, 21–24.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Hanson, K. A., Nagel, D. L. & Heidrick, M. L. (1991). *Int. J. Immunopharmacol.* **13**, 655–668.
Öztürk Yıldırım, S., Akkurt, M., Ur, F., Cesur, Z., Cesur, N. & Büyükgüngör, O. (2005). *Acta Cryst.* E**61**, o892–o894.
Öztürk Yıldırım, S., Akkurt, M., Ur, F., Cesur, Z., Cesur, N. & Heinemann, F. W. (2005). *Acta Cryst.* E**61**, o2357–o2359.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.
Ulusoy, N. (2002). *Arzneim.-Forsch. Drug. Res.* **52**, 565–571.

 doi:10.1107/S1600536807026712

supplementary materials

Acta Cryst. (2007). E**63**, o3103 [**doi:10.1107/S1600536807026712**]

2-[6-(4-Bromophenyl)imidazo[2,1-*b*]thiazol-3-yl]-*N*'-(1-ethylpropylidene)acetohydrazide

M. Akkurt, S.P. Yalçin, E. Gürsoy, N. U. Güzeldemirci and O. Büyükgüngör

Comment

Imidazo[2,1-*b*]thiazole derivatives have been reported in the literature as immunomodulatory (Hanson *et al.*, 1991), anti-helmintic (Amarouch *et al.*, 1987), antitubercular (Ulusoy, 2002) and anticancer (Andreani *et al.*, 1993) agents. In view of these observations, we have synthesized the title imidazo[2,1-*b*]thiazole derivative, (I), (Fig. 1), and we report here its crystal structure.

The thiazole and imidazole rings in (I) are essentially coplanar, with a dihedral angle of 0.7 (2)°. The benzene ring C1—C6 and the mean plane of the thiazole and imidazole rings system makes a dihedral angle of 2.99 (15)°. The values of the other geometric parameters in (I) are normal (Allen *et al.*, 1987). The mean C—S bond length [1.737 (5) Å] in (I) may be compared with the corresponding values in similar molecules [1.7588 (2) Å (Öztürk Yıldırım, Akkurt, Ur, Cesur, Cesur & Büyükgüngör, 2005), 1.783 (2) Å (Öztürk Yıldırım, Akkurt, Ur, Cesur, Cesur & Heinemann, 2005) and 1.729 (2) Å (Akkurt *et al.*, 2005)].

The crystal structure of (I) is stabilized by intermolecular C—H···O and N—H···O hydrogen bonding interactions (Table 1, Fig. 2).

Experimental

[6-(4-Bromophenyl)imidazo[2,1-*b*]thiazol-3-yl]acetic acid hydrazide (0.005 mol) and 3-pentanone (0.01 mol) were heated in 30 ml e thanol for 6 h. The precipitate obtained was purified and recrystallized from ethanol to yield colourless prisms of (I). IR [ν, cm^{-1}, KBr]: 3177, 3116 (N—H); 1663 (C═O). ^{1}H-NMR [δ, p.p.m., DMSO-d_6]: 0.96–1.05 (6*H*, m, CH_2CH_3), 2.22–2.33 (4*H*, m, CH_2CH_3), 3.89, 4.18 (2*H*, 2 s, CH_2CO), 7.02 (1*H*, s, imidazothiazole C_2—H), 7.54–7.57 (2*H*, m, Br—Ph $C_{3,5}$—H), 7.75–7.78 (2*H*, m, Br—Ph $C_{2,6}$—H), 8.21, 8.23 (1*H*, 2 s, imidazothiazole C_5—H), 10.35, 10.51 (1*H*, 2 s, CONH). APCI (+) m/*z* (%): 420 (MH^+, 97), 419 (100), 309 (15), 279 (8), 156 (13). Analysis calculated for $C_{18}H_{19}BrN_4OS$: C 51.56, H 4.57, N 13.36%. Found: C 51.48, H 4.15, N 13.50%.

Refinement

The H atom bound to N3 was found from a difference Fourier map and refined freely. All C-bound H atoms were positioned geometrically, with C—H = 0.93–0.97 Å, and refined using a riding model, with U_{iso}(H) = 1.2 or 1.5U_{eq}(methyl C). Atoms C15 and C16 were refined isotropically.

Figures

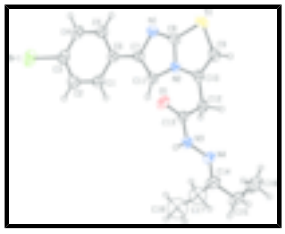


Fig. 1. View of (I), with the displacement ellipsoids for the non-H atoms drawn at the 30% probability level.

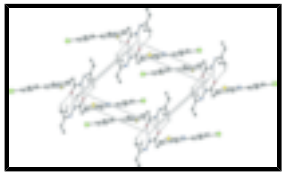


Fig. 2. A view of the packing and hydrogen bonding interactions for (I).

2-[6-(4-Bromophenyl)imidazo[2,1-*b*]thiazol-3-yl]-N'-(1- ethylpropylidene)acetohydrazide

Crystal data

$C_{18}H_{19}BrN_4OS$	$Z = 2$
$M_r = 419.34$	$F_{000} = 428$
Triclinic, $P\overline{1}$	$D_x = 1.469$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.9591$ (6) Å	Cell parameters from 27459 reflections
$b = 11.8636$ (10) Å	$\theta = 2.0$–28.0°
$c = 13.1247$ (11) Å	$\mu = 2.29$ mm^{-1}
$\alpha = 65.411$ (6)°	$T = 296$ K
$\beta = 78.892$ (7)°	Prism, colourless
$\gamma = 75.193$ (6)°	0.73 × 0.55 × 0.45 mm
$V = 947.99$ (15) Å^3	

Data collection

Stoe IPDSII diffractometer	4441 independent reflections
Monochromator: plane graphite	3359 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{int} = 0.082$
$T = 296$ K	$\theta_{max} = 27.8^\circ$
ω scans	$\theta_{min} = 2.0^\circ$
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$h = -9 \rightarrow 9$
$T_{min} = 0.285$, $T_{max} = 0.425$	$k = -15 \rightarrow 15$
17037 measured reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.061$

$wR(F^2) = 0.157$

$S = 1.02$

4441 reflections

222 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: difmap and geom

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2 + 1.3183P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 1.18$ e Å^{-3}

$\Delta\rho_{min} = -0.58$ e Å^{-3}

Extinction correction: none

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2$sigma(F^2) is used only for calculating –*R*-factor-obs *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and *R*-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.34386 (10)	0.34838 (5)	0.62926 (5)	0.0877 (3)
S1	−0.38374 (15)	0.10794 (12)	0.20860 (10)	0.0661 (4)
O1	0.2946 (4)	0.0228 (2)	0.0805 (2)	0.0620 (9)
N1	−0.1843 (4)	0.1789 (3)	0.3338 (3)	0.0514 (10)
N2	−0.0323 (4)	0.0263 (3)	0.2714 (2)	0.0409 (8)
N3	0.4446 (5)	−0.1704 (3)	0.0873 (3)	0.0476 (9)
N4	0.4402 (5)	−0.2985 (3)	0.1318 (3)	0.0499 (9)
C1	0.2832 (6)	0.1406 (4)	0.4558 (3)	0.0526 (12)
C2	0.3607 (6)	0.1905 (4)	0.5137 (3)	0.0576 (12)
C3	0.2373 (7)	0.2826 (4)	0.5476 (3)	0.0553 (14)
C4	0.0423 (7)	0.3269 (4)	0.5226 (3)	0.0569 (14)
C5	−0.0317 (6)	0.2779 (4)	0.4628 (3)	0.0528 (12)
C6	0.0875 (5)	0.1840 (3)	0.4283 (3)	0.0429 (10)
C7	0.0093 (5)	0.1322 (3)	0.3645 (3)	0.0416 (10)
C8	−0.2005 (5)	0.1129 (4)	0.2781 (3)	0.0472 (11)
C9	−0.2219 (6)	−0.0128 (4)	0.1743 (3)	0.0556 (12)
C10	−0.0436 (5)	−0.0466 (3)	0.2131 (3)	0.0442 (10)
C11	0.1039 (5)	0.0386 (3)	0.3270 (3)	0.0427 (10)
C12	0.1278 (5)	−0.1464 (3)	0.2006 (3)	0.0488 (11)
C13	0.2949 (5)	−0.0909 (3)	0.1179 (3)	0.0432 (10)
C14	0.5868 (7)	−0.3734 (4)	0.1055 (4)	0.0713 (16)
C15	0.5786 (9)	−0.5109 (4)	0.1570 (5)	0.091 (2)

C16	0.4022 (11)	−0.5455 (5)	0.2333 (7)	0.117 (3)
C17	0.7561 (11)	−0.3342 (7)	0.0056 (6)	0.114 (2)*
C18	0.8921 (15)	−0.3345 (10)	0.0640 (9)	0.161 (4)*
H1	0.36400	0.07660	0.43480	0.0630*
HN3	0.533 (6)	−0.136 (4)	0.042 (4)	0.055 (12)*
H2	0.49330	0.16260	0.52940	0.0690*
H4	−0.03900	0.38920	0.54570	0.0680*
H5	−0.16330	0.30820	0.44530	0.0630*
H9	−0.25680	−0.05030	0.13260	0.0670*
H11	0.23370	−0.00730	0.33710	0.0510*
H12A	0.08230	−0.20020	0.17520	0.0590*
H12B	0.17780	−0.19850	0.27330	0.0590*
H15A	0.58810	−0.53950	0.09660	0.1100*
H15B	0.69530	−0.55650	0.19780	0.1100*
H16A	0.39700	−0.52500	0.29740	0.1750*
H16B	0.40870	−0.63460	0.25790	0.1750*
H16C	0.28470	−0.49970	0.19490	0.1750*
H17A	0.80230	−0.39590	−0.02880	0.1370*
H17B	0.71370	−0.25130	−0.05160	0.1370*
H18A	0.84180	−0.27110	0.09520	0.2420*
H18B	1.01190	−0.31650	0.01530	0.2420*
H18C	0.92100	−0.41600	0.12380	0.2420*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1192 (5)	0.0840 (4)	0.0870 (4)	−0.0292 (3)	−0.0284 (3)	−0.0463 (3)
S1	0.0437 (5)	0.0868 (8)	0.0774 (7)	0.0001 (5)	−0.0194 (5)	−0.0427 (6)
O1	0.0670 (17)	0.0415 (14)	0.0719 (18)	−0.0176 (12)	0.0251 (14)	−0.0262 (13)
N1	0.0413 (16)	0.0578 (18)	0.0576 (18)	−0.0008 (13)	−0.0073 (13)	−0.0290 (15)
N2	0.0345 (13)	0.0475 (15)	0.0421 (14)	−0.0089 (11)	−0.0011 (11)	−0.0194 (12)
N3	0.0515 (17)	0.0403 (15)	0.0472 (16)	−0.0131 (13)	0.0056 (13)	−0.0154 (13)
N4	0.0593 (18)	0.0383 (15)	0.0482 (16)	−0.0082 (13)	−0.0050 (13)	−0.0139 (13)
C1	0.057 (2)	0.053 (2)	0.050 (2)	−0.0034 (17)	−0.0100 (16)	−0.0244 (17)
C2	0.060 (2)	0.060 (2)	0.056 (2)	−0.0087 (18)	−0.0158 (18)	−0.0231 (19)
C3	0.079 (3)	0.049 (2)	0.0434 (19)	−0.0227 (19)	−0.0082 (18)	−0.0165 (16)
C4	0.070 (3)	0.047 (2)	0.058 (2)	−0.0144 (18)	0.0023 (19)	−0.0265 (18)
C5	0.052 (2)	0.050 (2)	0.058 (2)	−0.0094 (16)	−0.0015 (16)	−0.0244 (18)
C6	0.0467 (18)	0.0420 (17)	0.0378 (16)	−0.0112 (14)	−0.0008 (13)	−0.0134 (14)
C7	0.0406 (17)	0.0428 (17)	0.0407 (16)	−0.0071 (13)	−0.0032 (13)	−0.0166 (14)
C8	0.0366 (16)	0.054 (2)	0.0498 (19)	−0.0031 (14)	−0.0070 (14)	−0.0212 (16)
C9	0.052 (2)	0.070 (2)	0.055 (2)	−0.0175 (18)	−0.0051 (16)	−0.0309 (19)
C10	0.0454 (18)	0.0487 (18)	0.0417 (17)	−0.0173 (14)	0.0030 (14)	−0.0191 (15)
C11	0.0352 (16)	0.0476 (18)	0.0459 (17)	−0.0063 (13)	−0.0070 (13)	−0.0183 (15)
C12	0.052 (2)	0.0473 (19)	0.0501 (19)	−0.0181 (16)	0.0071 (15)	−0.0220 (16)
C13	0.0479 (18)	0.0423 (18)	0.0412 (16)	−0.0112 (14)	0.0030 (14)	−0.0197 (14)
C14	0.074 (3)	0.044 (2)	0.080 (3)	−0.004 (2)	0.009 (2)	−0.020 (2)
C15	0.112 (4)	0.038 (2)	0.104 (4)	−0.002 (2)	−0.001 (3)	−0.020 (2)

C16	0.128 (5)	0.044 (3)	0.144 (6)	−0.024 (3)	0.019 (5)	−0.013 (3)

Geometric parameters (Å, °)

Br1—C3	1.899 (5)	C12—C13	1.508 (5)
S1—C8	1.730 (4)	C14—C15	1.495 (7)
S1—C9	1.744 (5)	C14—C17	1.581 (9)
O1—C13	1.228 (4)	C15—C16	1.456 (10)
N1—C7	1.388 (5)	C17—C18	1.326 (14)
N1—C8	1.309 (6)	C1—H1	0.9300
N2—C8	1.362 (6)	C2—H2	0.9300
N2—C10	1.396 (5)	C4—H4	0.9300
N2—C11	1.370 (5)	C5—H5	0.9300
N3—N4	1.389 (5)	C9—H9	0.9300
N3—C13	1.337 (5)	C11—H11	0.9300
N4—C14	1.267 (6)	C12—H12A	0.9700
N3—HN3	0.83 (5)	C12—H12B	0.9700
C1—C6	1.388 (6)	C15—H15A	0.9700
C1—C2	1.384 (6)	C15—H15B	0.9700
C2—C3	1.381 (7)	C16—H16A	0.9600
C3—C4	1.374 (7)	C16—H16B	0.9600
C4—C5	1.381 (6)	C16—H16C	0.9600
C5—C6	1.392 (6)	C17—H17A	0.9700
C6—C7	1.466 (5)	C17—H17B	0.9700
C7—C11	1.366 (5)	C18—H18A	0.9600
C9—C10	1.334 (6)	C18—H18B	0.9600
C10—C12	1.489 (5)	C18—H18C	0.9600
C8—S1—C9	89.5 (2)	C2—C1—H1	119.00
C7—N1—C8	103.6 (3)	C6—C1—H1	119.00
C8—N2—C10	115.3 (3)	C1—C2—H2	121.00
C8—N2—C11	106.2 (3)	C3—C2—H2	121.00
C10—N2—C11	138.4 (3)	C3—C4—H4	120.00
N4—N3—C13	119.5 (3)	C5—C4—H4	120.00
N3—N4—C14	118.8 (4)	C4—C5—H5	119.00
C13—N3—HN3	114 (3)	C6—C5—H5	119.00
N4—N3—HN3	126 (3)	S1—C9—H9	123.00
C2—C1—C6	121.5 (4)	C10—C9—H9	123.00
C1—C2—C3	118.7 (4)	N2—C11—H11	127.00
Br1—C3—C4	120.3 (4)	C7—C11—H11	127.00
C2—C3—C4	121.3 (4)	C10—C12—H12A	109.00
Br1—C3—C2	118.4 (4)	C10—C12—H12B	109.00
C3—C4—C5	119.3 (4)	C13—C12—H12A	109.00
C4—C5—C6	121.1 (4)	C13—C12—H12B	109.00
C1—C6—C5	118.2 (4)	H12A—C12—H12B	108.00
C5—C6—C7	121.1 (3)	C14—C15—H15A	108.00
C1—C6—C7	120.7 (4)	C14—C15—H15B	108.00
N1—C7—C11	111.0 (3)	C16—C15—H15A	108.00
N1—C7—C6	120.6 (3)	C16—C15—H15B	108.00
C6—C7—C11	128.5 (3)	H15A—C15—H15B	107.00

S1—C8—N2	110.6 (3)	C15—C16—H16A	109.00
S1—C8—N1	136.0 (3)	C15—C16—H16B	109.00
N1—C8—N2	113.5 (3)	C15—C16—H16C	109.00
S1—C9—C10	114.0 (3)	H16A—C16—H16B	109.00
N2—C10—C12	121.3 (3)	H16A—C16—H16C	110.00
C9—C10—C12	128.2 (4)	H16B—C16—H16C	109.00
N2—C10—C9	110.5 (3)	C14—C17—H17A	112.00
N2—C11—C7	105.7 (3)	C14—C17—H17B	112.00
C10—C12—C13	111.9 (3)	C18—C17—H17A	112.00
O1—C13—N3	121.1 (3)	C18—C17—H17B	112.00
N3—C13—C12	117.5 (3)	H17A—C17—H17B	110.00
O1—C13—C12	121.4 (3)	C17—C18—H18A	109.00
N4—C14—C17	126.0 (5)	C17—C18—H18B	109.00
N4—C14—C15	117.2 (5)	C17—C18—H18C	109.00
C15—C14—C17	115.6 (5)	H18A—C18—H18B	109.00
C14—C15—C16	116.4 (5)	H18A—C18—H18C	109.00
C14—C17—C18	98.4 (7)	H18B—C18—H18C	109.00
C8—S1—C9—C10	0.2 (3)	C6—C1—C2—C3	2.1 (6)
C9—S1—C8—N1	179.7 (4)	C1—C2—C3—Br1	178.9 (3)
C9—S1—C8—N2	0.3 (3)	C1—C2—C3—C4	−1.5 (6)
C8—N1—C7—C6	179.2 (3)	Br1—C3—C4—C5	179.8 (3)
C8—N1—C7—C11	−0.4 (4)	C2—C3—C4—C5	0.3 (6)
C7—N1—C8—S1	−178.9 (4)	C3—C4—C5—C6	0.5 (6)
C7—N1—C8—N2	0.5 (4)	C4—C5—C6—C7	−179.8 (4)
C11—N2—C10—C12	1.2 (6)	C4—C5—C6—C1	0.1 (6)
C10—N2—C8—S1	−0.7 (4)	C1—C6—C7—N1	−177.8 (4)
C10—N2—C8—N1	179.7 (3)	C5—C6—C7—C11	−178.3 (4)
C8—N2—C11—C7	0.2 (4)	C1—C6—C7—C11	1.8 (6)
C11—N2—C8—N1	−0.5 (4)	C5—C6—C7—N1	2.1 (5)
C11—N2—C8—S1	179.2 (2)	N1—C7—C11—N2	0.2 (4)
C8—N2—C10—C12	−179.0 (3)	C6—C7—C11—N2	−179.5 (3)
C10—N2—C11—C7	180.0 (4)	S1—C9—C10—C12	179.2 (3)
C11—N2—C10—C9	−178.9 (4)	S1—C9—C10—N2	−0.7 (4)
C8—N2—C10—C9	0.9 (4)	N2—C10—C12—C13	−73.2 (4)
N4—N3—C13—O1	179.7 (3)	C9—C10—C12—C13	106.9 (4)
N4—N3—C13—C12	0.2 (5)	C10—C12—C13—O1	9.8 (5)
C13—N3—N4—C14	−177.3 (4)	C10—C12—C13—N3	−170.7 (3)
N3—N4—C14—C15	178.7 (4)	N4—C14—C15—C16	−0.3 (8)
N3—N4—C14—C17	−14.5 (7)	C17—C14—C15—C16	−168.4 (6)
C2—C1—C6—C7	178.5 (4)	N4—C14—C17—C18	96.4 (8)
C2—C1—C6—C5	−1.4 (6)	C15—C14—C17—C18	−96.7 (8)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—HN3···O1^{i}	0.83 (5)	2.03 (5)	2.844 (4)	169 (4)
C17—H17B···O1^{i}	0.97	2.56	3.326 (9)	136

Symmetry codes: (i) −*x*+1, −*y*, −*z*.

Fig. 1

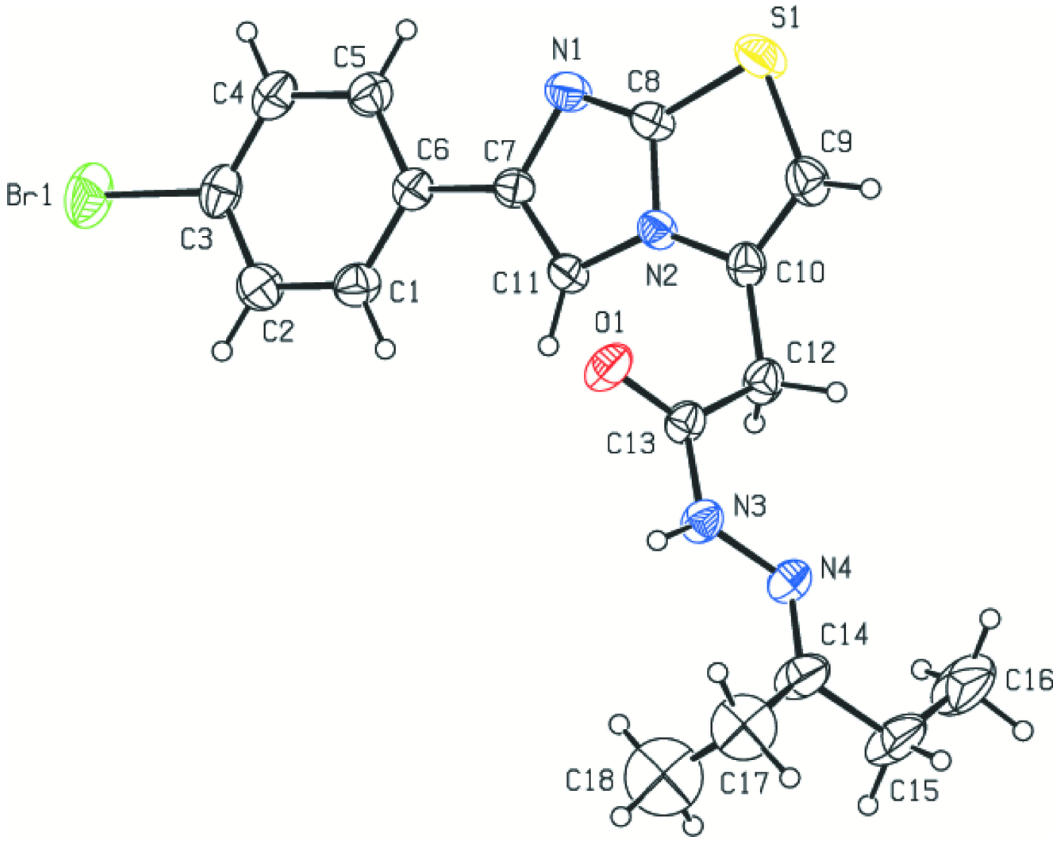

S1
N1
C8
C5
C4
C6
C7
C9
Br1
C3
N2
C10
C11
C1
C2
O1
C12
C13
N3
N4
C14
C16
C18
C17
C15

Fig. 2