



Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

3-[[6-(4-Chlorophenyl)imidazo[2,1-b]-[1,3,4]thiadiazol-2-yl]methyl]-1,2-benzoxazole

Afshan Banu,^a Mohamed Ziaulla,^a Noor Shahina Begum,^{a*} Ravi S. Lamani^b and I. M. Khazi^b^aDepartment of Studies in Chemistry, Bangalore University, Bangalore 560 001, India, and ^bDepartment of Chemistry, Karnatak University, Dharwad 580 003, India
Correspondence e-mail: noorsb@rediffmail.com

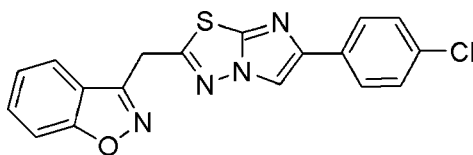
Received 1 January 2011; accepted 7 February 2011

Key indicators: single-crystal X-ray study; $T = 123$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.053; wR factor = 0.185; data-to-parameter ratio = 15.0.

In the title compound, $\text{C}_{18}\text{H}_{11}\text{ClN}_4\text{OS}$, the benzisoxazole and imidazothiadiazole rings are inclined at an angle of $23.81(7)^\circ$ with respect to each other. The imidazothiadiazole and chlorophenyl rings make a dihedral angle of $27.34(3)^\circ$. In the crystal, intermolecular $\text{C}-\text{H}\cdots\text{N}$ interactions generate a chain along the c axis and $\text{C}-\text{H}\cdots\text{O}$ interactions form centrosymmetric dimers resulting in an $R_2^2(26)$ graph-set motif. Moreover, the $\text{C}-\text{H}\cdots\text{N}$ and $\text{S}\cdots\text{N}$ [$3.206(4)$ Å] interactions links the molecules into $R(7)$ ring motifs. The packing is further stabilized by $\pi-\pi$ stacking interactions between the thiadiazole rings with a shortest centroid-centroid distance of $3.497(3)$ Å. In addition, $\text{C}-\text{H}\cdots\pi$ interactions are observed in the crystal structure

Related literature

For the preparation of the title compound see: Lamani *et al.* (2009). For the biological activity of benzisoxazole derivatives, see: Priya *et al.* (2005). For the use of five-membered heterocyclic ring 1,3,4-thiadiazoles in the design of compounds, see: Katritzky (1984); Diamond & Sevrain (2003a,b); Nakao *et al.* (2002a,b). For related structures, see: Sun & Zhang (2009). For hydrogen-bond motifs, see: Bernstein *et al.* (1995)



Experimental

Crystal data

 $\text{C}_{18}\text{H}_{11}\text{ClN}_4\text{OS}$
 $M_r = 366.83$ Monoclinic, $C2/c$
 $a = 38.419(7)$ Å $b = 5.7761(10)$ Å
 $c = 14.772(3)$ Å
 $\beta = 108.004(5)^\circ$
 $V = 3117.5(10)$ Å³
 $Z = 8$ Mo $K\alpha$ radiation
 $\mu = 0.39$ mm⁻¹
 $T = 123$ K
 $0.18 \times 0.16 \times 0.16$ mm

Data collection

Bruker SMART APEX CCD
detector diffractometer
Absorption correction: multi-scan
Bruker Smart Apex
 $T_{\min} = 0.933$, $T_{\max} = 0.940$ 8822 measured reflections
3379 independent reflections
2587 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.051$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.185$
 $S = 1.31$
3379 reflections226 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.74$ e Å⁻³
 $\Delta\rho_{\min} = -0.58$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

 $\text{Cg}1$ and $\text{Cg}2$ are the centroids of the $\text{C}7-\text{C}12$ and $\text{C}13-\text{C}18$ rings, respectively.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}9-\text{H}9\cdots\text{O}1^i$	0.93	2.39	3.232 (4)	150
$\text{C}2-\text{H}2\text{B}\cdots\text{N}1^{\text{ii}}$	0.97	2.49	3.352 (4)	148
$\text{C}5-\text{H}5\cdots\text{N}1^{\text{iii}}$	0.93	2.60	3.478 (4)	157
$\text{C}17-\text{H}17\cdots\text{Cg}1^{\text{iv}}$	0.93	2.78	3.470 (4)	131
$\text{C}11-\text{H}11\cdots\text{Cg}2^{\text{iv}}$	0.93	2.93	3.548 (4)	126

Symmetry codes: (i) $-x + \frac{1}{2}, -y + \frac{3}{2}, -z$; (ii) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$; (iii) $x, y - 1, z$; (iv) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT-Plus (Bruker, 1998); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997) and CAMERON (Watkin *et al.*, 1996); software used to prepare material for publication: WinGX (Farrugia, 1999).

NSB is thankful to the University Grants Commission (UGC), India, for financial assistance and the Department of Science and Technology, (DST), India, for the data-collection facility under the IRHPA-DST program.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2098).

References

- Bernstein, J., Davis, R. E., Shimon, L. & Chang, N.-L. (1995). *Angew. Chem.* **34**, 1555–1573.
- Bruker (1998). SMART and SAINT-Plus. Bruker AXS Inc., Madison, Wisconsin, USA.
- Diamond, S. & Sevrain, C. (2003a). *Chem Abstr.* **138**, 198554.
- Diamond, S. & Sevrain, C. (2003b). PCT Int. Appl. WO 2003016870.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Katritzky, A. R. (1984). In *Comprehensive Heterocyclic Chemistry*. Oxford: Pergamon.
- Lamani, R. S., Shetty, N. S., Ravindra, R. & Khazi, I. A. M. (2009). *Eur. J. Med. Chem.* **44**, 2828–2833.
- Nakao, H., Matsuzaki, Y., Tohnishi, M., Mmorimoto, M., Fujioka, S., Takemoto, T. & Mamezuka, K. (2002a). *Chem Abstr.* **137**, 384845.
- Nakao, H., Matsuzaki, Y., Tohnishi, M., Mmorimoto, M., Fujioka, S., Takemoto, T. & Mamezuka, K. (2002b). PCT Int. Appl. WO 2002092584.

Priya, B. S., Basappa., Swamy, S. N., Rangappa, K. S. (2005). *Bioorg. Med. Chem.* **13**, 2623–2628.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

Sun, Y. & Zhang, H.-H. (2009). *Acta Cryst.* **E65**, o1647.
Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.

supplementary materials

Acta Cryst. (2011). E67, o617-o618 [doi:10.1107/S1600536811004582]

3-{{[6-(4-Chlorophenyl)imidazo[2,1-*b*][1,3,4]thiadiazol-2-yl]methyl}-1,2-benzoxazole

A. Banu, M. Ziaulla, N. S. Begum, R. S. Lamani and I. M. Khazi

Comment

Imidazo[2,1-*b*][1,3,4]thiadiazole derivatives are reported to possess diverse pharmacological properties such as anticancer, antitubercular, antibacterial, antifungal, anticonvulsant, analgesic and antisecretory activities. Moreover, they are known to possess important biological activities (Priya *et al.*, 2005) and are useful in different therapies. Amongst them, five membered heterocyclic ring 1,3,4-thiadiazoles find wide application in designing compounds possessing useful properties (Katritzky *et al.*, 1984; Diamond & Sevrain, 2003*a,b*; Nakao *et al.*, 2002*a,b*). Due to the increasing importance of these heterocycles in biological and pharmaceutical fields, new chemical entities were synthesized by incorporating active pharmacophores in a single molecular framework so as to enhance their biological activities. In the title compound, the benzisoxazole (O1/N4/C3/C13–18) and imidazothiadiazole (S1/N1–N3/C1/C4–C6) rings are individually planar similar to those reported earlier (Sun & Zhang, 2009) with maximum deviations of 0.038 (3) Å for C1 and 0.016 (3) Å for C3 respectively. The mean planes of the benzisoxazole and imidazothiadiazole are inclined at an angle 23.81 (7)° with each other. The imidazothiadiazole and chlorophenyl rings make a dihedral angle of 27.34 (3)°. The thiadiazole moiety displays differences in the bond lengths between S1–C1/S1–C4 [1.756 (3)/1.736 (3)]. This can be attributed to the resonance effects of the imidazole ring which is stronger than that due to thiadiazole group. The crystal structure is stabilized by intermolecular C–H⋯N, C–H⋯O and S⋯N interactions. The C–H⋯N interaction generates chain like pattern along *c* axis. The C–H⋯O interaction forms centrosymmetric head-to-head dimers about inversion centers corresponding to R22(26) graph set motif (Bernstein *et al.*, 1995). The C–H⋯N interaction along with S⋯N [3.206 (4) Å] interaction results in a ring motif with a graph set *R*(7). The molecular packing is further stabilized by π - π stacking interactions between thiadiazole rings (*Cg*3: centroid of S1/C1/N2/N3/C4) with the shortest centroid–centroid distance 3.497 (3) Å. In addition, π -ring interactions of the type C–H⋯*Cg* (*Cg* being the centroids of rings C7–C12 and C13–C18) are also observed in the crystal structure; details have been given in Table 1.

Experimental

The title compound was synthesized by following the procedure reported earlier (Lamani *et al.*, 2009).

Refinement

The H atoms were placed at calculated positions in the riding model approximation with aromatic C–H = 0.93 Å and methylene C–H = 0.97 Å, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N/C})$.

Figures

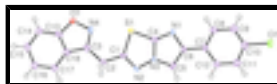


Fig. 1. ORTEP (Farrugia, 1997) view of the title compound, showing 50% probability ellipsoids and the atom numbering scheme.



Fig. 2. A unit cell packing of the title compound depicting the C—H...N, C—H...O and S...N intermolecular interactions with dotted lines. H-atoms not involved in hydrogen bonding have been excluded.

3-[[6-(4-Chlorophenyl)imidazo[2,1-b][1,3,4]thiadiazol-2-yl]methyl]- 1,2-benzoxazole

Crystal data

$C_{18}H_{11}ClN_4OS$	$F(000) = 1504$
$M_r = 366.83$	$D_x = 1.563 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: $-C 2yc$	Cell parameters from 3379 reflections
$a = 38.419 (7) \text{ \AA}$	$\theta = 2.2\text{--}27.0^\circ$
$b = 5.7761 (10) \text{ \AA}$	$\mu = 0.39 \text{ mm}^{-1}$
$c = 14.772 (3) \text{ \AA}$	$T = 123 \text{ K}$
$\beta = 108.004 (5)^\circ$	Block, yellow
$V = 3117.5 (10) \text{ \AA}^3$	$0.18 \times 0.16 \times 0.16 \text{ mm}$
$Z = 8$	

Data collection

Bruker SMART APEX CCD detector diffractometer	3379 independent reflections
Radiation source: fine-focus sealed tube graphite	2587 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.051$
Absorption correction: multi-scan Bruker Smart Apex	$\theta_{\text{max}} = 27.0^\circ$, $\theta_{\text{min}} = 2.2^\circ$
$T_{\text{min}} = 0.933$, $T_{\text{max}} = 0.940$	$h = -46 \rightarrow 48$
8822 measured reflections	$k = -6 \rightarrow 7$
	$l = -18 \rightarrow 14$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.053$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.185$	H-atom parameters constrained
$S = 1.31$	$w = 1/[\sigma^2(F_o^2) + (0.0894P)^2]$
3379 reflections	where $P = (F_o^2 + 2F_c^2)/3$
226 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.74 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.58 \text{ e \AA}^{-3}$

Special details

Experimental. The compound was synthesized by following the procedure given in Lamani *et al.*, (2009)

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness 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 threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R -factors(gt) *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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.19871 (8)	0.2236 (5)	0.1424 (2)	0.0151 (6)
C2	0.16451 (8)	0.1564 (5)	0.1657 (2)	0.0183 (7)
H2A	0.1565	0.0071	0.1366	0.022*
H2B	0.1711	0.1355	0.2341	0.022*
C3	0.13263 (8)	0.3171 (5)	0.1363 (2)	0.0166 (7)
C4	0.25323 (8)	0.4023 (5)	0.1246 (2)	0.0160 (7)
C5	0.28417 (8)	0.0835 (6)	0.1177 (2)	0.0167 (6)
H5	0.2910	-0.0704	0.1157	0.020*
C6	0.30436 (8)	0.2790 (5)	0.1142 (2)	0.0149 (6)
C7	0.34193 (8)	0.2930 (5)	0.1098 (2)	0.0148 (7)
C8	0.35464 (9)	0.4896 (5)	0.0746 (2)	0.0181 (7)
H8	0.3389	0.6139	0.0527	0.022*
C9	0.39034 (9)	0.5024 (5)	0.0718 (2)	0.0192 (7)
H9	0.3986	0.6340	0.0484	0.023*
C10	0.41322 (8)	0.3176 (6)	0.1039 (2)	0.0183 (7)
C11	0.40183 (9)	0.1192 (6)	0.1396 (2)	0.0206 (7)
H11	0.4178	-0.0038	0.1616	0.025*
C12	0.36610 (8)	0.1082 (6)	0.1418 (2)	0.0178 (7)
H12	0.3580	-0.0244	0.1649	0.021*
C13	0.07777 (9)	0.4766 (5)	0.1117 (2)	0.0176 (7)
C14	0.04157 (9)	0.5159 (6)	0.1076 (2)	0.0209 (7)
H14	0.0292	0.6519	0.0834	0.025*
C15	0.02526 (9)	0.3370 (6)	0.1424 (2)	0.0219 (7)
H15	0.0010	0.3519	0.1407	0.026*
C16	0.04440 (8)	0.1336 (6)	0.1800 (3)	0.0212 (7)
H16	0.0326	0.0188	0.2036	0.025*
C17	0.08036 (8)	0.1001 (6)	0.1828 (2)	0.0178 (7)
H17	0.0928	-0.0352	0.2074	0.021*
C18	0.09718 (8)	0.2764 (5)	0.1474 (2)	0.0166 (7)
O1	0.09977 (6)	0.6281 (4)	0.08271 (17)	0.0222 (5)
N1	0.28445 (7)	0.4813 (4)	0.11762 (19)	0.0161 (6)

supplementary materials

N2	0.22129 (7)	0.0628 (5)	0.13533 (19)	0.0171 (6)
N3	0.25177 (7)	0.1673 (4)	0.12454 (19)	0.0158 (6)
N4	0.13496 (7)	0.5207 (5)	0.1006 (2)	0.0208 (6)
S1	0.21240 (2)	0.51078 (13)	0.13431 (6)	0.0182 (2)
Cl1	0.45843 (2)	0.33439 (15)	0.10073 (6)	0.0267 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0141 (14)	0.0126 (15)	0.0175 (16)	0.0005 (12)	0.0032 (13)	0.0015 (12)
C2	0.0170 (15)	0.0154 (16)	0.0248 (18)	0.0016 (12)	0.0095 (14)	0.0034 (13)
C3	0.0197 (15)	0.0141 (15)	0.0155 (16)	-0.0028 (12)	0.0049 (13)	-0.0002 (12)
C4	0.0202 (15)	0.0121 (15)	0.0152 (16)	0.0008 (12)	0.0047 (13)	-0.0006 (12)
C5	0.0152 (14)	0.0138 (15)	0.0214 (16)	0.0032 (12)	0.0062 (13)	0.0002 (13)
C6	0.0131 (14)	0.0162 (16)	0.0153 (16)	-0.0011 (12)	0.0042 (13)	0.0011 (12)
C7	0.0137 (14)	0.0156 (16)	0.0159 (16)	-0.0034 (12)	0.0054 (12)	-0.0023 (12)
C8	0.0206 (16)	0.0157 (16)	0.0191 (17)	0.0021 (12)	0.0078 (14)	0.0006 (12)
C9	0.0252 (17)	0.0161 (17)	0.0176 (17)	-0.0052 (13)	0.0086 (14)	-0.0021 (12)
C10	0.0142 (14)	0.0231 (17)	0.0179 (17)	-0.0048 (12)	0.0051 (13)	-0.0056 (13)
C11	0.0231 (16)	0.0177 (17)	0.0220 (18)	0.0049 (13)	0.0084 (14)	-0.0019 (13)
C12	0.0193 (15)	0.0169 (16)	0.0178 (17)	0.0012 (13)	0.0067 (13)	0.0014 (13)
C13	0.0190 (16)	0.0158 (16)	0.0204 (17)	-0.0004 (12)	0.0096 (14)	0.0009 (13)
C14	0.0194 (16)	0.0200 (17)	0.0220 (18)	0.0035 (13)	0.0042 (14)	0.0000 (13)
C15	0.0177 (16)	0.0283 (19)	0.0209 (18)	-0.0017 (13)	0.0077 (14)	-0.0013 (14)
C16	0.0149 (15)	0.0216 (17)	0.0276 (19)	-0.0029 (13)	0.0075 (14)	0.0010 (14)
C17	0.0172 (15)	0.0163 (16)	0.0202 (17)	0.0005 (12)	0.0060 (13)	0.0023 (13)
C18	0.0136 (14)	0.0178 (16)	0.0183 (16)	0.0011 (12)	0.0049 (13)	-0.0003 (13)
O1	0.0200 (11)	0.0167 (12)	0.0325 (14)	0.0044 (9)	0.0120 (11)	0.0055 (10)
N1	0.0114 (12)	0.0167 (14)	0.0206 (14)	0.0006 (10)	0.0054 (11)	-0.0008 (11)
N2	0.0127 (12)	0.0178 (14)	0.0211 (15)	-0.0055 (10)	0.0059 (11)	0.0001 (11)
N3	0.0174 (13)	0.0115 (13)	0.0189 (15)	-0.0012 (10)	0.0059 (11)	0.0013 (10)
N4	0.0147 (13)	0.0244 (16)	0.0251 (16)	0.0015 (11)	0.0087 (12)	0.0010 (12)
S1	0.0184 (4)	0.0124 (4)	0.0257 (5)	-0.0008 (3)	0.0096 (4)	-0.0007 (3)
Cl1	0.0177 (4)	0.0329 (5)	0.0318 (5)	-0.0021 (3)	0.0110 (4)	-0.0057 (4)

Geometric parameters (\AA , $^\circ$)

C1—N2	1.297 (4)	C9—C10	1.371 (4)
C1—C2	1.508 (4)	C9—H9	0.9300
C1—S1	1.756 (3)	C10—C11	1.387 (5)
C2—C3	1.490 (4)	C10—Cl1	1.755 (3)
C2—H2A	0.9700	C11—C12	1.384 (4)
C2—H2B	0.9700	C11—H11	0.9300
C3—N4	1.304 (4)	C12—H12	0.9300
C3—C18	1.440 (4)	C13—O1	1.374 (4)
C4—N1	1.316 (4)	C13—C14	1.392 (4)
C4—N3	1.358 (4)	C13—C18	1.389 (4)
C4—S1	1.736 (3)	C14—C15	1.387 (5)
C5—C6	1.380 (4)	C14—H14	0.9300

C5—N3	1.369 (4)	C15—C16	1.406 (5)
C5—H5	0.9300	C15—H15	0.9300
C6—N1	1.406 (4)	C16—C17	1.383 (4)
C6—C7	1.468 (4)	C16—H16	0.9300
C7—C12	1.398 (4)	C17—C18	1.392 (4)
C7—C8	1.398 (4)	C17—H17	0.9300
C8—C9	1.387 (4)	O1—N4	1.436 (3)
C8—H8	0.9300	N2—N3	1.370 (3)
N2—C1—C2	119.1 (3)	C12—C11—C10	118.5 (3)
N2—C1—S1	116.7 (2)	C12—C11—H11	120.7
C2—C1—S1	124.0 (2)	C10—C11—H11	120.7
C3—C2—C1	117.9 (3)	C11—C12—C7	121.1 (3)
C3—C2—H2A	107.8	C11—C12—H12	119.4
C1—C2—H2A	107.8	C7—C12—H12	119.4
C3—C2—H2B	107.8	O1—C13—C14	125.8 (3)
C1—C2—H2B	107.8	O1—C13—C18	109.8 (3)
H2A—C2—H2B	107.2	C14—C13—C18	124.4 (3)
N4—C3—C18	112.3 (3)	C13—C14—C15	115.0 (3)
N4—C3—C2	121.8 (3)	C13—C14—H14	122.5
C18—C3—C2	125.9 (3)	C15—C14—H14	122.5
N1—C4—N3	112.7 (3)	C14—C15—C16	121.9 (3)
N1—C4—S1	138.5 (3)	C14—C15—H15	119.1
N3—C4—S1	108.8 (2)	C16—C15—H15	119.1
C6—C5—N3	104.3 (3)	C17—C16—C15	121.6 (3)
C6—C5—H5	127.8	C17—C16—H16	119.2
N3—C5—H5	127.8	C15—C16—H16	119.2
C5—C6—N1	111.2 (3)	C16—C17—C18	117.5 (3)
C5—C6—C7	128.2 (3)	C16—C17—H17	121.3
N1—C6—C7	120.6 (3)	C18—C17—H17	121.3
C12—C7—C8	118.3 (3)	C17—C18—C13	119.7 (3)
C12—C7—C6	120.2 (3)	C17—C18—C3	136.7 (3)
C8—C7—C6	121.5 (3)	C13—C18—C3	103.7 (3)
C9—C8—C7	121.1 (3)	C13—O1—N4	107.6 (2)
C9—C8—H8	119.4	C4—N1—C6	103.5 (2)
C7—C8—H8	119.4	C1—N2—N3	108.1 (3)
C10—C9—C8	118.8 (3)	C4—N3—N2	118.5 (3)
C10—C9—H9	120.6	C4—N3—C5	108.4 (3)
C8—C9—H9	120.6	N2—N3—C5	133.0 (3)
C9—C10—C11	122.1 (3)	C3—N4—O1	106.6 (2)
C9—C10—C11	118.8 (2)	C4—S1—C1	87.82 (14)
C11—C10—C11	119.1 (2)		
N2—C1—C2—C3	-155.9 (3)	O1—C13—C18—C3	-0.9 (3)
S1—C1—C2—C3	30.1 (4)	C14—C13—C18—C3	179.8 (3)
C1—C2—C3—N4	-7.1 (5)	N4—C3—C18—C17	-177.9 (4)
C1—C2—C3—C18	176.2 (3)	C2—C3—C18—C17	-0.9 (6)
N3—C5—C6—N1	-0.8 (3)	N4—C3—C18—C13	1.6 (4)
N3—C5—C6—C7	177.9 (3)	C2—C3—C18—C13	178.6 (3)
C5—C6—C7—C12	-22.8 (5)	C14—C13—O1—N4	179.2 (3)

supplementary materials

N1—C6—C7—C12	155.8 (3)	C18—C13—O1—N4	0.0 (3)
C5—C6—C7—C8	157.7 (3)	N3—C4—N1—C6	-0.8 (3)
N1—C6—C7—C8	-23.7 (4)	S1—C4—N1—C6	178.9 (3)
C12—C7—C8—C9	-0.3 (5)	C5—C6—N1—C4	1.0 (3)
C6—C7—C8—C9	179.2 (3)	C7—C6—N1—C4	-177.8 (3)
C7—C8—C9—C10	0.2 (5)	C2—C1—N2—N3	-173.3 (3)
C8—C9—C10—C11	-0.3 (5)	S1—C1—N2—N3	1.1 (3)
C8—C9—C10—C11	-179.8 (2)	N1—C4—N3—N2	177.4 (3)
C9—C10—C11—C12	0.5 (5)	S1—C4—N3—N2	-2.5 (3)
C11—C10—C11—C12	180.0 (2)	N1—C4—N3—C5	0.3 (4)
C10—C11—C12—C7	-0.7 (5)	S1—C4—N3—C5	-179.5 (2)
C8—C7—C12—C11	0.6 (5)	C1—N2—N3—C4	0.9 (4)
C6—C7—C12—C11	-179.0 (3)	C1—N2—N3—C5	177.1 (3)
O1—C13—C14—C15	-179.3 (3)	C6—C5—N3—C4	0.3 (3)
C18—C13—C14—C15	-0.1 (5)	C6—C5—N3—N2	-176.1 (3)
C13—C14—C15—C16	0.9 (5)	C18—C3—N4—O1	-1.7 (4)
C14—C15—C16—C17	-1.1 (5)	C2—C3—N4—O1	-178.8 (3)
C15—C16—C17—C18	0.4 (5)	C13—O1—N4—C3	1.1 (3)
C16—C17—C18—C13	0.4 (5)	N1—C4—S1—C1	-177.4 (4)
C16—C17—C18—C3	179.8 (4)	N3—C4—S1—C1	2.4 (2)
O1—C13—C18—C17	178.7 (3)	N2—C1—S1—C4	-2.1 (3)
C14—C13—C18—C17	-0.6 (5)	C2—C1—S1—C4	172.1 (3)

Hydrogen-bond geometry (\AA , $^\circ$)

Cg1 and Cg2 are the centroids of the C7—C12 and C13—C18 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C9—H9 \cdots O1 ⁱ	0.93	2.39	3.232 (4)	150
C2—H2B \cdots N1 ⁱⁱ	0.97	2.49	3.352 (4)	148
C5—H5 \cdots N1 ⁱⁱⁱ	0.93	2.60	3.478 (4)	157
C17—H17 \cdots Cg1 ^{iv}	0.93	2.78	3.470 (4)	131
C11—H11 \cdots Cg2 ^{iv}	0.93	2.93	3.548 (4)	126

Symmetry codes: (i) $-x+1/2, -y+3/2, -z$; (ii) $-x+1/2, y-1/2, -z+1/2$; (iii) $x, y-1, z$; (iv) $-x+1/2, y+1/2, -z+1/2$.

Fig. 1

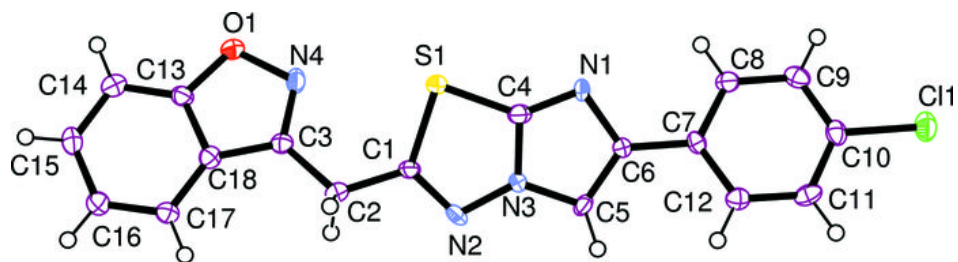
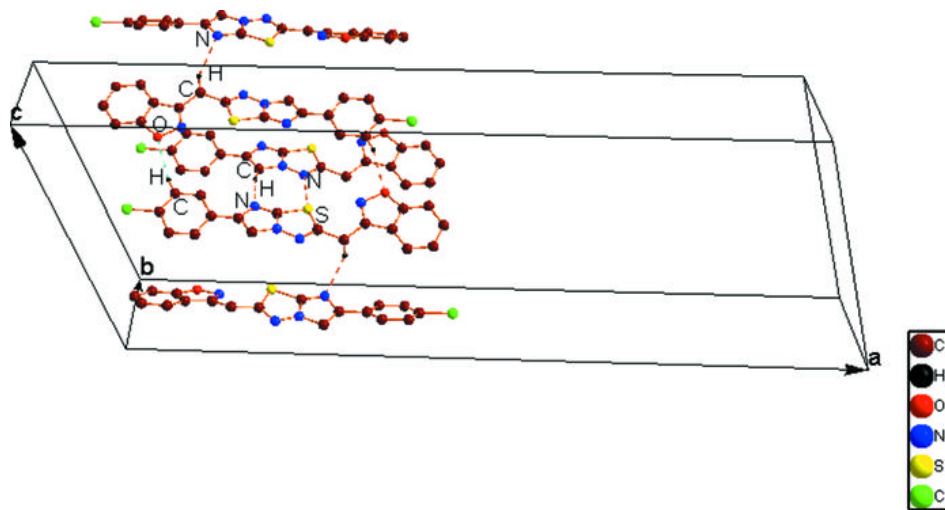


Fig. 2



Copyright of Acta Crystallographica: Section E (International Union of Crystallography - IUCr) is the property of International Union of Crystallography - IUCr and its content may not be copied or emailed to multiple sites or posted to a listserv without the copyright holder's express written permission. However, users may print, download, or email articles for individual use.