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4-{2-[2-(4-Chlorobenzylidene)hydrazinylidene]-3,6-dihydro-2*H*-1,3,4-thiadiazin-5-yl}-3-phenylsydnone

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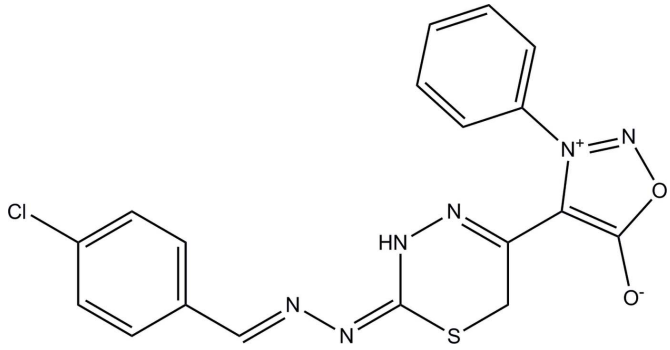
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.113; data-to-parameter ratio = 25.2.

The title compound, $C_{18}H_{13}ClN_6O_2S$, exists in *trans* and *cis* configurations with respect to the acyclic C=N bonds [C=N = 1.2837 (15) and 1.3000 (14) Å, respectively]. The 3,6-dihydro-2*H*-1,3,4-thiadiazine ring adopts a half-boat conformation. The sydnone ring is approximately planar [maximum deviation = 0.002 (1) Å] and forms dihedral angles of 50.45 (7) and 61.21 (6)° with the aromatic rings. In the crystal, intermolecular N—H···N, C—H···Cl and C—H···S hydrogen bonds link the molecules into layers parallel to *ab* plane. The crystal packing is stabilized by C—H···π interactions and further consolidated by π–π interactions involving the phenyl rings [centroid–centroid distance = 3.6306 (7) Å].



Experimental

Crystal data

$C_{18}H_{13}ClN_6O_2S$
M_r = 412.85
Triclinic, $P\overline{1}$
a = 7.3180 (3) Å
b = 10.1567 (5) Å
c = 12.4721 (6) Å
α = 96.686 (1)°
β = 95.285 (1)°
γ = 95.229 (1)°
V = 911.92 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 100 K
0.51 × 0.23 × 0.07 mm

Data collection

Bruker SMART APEXII DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.842, T_{max} = 0.976
18115 measured reflections
6480 independent reflections
5506 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.113
S = 1.05
6480 reflections
257 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Related literature

For background to sydnones and their biological activity, see: Newton & Ramsden (1982); Wagner & Hill (1974); Kalluraya & Rahiman (1997); Kalluraya *et al.* (2003). For related structures, see: Fun *et al.* (2010); Fun, Loh *et al.* (2011); Fun, Quah *et al.* (2011). For ring conformations, see: Cremer & Pople (1975). For bond-length data, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).

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

*Cg*2 is the centroid of the C1–C6 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
N3—H1*N*3···N2^{i}	0.84 (2)	2.03 (2)	2.8752 (14)	178 (2)
C9—H9*A*···Cl1^{ii}	0.97	2.78	3.4904 (13)	130
C18—H18*A*···S1^{iii}	0.93	2.86	3.6729 (12)	147
C17—H17*A*···*Cg*2^{iv}	0.93	2.64	3.5208 (15)	158

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2294).

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supplementary materials

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4-{2-[2-(4-Chlorobenzylidene)hydrazinylidene]-3,6-dihydro-2*H*-1,3,4-thiadiazin-5-yl}-3-phenylsydnone

H.-K. Fun, W.-S. Loh, Nithinchandra and B. Kalluraya

Comment

Sydnones are a class of mesoionic compounds containing a 1,2,3-oxadiazole ring system. A number of sydnone derivatives have shown diverse biological activities such as anti-inflammatory, analgesic and anti-arthritic (Newton & Ramsden, 1982; Wagner & Hill, 1974) properties. Sydnones possessing heterocyclic moieties at the 4-position are also known for a wide range of biological properties (Kalluraya & Rahiman, 1997). Encouraged by these reports and in continuation of our research for biologically active nitrogen-containing heterocycles, a thiadiazine moiety at the 4-position of the phenylsydnone was introduced. The title compound was synthesized by the condensation of 4-bromoacetyl-3-arylsydnones with *N*'-[(4-chlorophenyl)methylidene]thiocarbonohydrazide. 4-Bromoacetyl-3-arylsydnones were in turn obtained by the photochemical bromination of 4-acetyl-3-arylsydnones (Kalluraya *et al.*, 2003).

The title compound (Fig. 1) exists in *trans* and *cis* configurations with respect to the acyclic C7═N1 and C8═N2 bonds [C7═N1 = 1.2837 (15) Å and C8═N2 = 1.3000 (14) Å], respectively. The 3,6-dihydro-2*H*-1,3,4-thiadiazine ring (N3/N4/C10/C9/S1) adopts a half-boat conformation with the puckering parameter (Cremer & Pople, 1975), Q = 0.5266 (11) Å; Θ = 108.31 (12)°; φ = 138.02 (13)°. The sydnone ring (N5/N6/O1/C12/C11) is approximately planar with a maximum deviation of 0.002 (1) Å at atom N5 and forms dihedral angles of 50.45 (7)° and 61.21 (6)° with the phenyl rings (C1–C6 & C13–C18), respectively. Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges and are comparable to the related structures (Fun *et al.*, 2010; Fun & Loh *et al.*, 2011; Fun & Quah *et al.*, 2011).

In the crystal packing (Fig. 2), intermolecular N3—H1N3···N2, C9—H9A···Cl1 and C18—H18A···S1 hydrogen bonds (Table 1) link the molecules into layers parallel to *ab* plane. The crystal packing is stabilized by C—H···π interactions (Table 1) and further consolidated by π–π interactions (Table 1), involving the centroids of phenyl rings (*Cg*1; C13–C18) with the separation of $Cg1\cdots Cg1^{v}$ being 3.6306 (7) Å [symmetry code: (v) -1 - *x*, -*y*, 1 - *z*].

Experimental

To a solution of 4-bromoacetyl-3-(*p*-anisyl)sydnone (0.01 mol) and *N*'-[(4-chlorophenyl)methylidene]thiocarbonohydrazide (0.01 mol) in ethanol, a catalytic amount of anhydrous sodium acetate was added. The solution was stirred at room temperature for 2–3 h. The solid product that separated out was filtered and dried. It was then recrystallized from ethanol. Crystals suitable for X-ray analysis were obtained from 1:2 mixtures of DMF and ethanol by slow evaporation.

Refinement

H1N3 was located from the difference Fourier map and refined freely [N–H = 0.84 (2) Å]. The remaining H atoms were positioned geometrically and refined using a riding model with U_{iso}(H) = 1.2 U_{eq}(C) [C–H = 0.93 or 0.97 Å].

Figures

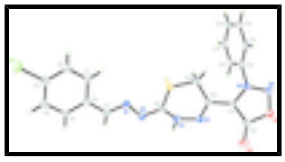

Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

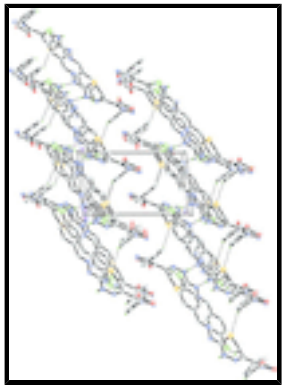

Fig. 2. The crystal packing of the title compound, viewed along the *b* axis. H atoms not involved in the intermolecular interactions (dashed lines) have been omitted for clarity.

4-{2-[2-(4-Chlorobenzylidene)hydrazinylidene]-3,6-dihydro-2*H*- 1,3,4-thiadiazin-5-yl}-3-phenyl-1,2,3-oxadiazol-3-ium-5-olate

Crystal data

$C_{18}H_{13}ClN_6O_2S$	$Z = 2$
$M_r = 412.85$	$F(000) = 424$
Triclinic, $P\overline{1}$	$D_x = 1.504$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.3180$ (3) Å	Cell parameters from 8568 reflections
$b = 10.1567$ (5) Å	$\theta = 2.8$–$35.0°$
$c = 12.4721$ (6) Å	$\mu = 0.35$ mm^{-1}
$\alpha = 96.686$ (1)°	$T = 100$ K
$\beta = 95.285$ (1)°	Plate, light purple
$\gamma = 95.229$ (1)°	0.51 × 0.23 × 0.07 mm
$V = 911.92$ (7) Å^3	

Data collection

Bruker SMART APEXII DUO CCD area-detector diffractometer	6480 independent reflections
Radiation source: fine-focus sealed tube	5506 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.022$
φ and ω scans	$\theta_{max} = 32.5°$, $\theta_{min} = 2.8°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)	$h = -11 \rightarrow 11$
$T_{min} = 0.842$, $T_{max} = 0.976$	$k = -15 \rightarrow 15$
18115 measured reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.039$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.113$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0611P)^2 + 0.3032P]$ where $P = (F_o^2 + 2F_c^2)/3$
6480 reflections	$(\Delta/\sigma)_{max} = 0.001$
257 parameters	$\Delta\rho_{max} = 0.53$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.27$ e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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 $F^2 > \sigma(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	1.07800 (5)	0.08403 (3)	−0.18284 (3)	0.03779 (9)
S1	0.17791 (4)	0.27870 (3)	0.20939 (2)	0.02534 (8)
O1	−0.27472 (13)	0.52923 (9)	0.54724 (7)	0.02723 (18)
O2	−0.14178 (14)	0.66439 (9)	0.43584 (8)	0.02957 (19)
N1	0.32516 (14)	0.31817 (9)	0.01686 (8)	0.02134 (17)
N2	0.16931 (14)	0.38648 (10)	0.02374 (7)	0.02176 (17)
N3	−0.07075 (13)	0.42674 (10)	0.12269 (8)	0.02133 (17)
N4	−0.14591 (13)	0.45733 (9)	0.21809 (7)	0.01985 (17)
N5	−0.27251 (13)	0.33810 (9)	0.45894 (7)	0.01958 (16)
N6	−0.32110 (15)	0.39514 (10)	0.55021 (8)	0.02548 (19)
C1	0.63437 (17)	0.17276 (12)	−0.03615 (9)	0.0237 (2)
H1A	0.5690	0.1433	0.0185	0.028*
C2	0.78848 (17)	0.11197 (12)	−0.06418 (10)	0.0265 (2)
H2A	0.8263	0.0413	−0.0295	0.032*
C3	0.88538 (17)	0.15913 (12)	−0.14545 (10)	0.0264 (2)

C4	0.83211 (18)	0.26371 (12)	−0.19913 (10)	0.0275 (2)
H4A	0.8994	0.2941	−0.2527	0.033*
C5	0.67620 (18)	0.32191 (11)	−0.17115 (9)	0.0250 (2)
H5A	0.6374	0.3911	−0.2073	0.030*
C6	0.57626 (16)	0.27820 (11)	−0.08939 (9)	0.02146 (19)
C7	0.41298 (16)	0.34357 (11)	−0.06406 (9)	0.0225 (2)
H7A	0.3715	0.4053	−0.1077	0.027*
C8	0.08764 (15)	0.36783 (10)	0.10979 (8)	0.01926 (18)
C9	−0.02848 (18)	0.25579 (12)	0.27750 (11)	0.0272 (2)
H9A	−0.1132	0.1856	0.2353	0.033*
H9B	0.0039	0.2276	0.3479	0.033*
C10	−0.12334 (14)	0.38080 (10)	0.29279 (9)	0.01908 (18)
C11	−0.19794 (15)	0.42203 (10)	0.39393 (9)	0.01953 (18)
C12	−0.19652 (16)	0.55221 (11)	0.45021 (9)	0.0229 (2)
C13	−0.30832 (14)	0.19503 (10)	0.43535 (9)	0.01922 (18)
C14	−0.22133 (15)	0.11515 (11)	0.50272 (9)	0.02130 (19)
H14A	−0.1436	0.1523	0.5641	0.026*
C15	−0.25405 (16)	−0.02255 (11)	0.47558 (10)	0.0241 (2)
H15A	−0.1976	−0.0784	0.5194	0.029*
C16	−0.36970 (17)	−0.07694 (12)	0.38406 (11)	0.0257 (2)
H16A	−0.3901	−0.1690	0.3667	0.031*
C17	−0.45555 (17)	0.00539 (12)	0.31792 (10)	0.0261 (2)
H17A	−0.5334	−0.0318	0.2566	0.031*
C18	−0.42526 (15)	0.14293 (12)	0.34325 (10)	0.0235 (2)
H18A	−0.4820	0.1988	0.2995	0.028*
H1N3	−0.095 (3)	0.481 (2)	0.0777 (16)	0.040 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.02970 (16)	0.03100 (16)	0.0513 (2)	0.00136 (11)	0.01490 (14)	−0.00771 (13)
S1	0.02671 (14)	0.02899 (15)	0.02507 (14)	0.01210 (10)	0.00651 (10)	0.01304 (10)
O1	0.0348 (5)	0.0217 (4)	0.0254 (4)	0.0064 (3)	0.0034 (3)	0.0011 (3)
O2	0.0342 (5)	0.0175 (4)	0.0367 (5)	0.0035 (3)	0.0001 (4)	0.0044 (3)
N1	0.0247 (4)	0.0201 (4)	0.0196 (4)	0.0045 (3)	0.0019 (3)	0.0024 (3)
N2	0.0257 (4)	0.0222 (4)	0.0183 (4)	0.0059 (3)	0.0016 (3)	0.0039 (3)
N3	0.0241 (4)	0.0227 (4)	0.0187 (4)	0.0064 (3)	0.0012 (3)	0.0067 (3)
N4	0.0212 (4)	0.0194 (4)	0.0196 (4)	0.0031 (3)	0.0011 (3)	0.0054 (3)
N5	0.0213 (4)	0.0185 (4)	0.0200 (4)	0.0044 (3)	0.0019 (3)	0.0051 (3)
N6	0.0314 (5)	0.0235 (4)	0.0228 (4)	0.0057 (4)	0.0055 (4)	0.0042 (3)
C1	0.0275 (5)	0.0233 (5)	0.0211 (5)	0.0033 (4)	0.0040 (4)	0.0037 (4)
C2	0.0280 (5)	0.0254 (5)	0.0262 (5)	0.0047 (4)	0.0037 (4)	0.0021 (4)
C3	0.0251 (5)	0.0236 (5)	0.0285 (5)	−0.0011 (4)	0.0061 (4)	−0.0051 (4)
C4	0.0320 (6)	0.0228 (5)	0.0259 (5)	−0.0057 (4)	0.0093 (4)	−0.0023 (4)
C5	0.0336 (6)	0.0194 (5)	0.0213 (5)	−0.0027 (4)	0.0054 (4)	0.0014 (4)
C6	0.0261 (5)	0.0193 (4)	0.0184 (4)	0.0010 (4)	0.0027 (4)	0.0007 (3)
C7	0.0286 (5)	0.0199 (5)	0.0192 (4)	0.0036 (4)	0.0022 (4)	0.0028 (3)
C8	0.0220 (4)	0.0168 (4)	0.0187 (4)	0.0023 (3)	−0.0007 (3)	0.0032 (3)

C9	0.0342 (6)	0.0197 (5)	0.0329 (6)	0.0097 (4)	0.0137 (5)	0.0118 (4)
C10	0.0200 (4)	0.0160 (4)	0.0223 (4)	0.0030 (3)	0.0022 (3)	0.0058 (3)
C11	0.0214 (4)	0.0167 (4)	0.0216 (4)	0.0038 (3)	0.0014 (3)	0.0059 (3)
C12	0.0240 (5)	0.0197 (5)	0.0251 (5)	0.0053 (4)	−0.0007 (4)	0.0040 (4)
C13	0.0198 (4)	0.0168 (4)	0.0222 (4)	0.0021 (3)	0.0038 (3)	0.0057 (3)
C14	0.0233 (5)	0.0209 (5)	0.0213 (5)	0.0043 (4)	0.0035 (4)	0.0070 (3)
C15	0.0247 (5)	0.0205 (5)	0.0301 (5)	0.0059 (4)	0.0074 (4)	0.0091 (4)
C16	0.0247 (5)	0.0189 (5)	0.0347 (6)	0.0008 (4)	0.0099 (4)	0.0039 (4)
C17	0.0227 (5)	0.0252 (5)	0.0290 (5)	−0.0025 (4)	0.0019 (4)	0.0018 (4)
C18	0.0205 (5)	0.0242 (5)	0.0259 (5)	0.0004 (4)	−0.0005 (4)	0.0074 (4)

Geometric parameters (Å, °)

Cl1—C3	1.7379 (13)	C4—C5	1.3861 (18)
S1—C8	1.7374 (10)	C4—H4A	0.9300
S1—C9	1.8097 (12)	C5—C6	1.3984 (16)
O1—N6	1.3788 (13)	C5—H5A	0.9300
O1—C12	1.4197 (15)	C6—C7	1.4607 (16)
O2—C12	1.2117 (14)	C7—H7A	0.9300
N1—C7	1.2837 (15)	C9—C10	1.5030 (15)
N1—N2	1.3921 (13)	C9—H9A	0.9700
N2—C8	1.3000 (14)	C9—H9B	0.9700
N3—C8	1.3659 (14)	C10—C11	1.4526 (15)
N3—N4	1.3712 (13)	C11—C12	1.4217 (15)
N3—H1N3	0.85 (2)	C13—C14	1.3870 (14)
N4—C10	1.2896 (13)	C13—C18	1.3881 (16)
N5—N6	1.3101 (14)	C14—C15	1.3935 (16)
N5—C11	1.3563 (13)	C14—H14A	0.9300
N5—C13	1.4434 (14)	C15—C16	1.3836 (18)
C1—C2	1.3874 (17)	C15—H15A	0.9300
C1—C6	1.4018 (16)	C16—C17	1.3912 (18)
C1—H1A	0.9300	C16—H16A	0.9300
C2—C3	1.3940 (17)	C17—C18	1.3886 (17)
C2—H2A	0.9300	C17—H17A	0.9300
C3—C4	1.3861 (19)	C18—H18A	0.9300
C8—S1—C9	97.34 (5)	N3—C8—S1	119.98 (8)
N6—O1—C12	111.31 (8)	C10—C9—S1	112.38 (8)
C7—N1—N2	112.59 (9)	C10—C9—H9A	109.1
C8—N2—N1	112.52 (9)	S1—C9—H9A	109.1
C8—N3—N4	126.88 (9)	C10—C9—H9B	109.1
C8—N3—H1N3	114.7 (14)	S1—C9—H9B	109.1
N4—N3—H1N3	111.8 (14)	H9A—C9—H9B	107.9
C10—N4—N3	118.20 (9)	N4—C10—C11	115.66 (9)
N6—N5—C11	115.55 (9)	N4—C10—C9	123.01 (10)
N6—N5—C13	117.95 (9)	C11—C10—C9	121.33 (9)
C11—N5—C13	126.46 (9)	N5—C11—C12	105.58 (9)
N5—N6—O1	104.02 (9)	N5—C11—C10	125.07 (9)
C2—C1—C6	120.65 (11)	C12—C11—C10	129.17 (10)
C2—C1—H1A	119.7	O2—C12—O1	120.14 (11)

C6—C1—H1A	119.7	O2—C12—C11	136.24 (12)
C1—C2—C3	118.54 (11)	O1—C12—C11	103.54 (9)
C1—C2—H2A	120.7	C14—C13—C18	122.57 (10)
C3—C2—H2A	120.7	C14—C13—N5	119.37 (10)
C4—C3—C2	122.18 (11)	C18—C13—N5	118.04 (9)
C4—C3—Cl1	118.32 (10)	C13—C14—C15	117.91 (10)
C2—C3—Cl1	119.49 (10)	C13—C14—H14A	121.0
C5—C4—C3	118.46 (11)	C15—C14—H14A	121.0
C5—C4—H4A	120.8	C16—C15—C14	120.63 (10)
C3—C4—H4A	120.8	C16—C15—H15A	119.7
C4—C5—C6	121.04 (11)	C14—C15—H15A	119.7
C4—C5—H5A	119.5	C15—C16—C17	120.33 (11)
C6—C5—H5A	119.5	C15—C16—H16A	119.8
C5—C6—C1	119.11 (11)	C17—C16—H16A	119.8
C5—C6—C7	118.29 (10)	C18—C17—C16	120.13 (11)
C1—C6—C7	122.59 (10)	C18—C17—H17A	119.9
N1—C7—C6	121.78 (10)	C16—C17—H17A	119.9
N1—C7—H7A	119.1	C13—C18—C17	118.43 (10)
C6—C7—H7A	119.1	C13—C18—H18A	120.8
N2—C8—N3	117.39 (9)	C17—C18—H18A	120.8
N2—C8—S1	122.56 (8)		

C7—N1—N2—C8	−175.59 (10)	S1—C9—C10—C11	−137.68 (9)
C8—N3—N4—C10	−32.21 (16)	N6—N5—C11—C12	0.24 (13)
C11—N5—N6—O1	−0.32 (13)	C13—N5—C11—C12	177.95 (10)
C13—N5—N6—O1	−178.24 (9)	N6—N5—C11—C10	175.72 (10)
C12—O1—N6—N5	0.28 (12)	C13—N5—C11—C10	−6.57 (17)
C6—C1—C2—C3	0.77 (18)	N4—C10—C11—N5	145.80 (11)
C1—C2—C3—C4	−0.37 (19)	C9—C10—C11—N5	−33.52 (17)
C1—C2—C3—Cl1	−179.55 (9)	N4—C10—C11—C12	−39.82 (16)
C2—C3—C4—C5	−0.58 (18)	C9—C10—C11—C12	140.87 (12)
Cl1—C3—C4—C5	178.61 (9)	N6—O1—C12—O2	−177.42 (10)
C3—C4—C5—C6	1.14 (18)	N6—O1—C12—C11	−0.15 (12)
C4—C5—C6—C1	−0.75 (17)	N5—C11—C12—O2	176.55 (13)
C4—C5—C6—C7	−179.85 (11)	C10—C11—C12—O2	1.3 (2)
C2—C1—C6—C5	−0.23 (17)	N5—C11—C12—O1	−0.04 (11)
C2—C1—C6—C7	178.83 (11)	C10—C11—C12—O1	−175.28 (10)
N2—N1—C7—C6	−177.30 (10)	N6—N5—C13—C14	−63.26 (14)
C5—C6—C7—N1	−172.94 (11)	C11—N5—C13—C14	119.08 (12)
C1—C6—C7—N1	8.00 (18)	N6—N5—C13—C18	118.73 (11)
N1—N2—C8—N3	−177.81 (9)	C11—N5—C13—C18	−58.93 (15)
N1—N2—C8—S1	5.18 (14)	C18—C13—C14—C15	0.06 (16)
N4—N3—C8—N2	−157.47 (11)	N5—C13—C14—C15	−177.86 (10)
N4—N3—C8—S1	19.62 (15)	C13—C14—C15—C16	0.09 (16)
C9—S1—C8—N2	−165.26 (10)	C14—C15—C16—C17	−0.21 (17)
C9—S1—C8—N3	17.80 (10)	C15—C16—C17—C18	0.17 (18)
C8—S1—C9—C10	−43.84 (10)	C14—C13—C18—C17	−0.10 (17)
N3—N4—C10—C11	177.00 (9)	N5—C13—C18—C17	177.85 (10)
N3—N4—C10—C9	−3.70 (16)	C16—C17—C18—C13	−0.01 (17)
S1—C9—C10—N4	43.07 (15)		

Hydrogen-bond geometry (Å, °)

Cg2 is the centroid of the C1–C6 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H1N3···N2^{i}	0.84 (2)	2.03 (2)	2.8752 (14)	178 (2)
C9—H9A···Cl1^{ii}	0.97	2.78	3.4904 (13)	130
C18—H18A···S1^{iii}	0.93	2.86	3.6729 (12)	147
C17—H17A···Cg2^{iv}	0.93	2.64	3.5208 (15)	158

Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) −*x*+1, −*y*, −*z*; (iii) *x*−1, *y*, *z*; (iv) −*x*, −*y*, −*z*.

Fig. 1

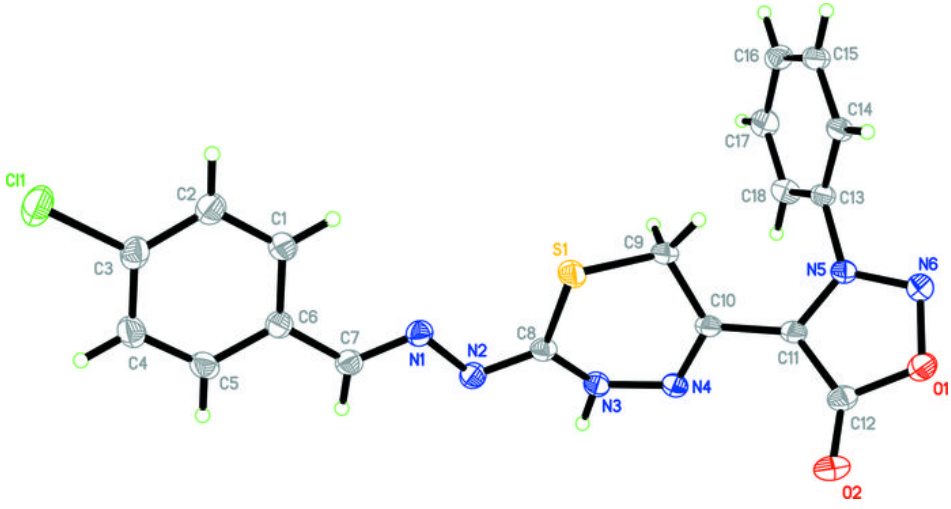
Cl1
C2
C1
C3
C6
C7
C4
C5
N1
N2
C8
S1
C9
N3
N4
C10
C11
N5
N6
C16
C15
C14
C17
C18
C13
O1
C12
O2

Fig. 2