

4-(4-Chlorophenyl)-N-[(E)-4-(dimethylamino)benzylidene]-1,3-thiazol-2-amine

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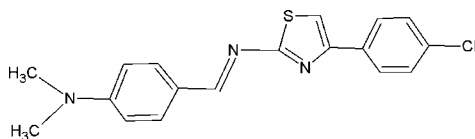
Received 25 June 2011; accepted 13 July 2011

Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.048; wR factor = 0.062; data-to-parameter ratio = 15.4.

The title compound, $\text{C}_{18}\text{H}_{16}\text{ClN}_3\text{S}$, adopts an extended molecular structure. The thiazole ring is inclined by 9.2 (1) and 15.3 (1)° with respect to the chlorophenyl and 4-(dimethylamino)phenyl rings, respectively, while the benzene ring planes make an angle of 19.0 (1)°. A weak intermolecular $\text{C}-\text{H}\cdots\pi$ contact is observed in the crystal structure.

Related literature

For related structures, see: Lynch *et al.* (1999; 2002). For medicinal applications of thiazole derivatives, see: Misra *et al.* (2004).



Experimental

Crystal data

 $\text{C}_{18}\text{H}_{16}\text{ClN}_3\text{S}$
 $M_r = 341.85$
Monoclinic, $P2_1$
 $a = 6.1169$ (7) Å
 $b = 7.4708$ (8) Å
 $c = 18.2536$ (18) Å
 $\beta = 97.975$ (11)° $V = 826.09$ (15) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 0.36$ mm⁻¹
 $T = 294$ K
0.24 × 0.18 × 0.16 mm

Data collection

Bruker APEXII CCD
diffractometer
Absorption correction: multi-scan
(*SADABS*; Bruker, 2004)
 $T_{\min} = 0.919$, $T_{\max} = 0.945$ 9063 measured reflections
3242 independent reflections
1355 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.084$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.062$
 $S = 0.78$
3242 reflections
210 parameters
1 restraintH-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.18$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.20$ e Å⁻³
Absolute structure: Flack (1983),
1483 Friedel pairs
Flack parameter: 0.06 (8)

Table 1

Hydrogen-bond geometry (Å, °).

Cg is the centroid of the C11–C16 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C18}-\text{H18B}\cdots\text{Cg}^i$	0.96	2.73	3.515 (5)	140

Symmetry code: (i) $-x + 1, y - \frac{1}{2}, -z + 2$.

Data collection: *APEX2* (Bruker, 2010); cell refinement: *SAINT-Plus* (Bruker, 2010); 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); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

We acknowledge the CCD facility, set up under the IRHPA–DST program at the IISc., Bangalore. RSR acknowledges the CSIR, Government of India, for funding under the scientist's pool scheme.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5251).

References

- Bruker (2004). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Bruker (2010). *APEX2* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
 Lynch, D. E., McClenaghan, I., Light, M. E. & Coles, S. J. (2002). *Cryst. Eng.* **5**, 123–136.
 Lynch, D. E., Nicholls, L. J., Smith, G., Byriel, K. A. & Kennard, C. H. L. (1999). *Acta Cryst.* **B55**, 758–766.
 Misra, R. N., Xiao, H.-Y., Kim, K. S., Lu, S., Han, W.-C., Barbosa, S. A., Hunt, J. T., Rawlins, D. B., Shan, W., Ahmed, S. Z., Qian, L., Chen, B.-C., Zhao, R., Bednarz, M. S., Kellar, K. A., Mulheron, J. G., Batorsky, R., Roongta, U., Kamath, A., Marathe, P., Ranadive, S. A., Sack, J. S., Tokarski, J. S., Pavletich, N. P., Lee, F. Y., Webster, K. R. & Kimball, S. D. (2004). *J. Med. Chem.* **47**, 1719–1728.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

supplementary materials

Acta Cryst. (2011). E67, o2115 [doi:10.1107/S1600536811028078]

4-(4-Chlorophenyl)-*N*-[(*E*)-4-(dimethylamino)benzylidene]-1,3-thiazol-2-amine

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Comment

The title compound, C₁₈H₁₆ClN₃S, (I), is a 2-amino-thiazole derivative. Few structures of such derivatives have been determined (Lynch *et al.*, 1999; 2002) and some of them have been shown to act as inhibitor of cyclin-dependent kinase (Misra *et al.*, 2004). The structure of (I) with adopted atom-numbering scheme is shown in Fig 1.

(I) adopts an extended structure. The thiazole ring is inclined with respect to chlorophenyl and dimethylaminophenyl rings by 9.2 (1)° and 15.3 (1)°, respectively, while both benzene ring planes make an angle of 19.0 (1)°. The dimethylamino group makes an angle of 4.0 (3)° with respect to the adjacent benzene ring. The crystal packing is governed by van der waals interactions only. Short intermolecular C—H···π contact is also observed (Table 1).

Experimental

A mixture of 2-amino-4-(4-chloro) phenyl thiazole (0.01 mol; CAS No. 2103–99-3) and paradimethyl amino benzaldehyde (0.01 mol) in ethanol (30 ml), and catalytic amount of glacial acetic acid (2 ml) in a clean conical flask was refluxed for 2 h. The resulting mixture was cooled, filtered and dried to get the title compound (m.p. 506–507°C). To obtain the suitable single crystals for X-ray diffraction, (I) was mixed with DMF (30 ml) and heated until completely dissolved. The mixture was left for slow evaporation.

Refinement

Hydrogen atoms were placed in their stereochemically expected positions and refined with the riding options. Methyl hydrogen atoms were fixed with reference to local electron density map. The distances with hydrogen atoms are as follows: C(aromatic/*sp*²)—H = 0.93 Å, C(methyl)—H = 0.96 Å, and $U_{\text{iso}} = 1.2 U_{\text{eq}}(\text{parent})$ [$1.5 U_{\text{eq}}(\text{parent})$ for methyl groups].

Figures

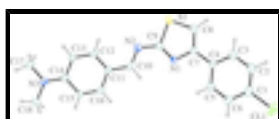


Fig. 1. A view of (I) with adopted atom-numbering scheme and non-H atoms shown as probability ellipsoids at 30% levels.

4-(4-Chlorophenyl)-*N*-[(*E*)-4-(dimethylamino)benzylidene]- 1,3-thiazol-2-amine

Crystal data

C₁₈H₁₆ClN₃S

$M_r = 341.85$

Monoclinic, $P2_1$

$F(000) = 356$

$D_x = 1.374 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

supplementary materials

Hall symbol: P 2₁b
 $a = 6.1169$ (7) Å
 $b = 7.4708$ (8) Å
 $c = 18.2536$ (18) Å
 $\beta = 97.975$ (11)°
 $V = 826.09$ (15) Å³
 $Z = 2$

Cell parameters from 1055 reflections
 $\theta = 2.2$ – 29.2 °
 $\mu = 0.36$ mm⁻¹
 $T = 294$ K
Needle, brown
 $0.24 \times 0.18 \times 0.16$ mm

Data collection

Bruker APEXII CCD
diffractometer
Radiation source: fine-focus sealed tube
graphite
 φ and ω scans
Absorption correction: multi-scan
(*SADABS*; Bruker, 2004)
 $T_{\min} = 0.919$, $T_{\max} = 0.945$
9063 measured reflections

3242 independent reflections
1355 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.084$
 $\theta_{\max} = 26.0$ °, $\theta_{\min} = 3.0$ °
 $h = -7 \rightarrow 7$
 $k = -9 \rightarrow 9$
 $l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.062$
 $S = 0.78$
3242 reflections
210 parameters
1 restraint
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.010P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.004$
 $\Delta\rho_{\max} = 0.18$ e Å⁻³
 $\Delta\rho_{\min} = -0.20$ e Å⁻³
Absolute structure: Flack (1983), 1483 Friedel pairs
Flack parameter: 0.06 (8)

Special details

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.

Weighted least-squares planes through the starred atoms (Nardelli, Musatti, Domiano & Andreotti Ric.Sci.(1965),15(II—A),807).
Equation of the plane: $m_1 * X + m_2 * Y + m_3 * Z = d$

Plane 1 $m_1 = -0.44990(0.00160)$ $m_2 = -0.87347(0.00086)$ $m_3 = -0.18611(0.00175)$ $D = -3.47756(0.01551)$ Atom d s/d/s (d/s)**2
C1 * -0.0082 0.0048 - 1.706 2.911 C2 * 0.0089 0.0046 1.925 3.707 C3 * -0.0021 0.0045 - 0.472 0.223 C4 * -0.0040 0.0039 - 1.036
1.072 C5 * 0.0051 0.0039 1.304 1.700 C6 * -0.0004 0.0040 - 0.096 0.009 C11 - 0.0062 0.0013 - 4.835 23.378 C7 - 0.0409 0.0039 -

10.501 110.265 ===== Sum((d/s)**2) for starred atoms 9.623 Chi-squared at 95% for 3 degrees of freedom: 7.81 The group of atoms deviates significantly from planarity

Plane 2 m1 = -0.34887(0.00131) m2 = -0.93392(0.00058) m3 = -0.07797(0.00194) D = -2.96690(0.02047) Atom d s d/s (d/s)**2
 N1 * 0.0036 0.0034 1.053 1.108 S1 * 0.0002 0.0012 0.201 0.041 C7 * -0.0021 0.0039 - 0.541 0.293 C8 * -0.0007 0.0043 - 0.157
 0.025 C9 * -0.0054 0.0042 - 1.283 1.647 N2 - 0.0838 0.0039 - 21.454 460.260 C4 - 0.0329 0.0039 - 8.470 71.739 =====
 Sum((d/s)**2) for starred atoms 3.113 Chi-squared at 95% for 2 degrees of freedom: 5.99 The group of atoms does not deviate significantly from planarity

Plane 3 m1 = 0.47925(0.00159) m2 = 0.86590(0.00089) m3 = -0.14330(0.00169) D = -0.77606(0.02916) Atom d s d/s (d/s)**2
 C11 * 0.0080 0.0041 1.980 3.920 C12 * -0.0093 0.0041 - 2.291 5.251 C13 * 0.0037 0.0043 0.856 0.733 C14 * 0.0043 0.0042 1.010
 1.021 C15 * -0.0044 0.0038 - 1.160 1.346 C16 * -0.0009 0.0040 - 0.219 0.048 N3 0.0139 0.0033 4.236 17.942 C10 0.0759 0.0041
 18.730 350.815 ===== Sum((d/s)**2) for starred atoms 12.318 Chi-squared at 95% for 3 degrees of freedom: 7.81 The
 group of atoms deviates significantly from planarity

Plane 4 m1 = 0.46397(0.00261) m2 = 0.88241(0.00119) m3 = -0.07795(0.00540) D = 0.57261(0.10767) Atom d s d/s (d/s)**2 N3 *
 0.0000 0.0033 0.000 0.000 C17 * 0.0000 0.0040 0.000 0.000 C18 * 0.0000 0.0041 0.000 0.000 C14 - 0.0851 0.0042 - 20.162 406.523
 ===== Sum((d/s)**2) for starred atoms 0.000 Dihedral angles formed by LSQ-planes Plane - plane angle (s.u.) angle (s.u.)
 1 2 9.17 (0.13) 170.83 (0.13) 1 3 19.04 (0.14) 160.96 (0.14) 1 4 15.20 (0.31) 164.80 (0.31) 2 3 15.27 (0.13) 164.73 (0.13) 2 4 11.51
 (0.27) 168.49 (0.27) 3 4 3.96 (0.31) 176.04 (0.31)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	-0.58295 (18)	0.55168 (16)	0.68740 (6)	0.0603 (4)
C11	-0.0164 (2)	0.44097 (17)	0.29270 (6)	0.0840 (5)
N1	-0.2184 (5)	0.4428 (5)	0.64682 (18)	0.0417 (9)
N2	-0.2363 (6)	0.4507 (5)	0.77983 (19)	0.0541 (10)
N3	0.3895 (6)	0.3460 (4)	1.0889 (2)	0.0448 (10)
C1	-0.1183 (8)	0.4555 (6)	0.3769 (2)	0.0504 (13)
C2	-0.3184 (7)	0.5363 (6)	0.3800 (2)	0.0577 (13)
H2	-0.4002	0.5824	0.3374	0.069*
C3	-0.3970 (6)	0.5480 (6)	0.4478 (2)	0.0490 (12)
H3	-0.5311	0.6045	0.4506	0.059*
C4	-0.2781 (6)	0.4765 (5)	0.5114 (2)	0.0340 (11)
C5	-0.0787 (6)	0.3928 (5)	0.5059 (2)	0.0445 (13)
H5	0.0023	0.3429	0.5478	0.053*
C6	0.0014 (7)	0.3830 (5)	0.4382 (2)	0.0473 (13)
H6	0.1356	0.3273	0.4349	0.057*
C7	-0.3576 (7)	0.4909 (5)	0.5840 (2)	0.0373 (12)
C8	-0.5606 (6)	0.5520 (6)	0.5945 (2)	0.0512 (12)
H8	-0.6706	0.5884	0.5571	0.061*
C9	-0.3158 (6)	0.4695 (6)	0.7050 (3)	0.0491 (13)
C10	-0.0454 (7)	0.3803 (5)	0.7958 (2)	0.0442 (13)

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H10	0.0264	0.3374	0.7577	0.053*
C11	0.0633 (7)	0.3650 (5)	0.8714 (3)	0.0369 (11)
C12	-0.0298 (6)	0.4390 (6)	0.9301 (2)	0.0422 (11)
H12	-0.1679	0.4928	0.9206	0.051*
C13	0.0767 (6)	0.4348 (6)	1.0015 (2)	0.0422 (12)
H13	0.0112	0.4879	1.0391	0.051*
C14	0.2839 (7)	0.3510 (6)	1.0185 (2)	0.0376 (12)
C15	0.3763 (7)	0.2732 (5)	0.9598 (2)	0.0415 (12)
H15	0.5122	0.2158	0.9690	0.050*
C16	0.2669 (7)	0.2815 (5)	0.8887 (2)	0.0466 (13)
H16	0.3318	0.2293	0.8508	0.056*
C17	0.2862 (6)	0.4146 (6)	1.1505 (2)	0.0654 (15)
H17C	0.1580	0.3443	1.1559	0.098*
H17B	0.2435	0.5370	1.1411	0.098*
H17A	0.3891	0.4078	1.1952	0.098*
C18	0.6027 (7)	0.2620 (6)	1.1087 (2)	0.0608 (14)
H18A	0.7059	0.3112	1.0790	0.091*
H18B	0.5894	0.1354	1.1002	0.091*
H18C	0.6543	0.2836	1.1600	0.091*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0511 (8)	0.0798 (10)	0.0498 (9)	0.0126 (8)	0.0057 (7)	-0.0004 (8)
C11	0.1220 (12)	0.0840 (10)	0.0528 (9)	-0.0034 (9)	0.0367 (9)	0.0026 (8)
N1	0.045 (2)	0.048 (2)	0.032 (2)	0.010 (2)	0.0036 (19)	-0.003 (2)
N2	0.047 (2)	0.072 (3)	0.044 (3)	0.005 (2)	0.009 (2)	0.002 (2)
N3	0.050 (3)	0.047 (3)	0.041 (3)	0.014 (2)	0.018 (2)	0.001 (2)
C1	0.072 (4)	0.039 (3)	0.043 (3)	-0.006 (3)	0.016 (3)	0.003 (3)
C2	0.074 (4)	0.056 (3)	0.043 (3)	0.009 (3)	0.006 (3)	0.019 (3)
C3	0.052 (3)	0.048 (3)	0.045 (3)	-0.003 (3)	-0.001 (3)	0.007 (3)
C4	0.040 (3)	0.028 (3)	0.035 (3)	-0.005 (2)	0.006 (2)	-0.002 (2)
C5	0.050 (3)	0.044 (3)	0.039 (3)	0.005 (2)	0.005 (3)	0.002 (2)
C6	0.053 (3)	0.041 (3)	0.049 (3)	0.001 (3)	0.015 (3)	-0.007 (3)
C7	0.043 (3)	0.026 (3)	0.042 (3)	-0.002 (2)	0.000 (2)	-0.004 (2)
C8	0.051 (3)	0.059 (3)	0.042 (3)	0.003 (3)	-0.002 (2)	-0.001 (3)
C9	0.048 (3)	0.045 (3)	0.052 (3)	0.009 (2)	-0.001 (3)	0.001 (3)
C10	0.057 (3)	0.040 (3)	0.039 (3)	-0.008 (3)	0.015 (3)	-0.006 (2)
C11	0.039 (3)	0.038 (3)	0.035 (3)	-0.003 (2)	0.008 (3)	-0.001 (2)
C12	0.037 (3)	0.046 (3)	0.046 (3)	0.003 (2)	0.013 (3)	-0.006 (3)
C13	0.041 (3)	0.053 (3)	0.034 (3)	0.006 (3)	0.011 (2)	0.001 (3)
C14	0.046 (3)	0.037 (3)	0.033 (3)	-0.001 (2)	0.016 (3)	0.006 (2)
C15	0.042 (3)	0.045 (3)	0.038 (3)	0.012 (2)	0.006 (3)	-0.008 (3)
C16	0.049 (3)	0.046 (3)	0.047 (3)	0.004 (2)	0.015 (3)	-0.004 (3)
C17	0.066 (3)	0.089 (4)	0.042 (3)	0.018 (3)	0.013 (3)	-0.003 (3)
C18	0.055 (4)	0.074 (4)	0.050 (4)	0.015 (3)	-0.005 (3)	0.001 (3)

Geometric parameters (Å, °)

S1—C8	1.720 (4)	C7—C8	1.362 (4)
S1—C9	1.733 (4)	C8—H8	0.9300
C11—C1	1.741 (4)	C10—C11	1.451 (5)
N1—C9	1.303 (4)	C10—H10	0.9300
N1—C7	1.378 (4)	C11—C16	1.390 (5)
N2—C10	1.277 (4)	C11—C12	1.394 (4)
N2—C9	1.393 (4)	C12—C13	1.375 (4)
N3—C14	1.357 (5)	C12—H12	0.9300
N3—C18	1.447 (5)	C13—C14	1.409 (5)
N3—C17	1.458 (4)	C13—H13	0.9300
C1—C6	1.361 (5)	C14—C15	1.404 (5)
C1—C2	1.373 (5)	C15—C16	1.377 (5)
C2—C3	1.392 (4)	C15—H15	0.9300
C2—H2	0.9300	C16—H16	0.9300
C3—C4	1.388 (5)	C17—H17C	0.9600
C3—H3	0.9300	C17—H17B	0.9600
C4—C5	1.386 (5)	C17—H17A	0.9600
C4—C7	1.477 (4)	C18—H18A	0.9600
C5—C6	1.394 (4)	C18—H18B	0.9600
C5—H5	0.9300	C18—H18C	0.9600
C6—H6	0.9300		
C8—S1—C9	88.9 (2)	N2—C10—C11	122.3 (4)
C9—N1—C7	109.8 (3)	N2—C10—H10	118.9
C10—N2—C9	116.7 (4)	C11—C10—H10	118.9
C14—N3—C18	122.9 (3)	C16—C11—C12	116.9 (4)
C14—N3—C17	121.4 (3)	C16—C11—C10	121.9 (4)
C18—N3—C17	115.6 (4)	C12—C11—C10	121.1 (4)
C6—C1—C2	121.5 (4)	C13—C12—C11	121.9 (4)
C6—C1—C11	118.9 (4)	C13—C12—H12	119.0
C2—C1—C11	119.6 (4)	C11—C12—H12	119.0
C1—C2—C3	118.9 (4)	C12—C13—C14	120.8 (4)
C1—C2—H2	120.6	C12—C13—H13	119.6
C3—C2—H2	120.6	C14—C13—H13	119.6
C4—C3—C2	120.9 (4)	N3—C14—C15	121.5 (4)
C4—C3—H3	119.5	N3—C14—C13	121.0 (4)
C2—C3—H3	119.5	C15—C14—C13	117.5 (4)
C5—C4—C3	118.6 (3)	C16—C15—C14	120.4 (4)
C5—C4—C7	120.0 (4)	C16—C15—H15	119.8
C3—C4—C7	121.5 (4)	C14—C15—H15	119.8
C4—C5—C6	120.6 (4)	C15—C16—C11	122.5 (4)
C4—C5—H5	119.7	C15—C16—H16	118.8
C6—C5—H5	119.7	C11—C16—H16	118.8
C1—C6—C5	119.5 (4)	N3—C17—H17C	109.5
C1—C6—H6	120.3	N3—C17—H17B	109.5
C5—C6—H6	120.3	H17C—C17—H17B	109.5
C8—C7—N1	116.1 (4)	N3—C17—H17A	109.5

supplementary materials

C8—C7—C4	124.8 (4)	H17C—C17—H17A	109.5
N1—C7—C4	119.1 (4)	H17B—C17—H17A	109.5
C7—C8—S1	109.7 (3)	N3—C18—H18A	109.5
C7—C8—H8	125.1	N3—C18—H18B	109.5
S1—C8—H8	125.1	H18A—C18—H18B	109.5
N1—C9—N2	130.3 (4)	N3—C18—H18C	109.5
N1—C9—S1	115.5 (3)	H18A—C18—H18C	109.5
N2—C9—S1	114.1 (3)	H18B—C18—H18C	109.5
C6—C1—C2—C3	1.7 (7)	C10—N2—C9—N1	-7.6 (7)
C11—C1—C2—C3	-179.6 (3)	C10—N2—C9—S1	175.8 (3)
C1—C2—C3—C4	-1.2 (7)	C8—S1—C9—N1	-0.6 (4)
C2—C3—C4—C5	0.0 (6)	C8—S1—C9—N2	176.5 (3)
C2—C3—C4—C7	178.9 (4)	C9—N2—C10—C11	175.4 (4)
C3—C4—C5—C6	0.8 (6)	N2—C10—C11—C16	177.2 (4)
C7—C4—C5—C6	-178.1 (4)	N2—C10—C11—C12	-4.8 (6)
C2—C1—C6—C5	-1.0 (7)	C16—C11—C12—C13	1.9 (6)
C11—C1—C6—C5	-179.7 (3)	C10—C11—C12—C13	-176.2 (4)
C4—C5—C6—C1	-0.3 (6)	C11—C12—C13—C14	-1.5 (7)
C9—N1—C7—C8	-0.7 (5)	C18—N3—C14—C15	0.2 (6)
C9—N1—C7—C4	178.3 (4)	C17—N3—C14—C15	-175.3 (4)
C5—C4—C7—C8	-172.4 (4)	C18—N3—C14—C13	-179.8 (4)
C3—C4—C7—C8	8.8 (6)	C17—N3—C14—C13	4.8 (6)
C5—C4—C7—N1	8.8 (5)	C12—C13—C14—N3	-179.8 (4)
C3—C4—C7—N1	-170.0 (4)	C12—C13—C14—C15	0.2 (6)
N1—C7—C8—S1	0.3 (5)	N3—C14—C15—C16	-179.4 (4)
C4—C7—C8—S1	-178.6 (3)	C13—C14—C15—C16	0.6 (6)
C9—S1—C8—C7	0.1 (3)	C14—C15—C16—C11	-0.2 (6)
C7—N1—C9—N2	-175.7 (4)	C12—C11—C16—C15	-1.0 (6)
C7—N1—C9—S1	0.8 (5)	C10—C11—C16—C15	177.0 (4)

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

Cg is the centroid of the C11–C16 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C18—H18B \cdots Cg ⁱ	0.96	2.73	3.515 (5)	140

Symmetry codes: (i) $-x+1, y-1/2, -z+2$.

Fig. 1

