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2-Amino-*N*-[3-(2-chlorobenzoyl)-5-ethylthiophen-2-yl]acetamide

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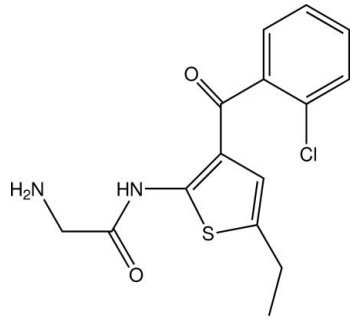
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.163; data-to-parameter ratio = 21.9.

In the title compound, $C_{15}H_{15}ClN_2O_2S$, the 2-aminoacetamide N—C(=O)—C—N unit is approximately planar, with an r.m.s. deviation of 0.020 (4) Å. The central thiophene ring makes dihedral angles of 7.84 (11) and 88.11 (11)°, respectively, with the 2-aminoacetamide unit and the 2-chlorophenyl ring. An intramolecular N—H···O hydrogen bond generates an S(6) ring motif. In the crystal, molecules are linked by an N—H···O hydrogen bond and weak C—H···O interactions into a chain along the c axis. A C—H···π interaction is also present.

Related literature

For bond-length data, see: Allen *et al.* (1987). For related literature on hydrogen-bond motifs, see: Bernstein *et al.* (1995). For background to and activities of etizolam and thiophene derivatives, see: Gewald & Schindler (1990); Jagadees Babu *et al.* (2011); Shafeeque *et al.* (1999); Nakamura & Mukasa (1992); Nakanishi *et al.* (1973); Ramanathan & Namboothiri (1978). For related structures, see: Dockendorff *et al.* (2006); Ferreira de Lima *et al.* (2009); Nogueira *et al.* (2010). For the stability of the temperature controller, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{15}H_{15}ClN_2O_2S$
M_r = 322.80
Monoclinic, $P2_1/c$
a = 13.9784 (11) Å
b = 13.5565 (11) Å
c = 8.3334 (7) Å
β = 91.233 (1)°
V = 1578.8 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 293 K
0.56 × 0.41 × 0.28 mm

Data collection

Bruker APEX DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.817, T_{max} = 0.902
16034 measured reflections
4184 independent reflections
3180 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.163
S = 1.05
4184 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

*Cg*1 is the centroid of the thiophene C8/C9/S1/C10/C11 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*1···O1	0.83	2.15	2.771 (2)	132
N2—H2*N*2···O2^{i}	0.87	2.48	3.118 (3)	131
C15—H15*B*···O2^{i}	0.97	2.37	3.120 (3)	134
C15—H15*A*···*Cg*1^{ii}	0.97	2.75	3.530 (2)	238

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

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: IS5060).

‡ Thomson Reuters ResearcherID: A-3561-2009.
§ Thomson Reuters ResearcherID: A-5085-2009.

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Acta Cryst. (2012). E**68**, o547–o548 [doi:10.1107/S1600536812003261]

2-Amino-*N*-[3-(2-chlorobenzoyl)-5-ethylthiophen-2-yl]acetamide

Hoong-Kun Fun, Suchada Chantrapromma, A. S. Dayananda, H. S. Yathirajan and A. R. Ramesha

S1. Comment

The title compound is an intermediate in the synthesis of a drug known as "etizolam" which possesses potent hypnotic properties (Nakamura & Mukasa, 1992). Thiophenes and their biheterocycles have received considerable attention during last two decades as they are endowed with variety of biological activities and have wide range of therapeutic properties (Gewald & Schindler, 1990; Ramanathan & Namboothiri, 1978). Thiophene derivatives possess different pharmacological and biological properties, of which the more potent properties are the anticonvulsant, anti-inflammatory and antibacterial activities (Jagadees Babu *et al.*, 2011; Shafeeque *et al.*, 1999). In view of the importance of thiophenes, the crystal structure of the title compound (I) is reported.

In the molecule of (I), $C_{15}H_{15}ClN_2O_2S$, the central thiophene ring makes a dihedral angle of 88.11 (11)° with the 2-chlorophenyl ring. The 2-aminoacetamide moiety is co-planar with the thiophene ring with an r.m.s. deviation of 0.067 (2) Å for the ten non-H atoms (C8–C11/C14-C15, S1, O2 N1 and N2) (Fig. 1) and with torsion angles C9–N1–C14–O2 = -1.6 (3)°, C9–N1–C14–C15 = 178.49 (18)° and N1–C14–C15–N2 = -6.9 (3)°. The orientation of the ethyl group with respect to the thiophene ring can be reflected by the torsion angle C11–C10–C12–C13 = 118.6 (4)° which indicates the (+)-anti-clinal conformation. An intramolecular N1—H1N1···O1 hydrogen bond generates an S(6) ring motif (Bernstein *et al.*, 1995). Bond distances of (I) are in normal range (Allen *et al.*, 1987) and comparable with the related structures (Dockendorff *et al.*, 2006; Ferreira de Lima *et al.*, 2009; Nogueira *et al.*, 2010).

In the crystal packing (Fig. 2), the molecules are linked by intermolecular N—H···O(acetamide) hydrogen bonds and weak C—H···O(acetamide) interactions (Table 1) into chains along the *c* axis. Weak C—H···π interactions are present (Table1).

S2. Experimental

The title compound was synthesized by the literature method (Nakanishi *et al.*, 1973). Yellow block-shaped single crystals of the title compound suitable for *X*-ray structure determination were recrystalized from C_2H_5OH/DMSO (1:1 *v*/*v*) by slow evaporation of the solvent at room temperature after several days (m.p. 417–419 K).

S3. Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with d(N—H) = 0.83 Å for NH, 0.87 Å for NH_2, and d(C—H) = 0.93 Å for aromatic, 0.97 Å for CH_2 and 0.96 Å for CH_3 groups. The U_{iso}(H) values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups.

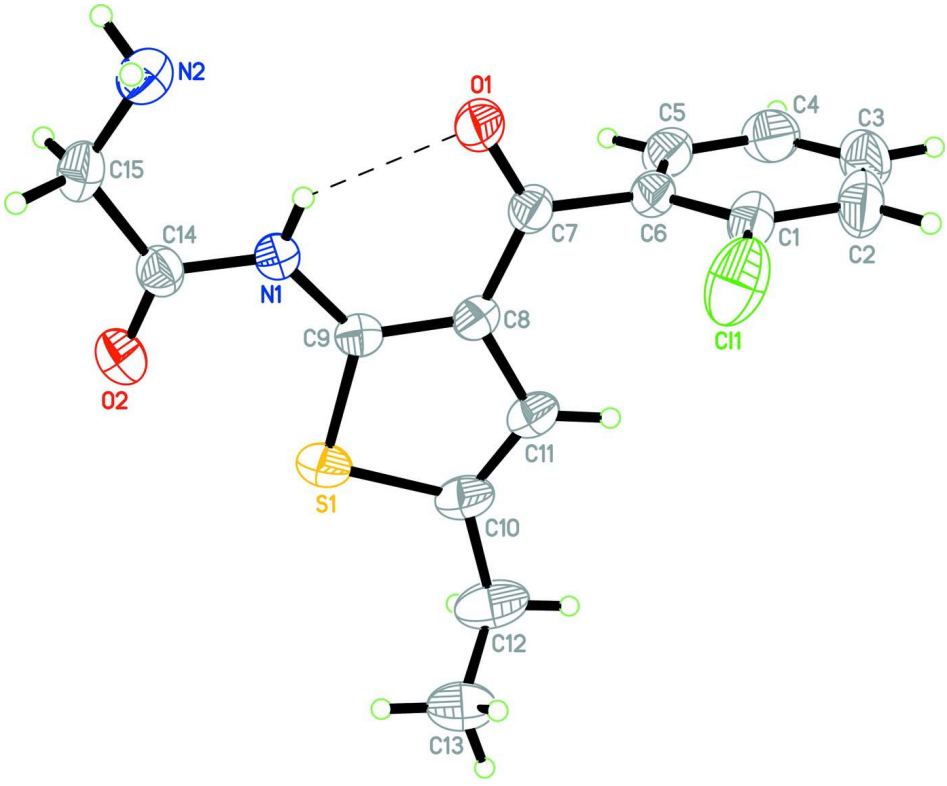

Figure 1

The molecular structure of the title compound, showing 40% probability displacement ellipsoids and the atom-numbering scheme. The intramolecular N—H···O hydrogen bond is shown as a dash line.

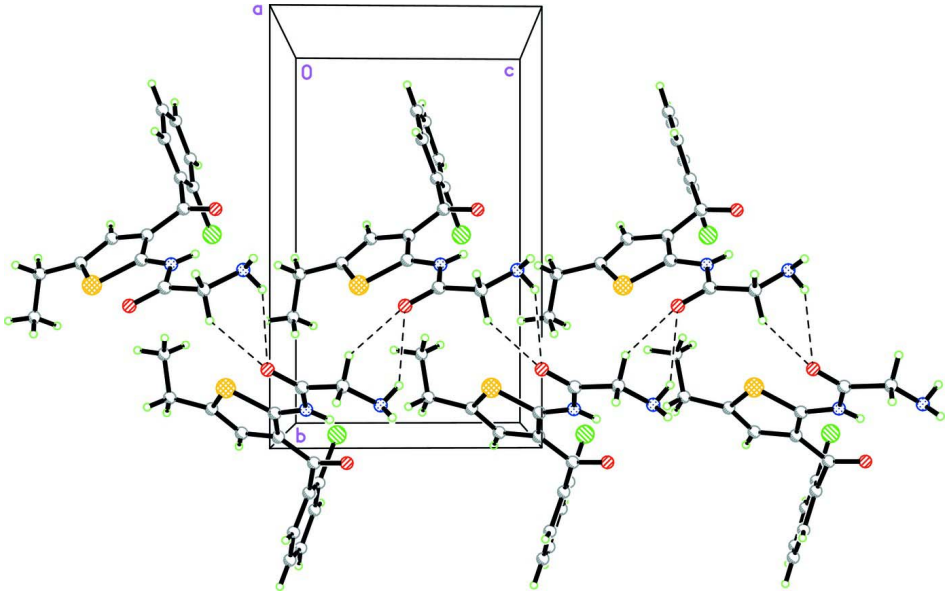

Figure 2

The crystal packing of the title compound viewed along the *a* axis, showing a chain running along the *c* axis. Hydrogen bonds are shown as dashed lines.

2-Amino-*N*-[3-(2-chlorobenzoyl)-5-ethylthiophen-2-yl]acetamide

Crystal data

$C_{15}H_{15}ClN_2O_2S$
$M_r = 322.80$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.9784$ (11) Å
$b = 13.5565$ (11) Å
$c = 8.3334$ (7) Å
$\beta = 91.233$ (1)°
$V = 1578.8$ (2) Å^3
$Z = 4$
$F(000) = 672$
$D_x = 1.358$ Mg m^{-3}
Melting point = 417–419 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4184 reflections
$\theta = 1.5$–29.0°
$\mu = 0.38$ mm^{-1}
$T = 293$ K
Block, yellow
0.56 × 0.41 × 0.28 mm

Data collection

Bruker APEX DUO CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.817$, $T_{max} = 0.902$
16034 measured reflections
4184 independent reflections
3180 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 29.0°$, $\theta_{min} = 1.5°$
$h = -18 \rightarrow 19$
$k = -18 \rightarrow 17$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.163$
$S = 1.05$
4184 reflections
191 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.079P)^2 + 0.4642P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ 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 esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.44203 (5)	0.00271 (7)	0.78182 (12)	0.1059 (3)
S1	0.12494 (4)	0.13080 (4)	1.17920 (6)	0.06549 (19)

O1	0.19142 (11)	−0.04825 (14)	0.72869 (17)	0.0736 (5)
O2	−0.03578 (13)	0.17865 (14)	1.0035 (2)	0.0834 (5)
N1	0.06864 (11)	0.08376 (12)	0.87282 (19)	0.0516 (4)
H1N1	0.0845	0.0597	0.7864	0.062*
N2	−0.02762 (16)	0.09813 (17)	0.5929 (3)	0.0771 (5)
H1N2	−0.0804	0.0735	0.5496	0.093*
H2N2	−0.0066	0.1416	0.5262	0.093*
C1	0.40677 (15)	−0.11245 (19)	0.8517 (3)	0.0658 (5)
C2	0.47451 (19)	−0.1860 (3)	0.8745 (3)	0.0863 (8)
H2A	0.5387	−0.1741	0.8543	0.104*
C3	0.4451 (2)	−0.2771 (2)	0.9274 (3)	0.0897 (8)
H3A	0.4899	−0.3274	0.9402	0.108*
C4	0.3506 (2)	−0.2951 (2)	0.9617 (3)	0.0834 (7)
H4A	0.3319	−0.3566	0.9988	0.100*
C5	0.28426 (17)	−0.22083 (18)	0.9404 (3)	0.0694 (6)
H5A	0.2206	−0.2324	0.9645	0.083*
C6	0.31130 (13)	−0.12879 (15)	0.8834 (2)	0.0545 (4)
C7	0.23554 (13)	−0.05129 (16)	0.8577 (2)	0.0540 (4)
C8	0.21449 (13)	0.01234 (14)	0.9924 (2)	0.0506 (4)
C9	0.13424 (13)	0.07179 (14)	0.9968 (2)	0.0497 (4)
C10	0.23183 (18)	0.07790 (18)	1.2498 (3)	0.0677 (6)
C11	0.26932 (16)	0.01788 (16)	1.1402 (2)	0.0606 (5)
H11A	0.3258	−0.0171	1.1580	0.073*
C12	0.2683 (3)	0.1027 (3)	1.4170 (3)	0.1028 (10)
H12A	0.2203	0.0829	1.4930	0.123*
H12B	0.3253	0.0639	1.4394	0.123*
C13	0.2909 (3)	0.2061 (3)	1.4438 (5)	0.1304 (15)
H13A	0.3160	0.2147	1.5510	0.196*
H13B	0.2339	0.2450	1.4296	0.196*
H13C	0.3378	0.2270	1.3684	0.196*
C14	−0.01269 (14)	0.13727 (14)	0.8807 (3)	0.0568 (4)
C15	−0.07268 (15)	0.14234 (17)	0.7292 (3)	0.0642 (5)
H15A	−0.1331	0.1092	0.7468	0.077*
H15B	−0.0865	0.2109	0.7050	0.077*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0672 (4)	0.1184 (7)	0.1321 (7)	−0.0118 (4)	0.0012 (4)	0.0488 (5)
S1	0.0777 (4)	0.0644 (3)	0.0544 (3)	−0.0016 (2)	0.0008 (2)	−0.0138 (2)
O1	0.0712 (9)	0.1004 (12)	0.0487 (7)	0.0291 (9)	−0.0113 (6)	−0.0111 (7)
O2	0.0772 (11)	0.0864 (12)	0.0864 (11)	0.0238 (9)	0.0016 (9)	−0.0235 (10)
N1	0.0509 (8)	0.0529 (9)	0.0509 (8)	0.0057 (7)	−0.0018 (6)	−0.0039 (6)
N2	0.0811 (13)	0.0784 (13)	0.0710 (12)	0.0116 (11)	−0.0191 (10)	−0.0050 (10)
C1	0.0517 (10)	0.0825 (15)	0.0631 (12)	0.0085 (10)	−0.0008 (9)	0.0073 (11)
C2	0.0599 (13)	0.119 (2)	0.0801 (16)	0.0295 (14)	−0.0003 (11)	0.0058 (16)
C3	0.095 (2)	0.0887 (19)	0.0849 (17)	0.0402 (16)	−0.0130 (14)	−0.0049 (15)
C4	0.099 (2)	0.0647 (14)	0.0851 (17)	0.0086 (13)	−0.0192 (14)	−0.0007 (12)

C5	0.0655 (13)	0.0703 (14)	0.0720 (13)	−0.0003 (10)	−0.0114 (10)	0.0000 (11)
C6	0.0497 (9)	0.0654 (12)	0.0483 (9)	0.0070 (8)	−0.0045 (7)	−0.0031 (8)
C7	0.0470 (9)	0.0654 (11)	0.0494 (9)	0.0045 (8)	−0.0027 (7)	0.0002 (8)
C8	0.0477 (9)	0.0560 (10)	0.0478 (9)	−0.0027 (7)	−0.0047 (7)	−0.0009 (7)
C9	0.0518 (9)	0.0492 (9)	0.0480 (9)	−0.0050 (7)	−0.0003 (7)	−0.0030 (7)
C10	0.0822 (14)	0.0698 (13)	0.0505 (10)	−0.0120 (11)	−0.0132 (10)	−0.0024 (9)
C11	0.0608 (11)	0.0649 (12)	0.0555 (10)	−0.0065 (9)	−0.0135 (9)	0.0017 (9)
C12	0.129 (3)	0.121 (2)	0.0574 (13)	−0.024 (2)	−0.0235 (15)	−0.0127 (15)
C13	0.131 (3)	0.144 (3)	0.114 (3)	0.016 (2)	−0.040 (2)	−0.072 (3)
C14	0.0534 (10)	0.0485 (10)	0.0686 (12)	0.0021 (8)	0.0015 (9)	−0.0005 (9)
C15	0.0538 (11)	0.0601 (12)	0.0784 (14)	0.0042 (9)	−0.0054 (9)	0.0132 (10)

Geometric parameters (Å, º)

Cl1—C1	1.741 (3)	C5—C6	1.390 (3)
S1—C9	1.7248 (18)	C5—H5A	0.9300
S1—C10	1.748 (3)	C6—C7	1.504 (3)
O1—C7	1.229 (2)	C7—C8	1.451 (3)
O2—C14	1.217 (3)	C8—C9	1.382 (3)
N1—C14	1.351 (2)	C8—C11	1.438 (3)
N1—C9	1.376 (2)	C10—C11	1.338 (3)
N1—H1N1	0.8253	C10—C12	1.511 (3)
N2—C15	1.441 (3)	C11—H11A	0.9300
N2—H1N2	0.8805	C12—C13	1.454 (5)
N2—H2N2	0.8655	C12—H12A	0.9700
C1—C6	1.384 (3)	C12—H12B	0.9700
C1—C2	1.386 (3)	C13—H13A	0.9600
C2—C3	1.376 (5)	C13—H13B	0.9600
C2—H2A	0.9300	C13—H13C	0.9600
C3—C4	1.379 (4)	C14—C15	1.502 (3)
C3—H3A	0.9300	C15—H15A	0.9700
C4—C5	1.378 (3)	C15—H15B	0.9700
C4—H4A	0.9300		
C9—S1—C10	91.49 (10)	N1—C9—C8	125.22 (16)
C14—N1—C9	125.06 (17)	N1—C9—S1	123.04 (14)
C14—N1—H1N1	119.8	C8—C9—S1	111.74 (13)
C9—N1—H1N1	114.9	C11—C10—C12	129.4 (3)
C15—N2—H1N2	96.0	C11—C10—S1	111.37 (15)
C15—N2—H2N2	112.5	C12—C10—S1	119.2 (2)
H1N2—N2—H2N2	106.7	C10—C11—C8	114.0 (2)
C6—C1—C2	121.2 (2)	C10—C11—H11A	123.0
C6—C1—Cl1	119.25 (17)	C8—C11—H11A	123.0
C2—C1—Cl1	119.6 (2)	C13—C12—C10	115.1 (3)
C3—C2—C1	118.8 (3)	C13—C12—H12A	108.5
C3—C2—H2A	120.6	C10—C12—H12A	108.5
C1—C2—H2A	120.6	C13—C12—H12B	108.5
C2—C3—C4	121.2 (2)	C10—C12—H12B	108.5

C2—C3—H3A	119.4	H12A—C12—H12B	107.5
C4—C3—H3A	119.4	C12—C13—H13A	109.5
C5—C4—C3	119.3 (3)	C12—C13—H13B	109.5
C5—C4—H4A	120.3	H13A—C13—H13B	109.5
C3—C4—H4A	120.3	C12—C13—H13C	109.5
C4—C5—C6	120.8 (2)	H13A—C13—H13C	109.5
C4—C5—H5A	119.6	H13B—C13—H13C	109.5
C6—C5—H5A	119.6	O2—C14—N1	121.8 (2)
C1—C6—C5	118.6 (2)	O2—C14—C15	122.17 (19)
C1—C6—C7	122.7 (2)	N1—C14—C15	116.03 (18)
C5—C6—C7	118.68 (18)	N2—C15—C14	113.44 (17)
O1—C7—C8	123.42 (18)	N2—C15—H15A	108.9
O1—C7—C6	119.14 (18)	C14—C15—H15A	108.9
C8—C7—C6	117.31 (16)	N2—C15—H15B	108.9
C9—C8—C11	111.39 (17)	C14—C15—H15B	108.9
C9—C8—C7	123.05 (16)	H15A—C15—H15B	107.7
C11—C8—C7	125.47 (18)		

C6—C1—C2—C3	1.0 (4)	C14—N1—C9—S1	−4.1 (3)
Cl1—C1—C2—C3	−179.0 (2)	C11—C8—C9—N1	178.71 (18)
C1—C2—C3—C4	−1.7 (4)	C7—C8—C9—N1	−4.8 (3)
C2—C3—C4—C5	0.9 (4)	C11—C8—C9—S1	−1.3 (2)
C3—C4—C5—C6	0.7 (4)	C7—C8—C9—S1	175.21 (15)
C2—C1—C6—C5	0.6 (3)	C10—S1—C9—N1	−178.53 (17)
Cl1—C1—C6—C5	−179.48 (17)	C10—S1—C9—C8	1.49 (16)
C2—C1—C6—C7	−179.0 (2)	C9—S1—C10—C11	−1.31 (19)
Cl1—C1—C6—C7	1.0 (3)	C9—S1—C10—C12	179.3 (2)
C4—C5—C6—C1	−1.4 (3)	C12—C10—C11—C8	−179.9 (3)
C4—C5—C6—C7	178.2 (2)	S1—C10—C11—C8	0.8 (3)
C1—C6—C7—O1	92.5 (3)	C9—C8—C11—C10	0.3 (3)
C5—C6—C7—O1	−87.0 (3)	C7—C8—C11—C10	−176.1 (2)
C1—C6—C7—C8	−91.3 (2)	C11—C10—C12—C13	118.6 (4)
C5—C6—C7—C8	89.1 (2)	S1—C10—C12—C13	−62.2 (4)
O1—C7—C8—C9	10.0 (3)	C9—N1—C14—O2	−1.6 (3)
C6—C7—C8—C9	−166.00 (18)	C9—N1—C14—C15	178.49 (18)
O1—C7—C8—C11	−174.0 (2)	O2—C14—C15—N2	173.2 (2)
C6—C7—C8—C11	10.0 (3)	N1—C14—C15—N2	−6.9 (3)
C14—N1—C9—C8	175.84 (19)		

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the thiophene C8/C9/S1/C10/C11 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*1···O1	0.83	2.15	2.771 (2)	132
N2—H2*N*2···O2^{i}	0.87	2.48	3.118 (3)	131

C15—H15*B*···O2^{i}	0.97	2.37	3.120 (3)	134
C15—H15*A*···*Cg*1^{ii}	0.97	2.75	3.530 (2)	238

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) −*x*, −*y*, −*z*+2.