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(*Z*)-2-(4-Chlorobenzylidene)benzo[*d*]-thiazolo[3,2-*a*]imidazol-3(2*H*)-one

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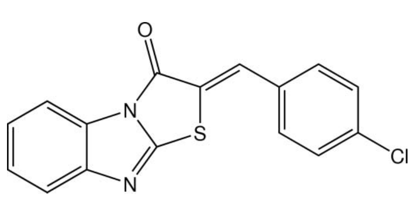
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.030; wR factor = 0.082; data-to-parameter ratio = 19.3.

The molecule of the title compound, $C_{16}H_9ClN_2OS$, is approximately planar, the dihedral angle between the thiazolo[3,2-*a*]benzimidazole ring system and the 4-chlorophenyl ring being 2.10 (5)°. An intramolecular C—H⋯S interaction generates an S(6) ring motif. In the crystal, molecules are stacked into columns along the b axis by π–π interactions with centroid–centroid distances of 3.6495 (7)–3.9546 (8) Å.

Related literature

For bond-length data, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For background to and the biological activity of thiazolo[3,2-*a*]benzimidazoles, see: Abdel-Aziz, El-Zahabi & Dawood (2010); Abdel-Aziz, Hamdy *et al.* (2007, 2008); Abdel-Aziz, Saleh & El-Zahabi (2010); Al-Rashood & Abdel-Aziz (2010); Chimirri *et al.* (1988); Farag *et al.* (2011); Hamdy *et al.* (2007); Mavrova *et al.* (2005). For the stability of the temperature controller, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{16}H_9ClN_2OS$
M_r = 312.77
Triclinic, $P\bar{1}$
a = 7.0182 (4) Å
b = 7.3443 (4) Å
c = 13.7142 (8) Å
α = 91.742 (1)°
β = 100.836 (1)°
γ = 112.878 (1)°
V = 635.47 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.46 mm^{-1}
T = 100 K
0.37 × 0.18 × 0.06 mm

Data collection

Bruker APEX DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.848, T_{max} = 0.973
14145 measured reflections
3660 independent reflections
3233 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.082
S = 1.05
3660 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C16—H16*A*⋯S1	0.93	2.50	3.2161 (13)	133

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: IS5117).

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§ Thomson Reuters ResearcherID: A-5085-2009.

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Acta Cryst. (2012). E**68**, o1393–o1394 [doi:10.1107/S1600536812015516]

(*Z*)-2-(4-Chlorobenzylidene)benzo[*d*]thiazolo[3,2-*a*]imidazol-3(2*H*)-one

Hoong-Kun Fun, Suchada Chantrapromma and Hatem A. Abdel-Aziz

S1. Comment

There are considerable interest in the chemistry of thiazolo[3,2-*a*]benzimidazoles and their unique pharmaceutical and medicinal applications have been reported. These activities including antibacterial, antifungal, anti-inflammatory, antiulcer, antiviral, anthelmintic and anticancer properties (Al-Rashood *et al.*, 2010; Chimirri *et al.*, 1988). The parasitological study in vitro has also shown that the analogs of the title compound exhibited higher activity than albendazole against *T. spiralis* (Mavrova *et al.*, 2005). These considerable biological activities as well as in continuation of our interests in the chemistry and biological activities of these compounds (Abdel-Aziz, Hamdy *et al.*, 2007, 2008; Abdel-Aziz, Saleh & El-Zahabi, 2010; Farag *et al.*, 2011; Hamdy *et al.*, 2007) have lead us to synthesize and present the X-ray structural analysis of the title compound (I).

In the molecular structure of (I), $C_{14}H_{11}ClN_4O_4$, the thiazolo[3,2-*a*]benzimidazole ring system is planar with an *r.m.s.* deviation 0.019 (12) Å for the thirteen non H-atoms (C1–C9/N1/N2/O1/S1) and the 4-chlorobenzilidene unit is also planar with an *r.m.s* deviation 0.002 (12) Å for the eight non H-atoms (C10–C16/Cl1). The dihedral between the mean plane through the thiazolo[3,2-*a*]benzimidazole ring system and 4-chlorophenyl ring is 2.10 (5)°. An intramolecular C—H···S weak interaction (Fig. 1 and Table 1) generates an S(6) ring motif (Bernstein *et al.*, 1995) which help to stabilize the planarity of the molecule. The bond distances agree with the literature values (Allen *et al.*, 1987).

In the crystal packing (Fig. 2), the molecules are stacked into column along the *b* axis by *π*–*π* interactions with the distances of $Cg1\cdots Cg1^{i}$ = 3.8297 (7) Å, $Cg2\cdots Cg4^{ii}$ = 3.9545 (8) Å, $Cg3\cdots Cg4^{i}$ = 3.7691 (8) Å and $Cg3\cdots Cg4^{ii}$ = 3.6495 (7) Å [symmetry codes: (i) 1-x, 1-y, -z; (ii) 1-x, -y, -z]. *Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of S1/C1/N2/C8/C9, C1/C2/C7/N1/N2, C2–C7 and C11–C16 rings, respectively.

S2. Experimental

The one-pot synthesis of the title compound was carried out by a cyclocondensation of 2-mercaptobenzimidazole, chloro-acetic acid, 4-chloro benzaldehyde, acetic anhydride and glacial acetic acid in the presence of sodium acetate to afford the title compound (Mavrova *et al.*, 2005; Abdel-Aziz, El-Zahabi & Dawood, 2010). Yellow needle-shaped single crystals of the title compound suitable for *x*-ray structure determination were recrystalized from ethanol by slow evaporation of the solvent at room temperature over several days.

S3. Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with d(C—H) = 0.93 Å for aromatic and CH atoms, and the U_{iso}(H) values were constrained to be $1.2U_{eq}$ of the carrier atoms

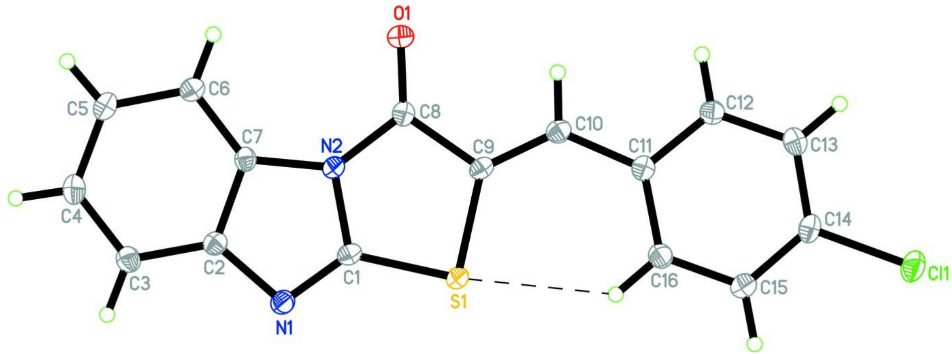

Figure 1

The molecular structure of the title compound with 50% probability displacement ellipsoids and the atom-numbering scheme. Intramolecular C—H···S weak interaction was shown as dashed line.

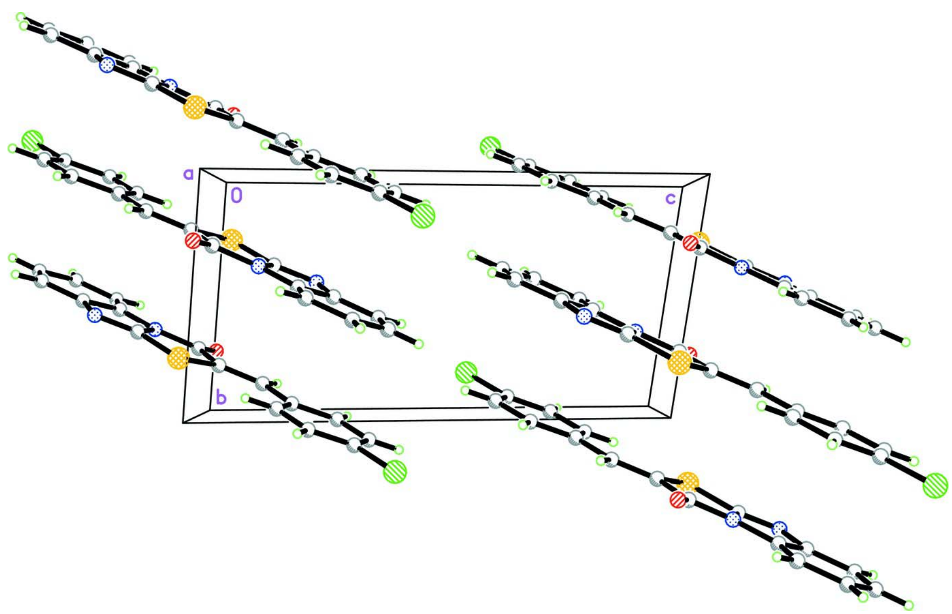

Figure 2

The crystal packing of the title compound viewed along the *a* axis.

(*Z*)-2-(4-Chlorobenzylidene)benzo[*d*]thiazolo[3,2- *a*]imidazol-3(2*H*)-one

Crystal data

$C_{16}H_9ClN_2OS$
M_r = 312.77
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.0182 (4) Å
b = 7.3443 (4) Å
c = 13.7142 (8) Å
α = 91.742 (1)°
β = 100.836 (1)°
γ = 112.878 (1)°
V = 635.47 (6) Å^3
Z = 2
F(000) = 320
D_x = 1.635 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3660 reflections
θ = 1.5–30.0°
μ = 0.46 mm^{-1}
T = 100 K
Needle, yellow
0.37 × 0.18 × 0.06 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)
$T_{min} = 0.848$, $T_{max} = 0.973$
14145 measured reflections
3660 independent reflections
3233 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 30.0°$, $\theta_{min} = 1.5°$
$h = -9 \rightarrow 9$
$k = -10 \rightarrow 10$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.082$
$S = 1.05$
3660 reflections
190 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
$w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 0.3855P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.56$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ 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 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}
S1	0.34693 (4)	0.25459 (4)	0.03735 (2)	0.01299 (8)
Cl1	−0.35675 (5)	−0.18707 (5)	−0.43869 (2)	0.02057 (9)
O1	0.88271 (14)	0.27130 (14)	−0.01062 (7)	0.01625 (18)
N1	0.58054 (16)	0.43157 (15)	0.22785 (8)	0.0138 (2)
N2	0.75134 (15)	0.36857 (15)	0.11464 (7)	0.01179 (19)
C1	0.56374 (18)	0.36129 (17)	0.13730 (9)	0.0123 (2)
C2	0.79803 (18)	0.49233 (17)	0.27094 (9)	0.0125 (2)
C3	0.90598 (19)	0.57701 (18)	0.36781 (9)	0.0147 (2)
H3A	0.8365	0.6030	0.4144	0.018*
C4	1.1227 (2)	0.62158 (18)	0.39238 (9)	0.0156 (2)
H4A	1.1988	0.6788	0.4566	0.019*
C5	1.22857 (19)	0.58244 (18)	0.32293 (9)	0.0149 (2)
H5A	1.3731	0.6138	0.3422	0.018*
C6	1.12230 (18)	0.49741 (18)	0.22550 (9)	0.0135 (2)

H6A	1.1918	0.4713	0.1789	0.016*
C7	0.90738 (18)	0.45404 (17)	0.20197 (9)	0.0117 (2)
C8	0.73740 (18)	0.28632 (17)	0.01951 (9)	0.0121 (2)
C9	0.51258 (18)	0.21858 (17)	−0.03702 (9)	0.0120 (2)
C10	0.45896 (18)	0.14096 (17)	−0.13349 (9)	0.0129 (2)
H10A	0.5708	0.1362	−0.1591	0.015*
C11	0.25559 (18)	0.06330 (17)	−0.20435 (9)	0.0125 (2)
C12	0.25076 (19)	−0.00568 (18)	−0.30184 (9)	0.0140 (2)
H12A	0.3757	0.0004	−0.3181	0.017*
C13	0.0643 (2)	−0.08267 (18)	−0.37443 (9)	0.0154 (2)
H13A	0.0636	−0.1272	−0.4388	0.018*
C14	−0.12171 (19)	−0.09177 (18)	−0.34886 (9)	0.0144 (2)
C15	−0.12333 (19)	−0.02595 (18)	−0.25342 (9)	0.0149 (2)
H15A	−0.2493	−0.0337	−0.2377	0.018*
C16	0.06430 (19)	0.05172 (18)	−0.18134 (9)	0.0141 (2)
H16A	0.0635	0.0965	−0.1173	0.017*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01026 (13)	0.01520 (14)	0.01318 (14)	0.00536 (10)	0.00154 (10)	−0.00024 (10)
Cl1	0.01474 (14)	0.02600 (17)	0.01591 (15)	0.00557 (12)	−0.00226 (11)	−0.00026 (11)
O1	0.0137 (4)	0.0197 (4)	0.0166 (4)	0.0080 (3)	0.0038 (3)	−0.0002 (3)
N1	0.0123 (4)	0.0143 (5)	0.0146 (5)	0.0056 (4)	0.0021 (4)	0.0006 (4)
N2	0.0103 (4)	0.0130 (4)	0.0123 (4)	0.0052 (3)	0.0018 (3)	0.0012 (4)
C1	0.0108 (5)	0.0127 (5)	0.0145 (5)	0.0056 (4)	0.0029 (4)	0.0021 (4)
C2	0.0126 (5)	0.0113 (5)	0.0140 (5)	0.0056 (4)	0.0024 (4)	0.0015 (4)
C3	0.0163 (5)	0.0142 (5)	0.0136 (5)	0.0065 (4)	0.0029 (4)	0.0007 (4)
C4	0.0176 (5)	0.0135 (5)	0.0134 (5)	0.0057 (4)	−0.0007 (4)	0.0004 (4)
C5	0.0129 (5)	0.0139 (5)	0.0163 (6)	0.0050 (4)	0.0001 (4)	0.0021 (4)
C6	0.0124 (5)	0.0131 (5)	0.0153 (5)	0.0056 (4)	0.0028 (4)	0.0021 (4)
C7	0.0131 (5)	0.0108 (5)	0.0108 (5)	0.0050 (4)	0.0013 (4)	0.0013 (4)
C8	0.0125 (5)	0.0104 (5)	0.0126 (5)	0.0044 (4)	0.0016 (4)	0.0013 (4)
C9	0.0096 (5)	0.0112 (5)	0.0155 (5)	0.0047 (4)	0.0023 (4)	0.0023 (4)
C10	0.0125 (5)	0.0121 (5)	0.0149 (5)	0.0059 (4)	0.0029 (4)	0.0024 (4)
C11	0.0130 (5)	0.0106 (5)	0.0135 (5)	0.0047 (4)	0.0017 (4)	0.0017 (4)
C12	0.0141 (5)	0.0141 (5)	0.0143 (5)	0.0062 (4)	0.0030 (4)	0.0013 (4)
C13	0.0176 (5)	0.0152 (5)	0.0125 (5)	0.0064 (4)	0.0020 (4)	0.0008 (4)
C14	0.0136 (5)	0.0125 (5)	0.0142 (5)	0.0042 (4)	−0.0009 (4)	0.0016 (4)
C15	0.0129 (5)	0.0158 (5)	0.0161 (6)	0.0059 (4)	0.0033 (4)	0.0027 (4)
C16	0.0148 (5)	0.0144 (5)	0.0131 (5)	0.0061 (4)	0.0028 (4)	0.0010 (4)

Geometric parameters (Å, º)

S1—C1	1.7411 (12)	C6—C7	1.3849 (16)
S1—C9	1.7692 (12)	C6—H6A	0.9300
Cl1—C14	1.7363 (12)	C8—C9	1.4981 (16)
O1—C8	1.2108 (14)	C9—C10	1.3480 (16)

N1—C1	1.2967 (15)	C10—C11	1.4556 (16)
N1—C2	1.4119 (15)	C10—H10A	0.9300
N2—C1	1.3903 (14)	C11—C12	1.4049 (16)
N2—C8	1.3909 (15)	C11—C16	1.4076 (16)
N2—C7	1.3980 (15)	C12—C13	1.3871 (17)
C2—C3	1.3895 (16)	C12—H12A	0.9300
C2—C7	1.4097 (16)	C13—C14	1.3917 (17)
C3—C4	1.3955 (17)	C13—H13A	0.9300
C3—H3A	0.9300	C14—C15	1.3850 (17)
C4—C5	1.3990 (17)	C15—C16	1.3888 (17)
C4—H4A	0.9300	C15—H15A	0.9300
C5—C6	1.3942 (17)	C16—H16A	0.9300
C5—H5A	0.9300		

C1—S1—C9	90.12 (5)	O1—C8—C9	126.82 (11)
C1—N1—C2	103.32 (10)	N2—C8—C9	107.93 (10)
C1—N2—C8	116.71 (10)	C10—C9—C8	119.68 (10)
C1—N2—C7	105.85 (9)	C10—C9—S1	128.06 (9)
C8—N2—C7	137.35 (10)	C8—C9—S1	112.26 (8)
N1—C1—N2	115.19 (10)	C9—C10—C11	130.90 (11)
N1—C1—S1	131.92 (9)	C9—C10—H10A	114.5
N2—C1—S1	112.88 (9)	C11—C10—H10A	114.5
C3—C2—C7	120.04 (11)	C12—C11—C16	118.15 (11)
C3—C2—N1	128.60 (11)	C12—C11—C10	117.52 (10)
C7—C2—N1	111.36 (10)	C16—C11—C10	124.33 (11)
C2—C3—C4	117.38 (11)	C13—C12—C11	121.66 (11)
C2—C3—H3A	121.3	C13—C12—H12A	119.2
C4—C3—H3A	121.3	C11—C12—H12A	119.2
C3—C4—C5	121.78 (11)	C12—C13—C14	118.53 (11)
C3—C4—H4A	119.1	C12—C13—H13A	120.7
C5—C4—H4A	119.1	C14—C13—H13A	120.7
C6—C5—C4	121.47 (11)	C15—C14—C13	121.46 (11)
C6—C5—H5A	119.3	C15—C14—Cl1	119.27 (9)
C4—C5—H5A	119.3	C13—C14—Cl1	119.26 (9)
C7—C6—C5	116.23 (11)	C14—C15—C16	119.61 (11)
C7—C6—H6A	121.9	C14—C15—H15A	120.2
C5—C6—H6A	121.9	C16—C15—H15A	120.2
C6—C7—N2	132.61 (11)	C15—C16—C11	120.58 (11)
C6—C7—C2	123.10 (11)	C15—C16—H16A	119.7
N2—C7—C2	104.28 (10)	C11—C16—H16A	119.7
O1—C8—N2	125.24 (11)		

C2—N1—C1—N2	0.05 (14)	C1—N2—C8—O1	−176.11 (12)
C2—N1—C1—S1	179.02 (10)	C7—N2—C8—O1	−0.2 (2)
C8—N2—C1—N1	177.22 (10)	C1—N2—C8—C9	3.12 (14)
C7—N2—C1—N1	0.13 (14)	C7—N2—C8—C9	178.99 (13)
C8—N2—C1—S1	−1.95 (13)	O1—C8—C9—C10	−3.77 (19)
C7—N2—C1—S1	−179.04 (8)	N2—C8—C9—C10	177.02 (11)

C9—S1—C1—N1	−178.97 (13)	O1—C8—C9—S1	176.23 (11)
C9—S1—C1—N2	0.01 (9)	N2—C8—C9—S1	−2.99 (12)
C1—N1—C2—C3	−179.20 (12)	C1—S1—C9—C10	−178.28 (12)
C1—N1—C2—C7	−0.20 (13)	C1—S1—C9—C8	1.72 (9)
C7—C2—C3—C4	0.23 (18)	C8—C9—C10—C11	179.37 (11)
N1—C2—C3—C4	179.15 (12)	S1—C9—C10—C11	−0.6 (2)
C2—C3—C4—C5	−0.26 (18)	C9—C10—C11—C12	178.99 (12)
C3—C4—C5—C6	0.22 (19)	C9—C10—C11—C16	−1.5 (2)
C4—C5—C6—C7	−0.14 (18)	C16—C11—C12—C13	0.28 (18)
C5—C6—C7—N2	−179.28 (12)	C10—C11—C12—C13	179.85 (11)
C5—C6—C7—C2	0.12 (18)	C11—C12—C13—C14	−0.30 (19)
C1—N2—C7—C6	179.25 (13)	C12—C13—C14—C15	0.04 (19)
C8—N2—C7—C6	3.1 (2)	C12—C13—C14—Cl1	179.84 (9)
C1—N2—C7—C2	−0.24 (12)	C13—C14—C15—C16	0.24 (19)
C8—N2—C7—C2	−176.40 (13)	Cl1—C14—C15—C16	−179.57 (9)
C3—C2—C7—C6	−0.17 (18)	C14—C15—C16—C11	−0.26 (19)
N1—C2—C7—C6	−179.26 (11)	C12—C11—C16—C15	0.01 (18)
C3—C2—C7—N2	179.38 (11)	C10—C11—C16—C15	−179.53 (11)
N1—C2—C7—N2	0.28 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16*A*···S1	0.93	2.50	3.2161 (13)	133