Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Acetyl-4-(phenylsulfanyl)imidazolidin-2-one

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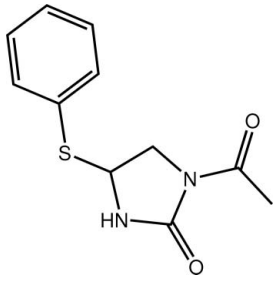
Received 20 February 2012; accepted 22 February 2012

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.028; wR factor = 0.073; data-to-parameter ratio = 14.6.

The five-membered ring in the title imidazolidinone derivative, $C_{11}H_{12}N_2O_2S$, adopts an envelope conformation with the S-bound C atom being the flap atom. Overall, the molecule has a U-shaped conformation as both rings are folded towards each other [dihedral angle = 31.66 (6)°]. An eight-membered amide $\{\cdots HNCO\}_2$ synthon leads to hydrogen-bonded dimeric aggregates in the crystal: these are additionally linked by C—H$\cdots\pi$ interactions.

Related literature

For the antitumour potential of imidazolidinones, see: Abdel-Aziz *et al.* (2012). For ring conformational analysis, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{11}H_{12}N_2O_2S$ M_r = 236.29
Monoclinic, $P2_1/n$
a = 7.0473 (1) Å
b = 14.3274 (3) Å
c = 10.7796 (2) Å
β = 96.921 (2)°
V = 1080.48 (3) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.56 mm^{-1}
T = 100 K
0.35 × 0.30 × 0.25 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.754, T_{max} = 1.000
8437 measured reflections
2186 independent reflections
2135 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.073
S = 1.01
2186 reflections
150 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

*Cg*1 is the centroid of the C6–C11 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H1$\cdots$O1^{i}	0.876 (19)	2.032 (19)	2.8989 (13)	169.8 (17)
C1—H1$A\cdots Cg1^{ii}$	0.98	2.72	3.6360 (13)	155

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; 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 *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

This work was supported by the Research Center of Pharmacy, King Saud University, Riyadh, Saudi Arabia. We also thank the Ministry of Higher Education (Malaysia) for funding structural studies through the High-Impact Research Scheme (grant No. UM.C/HIR/MOHE/SC/12).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5824).

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supplementary materials

Acta Cryst. (2012). E**68**, o908 [doi:10.1107/S1600536812007908]

1-Acetyl-4-(phenylsulfanyl)imidazolidin-2-one

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Comment

A recent study described the anti-tumor potential of imidazolidinones (Abdel-Aziz *et al.*, 2012). In continuation of these studies, herein, the crystal structure determination of an imidazolidinone derivative, 1-acetyl-4-(phenylthio)-imidazolidin-2-one (I) is described.

The five-membered ring in (I), Fig. 1, adopts an envelope conformation with the C4 atom being the flap atom. The puckering parameters (Cremer & Pople, 1975) are Q = 0.2364 (12) Å and φ_2 = 113.9 (3)°. The molecule has a U-shaped conformation whereby the five- and six-membered rings lie to the same side of the molecule and form a dihedral angle of 31.66 (6)°.

In the crystal packing, centrosymmetrically related molecules associate *via* N—H···O hydrogen bonds leading to the familiar eight-membered amide $\{\cdots HNCO\}_2$ synthon, Table 1. The dimers are connected into the three-dimensional architecture by C—H···π interactions, Fig. 2 and Table 1.

Experimental

At room temperature, trifluoroacetic acid (0.3 equiv.) was added drop wise to a stirred solution of 1-acetyl-4-methoxy-imidazolidin-2-one (1 equiv.) and thiophenol (1 equiv.) in dry CH_3CN (0.01 mol/l) over a period of 15 min. After being stirred for 2 h at room temperature, the mixture was quenched by adding ammonium chloride solution (5 ml). The product was extracted with ethylacetate, washed with brine and dried over anhydrous sodium sulfate. The product obtained after evaporation of solvent was purified by column chromatography using a mixture of hexane and $CHCl_3$ (1:1 *v*/*v*) as eluent. Crystals were obtained by slow evaporation of the eluent solution. Yield, 96%. m.p. 383–384 K. IR (KBr, cm^{-1}): *v* 3320 (N—H), 1760, 1710 (C═O). ^{1}H NMR ($CDCl_3$): δ 2.20 (s, 3H), 3.98 (m, 1H), 4.06 (m, 1H), 4.901 (m, 1H), 6.42 (s, 1H), 7.28 (d, 3H, J = 7.0 Hz), 7.45–7.46 (d, 2H, J = 5.5 Hz). ^{13}C NMR ($CDCl_3$): δ 23.21, 48.95, 56.17, 127.51, 129.07, 129.36, 129.46, 135.22, 155.12, 170.11.

Refinement

Carbon-bound H atoms were placed in calculated positions [C—H = 0.95 to 1.00 Å, U_{iso}(H) = 1.2–1.5U_{eq}(C)] and were included in the refinement in the riding model approximation. The H atom bonded to N was freely refined.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); 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 *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

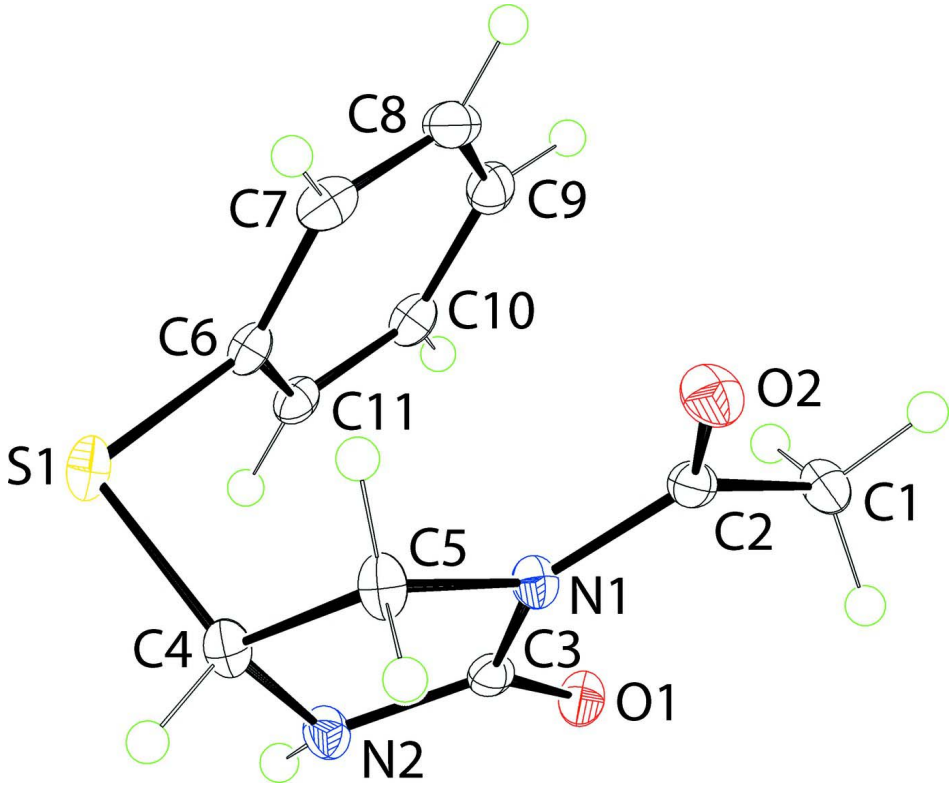

Figure 1

The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

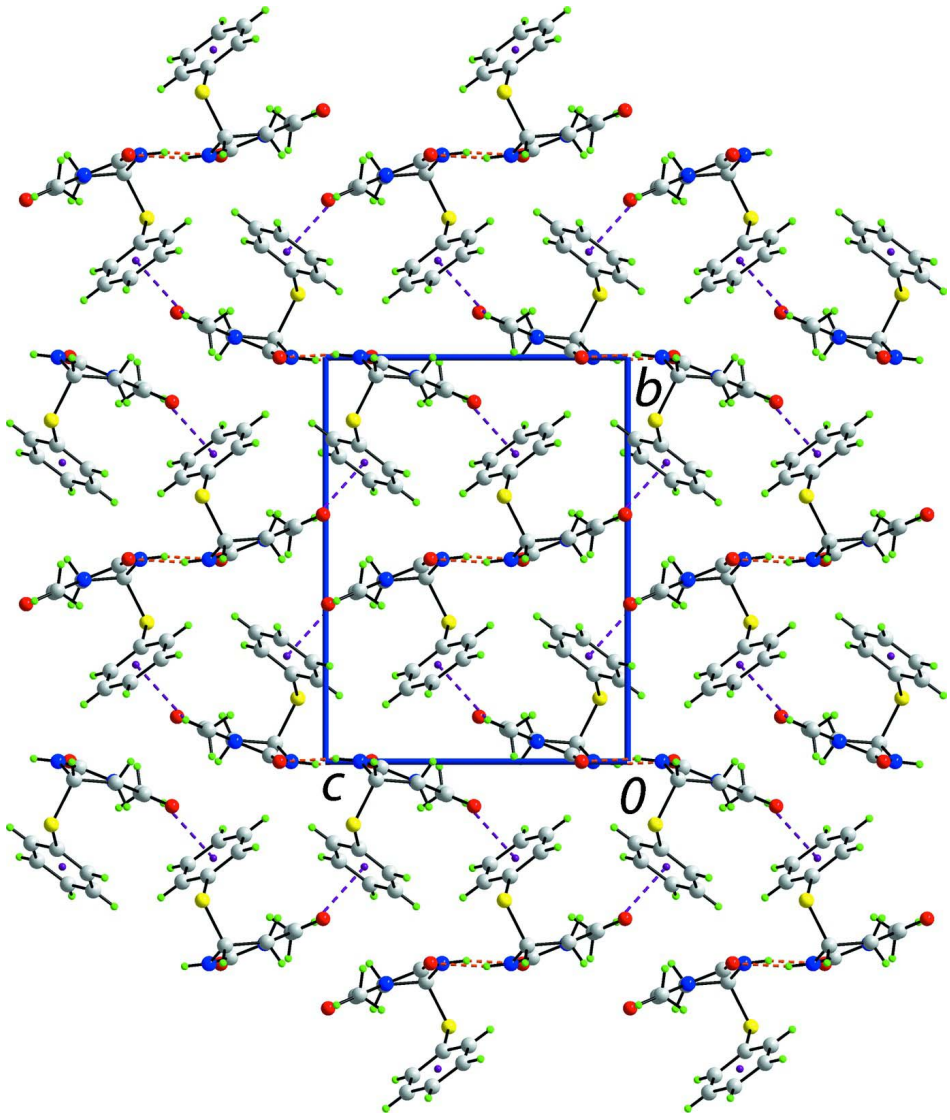

Figure 2

A view in projection down the *a* axis of the unit-cell contents for (I). The N—H···O and C—H···π interactions are shown as orange and purple dashed lines, respectively.

1-Acetyl-4-(phenylsulfanyl)imidazolidin-2-one

Crystal data

$C_{11}H_{12}N_2O_2S$
$M_r = 236.29$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.0473$ (1) Å
$b = 14.3274$ (3) Å
$c = 10.7796$ (2) Å
$\beta = 96.921$ (2)°
$V = 1080.48$ (3) Å^3
$Z = 4$

$F(000) = 496$
$D_x = 1.453$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.5418$ Å
Cell parameters from 6092 reflections
$\theta = 3.1$–$76.4°$
$\mu = 2.56$ mm^{-1}
$T = 100$ K
Prism, colourless
0.35 × 0.30 × 0.25 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.754, T_{max} = 1.000
8437 measured reflections
2186 independent reflections
2135 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
θ_{max} = 76.6°, θ_{min} = 5.2°
h = −8→8
k = −17→15
l = −10→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.073
S = 1.01
2186 reflections
150 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2 + 0.5578P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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.

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}
S1	0.90697 (4)	0.65626 (2)	0.40810 (3)	0.01816 (10)
O1	0.34661 (12)	0.49945 (6)	0.34757 (8)	0.01716 (19)
O2	0.48246 (13)	0.61074 (6)	0.00853 (8)	0.0195 (2)
N1	0.54386 (14)	0.54954 (7)	0.20071 (9)	0.0138 (2)
N2	0.67635 (15)	0.49985 (7)	0.38573 (9)	0.0161 (2)
C1	0.20799 (17)	0.57746 (9)	0.11228 (11)	0.0174 (3)
H1A	0.1359	0.6028	0.0363	0.026*
H1B	0.1814	0.6146	0.1846	0.026*
H1C	0.1696	0.5126	0.1237	0.026*
C2	0.41743 (17)	0.58111 (8)	0.10054 (10)	0.0142 (2)
C3	0.50542 (17)	0.51505 (8)	0.31596 (10)	0.0138 (2)
C4	0.83250 (17)	0.54464 (9)	0.33269 (11)	0.0163 (2)
H4	0.9445	0.5013	0.3399	0.020*
C5	0.75037 (17)	0.55287 (9)	0.19467 (11)	0.0169 (2)
H5A	0.7883	0.6124	0.1582	0.020*
H5B	0.7925	0.5003	0.1450	0.020*

C6	0.68485 (17)	0.71643 (8)	0.38907 (11)	0.0154 (2)
C7	0.63946 (19)	0.77629 (9)	0.28787 (11)	0.0192 (3)
H7	0.7304	0.7878	0.2314	0.023*
C8	0.4618 (2)	0.81908 (9)	0.26958 (12)	0.0209 (3)
H8	0.4305	0.8590	0.1997	0.025*
C9	0.32924 (19)	0.80386 (9)	0.35317 (12)	0.0201 (3)
H9	0.2073	0.8329	0.3402	0.024*
C10	0.37606 (18)	0.74601 (9)	0.45571 (11)	0.0180 (3)
H10	0.2862	0.7362	0.5134	0.022*
C11	0.55324 (17)	0.70240 (8)	0.47448 (11)	0.0158 (2)
H11	0.5848	0.6632	0.5450	0.019*
H1	0.675 (3)	0.4930 (13)	0.4664 (18)	0.032 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01240 (17)	0.02410 (18)	0.01774 (16)	−0.00284 (10)	0.00085 (11)	−0.00434 (11)
O1	0.0171 (5)	0.0213 (4)	0.0130 (4)	−0.0053 (3)	0.0016 (3)	0.0022 (3)
O2	0.0216 (5)	0.0235 (5)	0.0139 (4)	−0.0003 (4)	0.0039 (3)	0.0045 (3)
N1	0.0132 (5)	0.0171 (5)	0.0112 (4)	−0.0003 (4)	0.0018 (4)	0.0004 (4)
N2	0.0167 (5)	0.0189 (5)	0.0121 (5)	0.0000 (4)	−0.0005 (4)	0.0016 (4)
C1	0.0154 (6)	0.0203 (6)	0.0163 (5)	0.0016 (5)	0.0003 (4)	0.0031 (4)
C2	0.0178 (6)	0.0123 (5)	0.0122 (5)	0.0004 (4)	0.0003 (4)	−0.0004 (4)
C3	0.0181 (6)	0.0112 (5)	0.0117 (5)	−0.0011 (4)	0.0004 (4)	−0.0010 (4)
C4	0.0141 (6)	0.0199 (6)	0.0145 (5)	0.0016 (4)	0.0003 (4)	−0.0017 (4)
C5	0.0132 (6)	0.0239 (6)	0.0137 (5)	0.0005 (5)	0.0013 (4)	−0.0024 (5)
C6	0.0152 (6)	0.0160 (6)	0.0148 (5)	−0.0041 (4)	0.0018 (4)	−0.0045 (4)
C7	0.0252 (7)	0.0177 (6)	0.0158 (6)	−0.0051 (5)	0.0065 (5)	−0.0022 (4)
C8	0.0300 (7)	0.0150 (6)	0.0170 (6)	−0.0016 (5)	−0.0001 (5)	0.0010 (5)
C9	0.0189 (6)	0.0175 (6)	0.0231 (6)	0.0004 (5)	−0.0006 (5)	−0.0038 (5)
C10	0.0179 (6)	0.0189 (6)	0.0178 (6)	−0.0042 (5)	0.0046 (5)	−0.0045 (5)
C11	0.0187 (6)	0.0159 (6)	0.0128 (5)	−0.0046 (5)	0.0015 (4)	−0.0015 (4)

Geometric parameters (Å, º)

S1—C6	1.7771 (13)	C4—H4	1.0000
S1—C4	1.8413 (13)	C5—H5A	0.9900
O1—C3	1.2290 (15)	C5—H5B	0.9900
O2—C2	1.2181 (14)	C6—C7	1.3943 (18)
N1—C3	1.3936 (14)	C6—C11	1.3978 (16)
N1—C2	1.3902 (15)	C7—C8	1.3864 (19)
N1—C5	1.4654 (15)	C7—H7	0.9500
N2—C3	1.3586 (16)	C8—C9	1.3913 (18)
N2—C4	1.4496 (15)	C8—H8	0.9500
N2—H1	0.876 (19)	C9—C10	1.3891 (18)
C1—C2	1.4975 (16)	C9—H9	0.9500
C1—H1A	0.9800	C10—C11	1.3891 (18)
C1—H1B	0.9800	C10—H10	0.9500
C1—H1C	0.9800	C11—H11	0.9500
C4—C5	1.5346 (16)		

C6—S1—C4	99.80 (6)	N1—C5—C4	102.41 (9)
C3—N1—C2	129.24 (10)	N1—C5—H5A	111.3
C3—N1—C5	110.61 (10)	C4—C5—H5A	111.3
C2—N1—C5	120.12 (10)	N1—C5—H5B	111.3
C3—N2—C4	112.04 (10)	C4—C5—H5B	111.3
C3—N2—H1	116.8 (12)	H5A—C5—H5B	109.2
C4—N2—H1	122.8 (12)	C7—C6—C11	119.73 (12)
C2—C1—H1A	109.5	C7—C6—S1	120.30 (9)
C2—C1—H1B	109.5	C11—C6—S1	119.96 (10)
H1A—C1—H1B	109.5	C8—C7—C6	120.09 (11)
C2—C1—H1C	109.5	C8—C7—H7	120.0
H1A—C1—H1C	109.5	C6—C7—H7	120.0
H1B—C1—H1C	109.5	C7—C8—C9	120.26 (12)
O2—C2—N1	118.50 (11)	C7—C8—H8	119.9
O2—C2—C1	123.53 (11)	C9—C8—H8	119.9
N1—C2—C1	117.97 (10)	C8—C9—C10	119.68 (12)
O1—C3—N2	126.42 (10)	C8—C9—H9	120.2
O1—C3—N1	126.36 (11)	C10—C9—H9	120.2
N2—C3—N1	107.20 (10)	C11—C10—C9	120.49 (11)
N2—C4—C5	101.59 (9)	C11—C10—H10	119.8
N2—C4—S1	113.57 (8)	C9—C10—H10	119.8
C5—C4—S1	114.55 (9)	C10—C11—C6	119.70 (11)
N2—C4—H4	108.9	C10—C11—H11	120.1
C5—C4—H4	108.9	C6—C11—H11	120.1
S1—C4—H4	108.9		

C3—N1—C2—O2	178.27 (11)	C3—N1—C5—C4	−16.59 (12)
C5—N1—C2—O2	0.41 (17)	C2—N1—C5—C4	161.64 (10)
C3—N1—C2—C1	−1.26 (18)	N2—C4—C5—N1	23.05 (12)
C5—N1—C2—C1	−179.12 (10)	S1—C4—C5—N1	−99.80 (10)
C4—N2—C3—O1	−167.06 (11)	C4—S1—C6—C7	−95.17 (10)
C4—N2—C3—N1	14.33 (13)	C4—S1—C6—C11	83.57 (10)
C2—N1—C3—O1	5.9 (2)	C11—C6—C7—C8	−2.31 (18)
C5—N1—C3—O1	−176.12 (11)	S1—C6—C7—C8	176.44 (9)
C2—N1—C3—N2	−175.53 (11)	C6—C7—C8—C9	1.12 (19)
C5—N1—C3—N2	2.49 (13)	C7—C8—C9—C10	0.44 (19)
C3—N2—C4—C5	−23.91 (13)	C8—C9—C10—C11	−0.80 (19)
C3—N2—C4—S1	99.60 (10)	C9—C10—C11—C6	−0.39 (18)
C6—S1—C4—N2	−55.80 (9)	C7—C6—C11—C10	1.94 (18)
C6—S1—C4—C5	60.32 (9)	S1—C6—C11—C10	−176.81 (9)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C6–C11 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1···O1^{i}	0.876 (19)	2.032 (19)	2.8989 (13)	169.8 (17)
C1—H1*A*···*Cg*1^{ii}	0.98	2.72	3.6360 (13)	155

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