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2,5-Dichloro-*N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)-benzenesulfonamide

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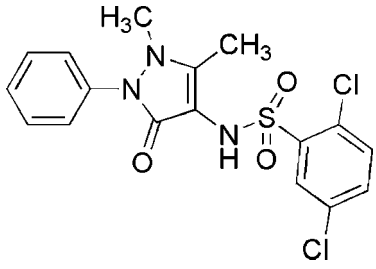
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.007 Å; R factor = 0.096; wR factor = 0.270; data-to-parameter ratio = 13.2.

In the title compound, $C_{17}H_{15}Cl_2N_3O_3S$, the dihedral angle between the mean planes of the pyrazole and phenyl rings is 41.5 (2)°. The dichlorobenzene ring and the pyrazole residue form a C—N—S—C torsion angle of 70.3 (3)°. One intermolecular N—H···O and two intermolecular C—H···O hydrogen bonds are observed in the crystal structure.

Related literature

For related literature, see: Bernardo *et al.* (1996); Chiaramonte *et al.* (2003); Punniyamurthy *et al.* (1995); Torayama *et al.* (1997); Xue *et al.* (2000).



Experimental

Crystal data

$C_{17}H_{15}Cl_2N_3O_3S$
M_r = 412.28
Triclinic, $P\overline{1}$
a = 8.009 (2) Å
b = 10.697 (3) Å
c = 11.201 (5) Å
α = 102.17 (3)°
β = 92.23 (2)°
γ = 108.69 (3)°
V = 882.7 (5) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 4.63 mm^{-1}
T = 299 (2) K
0.45 × 0.38 × 0.13 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.180, T_{max} = 0.545
3679 measured reflections
3139 independent reflections
2692 reflections with $I > 2\sigma(I)$
R_{int} = 0.102
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.096
$wR(F^2)$ = 0.270
S = 1.20
3139 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.93 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O3^{i}	0.86	2.03	2.846 (4)	157
C3—H3···O1^{ii}	0.93	2.51	3.392 (5)	158
C11—H11···O2^{i}	0.93	2.48	3.360 (6)	157

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

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

The authors thank Professor Dr Hartmut Fuess, Technische Universität Darmstadt, for diffractometer time.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2079).

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supplementary materials

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2,5-Dichloro-*N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)benzenesulfonamide

L. E. da Silva, P. T. de Sousa Jr, V. C. da Silva, T. A. N. Ribeiro, S. Foro and E. L. Dall'Oglio

Comment

4-aminoantipyrine and its complexes are known for their variety of applications in the area of catalysis (Bernardo *et al.*, 1996; Punniyamurthy *et al.*, 1995), clinical applications (Chiaramonte *et al.*, 2003), and pharmacology (Torayama *et al.*, 1997). We have focused our research on investigation of different heterocyclic systems based on sulfonamide pharmacophoric group and metal complexes searching new lead compounds with antiparasitic activity. In the light of this interest, we describe here an crystallographic study of the title compound, (I).

The C7—N1—S1—C1 torsion angle between the pyrazole moiety and the dichlorbenzene ring is 70.3 (3)°. The phenyl ring and the pyrazole residue are twisted to each other by an angle of 41.5 (2)° between the mean planes. The N—H H atom has an intermolecular hydrogen bond to O3 [N—H···O = 2.03 Å]. The two sulfonamide oxygen atoms O1 and O2 are involved in non-classical intermolecular hydrogen bonds with C3 and C11 [C—H···O = 2.51 Å, C—H···O = 2.48 Å, respectively] (Table 1).

Experimental

Compound (I) was prepared according to a literature procedure (Xue *et al.*, 2000). Suitable crystals were obtained by re-crystallization from methanol-dichloromethane (1:1).

Refinement

The C—H atoms were positioned with idealized geometry and refined using a riding model with C—H in the range 0.93–0.96 Å. The N—H H atoms were initially located in difference map, which shows that the nitrogen atom is nearly planar. Finally the N—H atoms were positioned with idealized geometry and refined using a riding model with N—H = 0.86 Å. All H atoms were refined with isotropic displacement parameters (set to 1.2 times of the U_{eq} of the parent atom). All crystals investigated exhibits very broad reflection profiles and thus were of low crystal quality, which might be the reason for the bad reliability factors.

Figures

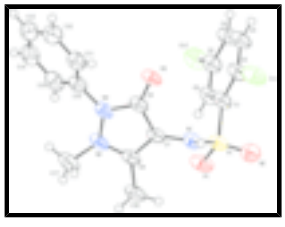


Fig. 1. Molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level.

2,5-Dichloro*N*-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*- pyrazol-4-yl)benzenesulfonamide

Crystal data

$C_{17}H_{15}Cl_2N_3O_3S$	$Z = 2$
$M_r = 412.28$	$F_{000} = 424$
Triclinic, $P\overline{1}$	$D_x = 1.551$ Mg m^{-3}
Hall symbol: -P 1	Cu $K\alpha$ radiation $\lambda = 1.54180$ Å
$a = 8.009$ (2) Å	Cell parameters from 25 reflections
$b = 10.697$ (3) Å	$\theta = 5.3$–18.7º
$c = 11.201$ (5) Å	$\mu = 4.63$ mm^{-1}
$\alpha = 102.17$ (3)º	$T = 299$ (2) K
$\beta = 92.23$ (2)º	Prism, colorless
$\gamma = 108.69$ (3)º	0.45 × 0.38 × 0.13 mm
$V = 882.7$ (5) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.102$
Radiation source: fine-focus sealed tube	$\theta_{max} = 66.9$º
Monochromator: graphite	$\theta_{min} = 4.1$º
$T = 299(2)$ K	$h = -9 \rightarrow 9$
$\omega/2\theta$ scans	$k = -12 \rightarrow 12$
Absorption correction: Psi-scan (North *et al.*, 1968)	$l = -13 \rightarrow 2$
$T_{min} = 0.180$, $T_{max} = 0.545$	3 standard reflections
3679 measured reflections	every 120 min
3139 independent reflections	intensity decay: 1.0%
2692 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.096$	H-atom parameters constrained
$wR(F^2) = 0.270$	$w = 1/[\sigma^2(F_o^2) + (0.2P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.20$	$(\Delta/\sigma)_{max} < 0.001$
3139 reflections	$\Delta\rho_{max} = 1.15$ e Å^{-3}
237 parameters	$\Delta\rho_{min} = -0.93$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.2506 (5)	0.6027 (4)	0.3252 (4)	0.0406 (9)
C2	0.4235 (5)	0.6088 (4)	0.3586 (4)	0.0447 (9)
C3	0.5105 (6)	0.5429 (5)	0.2785 (5)	0.0520 (11)
H3	0.6247	0.5465	0.3027	0.062*
C4	0.4290 (6)	0.4715 (5)	0.1624 (5)	0.0525 (11)
H4	0.4874	0.4265	0.1079	0.063*
C5	0.2600 (6)	0.4674 (4)	0.1280 (4)	0.0449 (9)
C6	0.1701 (6)	0.5323 (4)	0.2073 (4)	0.0443 (10)
H6	0.0565	0.5290	0.1821	0.053*
C7	0.2173 (5)	0.9206 (4)	0.3645 (4)	0.0371 (8)
C8	0.0806 (5)	0.9498 (4)	0.3131 (4)	0.0414 (9)
C9	0.3788 (5)	0.9952 (4)	0.3207 (4)	0.0381 (8)
C10	0.4284 (6)	1.1241 (4)	0.1575 (4)	0.0430 (9)
C11	0.6038 (6)	1.2059 (4)	0.1939 (5)	0.0488 (10)
H11	0.6519	1.2274	0.2756	0.059*
C12	0.7050 (7)	1.2546 (5)	0.1065 (5)	0.0589 (12)
H12	0.8241	1.3066	0.1289	0.071*
C13	0.6322 (8)	1.2275 (5)	−0.0142 (5)	0.0616 (13)
H13	0.7017	1.2620	−0.0721	0.074*
C14	0.4574 (8)	1.1494 (5)	−0.0480 (5)	0.0605 (12)
H14	0.4082	1.1317	−0.1289	0.073*
C15	0.3541 (7)	1.0971 (5)	0.0370 (4)	0.0511 (10)
H15	0.2355	1.0441	0.0139	0.061*
C16	−0.1099 (6)	0.9038 (5)	0.3355 (5)	0.0557 (12)
H16A	−0.1217	0.8644	0.4055	0.067*
H16B	−0.1795	0.8374	0.2645	0.067*
H16C	−0.1508	0.9802	0.3510	0.067*
C17	0.0771 (7)	1.1450 (5)	0.2313 (6)	0.0620 (13)
H17C	0.1435	1.1976	0.1785	0.074*
H17B	0.0936	1.2011	0.3128	0.074*
H17A	−0.0466	1.1110	0.2005	0.074*
N1	0.2147 (4)	0.8422 (3)	0.4515 (3)	0.0377 (7)
H1A	0.2656	0.8841	0.5246	0.045*

N2	0.1397 (4)	1.0301 (4)	0.2342 (4)	0.0456 (9)
N3	0.3272 (4)	1.0676 (4)	0.2471 (3)	0.0434 (8)
O1	−0.0439 (4)	0.6444 (3)	0.3520 (3)	0.0525 (8)
O2	0.1325 (4)	0.6469 (3)	0.5388 (3)	0.0546 (8)
O3	0.5322 (3)	0.9969 (3)	0.3430 (3)	0.0441 (7)
Cl1	0.53256 (15)	0.69729 (13)	0.50285 (11)	0.0617 (5)
Cl2	0.15602 (17)	0.37735 (13)	−0.01848 (11)	0.0634 (5)
S1	0.12324 (12)	0.67997 (9)	0.42367 (9)	0.0404 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0293 (19)	0.0222 (17)	0.064 (2)	0.0068 (14)	−0.0029 (16)	0.0015 (15)
C2	0.031 (2)	0.0317 (19)	0.065 (2)	0.0093 (16)	−0.0046 (17)	0.0002 (17)
C3	0.031 (2)	0.039 (2)	0.082 (3)	0.0129 (18)	0.0001 (19)	0.005 (2)
C4	0.040 (2)	0.036 (2)	0.079 (3)	0.0144 (19)	0.008 (2)	0.004 (2)
C5	0.041 (2)	0.0269 (18)	0.060 (2)	0.0090 (16)	−0.0018 (17)	0.0019 (16)
C6	0.032 (2)	0.0279 (18)	0.068 (3)	0.0088 (15)	−0.0054 (17)	0.0036 (17)
C7	0.0240 (18)	0.0249 (17)	0.057 (2)	0.0073 (14)	0.0007 (15)	0.0002 (15)
C8	0.0286 (19)	0.0292 (18)	0.063 (2)	0.0134 (15)	0.0006 (16)	−0.0013 (16)
C9	0.0275 (19)	0.0260 (17)	0.056 (2)	0.0094 (15)	−0.0015 (15)	−0.0007 (15)
C10	0.037 (2)	0.0302 (19)	0.060 (2)	0.0135 (16)	0.0013 (17)	0.0030 (16)
C11	0.044 (2)	0.033 (2)	0.067 (3)	0.0127 (18)	0.0016 (19)	0.0065 (18)
C12	0.050 (3)	0.038 (2)	0.087 (3)	0.010 (2)	0.013 (2)	0.018 (2)
C13	0.072 (3)	0.042 (2)	0.083 (3)	0.028 (2)	0.025 (3)	0.023 (2)
C14	0.078 (4)	0.047 (3)	0.064 (3)	0.033 (3)	0.007 (2)	0.011 (2)
C15	0.050 (3)	0.037 (2)	0.062 (3)	0.0172 (19)	−0.006 (2)	0.0024 (18)
C16	0.026 (2)	0.053 (3)	0.091 (3)	0.0184 (19)	0.005 (2)	0.014 (2)
C17	0.044 (3)	0.046 (3)	0.101 (4)	0.024 (2)	0.000 (2)	0.016 (3)
N1	0.0257 (15)	0.0237 (15)	0.0546 (18)	0.0039 (12)	−0.0041 (12)	−0.0013 (13)
N2	0.0238 (17)	0.0402 (19)	0.072 (2)	0.0145 (15)	−0.0032 (14)	0.0084 (16)
N3	0.0253 (16)	0.0352 (17)	0.067 (2)	0.0090 (14)	−0.0029 (14)	0.0091 (15)
O1	0.0225 (14)	0.0358 (15)	0.084 (2)	0.0042 (12)	−0.0057 (13)	−0.0066 (14)
O2	0.0431 (18)	0.0384 (16)	0.079 (2)	0.0088 (13)	0.0110 (14)	0.0131 (15)
O3	0.0249 (14)	0.0383 (15)	0.0647 (17)	0.0119 (12)	−0.0030 (11)	0.0022 (12)
Cl1	0.0370 (7)	0.0592 (8)	0.0747 (8)	0.0170 (5)	−0.0131 (5)	−0.0118 (6)
Cl2	0.0586 (8)	0.0551 (8)	0.0669 (8)	0.0218 (6)	−0.0068 (6)	−0.0079 (5)
S1	0.0240 (6)	0.0258 (6)	0.0648 (7)	0.0048 (4)	0.0011 (4)	0.0029 (4)

Geometric parameters (Å, °)

C1—C6	1.389 (6)	C11—C12	1.376 (7)
C1—C2	1.397 (5)	C11—H11	0.9300
C1—S1	1.785 (4)	C12—C13	1.385 (8)
C2—C3	1.373 (7)	C12—H12	0.9300
C2—Cl1	1.727 (4)	C13—C14	1.370 (8)
C3—C4	1.377 (7)	C13—H13	0.9300
C3—H3	0.9300	C14—C15	1.376 (8)
C4—C5	1.378 (6)	C14—H14	0.9300

C4—H4	0.9300	C15—H15	0.9300
C5—C6	1.378 (6)	C16—H16A	0.9600
C5—Cl2	1.739 (4)	C16—H16B	0.9600
C6—H6	0.9300	C16—H16C	0.9600
C7—C8	1.368 (5)	C17—N2	1.473 (5)
C7—N1	1.410 (5)	C17—H17C	0.9600
C7—C9	1.450 (5)	C17—H17B	0.9600
C8—N2	1.355 (6)	C17—H17A	0.9600
C8—C16	1.495 (6)	N1—S1	1.608 (3)
C9—O3	1.237 (4)	N1—H1A	0.8600
C9—N3	1.377 (5)	N2—N3	1.418 (4)
C10—C15	1.386 (7)	O1—S1	1.429 (3)
C10—C11	1.386 (6)	O2—S1	1.412 (4)
C10—N3	1.427 (6)		
C6—C1—C2	118.6 (4)	C14—C13—C12	119.7 (5)
C6—C1—S1	116.8 (3)	C14—C13—H13	120.1
C2—C1—S1	124.6 (3)	C12—C13—H13	120.1
C3—C2—C1	121.0 (4)	C13—C14—C15	120.5 (5)
C3—C2—Cl1	118.1 (3)	C13—C14—H14	119.8
C1—C2—Cl1	120.9 (3)	C15—C14—H14	119.8
C2—C3—C4	120.1 (4)	C14—C15—C10	119.4 (5)
C2—C3—H3	119.9	C14—C15—H15	120.3
C4—C3—H3	119.9	C10—C15—H15	120.3
C3—C4—C5	119.2 (4)	C8—C16—H16A	109.5
C3—C4—H4	120.4	C8—C16—H16B	109.5
C5—C4—H4	120.4	H16A—C16—H16B	109.5
C4—C5—C6	121.5 (4)	C8—C16—H16C	109.5
C4—C5—Cl2	119.5 (4)	H16A—C16—H16C	109.5
C6—C5—Cl2	119.0 (3)	H16B—C16—H16C	109.5
C5—C6—C1	119.5 (4)	N2—C17—H17C	109.5
C5—C6—H6	120.2	N2—C17—H17B	109.5
C1—C6—H6	120.2	H17C—C17—H17B	109.5
C8—C7—N1	129.1 (4)	N2—C17—H17A	109.5
C8—C7—C9	107.5 (4)	H17C—C17—H17A	109.5
N1—C7—C9	123.3 (3)	H17B—C17—H17A	109.5
N2—C8—C7	110.5 (4)	C7—N1—S1	124.6 (3)
N2—C8—C16	121.7 (4)	C7—N1—H1A	117.7
C7—C8—C16	127.8 (4)	S1—N1—H1A	117.7
O3—C9—N3	125.7 (4)	C8—N2—N3	106.6 (3)
O3—C9—C7	129.0 (4)	C8—N2—C17	120.7 (4)
N3—C9—C7	105.2 (3)	N3—N2—C17	113.2 (3)
C15—C10—C11	120.9 (4)	C9—N3—N2	109.5 (3)
C15—C10—N3	121.0 (4)	C9—N3—C10	124.7 (3)
C11—C10—N3	118.1 (4)	N2—N3—C10	120.9 (3)
C12—C11—C10	118.5 (5)	O2—S1—O1	120.7 (2)
C12—C11—H11	120.8	O2—S1—N1	105.36 (19)
C10—C11—H11	120.8	O1—S1—N1	107.72 (18)
C11—C12—C13	121.0 (5)	O2—S1—C1	109.1 (2)
C11—C12—H12	119.5	O1—S1—C1	104.75 (19)

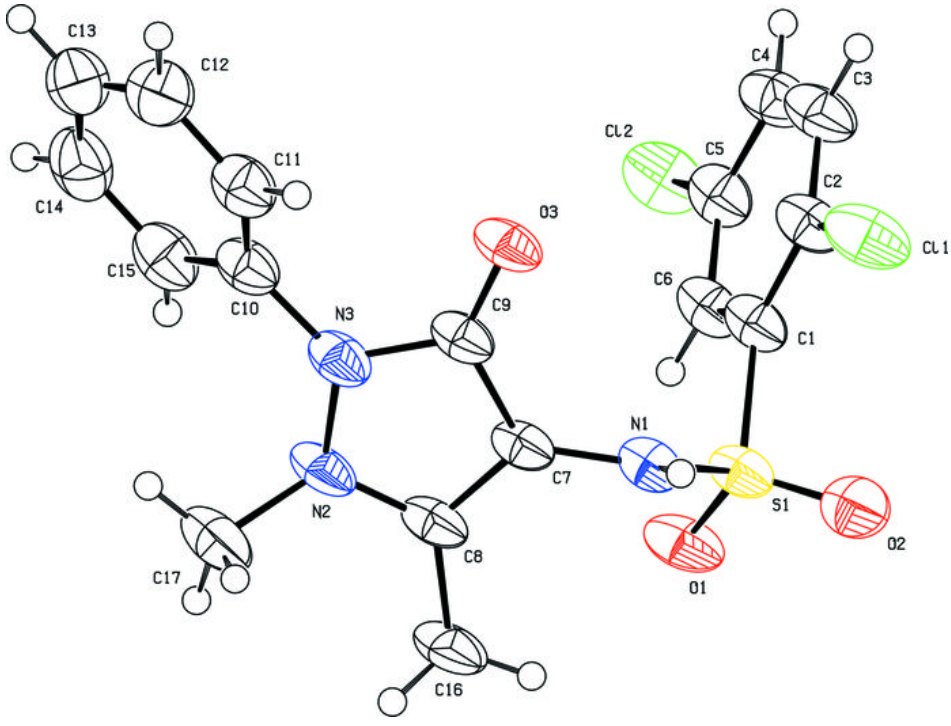
C13—C12—H12	119.5	N1—S1—C1	108.86 (18)
C6—C1—C2—C3	−2.2 (6)	N3—C10—C15—C14	−177.8 (4)
S1—C1—C2—C3	177.9 (3)	C8—C7—N1—S1	70.4 (5)
C6—C1—C2—Cl1	178.8 (3)	C9—C7—N1—S1	−114.7 (4)
S1—C1—C2—Cl1	−1.0 (5)	C7—C8—N2—N3	−7.3 (5)
C1—C2—C3—C4	1.2 (7)	C16—C8—N2—N3	172.7 (4)
Cl1—C2—C3—C4	−179.8 (4)	C7—C8—N2—C17	−138.1 (4)
C2—C3—C4—C5	0.1 (7)	C16—C8—N2—C17	41.8 (6)
C3—C4—C5—C6	−0.5 (7)	O3—C9—N3—N2	174.6 (4)
C3—C4—C5—Cl2	−180.0 (4)	C7—C9—N3—N2	−5.8 (4)
C4—C5—C6—C1	−0.5 (6)	O3—C9—N3—C10	19.4 (6)
Cl2—C5—C6—C1	179.0 (3)	C7—C9—N3—C10	−161.1 (4)
C2—C1—C6—C5	1.8 (6)	C8—N2—N3—C9	8.2 (5)
S1—C1—C6—C5	−178.3 (3)	C17—N2—N3—C9	143.2 (4)
N1—C7—C8—N2	179.3 (4)	C8—N2—N3—C10	164.6 (4)
C9—C7—C8—N2	3.7 (5)	C17—N2—N3—C10	−60.5 (5)
N1—C7—C8—C16	−0.7 (7)	C15—C10—N3—C9	127.2 (4)
C9—C7—C8—C16	−176.3 (4)	C11—C10—N3—C9	−52.3 (6)
C8—C7—C9—O3	−179.0 (4)	C15—C10—N3—N2	−25.4 (6)
N1—C7—C9—O3	5.1 (6)	C11—C10—N3—N2	155.0 (4)
C8—C7—C9—N3	1.4 (4)	C7—N1—S1—O2	−172.8 (3)
N1—C7—C9—N3	−174.4 (3)	C7—N1—S1—O1	−42.8 (4)
C15—C10—C11—C12	−3.1 (6)	C7—N1—S1—C1	70.3 (3)
N3—C10—C11—C12	176.5 (4)	C6—C1—S1—O2	132.0 (3)
C10—C11—C12—C13	2.6 (7)	C2—C1—S1—O2	−48.2 (4)
C11—C12—C13—C14	−0.9 (8)	C6—C1—S1—O1	1.5 (4)
C12—C13—C14—C15	−0.5 (7)	C2—C1—S1—O1	−178.7 (4)
C13—C14—C15—C10	0.0 (7)	C6—C1—S1—N1	−113.5 (3)
C11—C10—C15—C14	1.8 (6)	C2—C1—S1—N1	66.3 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O3^{i}	0.86	2.03	2.846 (4)	157
C3—H3···O1^{ii}	0.93	2.51	3.392 (5)	158
C11—H11···O2^{i}	0.93	2.48	3.360 (6)	157

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

Fig. 1


C13
C12
C11
C14
C15
C10
N3
O3
C9
C4
C3
CL2
C5
C2
CL1
C6
C1
N1
C7
S1
O2
O1
N2
C8
C17
C16