Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)-4-methylbenzenesulfonamide

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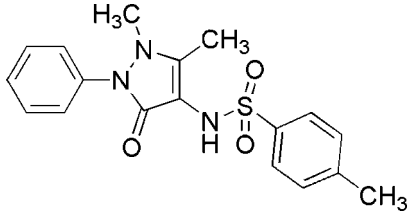
Received 20 November 2007; accepted 21 November 2007

Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.108; data-to-parameter ratio = 13.6.

In the title compound, $C_{18}H_{19}N_3O_3S$, the phenyl ring and the pyrazole ring are twisted with respect to each other by an angle of 49.11 (7)°. The C—N—S—C torsion angle is −122.5 (2)°. The methyl group bonded to the N atom of the pyrazole ring has a large deviation from the mean ring plane of 0.603 (3) Å. One intermolecular N—H···O and two non-classical intermolecular C—H···O hydrogen bonds are observed in the crystal structure.

Related literature

For related literature, see: Xue *et al.* (2000); Alves & Duarte (2002).



Experimental

Crystal data

$C_{18}H_{19}N_3O_3S$
M_r = 357.42
Triclinic, $P\overline{1}$
a = 9.202 (1) Å
b = 9.892 (1) Å
c = 10.067 (1) Å
α = 103.688 (9)°
β = 90.360 (9)°
γ = 104.300 (9)°
V = 860.71 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 299 (2) K
0.50 × 0.20 × 0.16 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.902, T_{max} = 0.967
10096 measured reflections
3519 independent reflections
2600 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.109
S = 1.07
3519 reflections
259 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O3^{i}	0.87 (2)	1.97 (2)	2.826 (2)	167.1 (18)
C2—H2···O1^{ii}	0.92 (2)	2.54 (2)	3.270 (2)	136.4 (16)
C12—H12···O2^{iii}	0.97 (2)	2.43 (2)	3.245 (2)	141.9 (17)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; 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: *SHELXS97*.

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: BT2634).

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supporting information

Acta Cryst. (2008). E**64**, o52 [https://doi.org/10.1107/S1600536807061594]

N-(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)-4-methylbenzenesulfonamide

Luiz Everson da Silva, Paulo Teixeira de Sousa Jr, Evandro Luiz Dall'Oglio and Sabine Foro

S1. Comment

Pyrazolone derivatives, as dypirone, known as a non-steroidal anti-inflammatory drug show analgesic property and have been widely used in Europa and Latin America (Alves & Duarte, 2002). The crystal elucidation of the title compound is a strategy to find new 4-aminoantypirine derivatives with biological significance.

The pyrazole moiety forms a C8—N1—S1—C1 torsion angle with the toluene ring of -122.5 (2)° and a dihedral angle between the mean planes of 49.11 (7)° with the phenyl ring showing the nonplanarity of the system. The methyl group with C18 bounded to the nitrogen atom N2 of the pyrazole ring has a high deviation from the mean plane of -0.603 (3) Å. The NH group has an intermolecular hydrogen bond to the oxygen atom O3 [N—H···O = 1.97 (2) Å]. Both sulfonamide oxygen atoms O1 and O2 are involved in non-classical intermolecular hydrogen bonds with C2 and C12 [C—H···O = 2.54 (2) Å, C—H···O = 2.43 (2) Å, respectively] (Table 1).

S2. Experimental

The ligand was obtained according to the procedure previously described (Xue *et al.*, 2000). Single crystals of (I) suitable for X-ray data collection appeared after a few days from methanol-dichloromethane (1:1).

S3. Refinement

The H atoms of the methyl groups were positioned with idealized geometry using a riding model with C—H = 0.96 Å. The other H atoms were located in difference map, and their positional parameters were refined freely with N—H = 0.87 (2) %A and C—H = 0.92 (2)–0.97 (2) Å. All H atoms were refined with isotropic displacement parameters (set to 1.2 times of the U_{eq} of the parent atom).

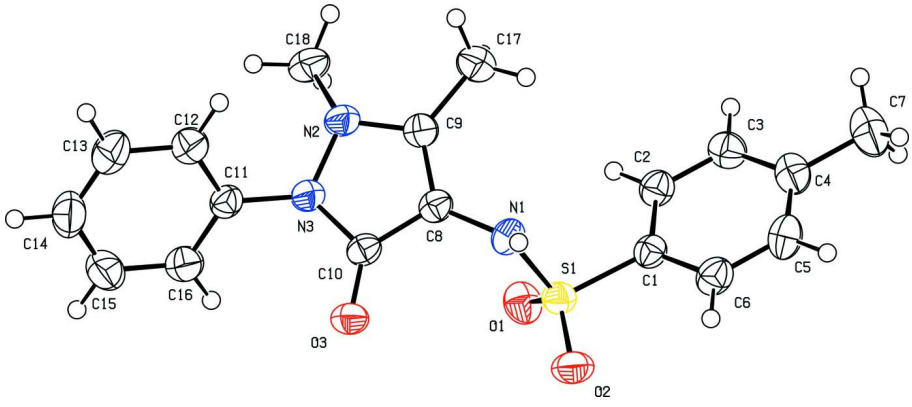

Figure 1

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

N-(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro- 1*H*-pyrazol-4-yl)-4-methylbenzenesulfonamide

Crystal data

$C_{18}H_{19}N_3O_3S$
$M_r = 357.42$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.202$ (1) Å
$b = 9.892$ (1) Å
$c = 10.067$ (1) Å
$\alpha = 103.688$ (9)°
$\beta = 90.360$ (9)°
$\gamma = 104.300$ (9)°
$V = 860.71$ (15) Å^3
$Z = 2$
$F(000) = 376$
$D_x = 1.379$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4280 reflections
$\theta = 2.0$–$25.6°$
$\mu = 0.21$ mm^{-1}
$T = 299$ K
Rod, colorless
0.50 × 0.20 × 0.16 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
Radiation source: fine-focus sealed tube
Graphite monochromator
Rotation method data acquisition using ω and phi scans.
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min} = 0.902$, $T_{max} = 0.967$
10096 measured reflections
3519 independent reflections
2600 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.3°$
$h = -11 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.109$
$S = 1.07$
3519 reflections
259 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
$w = 1/[\sigma^2(F_o^2) + (0.0545P)^2 + 0.208P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.041$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.15033 (19)	0.83574 (19)	0.62802 (18)	0.0331 (4)
C2	0.0708 (2)	0.8120 (2)	0.50358 (19)	0.0381 (4)
H2	0.015 (2)	0.875 (2)	0.491 (2)	0.046*
C3	0.0712 (2)	0.6926 (2)	0.4009 (2)	0.0416 (5)
H3	0.016 (2)	0.677 (2)	0.319 (2)	0.050*
C4	0.1508 (2)	0.5953 (2)	0.4180 (2)	0.0429 (5)
C5	0.2301 (3)	0.6212 (2)	0.5424 (2)	0.0478 (5)
H5	0.280 (3)	0.554 (3)	0.562 (2)	0.057*
C6	0.2306 (2)	0.7402 (2)	0.6482 (2)	0.0429 (5)
H6	0.285 (2)	0.756 (2)	0.731 (2)	0.051*
C7	0.1510 (3)	0.4657 (2)	0.3046 (2)	0.0620 (6)
H7A	0.2306	0.4904	0.2466	0.074*
H7B	0.0563	0.4340	0.2517	0.074*
H7C	0.1663	0.3898	0.3430	0.074*
C8	−0.12615 (19)	1.02665 (19)	0.81942 (17)	0.0330 (4)
C9	−0.2574 (2)	0.9894 (2)	0.74125 (17)	0.0347 (4)
C10	−0.11502 (19)	1.16193 (19)	0.91546 (17)	0.0327 (4)
C11	−0.3116 (2)	1.2945 (2)	0.98271 (17)	0.0343 (4)
C12	−0.4544 (2)	1.2434 (2)	1.0227 (2)	0.0416 (5)
H12	−0.510 (2)	1.144 (2)	0.988 (2)	0.050*
C13	−0.5179 (3)	1.3360 (3)	1.1144 (2)	0.0525 (6)
H13	−0.617 (3)	1.300 (3)	1.140 (2)	0.063*
C14	−0.4392 (3)	1.4765 (3)	1.1678 (2)	0.0583 (6)
H14	−0.482 (3)	1.542 (3)	1.228 (2)	0.070*
C15	−0.2969 (3)	1.5266 (3)	1.1285 (2)	0.0559 (6)
H15	−0.247 (3)	1.622 (3)	1.159 (2)	0.067*
C16	−0.2324 (2)	1.4360 (2)	1.0346 (2)	0.0446 (5)
H16	−0.136 (3)	1.466 (2)	1.005 (2)	0.054*
C17	−0.3153 (2)	0.8652 (2)	0.6214 (2)	0.0472 (5)
H17A	−0.2589	0.7950	0.6183	0.057*
H17B	−0.3051	0.8980	0.5386	0.057*
H17C	−0.4194	0.8226	0.6299	0.057*
C18	−0.4369 (2)	1.1268 (2)	0.6960 (2)	0.0441 (5)
H18A	−0.5081	1.0412	0.6456	0.053*
H18B	−0.3786	1.1736	0.6332	0.053*
H18C	−0.4896	1.1908	0.7498	0.053*
N1	−0.02275 (17)	0.94195 (17)	0.81689 (15)	0.0349 (4)
H1N	−0.024 (2)	0.889 (2)	0.875 (2)	0.042*
N2	−0.33766 (17)	1.08873 (17)	0.78608 (15)	0.0374 (4)
N3	−0.24404 (16)	1.20148 (16)	0.88633 (15)	0.0361 (4)
O1	0.15031 (16)	1.10496 (14)	0.70246 (14)	0.0467 (4)
O2	0.25442 (14)	0.99605 (15)	0.86636 (13)	0.0478 (4)
O3	−0.01857 (14)	1.23296 (14)	1.00850 (13)	0.0403 (3)
S1	0.14404 (5)	0.98554 (5)	0.76144 (4)	0.03506 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0302 (9)	0.0337 (9)	0.0365 (9)	0.0078 (7)	0.0056 (7)	0.0112 (8)
C2	0.0388 (10)	0.0400 (11)	0.0389 (10)	0.0138 (9)	0.0014 (8)	0.0126 (8)
C3	0.0436 (11)	0.0444 (11)	0.0353 (10)	0.0083 (9)	0.0031 (9)	0.0100 (9)
C4	0.0466 (11)	0.0370 (11)	0.0441 (11)	0.0076 (9)	0.0160 (9)	0.0110 (9)
C5	0.0524 (13)	0.0464 (12)	0.0541 (12)	0.0253 (10)	0.0102 (10)	0.0171 (10)
C6	0.0415 (11)	0.0518 (12)	0.0402 (10)	0.0182 (10)	0.0015 (9)	0.0139 (9)
C7	0.0764 (17)	0.0471 (13)	0.0580 (14)	0.0161 (12)	0.0197 (12)	0.0034 (11)
C8	0.0306 (9)	0.0390 (10)	0.0305 (9)	0.0090 (8)	0.0037 (7)	0.0105 (8)
C9	0.0341 (9)	0.0394 (10)	0.0303 (9)	0.0078 (8)	0.0037 (7)	0.0094 (8)
C10	0.0293 (9)	0.0380 (10)	0.0321 (9)	0.0077 (8)	0.0026 (7)	0.0118 (8)
C11	0.0326 (9)	0.0393 (10)	0.0333 (9)	0.0133 (8)	0.0000 (7)	0.0093 (8)
C12	0.0395 (11)	0.0431 (11)	0.0424 (10)	0.0106 (9)	0.0030 (8)	0.0107 (9)
C13	0.0460 (13)	0.0643 (15)	0.0523 (13)	0.0217 (11)	0.0136 (10)	0.0162 (11)
C14	0.0621 (15)	0.0639 (15)	0.0524 (13)	0.0344 (13)	0.0064 (11)	0.0016 (11)
C15	0.0616 (15)	0.0409 (12)	0.0602 (14)	0.0169 (11)	−0.0104 (12)	−0.0006 (11)
C16	0.0380 (11)	0.0426 (11)	0.0515 (12)	0.0084 (9)	−0.0009 (9)	0.0098 (9)
C17	0.0458 (12)	0.0487 (12)	0.0410 (11)	0.0091 (10)	−0.0031 (9)	0.0026 (9)
C18	0.0345 (10)	0.0566 (13)	0.0415 (10)	0.0104 (9)	−0.0033 (8)	0.0142 (9)
N1	0.0347 (8)	0.0386 (9)	0.0365 (8)	0.0131 (7)	0.0057 (7)	0.0147 (7)
N2	0.0317 (8)	0.0445 (9)	0.0344 (8)	0.0105 (7)	−0.0045 (6)	0.0057 (7)
N3	0.0307 (8)	0.0409 (9)	0.0345 (8)	0.0099 (7)	−0.0013 (6)	0.0043 (7)
O1	0.0529 (9)	0.0362 (7)	0.0511 (8)	0.0088 (6)	0.0111 (7)	0.0138 (6)
O2	0.0348 (7)	0.0570 (9)	0.0443 (8)	0.0050 (6)	−0.0057 (6)	0.0059 (7)
O3	0.0348 (7)	0.0408 (7)	0.0412 (7)	0.0064 (6)	−0.0068 (6)	0.0058 (6)
S1	0.0318 (3)	0.0350 (3)	0.0358 (2)	0.00564 (18)	0.00188 (18)	0.00684 (18)

Geometric parameters (Å, º)

C1—C6	1.384 (3)	C11—C12	1.386 (3)
C1—C2	1.387 (3)	C11—N3	1.429 (2)
C1—S1	1.7620 (18)	C12—C13	1.380 (3)
C2—C3	1.375 (3)	C12—H12	0.97 (2)
C2—H2	0.92 (2)	C13—C14	1.375 (3)
C3—C4	1.385 (3)	C13—H13	0.96 (2)
C3—H3	0.93 (2)	C14—C15	1.377 (3)
C4—C5	1.382 (3)	C14—H14	0.94 (2)
C4—C7	1.502 (3)	C15—C16	1.384 (3)
C5—C6	1.387 (3)	C15—H15	0.92 (3)
C5—H5	0.95 (2)	C16—H16	0.94 (2)
C6—H6	0.92 (2)	C17—H17A	0.9600
C7—H7A	0.9600	C17—H17B	0.9600
C7—H7B	0.9600	C17—H17C	0.9600
C7—H7C	0.9600	C18—N2	1.456 (2)
C8—C9	1.358 (2)	C18—H18A	0.9600
C8—N1	1.411 (2)	C18—H18B	0.9600

C8—C10	1.433 (2)	C18—H18C	0.9600
C9—N2	1.367 (2)	N1—S1	1.6281 (16)
C9—C17	1.488 (3)	N1—H1N	0.87 (2)
C10—O3	1.236 (2)	N2—N3	1.409 (2)
C10—N3	1.389 (2)	O1—S1	1.4318 (14)
C11—C16	1.381 (3)	O2—S1	1.4284 (14)

C6—C1—C2	120.13 (18)	C14—C13—C12	120.4 (2)
C6—C1—S1	120.34 (14)	C14—C13—H13	121.2 (14)
C2—C1—S1	119.51 (14)	C12—C13—H13	118.3 (14)
C3—C2—C1	119.68 (19)	C13—C14—C15	120.1 (2)
C3—C2—H2	120.0 (13)	C13—C14—H14	121.8 (16)
C1—C2—H2	120.3 (13)	C15—C14—H14	118.0 (16)
C2—C3—C4	121.46 (19)	C14—C15—C16	120.3 (2)
C2—C3—H3	118.7 (13)	C14—C15—H15	120.4 (16)
C4—C3—H3	119.8 (13)	C16—C15—H15	119.2 (16)
C5—C4—C3	118.02 (18)	C11—C16—C15	119.2 (2)
C5—C4—C7	121.1 (2)	C11—C16—H16	117.9 (13)
C3—C4—C7	120.87 (19)	C15—C16—H16	122.8 (14)
C4—C5—C6	121.73 (19)	C9—C17—H17A	109.5
C4—C5—H5	121.0 (14)	C9—C17—H17B	109.5
C6—C5—H5	117.0 (14)	H17A—C17—H17B	109.5
C1—C6—C5	118.98 (19)	C9—C17—H17C	109.5
C1—C6—H6	120.6 (14)	H17A—C17—H17C	109.5
C5—C6—H6	120.4 (14)	H17B—C17—H17C	109.5
C4—C7—H7A	109.5	N2—C18—H18A	109.5
C4—C7—H7B	109.5	N2—C18—H18B	109.5
H7A—C7—H7B	109.5	H18A—C18—H18B	109.5
C4—C7—H7C	109.5	N2—C18—H18C	109.5
H7A—C7—H7C	109.5	H18A—C18—H18C	109.5
H7B—C7—H7C	109.5	H18B—C18—H18C	109.5
C9—C8—N1	126.38 (17)	C8—N1—S1	122.21 (13)
C9—C8—C10	108.83 (16)	C8—N1—H1N	121.7 (13)
N1—C8—C10	124.56 (16)	S1—N1—H1N	110.7 (13)
C8—C9—N2	109.58 (16)	C9—N2—N3	106.85 (14)
C8—C9—C17	129.48 (18)	C9—N2—C18	123.39 (15)
N2—C9—C17	120.92 (17)	N3—N2—C18	117.59 (15)
O3—C10—N3	124.10 (17)	C10—N3—N2	109.26 (14)
O3—C10—C8	130.98 (17)	C10—N3—C11	124.48 (14)
N3—C10—C8	104.90 (15)	N2—N3—C11	118.75 (14)
C16—C11—C12	120.73 (18)	O2—S1—O1	119.94 (9)
C16—C11—N3	118.91 (17)	O2—S1—N1	109.23 (8)
C12—C11—N3	120.36 (17)	O1—S1—N1	107.43 (8)
C13—C12—C11	119.2 (2)	O2—S1—C1	106.91 (9)
C13—C12—H12	119.7 (13)	O1—S1—C1	107.94 (8)
C11—C12—H12	121.1 (13)	N1—S1—C1	104.32 (8)

C6—C1—C2—C3	0.5 (3)	C10—C8—N1—S1	−73.9 (2)

S1—C1—C2—C3	−177.76 (14)	C8—C9—N2—N3	6.99 (19)
C1—C2—C3—C4	−0.7 (3)	C17—C9—N2—N3	−171.68 (15)
C2—C3—C4—C5	0.3 (3)	C8—C9—N2—C18	148.18 (17)
C2—C3—C4—C7	−179.63 (18)	C17—C9—N2—C18	−30.5 (3)
C3—C4—C5—C6	0.3 (3)	O3—C10—N3—N2	−172.84 (16)
C7—C4—C5—C6	−179.82 (19)	C8—C10—N3—N2	5.62 (18)
C2—C1—C6—C5	0.0 (3)	O3—C10—N3—C11	−23.8 (3)
S1—C1—C6—C5	178.27 (15)	C8—C10—N3—C11	154.70 (16)
C4—C5—C6—C1	−0.4 (3)	C9—N2—N3—C10	−7.89 (19)
N1—C8—C9—N2	171.06 (16)	C18—N2—N3—C10	−151.70 (15)
C10—C8—C9—N2	−3.6 (2)	C9—N2—N3—C11	−159.01 (15)
N1—C8—C9—C17	−10.4 (3)	C18—N2—N3—C11	57.2 (2)
C10—C8—C9—C17	174.95 (17)	C16—C11—N3—C10	64.2 (2)
C9—C8—C10—O3	176.98 (18)	C12—C11—N3—C10	−116.1 (2)
N1—C8—C10—O3	2.2 (3)	C16—C11—N3—N2	−149.34 (17)
C9—C8—C10—N3	−1.34 (18)	C12—C11—N3—N2	30.4 (2)
N1—C8—C10—N3	−176.10 (15)	C8—N1—S1—O2	123.46 (15)
C16—C11—C12—C13	0.6 (3)	C8—N1—S1—O1	−8.10 (16)
N3—C11—C12—C13	−179.08 (17)	C8—N1—S1—C1	−122.52 (15)
C11—C12—C13—C14	−1.3 (3)	C6—C1—S1—O2	11.34 (18)
C12—C13—C14—C15	0.9 (4)	C2—C1—S1—O2	−170.41 (14)
C13—C14—C15—C16	0.3 (4)	C6—C1—S1—O1	141.64 (16)
C12—C11—C16—C15	0.6 (3)	C2—C1—S1—O1	−40.11 (17)
N3—C11—C16—C15	−179.73 (18)	C6—C1—S1—N1	−104.31 (16)
C14—C15—C16—C11	−1.0 (3)	C2—C1—S1—N1	73.94 (16)
C9—C8—N1—S1	112.28 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O3^{i}	0.87 (2)	1.97 (2)	2.826 (2)	167.1 (18)
C2—H2···O1^{ii}	0.92 (2)	2.54 (2)	3.270 (2)	136.4 (16)
C12—H12···O2^{iii}	0.97 (2)	2.43 (2)	3.245 (2)	141.9 (17)

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