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(1*S*)-Benzyl 3-methyl-5-oxo-4-phenylhydrazono-4,5-dihydro-1*H*-pyrazole-1-dithiocarboxylate

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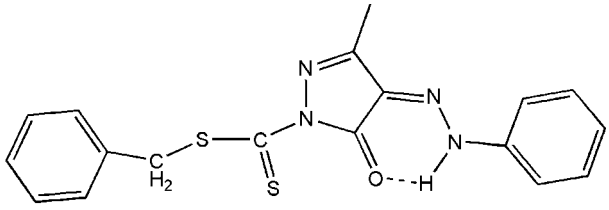
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.045; wR factor = 0.120; data-to-parameter ratio = 13.3.

The title compound, $C_{18}H_{16}N_4OS_2$, has been synthesized by the condensation reaction of ethyl 3-oxo-2-(phenylhydrazono)butanoate and (*S*)-benzyl dithiocarbazate. The pyrazolone structure is stabilized by a strong N—H···O=C intramolecular hydrogen bond.

Related literature

For related literature, see: Bao *et al.* (2006); Bose *et al.* (2005); Caruso *et al.* (2000); Clark & Bookland (2005); Ito *et al.* (2001); Kees *et al.* (1996); Knorr (1884); Omotowa & Mesubi (1997); Shi *et al.* (2005); Whitaker (1995).



Experimental

Crystal data

$C_{18}H_{16}N_4OS_2$
M_r = 368.47
Triclinic, $P\overline{1}$
a = 9.143 (6) Å
b = 10.079 (6) Å
c = 10.217 (6) Å
α = 84.059 (10)°
β = 79.410 (11)°
γ = 77.095 (9)°
V = 900.2 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 294 (2) K
0.24 × 0.22 × 0.16 mm

Data collection

Bruker SMART CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker 2001)
T_{min} = 0.930, T_{max} = 0.952
4385 measured reflections
3062 independent reflections
1974 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.120
S = 1.03
3062 reflections
231 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O1	0.90 (3)	2.13 (3)	2.823 (4)	133 (3)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2028).

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supplementary materials

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(1*S*)-Benzyl 3-methyl-5-oxo-4-phenylhydrazono-4,5-dihydro-1*H*-pyrazole-1-dithiocarboxylate

Y.-H. Liu, Y. Zhao, X.-L. Liu, B.-W. Tong and J. Ye

Comment

Pyrazolones constitute a group of organic compounds that have been extensively studied due to their properties and applications. Since the synthesis of antipyrine (2,3-dimethyl-1-phenyl-5-pyrazolone) by Knorr (Knorr,1884), a great deal of attention has been paid to the properties of these compounds and a series of drugs have been synthesized. For examples anti-inflammatory drugs (Clark & Bookland, 2005), compounds with antifungal compounds (Omotowa & Mesubi, 1997), antitumor (Caruso *et al.*, 2000) and antihyperglycemic (Kees *et al.*, 1996). Although the use of pyrazolones as drugs has warranted significant attention, many more applications have been devised for this group of molecules outside the pharmaceutical field. They have been applied to the solvent extraction of metal ions (Bose *et al.*, 2005), for analytical purposes (Ito *et al.*, 2001), in the preparation of azo colorants (Whitaker, 1995), as ligands in complexes with catalytic activity (Bao *et al.*, 2006) and in the synthesis of rare earth metal complexes with interesting photophysical properties (Shi *et al.*, 2005). In present work, we report the preparation the title compound (I), and its crystal structure.

Determination of its crystal structure (Fig.1), the title compound shows one larger conjugation system in the molecule with eight carbon atoms (C11–C18),four nitrogen atoms (N1–N4) and one oxygen (O1),which is further confirmed by by UV spectroscopy.

In the title compound, the dihedral angle between this conjugation system with plane of C7—S1—C8═S2 is 13.1°. The benzene ring (C13–C18) is involved in the conjugation system (Table 1). An intramolecular N—H···O═ C hydrogen bonds is also present in the crystal structure of (I) (Table 2).

Experimental

The title compound was synthesized by refluxing an ethanol solution of ethyl 3-oxo-2-(phenylhydrazono)butanate and *S*-benzyldithiocarbazate (1:1) for 24 h. After 12 h at room temperature for 12 h, The precipitatewas colleceted by filtration and recrystallized from ethanol (yield 82.2%)·The yellow crystals suitable for X-ray analysis were obtained by slow evaporation of a dichloromethane solution at 278 K (m.p. 344.1–345.8 K). Analysis calculated for $C_{18}H_{16}N_4OS_2$: C 58.67, H 4.36, N 15.21%; found: C 58.66, H 4.35, N 15.21%. IR (KBr,cm^{-1}): 3214(s, NH), 1619 (*versus*, O═C), 1545 (s, N═C), 1280(w, S═C). UV (λ_{max}, in $CHCl_3$, nm): 404 (K-band, 1.92×10^4). ^{1}HNMR (600 MHz, $CDCl_3$): δ: 10.47 (m, 10H, ArH), 6.83 (s, H, NH), 4.06 (s, 2H, $ArCH_2$), 1.19 (s, 3H, CH_3).

Refinement

The H atoms were placed in calculated positions and refined as riding, with C—H = 0.93–0.97 Å with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(methyl C) except for N4, (N—H = 0.90 Å), which was refined.

Figures

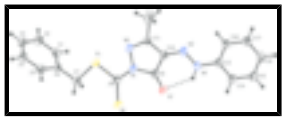


Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. The dashed line indicates the intramolecular hydrogen bond.

(1*S*)-Benzyl 3-methyl-5-oxo-4-phenylhydrazono-4,5-dihydro-1*H*-pyrazole-1-dithiocarboxylate

Crystal data

$C_{18}H_{16}N_4OS_2$	$Z = 2$
$M_r = 368.47$	$F_{000} = 384$
Triclinic, $P\bar{1}$	$D_x = 1.359$ Mg m^{-3}
$a = 9.143$ (6) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 10.079$ (6) Å	Cell parameters from 1587 reflections
$c = 10.217$ (6) Å	$\theta = 2.8$–28.1°
$\alpha = 84.059$ (10)°	$\mu = 0.31$ mm^{-1}
$\beta = 79.410$ (11)°	$T = 294$ (2) K
$\gamma = 77.095$ (9)°	Prism, yellow
$V = 900.2$ (10) Å^3	0.24 × 0.22 × 0.16 mm

Data collection

Bruker SMART CCD area detector diffractometer	3062 independent reflections
Radiation source: fine-focus sealed tube	1974 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.034$
$T = 294$(2) K	$\theta_{max} = 25.0^\circ$
φ and ω scans	$\theta_{min} = 2.0^\circ$
Absorption correction: multi-scan (SADABS; Bruker 2001)	$h = -10 \rightarrow 10$
$T_{min} = 0.930$, $T_{max} = 0.952$	$k = -11 \rightarrow 11$
4385 measured reflections	$l = -12 \rightarrow 5$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.120$	$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.22P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
3062 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}

231 parameters	$\Delta\rho_{min} = -0.24$ 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}
S1	0.33476 (11)	0.39781 (8)	0.74742 (8)	0.0596 (3)
S2	0.44038 (11)	0.13389 (8)	0.60963 (9)	0.0608 (3)
O1	0.6843 (2)	−0.0198 (2)	0.7830 (2)	0.0559 (6)
N1	0.5025 (3)	0.1812 (2)	0.8440 (2)	0.0447 (6)
N2	0.4614 (3)	0.2616 (2)	0.9587 (2)	0.0483 (7)
N4	0.8444 (3)	−0.1042 (2)	0.9988 (3)	0.0468 (7)
H4	0.834 (4)	−0.121 (3)	0.916 (3)	0.060 (10)*
N3	0.7573 (3)	0.0034 (2)	1.0579 (2)	0.0457 (6)
C1	0.2451 (4)	0.6887 (3)	0.5723 (3)	0.0569 (9)
H1	0.3505	0.6713	0.5498	0.068*
C2	0.1642 (4)	0.8227 (3)	0.5820 (3)	0.0603 (9)
H2	0.2156	0.8941	0.5675	0.072*
C3	0.0083 (4)	0.8492 (3)	0.6129 (3)	0.0585 (10)
H3	−0.0456	0.9387	0.6204	0.070*
C4	−0.0681 (4)	0.7445 (4)	0.6329 (3)	0.0593 (10)
H4A	−0.1738	0.7630	0.6509	0.071*
C5	0.0129 (4)	0.6110 (3)	0.6263 (3)	0.0570 (9)
H5	−0.0389	0.5399	0.6425	0.068*
C6	0.1716 (4)	0.5822 (3)	0.5954 (3)	0.0469 (8)
C7	0.2581 (4)	0.4350 (3)	0.5920 (3)	0.0625 (10)
H7A	0.3396	0.4238	0.5158	0.075*
H7B	0.1906	0.3747	0.5864	0.075*
C8	0.4323 (3)	0.2265 (3)	0.7332 (3)	0.0418 (7)
C9	0.6219 (3)	0.0678 (3)	0.8612 (3)	0.0445 (8)
C10	0.6526 (3)	0.0813 (3)	0.9940 (3)	0.0425 (7)
C11	0.5485 (3)	0.2025 (3)	1.0448 (3)	0.0437 (7)
C12	0.5357 (4)	0.2564 (3)	1.1777 (3)	0.0638 (10)
H12A	0.6328	0.2712	1.1885	0.096*
H12B	0.5036	0.1916	1.2466	0.096*
H12C	0.4623	0.3410	1.1837	0.096*

C13	0.9598 (3)	−0.1901 (3)	1.0616 (3)	0.0428 (7)
C14	1.0467 (4)	−0.3042 (3)	0.9965 (3)	0.0541 (9)
H14	1.0282	−0.3227	0.9144	0.065*
C15	1.1615 (4)	−0.3898 (3)	1.0562 (3)	0.0573 (9)
H15	1.2187	−0.4669	1.0145	0.069*
C16	1.1911 (4)	−0.3614 (3)	1.1758 (3)	0.0572 (9)
H16	1.2703	−0.4174	1.2133	0.069*
C17	1.1033 (4)	−0.2496 (3)	1.2406 (3)	0.0573 (9)
H17	1.1220	−0.2318	1.3228	0.069*
C18	0.9873 (4)	−0.1637 (3)	1.1837 (3)	0.0511 (8)
H18	0.9283	−0.0886	1.2277	0.061*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0772 (7)	0.0387 (5)	0.0614 (5)	0.0107 (4)	−0.0292 (5)	−0.0144 (4)
S2	0.0757 (7)	0.0447 (5)	0.0598 (5)	0.0029 (4)	−0.0162 (5)	−0.0183 (4)
O1	0.0515 (14)	0.0453 (12)	0.0669 (14)	0.0049 (11)	−0.0095 (11)	−0.0186 (11)
N1	0.0448 (15)	0.0350 (13)	0.0510 (15)	0.0026 (12)	−0.0093 (12)	−0.0085 (11)
N2	0.0509 (16)	0.0380 (14)	0.0539 (15)	−0.0009 (12)	−0.0094 (13)	−0.0112 (12)
N4	0.0443 (16)	0.0416 (15)	0.0530 (16)	−0.0007 (12)	−0.0127 (14)	−0.0058 (12)
N3	0.0385 (15)	0.0403 (14)	0.0558 (15)	−0.0055 (12)	−0.0062 (13)	−0.0003 (12)
C1	0.048 (2)	0.057 (2)	0.065 (2)	−0.0052 (18)	−0.0161 (18)	−0.0035 (17)
C2	0.070 (3)	0.0450 (19)	0.067 (2)	−0.0127 (19)	−0.015 (2)	−0.0014 (16)
C3	0.071 (3)	0.0417 (19)	0.057 (2)	0.0040 (19)	−0.0124 (19)	−0.0039 (15)
C4	0.048 (2)	0.062 (2)	0.062 (2)	0.0038 (19)	−0.0079 (17)	−0.0162 (17)
C5	0.065 (2)	0.0486 (19)	0.060 (2)	−0.0138 (18)	−0.0120 (18)	−0.0068 (16)
C6	0.053 (2)	0.0397 (17)	0.0463 (17)	0.0023 (16)	−0.0168 (16)	−0.0068 (13)
C7	0.073 (2)	0.0491 (19)	0.064 (2)	0.0084 (18)	−0.0283 (19)	−0.0128 (16)
C8	0.0382 (17)	0.0370 (16)	0.0494 (17)	−0.0064 (14)	−0.0067 (14)	−0.0037 (13)
C9	0.0366 (18)	0.0368 (17)	0.0585 (19)	−0.0066 (14)	−0.0042 (15)	−0.0049 (14)
C10	0.0375 (18)	0.0363 (16)	0.0526 (18)	−0.0071 (14)	−0.0061 (15)	−0.0011 (13)
C11	0.0427 (18)	0.0392 (16)	0.0492 (18)	−0.0072 (15)	−0.0085 (15)	−0.0053 (13)
C12	0.069 (2)	0.061 (2)	0.061 (2)	−0.0040 (19)	−0.0133 (19)	−0.0182 (17)
C13	0.0380 (18)	0.0399 (17)	0.0496 (18)	−0.0082 (14)	−0.0077 (15)	0.0020 (13)
C14	0.059 (2)	0.0480 (19)	0.0540 (19)	−0.0034 (17)	−0.0136 (17)	−0.0090 (15)
C15	0.059 (2)	0.0425 (18)	0.063 (2)	0.0062 (17)	−0.0100 (18)	−0.0073 (15)
C16	0.050 (2)	0.054 (2)	0.060 (2)	0.0001 (17)	−0.0096 (17)	0.0084 (16)
C17	0.059 (2)	0.061 (2)	0.0515 (19)	−0.0065 (18)	−0.0160 (17)	−0.0034 (16)
C18	0.048 (2)	0.0502 (19)	0.0519 (18)	−0.0014 (16)	−0.0087 (16)	−0.0095 (14)

Geometric parameters (Å, °)

S1—C8	1.765 (3)	C5—H5	0.9300
S1—C7	1.823 (3)	C6—C7	1.518 (4)
S2—C8	1.628 (3)	C7—H7A	0.9700
O1—C9	1.223 (3)	C7—H7B	0.9700
N1—C8	1.390 (4)	C9—C10	1.460 (4)
N1—C9	1.415 (3)	C10—C11	1.448 (4)

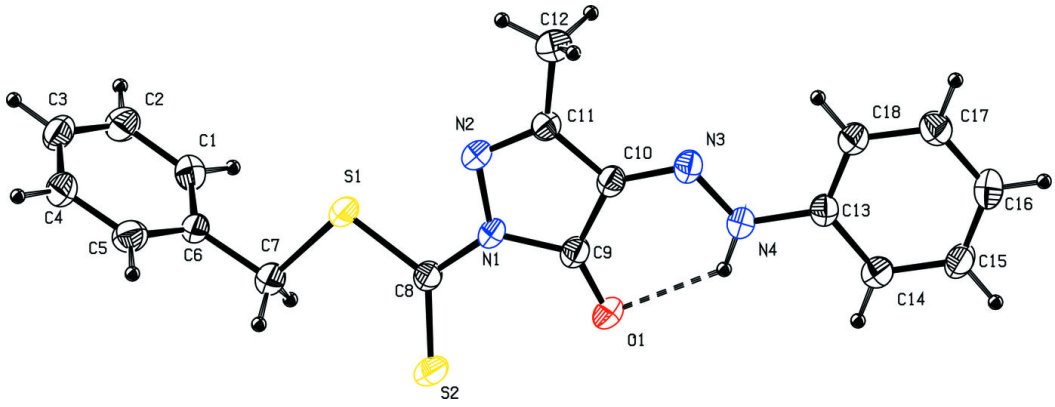
N1—N2	1.439 (3)	C11—C12	1.489 (4)
N2—C11	1.303 (4)	C12—H12A	0.9600
N4—N3	1.322 (3)	C12—H12B	0.9600
N4—C13	1.414 (4)	C12—H12C	0.9600
N4—H4	0.90 (3)	C13—C18	1.380 (4)
N3—C10	1.322 (4)	C13—C14	1.397 (4)
C1—C6	1.368 (5)	C14—C15	1.393 (4)
C1—C2	1.391 (4)	C14—H14	0.9300
C1—H1	0.9300	C15—C16	1.369 (5)
C2—C3	1.373 (5)	C15—H15	0.9300
C2—H2	0.9300	C16—C17	1.381 (4)
C3—C4	1.369 (5)	C16—H16	0.9300
C3—H3	0.9300	C17—C18	1.387 (4)
C4—C5	1.385 (4)	C17—H17	0.9300
C4—H4A	0.9300	C18—H18	0.9300
C5—C6	1.397 (5)		
C8—S1—C7	101.82 (14)	S2—C8—S1	125.74 (18)
C8—N1—C9	129.6 (2)	O1—C9—N1	128.1 (3)
C8—N1—N2	119.0 (2)	O1—C9—C10	128.7 (3)
C9—N1—N2	111.3 (2)	N1—C9—C10	103.2 (2)
C11—N2—N1	107.2 (2)	N3—C10—C11	124.6 (3)
N3—N4—C13	120.3 (3)	N3—C10—C9	128.4 (3)
N3—N4—H4	120 (2)	C11—C10—C9	107.0 (2)
C13—N4—H4	119 (2)	N2—C11—C10	111.2 (3)
N4—N3—C10	117.7 (3)	N2—C11—C12	122.2 (3)
C6—C1—C2	120.9 (3)	C10—C11—C12	126.5 (3)
C6—C1—H1	119.5	C11—C12—H12A	109.5
C2—C1—H1	119.5	C11—C12—H12B	109.5
C3—C2—C1	119.8 (4)	H12A—C12—H12B	109.5
C3—C2—H2	120.1	C11—C12—H12C	109.5
C1—C2—H2	120.1	H12A—C12—H12C	109.5
C4—C3—C2	120.3 (3)	H12B—C12—H12C	109.5
C4—C3—H3	119.8	C18—C13—C14	120.2 (3)
C2—C3—H3	119.8	C18—C13—N4	121.7 (3)
C3—C4—C5	119.7 (3)	C14—C13—N4	118.1 (3)
C3—C4—H4A	120.2	C15—C14—C13	119.0 (3)
C5—C4—H4A	120.2	C15—C14—H14	120.5
C4—C5—C6	120.7 (3)	C13—C14—H14	120.5
C4—C5—H5	119.7	C16—C15—C14	120.6 (3)
C6—C5—H5	119.7	C16—C15—H15	119.7
C1—C6—C5	118.5 (3)	C14—C15—H15	119.7
C1—C6—C7	121.7 (3)	C15—C16—C17	120.0 (3)
C5—C6—C7	119.8 (3)	C15—C16—H16	120.0
C6—C7—S1	105.5 (2)	C17—C16—H16	120.0
C6—C7—H7A	110.6	C16—C17—C18	120.4 (3)
S1—C7—H7A	110.6	C16—C17—H17	119.8
C6—C7—H7B	110.6	C18—C17—H17	119.8
S1—C7—H7B	110.6	C13—C18—C17	119.7 (3)
H7A—C7—H7B	108.8	C13—C18—H18	120.1

N1—C8—S2	124.5 (2)	C17—C18—H18	120.1
N1—C8—S1	109.79 (19)		
C8—N1—N2—C11	−176.3 (3)	N2—N1—C9—C10	0.3 (3)
C9—N1—N2—C11	−0.4 (3)	N4—N3—C10—C11	−179.9 (3)
C13—N4—N3—C10	179.1 (3)	N4—N3—C10—C9	−2.3 (5)
C6—C1—C2—C3	−1.1 (5)	O1—C9—C10—N3	1.6 (6)
C1—C2—C3—C4	−0.7 (5)	N1—C9—C10—N3	−178.0 (3)
C2—C3—C4—C5	2.2 (5)	O1—C9—C10—C11	179.6 (3)
C3—C4—C5—C6	−1.9 (5)	N1—C9—C10—C11	−0.1 (3)
C2—C1—C6—C5	1.4 (5)	N1—N2—C11—C10	0.4 (3)
C2—C1—C6—C7	−177.0 (3)	N1—N2—C11—C12	−178.8 (3)
C4—C5—C6—C1	0.1 (5)	N3—C10—C11—N2	177.8 (3)
C4—C5—C6—C7	178.5 (3)	C9—C10—C11—N2	−0.2 (4)
C1—C6—C7—S1	75.7 (3)	N3—C10—C11—C12	−3.1 (5)
C5—C6—C7—S1	−102.7 (3)	C9—C10—C11—C12	178.9 (3)
C8—S1—C7—C6	−179.9 (2)	N3—N4—C13—C18	−1.4 (5)
C9—N1—C8—S2	18.1 (5)	N3—N4—C13—C14	178.6 (3)
N2—N1—C8—S2	−167.0 (2)	C18—C13—C14—C15	−0.4 (5)
C9—N1—C8—S1	−161.8 (3)	N4—C13—C14—C15	179.6 (3)
N2—N1—C8—S1	13.1 (3)	C13—C14—C15—C16	−1.3 (5)
C7—S1—C8—N1	178.5 (2)	C14—C15—C16—C17	2.2 (5)
C7—S1—C8—S2	−1.4 (3)	C15—C16—C17—C18	−1.6 (5)
C8—N1—C9—O1	−4.1 (5)	C14—C13—C18—C17	1.1 (5)
N2—N1—C9—O1	−179.3 (3)	N4—C13—C18—C17	−178.9 (3)
C8—N1—C9—C10	175.6 (3)	C16—C17—C18—C13	−0.1 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···O1	0.90 (3)	2.13 (3)	2.823 (4)	133 (3)

Fig. 1


C12
C3
C2
C1
N2
C11
C18
C17
S1
C10
N3
C4
C5
C6
C7
C8
N1
C9
N4
C13
C16
C15
C14
O1
S2