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N′-[Bis(benzylsulfanyl)methylene]-2-furohydrazide

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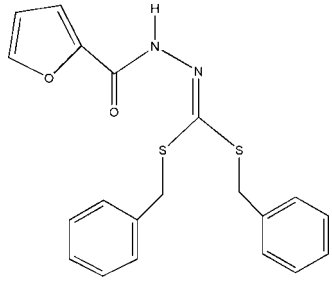
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.092; data-to-parameter ratio = 23.3.

In the title compound, $C_{20}H_{18}N_2O_2S_2$, the dihedral angles between the 2-furoic acid group and the two benzyl groups are 72.4 (9) and 75.8 (8)°, while the angle between the mean planes of the two benzyl groups is 48.9 (2)°. The crystal packing is stabilized by intermolecular C—H···O interactions between the extended O atom of a 2-furoic acid group and H atoms from nearby benzyl and 2-furoic acid groups in the unit cell, linking the molecules into chains in a zigzag pattern, diagonally across the *ac* plane containing the 2-fuoric acid rings. Additional intermolecular interactions occur between the π orbitals of one benzyl ring and H atoms from a nearby benzyl ring at the opposite end of the molecule. Additional intramolecular interactions between the hydrazide H atom and both an O atom from a nearby furoic acid group and an S atom from a close sulfanyl group provide added stability to the molecule.

Related literature

For a related structure, see: Boschi *et al.* (2003). For related background (biological, anticancer and antimicrobial activity), see: Bharti *et al.* (2000); Chan *et al.* (2003).



Experimental

Crystal data

$C_{20}H_{18}N_2O_2S_2$
M_r = 382.48
Triclinic, $P\overline{1}$
a = 9.2058 (14) Å
b = 9.2663 (14) Å
c = 11.3877 (17) Å
α = 109.983 (2)°
β = 94.781 (2)°
γ = 90.201 (3)°
V = 909.2 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 100 K
0.50 × 0.48 × 0.31 mm

Data collection

Bruker SMART CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1999)
T_{min} = 0.752, T_{max} = 0.908
10879 measured reflections
5473 independent reflections
5150 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.092
S = 1.05
5473 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

*Cg*1 is the centroid of a benzyl ring.

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*A*···O2	0.86	2.22	2.6310 (12)	109
N2—H2*A*···S1*B*	0.86	2.37	2.8132 (10)	113
C4—H4*A*···O1^{i}	0.93	2.48	3.3823 (15)	164
C4*A*—H4*AA*···O1^{ii}	0.93	2.51	3.3136 (15)	145
C5*B*—H5*BA*···*Cg*1^{iii}	0.95	2.81	3.4504 (14)	127

Symmetry codes: (i) $-x+3, -y+2, -z+1$; (ii) $-x+2, -y+1, -z$; (iii) $-x+1, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 2006); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); 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: ZL2079).

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supplementary materials

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N'-[Bis(benzylsulfanyl)methylene]-2-furohydrazide

R. J. Butcher, J. P. Jasinski, S. K. Kushawaha, M. K. Bharty and N. K. Singh

Comment

Dithiocarbazate derivatives have been widely studied in radiopharmaceutical applications (Boschi *et al.* 2003) and have potential biological activity as anticancer and antimicrobial drugs (Bharti *et al.* 2000). This functional group is of particular interest and can coordinate to metals to give structures with different geometries and properties. As a part of our ongoing research on the dithio derivatives of acid hydrazides, we report here the crystal structure of the title compound, $C_{20}H_{118}N_2O_2S_2$, a new bis benzyl sulfanyl methylene hydrazide.

The dihedral angle between the 2-furoic acid group and the two benzyl groups is 72.4 (9)° and 75.8 (8)°, respectively, while the angle between the mean planes of the two benzyl groups is 48.9 (2)° (Fig. 1). Bond angles around C1 clearly indicate planar sp^2 behavior. Crystal packing is stabilized by intermolecular C—H···O packing interactions between the extended oxygen atom (O1) of a 2-furoic acid group and hydrogen atoms, both from nearby benzyl (H4AA) and 2-furoic acid groups (H4A) in the unit cell, which link the molecules into chains in a zigzag-like pattern, diagonally across the *ac* plane containing the 2-furoic acid rings (Fig. 2). Additional intermolecular interactions occur between the *Cg*1-π orbitals of one benzyl ring and hydrogen atoms from a nearby benzyl ring at the opposite end of the molecule (Table 1). Additional intramolecular interactions between the hydrazide hydrogen atom (H2A) and both the oxygen from a nearby furoic acid group and a sulfur atom from a close sulfanyl group provide added stability.

Experimental

Potassium 2-furoic acid hydrazide carbodithioate was prepared by adding carbon disulfide (0.04 mol, 2.4 ml) to a solution of furan-2-carboxylic acid hydrazide (0.02 mol, 2.52 g) and potassium hydroxide (0.02 mol, 1.12 g) in methanol (30 ml) and stirring the reaction mixture for 2 h. The solid that separated was filtered off, washed with a 10% (*v*/*v*) mixture of ethanol-ether and dried *in vacuo*. yield 1.44 g, 60%, m.p. 438 K. The title ompound was prepared by drop wise addition of benzyl chloride (0.02 mol, 2.53 g) to a suspension of a potassium salt of 2-furoic acid hydrazide carbodithioate (0.01 mol, 2.28 g) in methanol (20 ml) and stirring the reaction mixture for a period of 5–6 h. The reaction mixture was filtered and the solution was evaporated almost to dryness. The solid was washed several times with carbon tetrachloride and then with chloroform and recrystalized from methanol. Transparent white shining crystals of the title compound (m.p. 388 K), suitable for X-ray analysis were obtained by slow evaporation of the methanol solution over a period of three weeks (yield 1.91 g, 50%): Analysis found: C 62.82, H 4.75, N 7.40, S 16.85; $C_{20}H_{18}N_2O_2S_2$ requires: C 62.74, H 4.70, N 7.32, S 16.73.

Refinement

The amide hydrogen atom (H2A) was located in a difference Fourier map and along with all other H atoms were placed in their calculated positions and then refined using the riding model with N—H = 0.86 Å; C—H = 0.93 to 0.97 Å, and U_{iso}(H) = 1.18–1.22U_{eq}(C,*N*). The maximum residual electron density peaks of 0.486 and −0.297 e Å^3, were located at 0.68Å from CA2 and 0.27Å from H6A.

Figures

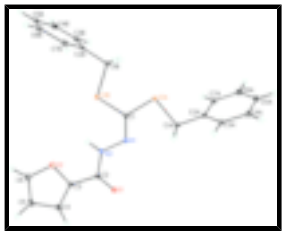

Fig. 1. Molecular structure of the title compound showing atom labeling and 50% probability displacement ellipsoids.

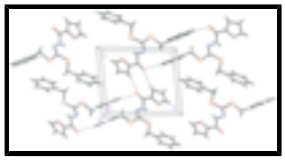

Fig. 2. Packing diagram of $C_{20}H_{18}N_2O_2S_2$, viewed down the *b* axis. Dashed lines indicate intermolecular hydrogen bonding.

N'-[Bis(benzylsulfanyl)methylene]-2-furohydrazide

Crystal data

$C_{20}H_{18}N_2O_2S_2$	$Z = 2$
$M_r = 382.48$	$F_{000} = 400$
Triclinic, $P\overline{1}$	$D_x = 1.397$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.2058$ (14) Å	Cell parameters from 8953 reflections
$b = 9.2663$ (14) Å	$\theta = 2.2$–30.6º
$c = 11.3877$ (17) Å	$\mu = 0.31$ mm^{-1}
$\alpha = 109.983$ (2)º	$T = 100$ K
$\beta = 94.781$ (2)º	Prism, colorless
$\gamma = 90.201$ (3)º	0.50 × 0.48 × 0.31 mm
$V = 909.2$ (2) Å^3	

Data collection

Bruker SMART CCD area detector diffractometer	5473 independent reflections
Radiation source: fine-focus sealed tube	5150 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.016$
$T = 100$ K	$\theta_{max} = 30.5$º
φ and ω scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1999)	$h = -12 \rightarrow 13$
$T_{min} = 0.752$, $T_{max} = 0.908$	$k = -13 \rightarrow 13$
10879 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H-atom parameters constrained
$wR(F^2) = 0.092$	$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.3812P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.002$
5473 reflections	$\Delta\rho_{max} = 0.48$ e Å^{-3}
235 parameters	$\Delta\rho_{min} = -0.29$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. Spectroscopic analysis: IR(KBr,ν cm^{-1}): 3310, (–NH); 1680, (C=O); 1583, (Thiomide I[β(NH + ν(CN)]; 1277, (Thioamide II [ν(CN) + β(NH)]; 754, (Thioamide IV, /n (C—S); 1074 /n (N—N). ^{1}H NMR ($CDCl_3$,δ, p.p.m.): 9.70, (s, 1H, NH); 4.25, (d, 2H, –CH_2); 7.76–7.89, (m, 3H, furan ring); 7.31–7.46, (m, 5H, phenyl); ^{13}C NMR ($CDCl_3$, δ, p.p.m.): 178.61, (C—S); 160.30, (C=O); 145.40, (C3); 115.92, (C4); 112.52, (C5); 144.36, (C6); 153.12, (C2A); 112.34, (C3A,7 A); 129.76, (C4A,6 A); 127.78, (C5A); 36.86, (CH_2).

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 $F^2 > 2$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}
S1A	0.83197 (3)	0.46195 (3)	0.31516 (2)	0.01799 (7)
S1B	0.83350 (3)	0.69808 (3)	0.57280 (2)	0.01936 (7)
O1	1.31416 (9)	0.81929 (11)	0.44309 (8)	0.02540 (18)
O2	1.15179 (9)	1.05449 (10)	0.71366 (8)	0.02291 (17)
N1	1.03648 (10)	0.68224 (11)	0.41270 (8)	0.01901 (18)
N2	1.08610 (10)	0.81545 (11)	0.50926 (9)	0.01960 (18)
H2A	1.0290	0.8610	0.5657	0.024*
C1	0.91710 (12)	0.62306 (12)	0.43136 (9)	0.01711 (18)
C2	1.22268 (12)	0.87532 (12)	0.51658 (10)	0.01811 (19)
C3	1.25246 (12)	1.01706 (12)	0.62573 (10)	0.01824 (19)
C4	1.36458 (13)	1.12278 (13)	0.66080 (11)	0.0227 (2)
H4A	1.4459	1.1235	0.6177	0.027*
C5	1.33189 (15)	1.23308 (14)	0.77784 (12)	0.0270 (2)
H5A	1.3882	1.3201	0.8257	0.032*
C6	1.20373 (15)	1.18689 (14)	0.80570 (12)	0.0273 (2)
H6A	1.1575	1.2380	0.8773	0.033*

C1A	0.95464 (12)	0.43706 (14)	0.19310 (10)	0.0206 (2)
H1AA	0.9687	0.5337	0.1794	0.025*
H1AB	1.0488	0.4057	0.2190	0.025*
C2A	0.89122 (11)	0.31695 (12)	0.07338 (10)	0.01711 (19)
C3A	0.84726 (12)	0.35829 (13)	−0.03044 (10)	0.0194 (2)
H3AA	0.8530	0.4610	−0.0239	0.023*
C4A	0.79483 (13)	0.24774 (14)	−0.14391 (10)	0.0231 (2)
H4AA	0.7684	0.2762	−0.2133	0.028*
C5A	0.78214 (13)	0.09491 (14)	−0.15297 (11)	0.0247 (2)
H5AA	0.7470	0.0207	−0.2285	0.030*
C6A	0.82198 (13)	0.05301 (13)	−0.04922 (12)	0.0250 (2)
H6AA	0.8114	−0.0490	−0.0547	0.030*
C7A	0.87777 (13)	0.16316 (13)	0.06314 (11)	0.0217 (2)
H7AA	0.9063	0.1340	0.1318	0.026*
C1B	0.66064 (12)	0.59096 (14)	0.54544 (10)	0.0215 (2)
H1BA	0.5962	0.6137	0.4827	0.026*
H1BB	0.6758	0.4813	0.5174	0.026*
C2B	0.59769 (11)	0.64384 (12)	0.67084 (10)	0.01821 (19)
C3B	0.62147 (12)	0.56157 (13)	0.75201 (11)	0.0217 (2)
H3BA	0.6725	0.4712	0.7275	0.026*
C4B	0.56896 (13)	0.61435 (14)	0.87003 (11)	0.0234 (2)
H4BA	0.5854	0.5592	0.9242	0.028*
C5B	0.49201 (13)	0.74924 (14)	0.90733 (11)	0.0234 (2)
H5BA	0.4572	0.7843	0.9862	0.028*
C6B	0.46754 (13)	0.83113 (14)	0.82611 (11)	0.0235 (2)
H6BA	0.4158	0.9211	0.8505	0.028*
C7B	0.52029 (12)	0.77887 (13)	0.70825 (11)	0.0207 (2)
H7BA	0.5039	0.8342	0.6542	0.025*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.01715 (12)	0.02079 (13)	0.01268 (11)	−0.00613 (9)	0.00220 (9)	0.00130 (9)
S1B	0.01660 (12)	0.02282 (13)	0.01414 (12)	−0.00608 (9)	0.00312 (9)	0.00017 (9)
O1	0.0206 (4)	0.0314 (4)	0.0182 (4)	−0.0067 (3)	0.0048 (3)	0.0001 (3)
O2	0.0243 (4)	0.0205 (4)	0.0195 (4)	−0.0025 (3)	0.0052 (3)	0.0004 (3)
N1	0.0188 (4)	0.0197 (4)	0.0148 (4)	−0.0059 (3)	0.0013 (3)	0.0012 (3)
N2	0.0186 (4)	0.0192 (4)	0.0164 (4)	−0.0057 (3)	0.0042 (3)	−0.0003 (3)
C1	0.0178 (4)	0.0188 (4)	0.0126 (4)	−0.0030 (3)	0.0014 (3)	0.0027 (3)
C2	0.0182 (5)	0.0200 (5)	0.0150 (4)	−0.0044 (4)	0.0002 (4)	0.0048 (4)
C3	0.0184 (5)	0.0190 (5)	0.0163 (4)	−0.0025 (4)	0.0012 (4)	0.0048 (4)
C4	0.0226 (5)	0.0229 (5)	0.0209 (5)	−0.0069 (4)	−0.0016 (4)	0.0065 (4)
C5	0.0328 (6)	0.0196 (5)	0.0238 (5)	−0.0061 (4)	−0.0034 (5)	0.0028 (4)
C6	0.0348 (6)	0.0197 (5)	0.0212 (5)	−0.0008 (4)	0.0028 (5)	−0.0012 (4)
C1A	0.0184 (5)	0.0274 (5)	0.0131 (4)	−0.0067 (4)	0.0024 (4)	0.0032 (4)
C2A	0.0151 (4)	0.0206 (5)	0.0136 (4)	−0.0017 (3)	0.0033 (3)	0.0029 (4)
C3A	0.0215 (5)	0.0199 (5)	0.0158 (4)	−0.0022 (4)	0.0027 (4)	0.0049 (4)
C4A	0.0245 (5)	0.0277 (6)	0.0150 (5)	−0.0029 (4)	0.0006 (4)	0.0049 (4)

C5A	0.0228 (5)	0.0236 (5)	0.0198 (5)	−0.0034 (4)	0.0033 (4)	−0.0029 (4)
C6A	0.0244 (5)	0.0169 (5)	0.0303 (6)	0.0004 (4)	0.0055 (4)	0.0032 (4)
C7A	0.0212 (5)	0.0227 (5)	0.0222 (5)	0.0011 (4)	0.0026 (4)	0.0087 (4)
C1B	0.0172 (5)	0.0261 (5)	0.0162 (4)	−0.0073 (4)	0.0032 (4)	0.0003 (4)
C2B	0.0138 (4)	0.0210 (5)	0.0162 (4)	−0.0047 (3)	0.0022 (3)	0.0015 (4)
C3B	0.0190 (5)	0.0219 (5)	0.0228 (5)	0.0003 (4)	0.0043 (4)	0.0053 (4)
C4B	0.0216 (5)	0.0287 (6)	0.0204 (5)	−0.0018 (4)	0.0034 (4)	0.0089 (4)
C5B	0.0196 (5)	0.0282 (6)	0.0184 (5)	−0.0037 (4)	0.0055 (4)	0.0020 (4)
C6B	0.0190 (5)	0.0222 (5)	0.0256 (5)	0.0004 (4)	0.0066 (4)	0.0024 (4)
C7B	0.0175 (5)	0.0223 (5)	0.0218 (5)	−0.0018 (4)	0.0027 (4)	0.0065 (4)

Geometric parameters (Å, °)

S1A—C1	1.7500 (11)	C3A—C4A	1.3928 (15)
S1A—C1A	1.8179 (11)	C3A—H3AA	0.9300
S1B—C1	1.7648 (11)	C4A—C5A	1.3881 (17)
S1B—C1B	1.8192 (11)	C4A—H4AA	0.9300
O1—C2	1.2259 (14)	C5A—C6A	1.3868 (18)
O2—C6	1.3659 (14)	C5A—H5AA	0.9300
O2—C3	1.3789 (13)	C6A—C7A	1.3917 (17)
N1—C1	1.2915 (14)	C6A—H6AA	0.9300
N1—N2	1.3879 (12)	C7A—H7AA	0.9300
N2—C2	1.3571 (14)	C1B—C2B	1.5090 (15)
N2—H2A	0.8600	C1B—H1BA	0.9700
C2—C3	1.4731 (15)	C1B—H1BB	0.9700
C3—C4	1.3570 (15)	C2B—C3B	1.3902 (16)
C4—C5	1.4316 (17)	C2B—C7B	1.3954 (16)
C4—H4A	0.9300	C3B—C4B	1.3927 (16)
C5—C6	1.3518 (19)	C3B—H3BA	0.9300
C5—H5A	0.9300	C4B—C5B	1.3922 (17)
C6—H6A	0.9300	C4B—H4BA	0.9300
C1A—C2A	1.5046 (15)	C5B—C6B	1.3886 (18)
C1A—H1AA	0.9700	C5B—H5BA	0.9300
C1A—H1AB	0.9700	C6B—C7B	1.3920 (16)
C2A—C3A	1.3925 (15)	C6B—H6BA	0.9300
C2A—C7A	1.3937 (16)	C7B—H7BA	0.9300
C1—S1A—C1A	99.49 (5)	C5A—C4A—C3A	119.75 (11)
C1—S1B—C1B	105.31 (5)	C5A—C4A—H4AA	120.1
C6—O2—C3	106.42 (9)	C3A—C4A—H4AA	120.1
C1—N1—N2	114.05 (9)	C6A—C5A—C4A	119.89 (10)
C2—N2—N1	121.44 (9)	C6A—C5A—H5AA	120.1
C2—N2—H2A	119.3	C4A—C5A—H5AA	120.1
N1—N2—H2A	119.3	C5A—C6A—C7A	120.21 (11)
N1—C1—S1A	120.42 (8)	C5A—C6A—H6AA	119.9
N1—C1—S1B	122.38 (8)	C7A—C6A—H6AA	119.9
S1A—C1—S1B	117.20 (6)	C6A—C7A—C2A	120.43 (11)
O1—C2—N2	125.12 (10)	C6A—C7A—H7AA	119.8
O1—C2—C3	122.36 (10)	C2A—C7A—H7AA	119.8
N2—C2—C3	112.51 (9)	C2B—C1B—S1B	104.83 (7)

C4—C3—O2	110.42 (10)	C2B—C1B—H1BA	110.8
C4—C3—C2	132.44 (10)	S1B—C1B—H1BA	110.8
O2—C3—C2	117.14 (9)	C2B—C1B—H1BB	110.8
C3—C4—C5	105.83 (11)	S1B—C1B—H1BB	110.8
C3—C4—H4A	127.1	H1BA—C1B—H1BB	108.9
C5—C4—H4A	127.1	C3B—C2B—C7B	119.53 (10)
C6—C5—C4	107.05 (10)	C3B—C2B—C1B	120.15 (10)
C6—C5—H5A	126.5	C7B—C2B—C1B	120.27 (10)
C4—C5—H5A	126.5	C2B—C3B—C4B	120.07 (11)
C5—C6—O2	110.29 (11)	C2B—C3B—H3BA	120.0
C5—C6—H6A	124.9	C4B—C3B—H3BA	120.0
O2—C6—H6A	124.9	C5B—C4B—C3B	120.34 (11)
C2A—C1A—S1A	109.68 (7)	C5B—C4B—H4BA	119.8
C2A—C1A—H1AA	109.7	C3B—C4B—H4BA	119.8
S1A—C1A—H1AA	109.7	C6B—C5B—C4B	119.65 (11)
C2A—C1A—H1AB	109.7	C6B—C5B—H5BA	120.2
S1A—C1A—H1AB	109.7	C4B—C5B—H5BA	120.2
H1AA—C1A—H1AB	108.2	C5B—C6B—C7B	120.12 (11)
C3A—C2A—C7A	118.85 (10)	C5B—C6B—H6BA	119.9
C3A—C2A—C1A	119.96 (10)	C7B—C6B—H6BA	119.9
C7A—C2A—C1A	121.18 (10)	C6B—C7B—C2B	120.28 (11)
C2A—C3A—C4A	120.83 (10)	C6B—C7B—H7BA	119.9
C2A—C3A—H3AA	119.6	C2B—C7B—H7BA	119.9
C4A—C3A—H3AA	119.6		
C1—N1—N2—C2	166.99 (10)	S1A—C1A—C2A—C3A	113.50 (10)
N2—N1—C1—S1A	175.81 (8)	S1A—C1A—C2A—C7A	−67.69 (12)
N2—N1—C1—S1B	−4.57 (14)	C7A—C2A—C3A—C4A	−1.93 (16)
C1A—S1A—C1—N1	−2.02 (11)	C1A—C2A—C3A—C4A	176.90 (10)
C1A—S1A—C1—S1B	178.35 (7)	C2A—C3A—C4A—C5A	1.86 (17)
C1B—S1B—C1—N1	173.39 (10)	C3A—C4A—C5A—C6A	−0.14 (18)
C1B—S1B—C1—S1A	−6.99 (8)	C4A—C5A—C6A—C7A	−1.47 (18)
N1—N2—C2—O1	−1.29 (18)	C5A—C6A—C7A—C2A	1.39 (18)
N1—N2—C2—C3	179.69 (10)	C3A—C2A—C7A—C6A	0.31 (16)
C6—O2—C3—C4	−0.17 (13)	C1A—C2A—C7A—C6A	−178.51 (10)
C6—O2—C3—C2	178.91 (10)	C1—S1B—C1B—C2B	174.10 (8)
O1—C2—C3—C4	10.0 (2)	S1B—C1B—C2B—C3B	−94.13 (11)
N2—C2—C3—C4	−170.94 (12)	S1B—C1B—C2B—C7B	83.28 (11)
O1—C2—C3—O2	−168.84 (11)	C7B—C2B—C3B—C4B	−0.35 (16)
N2—C2—C3—O2	10.22 (14)	C1B—C2B—C3B—C4B	177.07 (10)
O2—C3—C4—C5	−0.02 (13)	C2B—C3B—C4B—C5B	0.23 (17)
C2—C3—C4—C5	−178.92 (12)	C3B—C4B—C5B—C6B	0.09 (17)
C3—C4—C5—C6	0.21 (14)	C4B—C5B—C6B—C7B	−0.28 (17)
C4—C5—C6—O2	−0.33 (15)	C5B—C6B—C7B—C2B	0.15 (17)
C3—O2—C6—C5	0.32 (14)	C3B—C2B—C7B—C6B	0.17 (16)
C1—S1A—C1A—C2A	−171.49 (8)	C1B—C2B—C7B—C6B	−177.26 (10)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

N2—H2A···O2	0.86	2.22	2.6310 (12)	109
N2—H2A···S1B	0.86	2.37	2.8132 (10)	113
C4—H4A···O1^{i}	0.93	2.48	3.3823 (15)	164
C4A—H4AA···O1^{ii}	0.93	2.51	3.3136 (15)	145
C5B—H5BA···Cg1^{iii}	0.95	2.81	3.4504 (14)	127

Symmetry codes: (i) −*x*+3, −*y*+2, −*z*+1; (ii) −*x*+2, −*y*+1, −*z*; (iii) −*x*+1, −*y*+1, −*z*+1.

Fig. 1

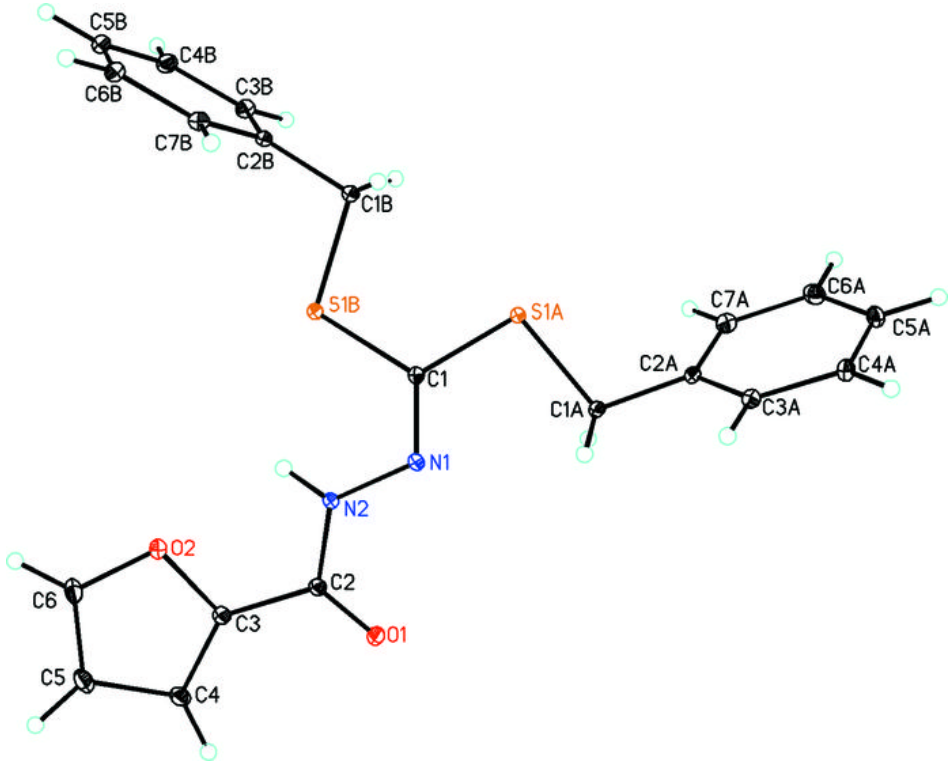
C5B
C4B
C3B
C6B
C7B
C2B
C1B
S1B
S1A
C7A
C6A
C5A
C2A
C4A
C1
C3A
C1A
N1
N2
O2
C2
C6
C3
O1
C5
C4

Fig. 2