

Crystal structure of (*E*)-2-[1-(benzo[*d*]-[1,3]dioxol-5-yl)ethylidene]-*N*-methylhydrazine-1-carbothioamide

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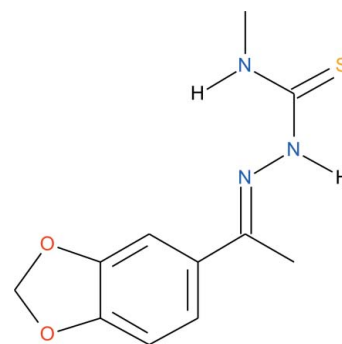
In the title compound, C₁₁H₁₃N₃O₂S, there is a short intramolecular N—H...N contact. The benzo[*d*][1,3]dioxole ring system is approximately planar (r.m.s. deviation = 0.025 Å) and makes a dihedral angle of 56.83 (6)° with the mean plane of the methylthiosemicarbazone fragment [—N—N—C(=S)—N—C; maximum deviation = 0.1111 (14) Å for the imino N atom]. In the crystal, molecules are linked *via* pairs of N—H...S hydrogen bonds, forming inversion dimers. The dimers are connected by N—H...S hydrogen bonds into layers parallel to (100). The H atoms of both methyl groups are disordered over two sets of sites and were refined with occupancy ratios of 0.5:0.5 and 0.75:0.25.

Keywords: crystal structure; thiosemicarbazone; 3',4'-(methylenedioxy)acetophenone; 4-methylthiosemicarbazone; hydrogen bonding; two-dimensional network.

CCDC reference: 1036961

1. Related literature

For one of the first reports of the synthesis of thiosemicarbazone derivatives, see: Freund & Schander (1902). For one of the first reports of 3,4-methylenedioxyacetophenone and its extraction from the South American rosewood tree, see: Mors *et al.* (1957). For the crystal structure of a derivative of the title compound, 1-(2*H*-1,3-benzodioxol-5-yl)ethanone thiosemicarbazone, see: Oliveira *et al.* (2013).



2. Experimental

2.1. Crystal data

C₁₁H₁₃N₃O₂S
M_r = 251.30
 Monoclinic, *P*2₁/*c*
a = 8.7927 (4) Å
b = 12.5979 (6) Å
c = 10.9254 (4) Å
 β = 106.098 (3)°

V = 1162.75 (9) Å³
Z = 4
 Mo *K*α radiation
 μ = 0.27 mm⁻¹
T = 200 K
 0.2 × 0.1 × 0.1 mm

2.2. Data collection

Stoe IPDS-1 diffractometer
 12631 measured reflections
 2530 independent reflections

2166 reflections with *I* > 2σ(*I*)
*R*_{int} = 0.034

2.3. Refinement

R[*F*² > 2σ(*F*²)] = 0.038
wR(*F*²) = 0.096
S = 1.06
 2530 reflections

157 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max}$ = 0.22 e Å⁻³
 $\Delta\rho_{\min}$ = -0.21 e Å⁻³

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

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N3—H1N3...N1	0.88	2.17	2.6080 (19)	110
N2—H1N2...S1 ⁱ	0.88	2.62	3.4871 (14)	168
N3—H1N3...S1 ⁱⁱ	0.88	2.86	3.4973 (14)	131

Symmetry codes: (i) $-x + 1, -y + 1, -z + 2$; (ii) $x, -y + \frac{3}{2}, z - \frac{1}{2}$.

Data collection: *X*-AREA (Stoe & Cie, 2008); cell refinement: *X*-AREA; data reduction: *X*-RED32 (Stoe & Cie, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SU5032).

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supporting information

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Crystal structure of (*E*)-2-[1-(benzo[*d*][1,3]dioxol-5-yl)ethylidene]-*N*-methylhydrazine-1-carbothioamide

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S1. Structural commentary

In our research we are interested in the synthesis of thiosemicarbazone derivatives of natural products. Herein, we report the synthesis and crystal structure of 1-(2*H*-1,3-benzodioxol-5-yl)ethanone 4-methylthiosemicarbazone, a product of the reaction between 3',4'-(methylenedioxy)acetophenone and 4-methylthiosemicarbazide. The ketone is a natural product obtained from the South American rosewood trees that belong to the *Lauraceae* family (Mors *et al.*, 1957).

In the title molecule, Fig. 1, the torsion angle for the N1–N2–C10–N3 entity is 10.2 (2)°. The maximum deviation from the mean plane of the non-H atoms for the C1–C9/O1–O2 fragment and for the C10–C11/N1–N3/S1 fragment amount to 0.2844 (14) Å and 0.1111 (12) Å, respectively, and the angle between their mean planes is 55.39 (4)°. The molecule has two disordered methyl groups. The H atoms of the terminal methyl substituent, C11, are disordered over two sets of sites with an occupancy ratio of 0.75:0.25, those of the other methyl substituent, C9, attached to the Schiff base are disordered over two sets of sites with an occupancy ratio of 0.5:0.5 (Fig. 1).

In the crystal, the molecules are linked *via* pairs of N2–H1N2···S1 hydrogen bonds into inversion dimers. These dimers are connected by weak N3–H1N3···S1 hydrogen bonds into layers, that are parallel to the *bc* plane. Finally, an intramolecular N3–H1N3···N1 hydrogen bond is also observed (Figs. 2 and 3, and Table 1).

S2. Synthesis and crystallization

The synthesis of the title compound was adapted from a previously reported procedure (Freund & Schander, 1902). In a hydrochloric acid catalyzed reaction, a mixture of 3',4'-(methylenedioxy)acetophenone (10 mmol) and 4-Methyl-3-thiosemicarbazide (10 mmol) in ethanol (80 ml) was refluxed for 6 h. After cooling and filtering, the title compound was obtained. Colourless crystals were obtained in DMSO by the slow evaporation of the solvent.

S3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The NH H atoms were located in a difference Fourier map and were refined as riding atoms with N–H = 0.88 Å and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{N})$. The C-bound H atoms were positioned with idealized geometry and refined as riding atoms: C–H = 0.95–0.99 Å with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and = $1.2U_{\text{eq}}(\text{C})$ for other H atoms. The H atoms of methyl groups, C9 and C11, are disordered over two positions and were refined in two different orientations rotated by 60° with occupancy ratios of 0.5:0.5 and 0.75:0.25, respectively.

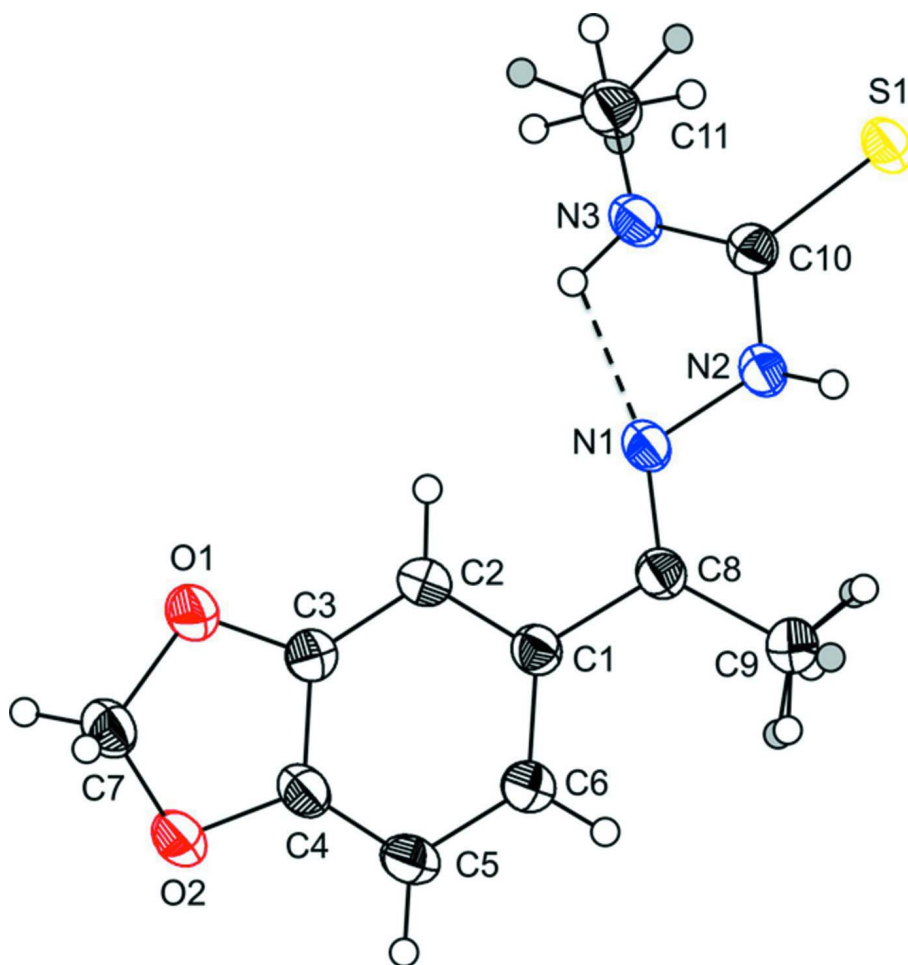
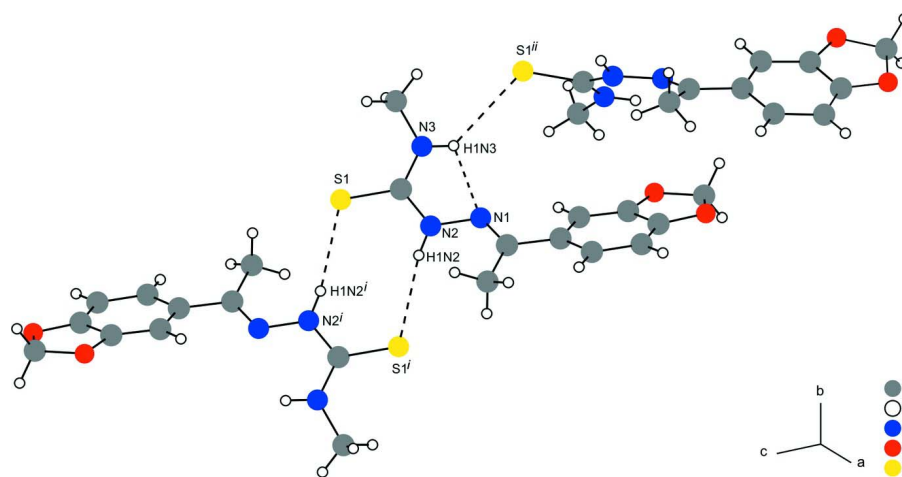


Figure 1

The molecular structure of the title compound with atom labelling. Displacement ellipsoids are drawn at the 40% probability level. Disordered H atoms are shown with white and light gray interior colours and the short intramolecular N-H \cdots N contact is shown as a dashed line (see Table 1 for details).

**Figure 2**

A view of the intramolecular and intermolecular hydrogen bonds (dashed lines) in the crystal structure of the title compound (see Table 1 for details of the hydrogen bonding and the symmetry codes; disordered H atoms are not shown for clarity).

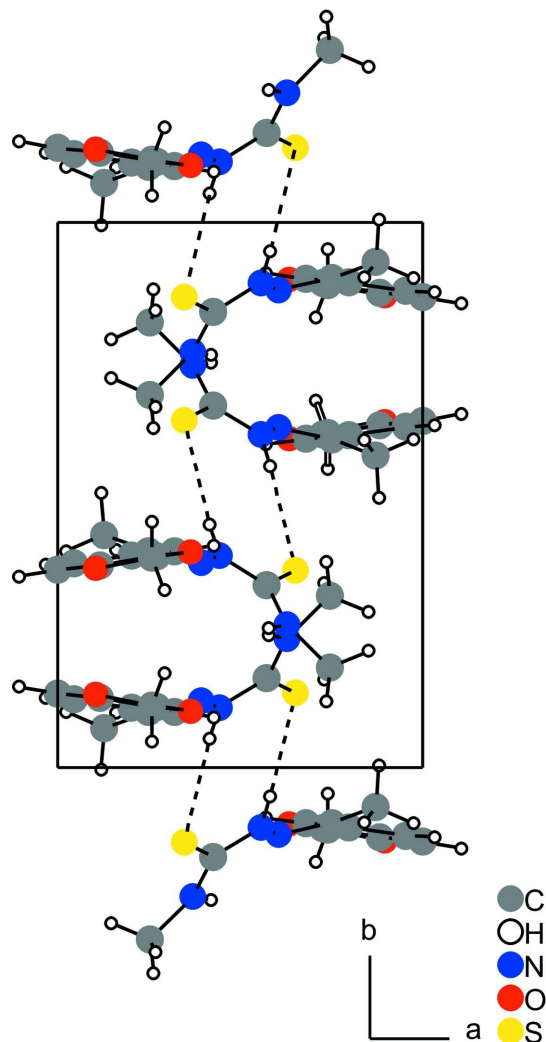


Figure 3

A partial view along the *c* axis of the crystal packing of the title compound. The N2—H1N2...S1 hydrogen bonds are shown as dashed lines (see Table 1 for details; disordered H atoms are not shown for clarity).

(*E*)-2-[1-(Benzo[*d*][1,3]dioxol-5-yl)ethylidene]-*N*-methylhydrazine-1-carbothioamide

Crystal data

$C_{11}H_{13}N_3O_2S$

$M_r = 251.30$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 8.7927(4)\ \text{\AA}$

$b = 12.5979(6)\ \text{\AA}$

$c = 10.9254(4)\ \text{\AA}$

$\beta = 106.098(3)^\circ$

$V = 1162.75(9)\ \text{\AA}^3$

$Z = 4$

$F(000) = 528$

$D_x = 1.436\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

$\theta = 2.4\text{--}27.0^\circ$

$\mu = 0.27\ \text{mm}^{-1}$

$T = 200\ \text{K}$

Prism, colourless

$0.2 \times 0.1 \times 0.1\ \text{mm}$

Data collection

Stoe IPDS-1 diffractometer	2530 independent reflections
Radiation source: fine-focus sealed tube, Stoe IPDS-1	2166 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\text{int}} = 0.034$
φ scans	$\theta_{\text{max}} = 27.0^\circ$, $\theta_{\text{min}} = 2.4^\circ$
12631 measured reflections	$h = -11 \rightarrow 11$
	$k = -16 \rightarrow 16$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.038$	$w = 1/[\sigma^2(F_o^2) + (0.0452P)^2 + 0.3583P]$
$wR(F^2) = 0.096$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2530 reflections	$\Delta\rho_{\text{max}} = 0.22 \text{ e } \text{\AA}^{-3}$
157 parameters	$\Delta\rho_{\text{min}} = -0.21 \text{ e } \text{\AA}^{-3}$
0 restraints	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $F_c^* = kFc[1 + 0.001x Fc^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.012 (3)
Secondary atom site location: difference Fourier map	

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.79760 (18)	0.61024 (12)	0.64282 (15)	0.0335 (3)	
C2	0.67988 (19)	0.60308 (14)	0.52567 (16)	0.0376 (4)	
H2	0.5718	0.5929	0.5224	0.045*	
C3	0.72677 (19)	0.61135 (13)	0.41723 (15)	0.0363 (4)	
C4	0.8828 (2)	0.62849 (14)	0.41992 (16)	0.0389 (4)	
C5	0.9996 (2)	0.63636 (16)	0.53155 (17)	0.0459 (4)	
H5	1.1066	0.6488	0.5329	0.055*	
C6	0.9547 (2)	0.62527 (14)	0.64410 (17)	0.0396 (4)	
H6	1.0337	0.6281	0.7235	0.048*	
O1	0.63513 (15)	0.60420 (12)	0.29353 (11)	0.0499 (3)	
C7	0.7408 (2)	0.61449 (15)	0.21584 (17)	0.0429 (4)	
H7A	0.7070	0.6739	0.1551	0.052*	
H7B	0.7407	0.5485	0.1666	0.052*	
O2	0.89564 (15)	0.63434 (12)	0.29772 (12)	0.0513 (4)	
C8	0.75138 (18)	0.60240 (12)	0.76304 (15)	0.0335 (3)	

N1	0.60559 (16)	0.62379 (11)	0.75398 (13)	0.0359 (3)	
N2	0.55651 (16)	0.61080 (11)	0.86408 (13)	0.0368 (3)	
H1N2	0.5828	0.5535	0.9113	0.055*	
C9	0.8720 (2)	0.57270 (15)	0.88417 (17)	0.0433 (4)	
H9A	0.8400	0.6009	0.9568	0.065*	0.50
H9B	0.9750	0.6025	0.8843	0.065*	0.50
H9C	0.8802	0.4952	0.8907	0.065*	0.50
H9D	0.9568	0.5315	0.8644	0.065*	0.50
H9E	0.8218	0.5299	0.9370	0.065*	0.50
H9F	0.9166	0.6372	0.9305	0.065*	0.50
C10	0.42636 (18)	0.66446 (12)	0.87292 (15)	0.0328 (3)	
N3	0.37103 (17)	0.73745 (11)	0.78479 (14)	0.0407 (3)	
H1N3	0.4212	0.7432	0.7257	0.061*	
S1	0.34744 (5)	0.63743 (3)	0.99435 (4)	0.03782 (15)	
C11	0.2532 (2)	0.81607 (15)	0.79064 (19)	0.0491 (5)	
H11A	0.2636	0.8777	0.7387	0.074*	0.25
H11B	0.2690	0.8384	0.8792	0.074*	0.25
H11C	0.1473	0.7854	0.7579	0.074*	0.25
H11D	0.1896	0.7900	0.8452	0.074*	0.75
H11E	0.1842	0.8292	0.7047	0.074*	0.75
H11F	0.3059	0.8823	0.8260	0.074*	0.75

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0351 (8)	0.0332 (8)	0.0342 (8)	0.0027 (6)	0.0129 (6)	0.0018 (6)
C2	0.0319 (8)	0.0451 (9)	0.0384 (9)	0.0008 (6)	0.0142 (7)	0.0023 (7)
C3	0.0353 (8)	0.0395 (8)	0.0343 (8)	0.0004 (6)	0.0098 (6)	-0.0001 (6)
C4	0.0409 (9)	0.0447 (9)	0.0355 (8)	-0.0020 (7)	0.0179 (7)	0.0002 (7)
C5	0.0339 (8)	0.0634 (12)	0.0439 (10)	-0.0059 (8)	0.0164 (7)	-0.0005 (8)
C6	0.0346 (8)	0.0483 (9)	0.0369 (9)	-0.0010 (7)	0.0114 (7)	0.0003 (7)
O1	0.0403 (7)	0.0789 (9)	0.0314 (6)	-0.0050 (6)	0.0111 (5)	-0.0002 (6)
C7	0.0473 (10)	0.0492 (10)	0.0354 (9)	-0.0048 (8)	0.0167 (7)	-0.0046 (7)
O2	0.0435 (7)	0.0788 (10)	0.0360 (7)	-0.0057 (6)	0.0182 (6)	0.0010 (6)
C8	0.0354 (8)	0.0328 (7)	0.0343 (8)	0.0018 (6)	0.0129 (6)	0.0027 (6)
N1	0.0384 (7)	0.0407 (7)	0.0326 (7)	0.0052 (6)	0.0165 (6)	0.0050 (5)
N2	0.0391 (7)	0.0416 (7)	0.0334 (7)	0.0071 (6)	0.0164 (6)	0.0084 (6)
C9	0.0388 (9)	0.0531 (10)	0.0379 (9)	0.0000 (7)	0.0101 (7)	0.0081 (7)
C10	0.0328 (7)	0.0335 (7)	0.0327 (8)	-0.0019 (6)	0.0102 (6)	-0.0010 (6)
N3	0.0420 (8)	0.0443 (8)	0.0426 (8)	0.0101 (6)	0.0229 (6)	0.0111 (6)
S1	0.0437 (2)	0.0414 (2)	0.0333 (2)	0.00154 (17)	0.01874 (17)	0.00216 (16)
C11	0.0513 (10)	0.0473 (10)	0.0551 (11)	0.0162 (8)	0.0255 (9)	0.0119 (8)

Geometric parameters (Å, °)

C1—C6	1.390 (2)	N2—C10	1.355 (2)
C1—C2	1.408 (2)	N2—H1N2	0.8800
C1—C8	1.482 (2)	C9—H9A	0.9800

C2—C3	1.362 (2)	C9—H9B	0.9800
C2—H2	0.9500	C9—H9C	0.9800
C3—O1	1.371 (2)	C9—H9D	0.9800
C3—C4	1.381 (2)	C9—H9E	0.9800
C4—C5	1.362 (3)	C9—H9F	0.9800
C4—O2	1.372 (2)	C10—N3	1.323 (2)
C5—C6	1.399 (2)	C10—S1	1.6935 (16)
C5—H5	0.9500	N3—C11	1.448 (2)
C6—H6	0.9500	N3—H1N3	0.8800
O1—C7	1.427 (2)	C11—H11A	0.9800
C7—O2	1.429 (2)	C11—H11B	0.9800
C7—H7A	0.9900	C11—H11C	0.9800
C7—H7B	0.9900	C11—H11D	0.9800
C8—N1	1.287 (2)	C11—H11E	0.9800
C8—C9	1.496 (2)	C11—H11F	0.9800
N1—N2	1.3957 (18)		
C6—C1—C2	119.71 (15)	H9B—C9—H9D	56.3
C6—C1—C8	121.06 (14)	H9C—C9—H9D	56.3
C2—C1—C8	119.22 (14)	C8—C9—H9E	109.5
C3—C2—C1	117.53 (15)	H9A—C9—H9E	56.3
C3—C2—H2	121.2	H9B—C9—H9E	141.1
C1—C2—H2	121.2	H9C—C9—H9E	56.3
C2—C3—O1	127.99 (15)	H9D—C9—H9E	109.5
C2—C3—C4	122.14 (16)	C8—C9—H9F	109.5
O1—C3—C4	109.88 (15)	H9A—C9—H9F	56.3
C5—C4—O2	128.48 (15)	H9B—C9—H9F	56.3
C5—C4—C3	121.85 (16)	H9C—C9—H9F	141.1
O2—C4—C3	109.67 (15)	H9D—C9—H9F	109.5
C4—C5—C6	116.98 (16)	H9E—C9—H9F	109.5
C4—C5—H5	121.5	N3—C10—N2	116.24 (14)
C6—C5—H5	121.5	N3—C10—S1	124.21 (12)
C1—C6—C5	121.76 (16)	N2—C10—S1	119.53 (12)
C1—C6—H6	119.1	C10—N3—C11	124.52 (14)
C5—C6—H6	119.1	C10—N3—H1N3	115.7
C3—O1—C7	106.19 (13)	C11—N3—H1N3	119.1
O1—C7—O2	107.93 (13)	N3—C11—H11A	109.5
O1—C7—H7A	110.1	N3—C11—H11B	109.5
O2—C7—H7A	110.1	H11A—C11—H11B	109.5
O1—C7—H7B	110.1	N3—C11—H11C	109.5
O2—C7—H7B	110.1	H11A—C11—H11C	109.5
H7A—C7—H7B	108.4	H11B—C11—H11C	109.5
C4—O2—C7	106.18 (13)	N3—C11—H11D	109.5
N1—C8—C1	115.47 (14)	H11A—C11—H11D	141.1
N1—C8—C9	124.57 (15)	H11B—C11—H11D	56.3
C1—C8—C9	119.95 (14)	H11C—C11—H11D	56.3
C8—N1—N2	116.66 (13)	N3—C11—H11E	109.5
C10—N2—N1	118.15 (13)	H11A—C11—H11E	56.3

C10—N2—H1N2	117.2	H11B—C11—H11E	141.1
N1—N2—H1N2	120.5	H11C—C11—H11E	56.3
C8—C9—H9A	109.5	H11D—C11—H11E	109.5
C8—C9—H9B	109.5	N3—C11—H11F	109.5
H9A—C9—H9B	109.5	H11A—C11—H11F	56.3
C8—C9—H9C	109.5	H11B—C11—H11F	56.3
H9A—C9—H9C	109.5	H11C—C11—H11F	141.1
H9B—C9—H9C	109.5	H11D—C11—H11F	109.5
C8—C9—H9D	109.5	H11E—C11—H11F	109.5
H9A—C9—H9D	141.1		
C6—C1—C2—C3	0.0 (2)	C5—C4—O2—C7	176.38 (19)
C8—C1—C2—C3	179.57 (15)	C3—C4—O2—C7	-2.97 (19)
C1—C2—C3—O1	178.21 (16)	O1—C7—O2—C4	3.96 (19)
C1—C2—C3—C4	-1.4 (3)	C6—C1—C8—N1	157.83 (16)
C2—C3—C4—C5	1.1 (3)	C2—C1—C8—N1	-21.7 (2)
O1—C3—C4—C5	-178.57 (17)	C6—C1—C8—C9	-21.4 (2)
C2—C3—C4—O2	-179.47 (16)	C2—C1—C8—C9	159.10 (16)
O1—C3—C4—O2	0.8 (2)	N1—C8—N1—N2	0 (79)
O2—C4—C5—C6	-178.68 (17)	C1—C8—N1—N2	176.24 (13)
C3—C4—C5—C6	0.6 (3)	C9—C8—N1—N2	-4.6 (2)
C2—C1—C6—C5	1.7 (3)	C8—N1—N2—C10	157.92 (15)
C8—C1—C6—C5	-177.83 (16)	N1—N2—C10—N3	-10.2 (2)
C4—C5—C6—C1	-2.0 (3)	N1—N2—C10—S1	171.13 (11)
C2—C3—O1—C7	-178.00 (18)	N2—C10—N3—C11	-167.92 (17)
C4—C3—O1—C7	1.7 (2)	S1—C10—N3—C11	10.7 (3)
C3—O1—C7—O2	-3.47 (19)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N3—H1N3 \cdots N1	0.88	2.17	2.6080 (19)	110
N2—H1N2 \cdots S1 ⁱ	0.88	2.62	3.4871 (14)	168
N3—H1N3 \cdots S1 ⁱⁱ	0.88	2.86	3.4973 (14)	131

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