

Methyl 2-[(Z)-5-methyl-2-oxoindolin-3-ylidene]-hydrazinecarbodithioate

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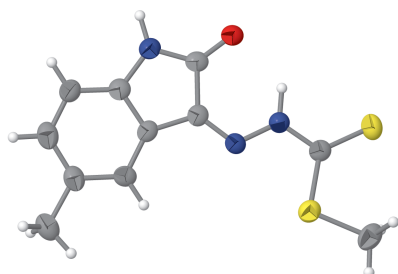
Keywords: crystal structure; dithiocarbazate; 5-methylisatin; C=O...C=O interaction.

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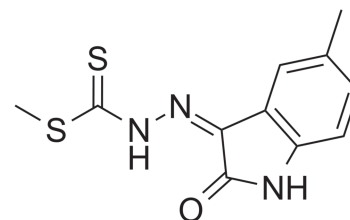
Structural data: full structural data are available from iucrdata.iucr.org

The title dithiocarbazate imine, C₁₁H₁₁N₃OS₂, was obtained from the condensation reaction of *S*-methylthiocarbazate (SMDTC) and 5-methylisatin. It shows a *Z* configuration about the imine C=N bond, which is associated with an intramolecular N–H...O hydrogen bond that closes an *S*(6) ring. In the crystal, inversion dimers linked by pairwise N–H...O hydrogen bonds generate *R*₂²(8) loops. The extended structure features C–H...S contacts as well as reciprocal carbonyl–carbonyl (C=O...C=O) interactions.

3D view



Chemical scheme



Structure description

In medicinal chemistry, isatin (1*H*-indole-2,3-dione, C₈H₅NO₂) and its derivatives represent an important class of heterocyclic compounds with potential pharmacological properties (Shu *et al.*, 2024). Taking advantage of the versatile reactivity of the isatin nucleus, a huge library of isatin derivatives with various applications is now available. Most of these derivatives have been obtained by utilizing either the high reactivity of its 3-carbonyl group or the nucleophilic nature of its NH group. The NH group can undergo *N*-acylation, *N*-arylation or *N*-alkylation, whereas the C3 carbonyl group can be utilized in the synthesis of hydrazone or imine derivatives as well as oxindoles and spirocyclic compounds (Nath *et al.*, 2020). These derivatives are reported to possess several biological activities and find applications in the field of crystal engineering, supramolecular chemistry and materials science (Mehreen *et al.*, 2022a; Ahmed *et al.*, 2019).

Recently, chemists have recognized both one-sided and reciprocal carbonyl–carbonyl interactions as non-covalent interactions of significant interest due to their ability to influence the geometries of small molecules and affect the three dimensional structures of peptides, peptoids, proteins and polyesters (Rahim *et al.*, 2017). Very recently, the use of isatin-derived compounds as potent α -glucosidase inhibitors in managing diabetes has been reported, highlighting the role of C=O...C=O interactions in inhibiting

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N4-H4\cdots O2$	0.98 (2)	2.01 (6)	2.754 (6)	130 (6)
$N1-H1\cdots O2^i$	0.98 (2)	1.85 (2)	2.825 (6)	171 (7)

Symmetry code: (i) $-x + 2, -y + 1, -z$.

α -glucosidase and controlling postprandial hyperglycemia (Mehreen *et al.*, 2022b). As a continuation of our research interests in isatin derivatives, we now report the synthesis and crystal structure of the title compound, $C_{11}H_{11}N_3OS_2$.

The asymmetric unit of the title compound (Fig. 1) comprises one molecule and crystallizes in the monoclinic space group $P2_1/c$. The methyl hydrazinecarbodithioate chain connects to the nine-membered 5-methylisatin ring at C3 and adopts a near planar geometry (r.m.s. deviation from planarity = 0.033 Å). The essentially planar conformation of the molecule is associated with the formation of an intramolecular $N4-H4\cdots O2$ hydrogen bond (Table 1), which closes an $S(6)$ loop. In the solid state, the compound exists in its thione tautomeric form with the dithiocarbazate fragment adopting a Z conformation about the $C=N$ bond with respect to the 5-methylisatin moiety, while the S -methyl group adopts a *syn* conformation relative to the azomethine nitrogen atom. Otherwise, the bond lengths and angles in the title compound may be regarded as normal.

In the crystal, the molecules of the title compound form inversion dimers through pairwise $N1-H1\cdots O2$ hydrogen bonds (Table 1) in the common $R_2^2(8)$ motif. There are additional weak, non-classical $C7-H7\cdots S11$ hydrogen bonds, which link molecules into $C(10)$ chains propagating along [010]. The combination of the chains and inversion dimers forms corrugated sheets lying in the (102) plane (Fig. 2). The aforementioned sheets stack by way of reciprocal carbonyl-carbonyl interactions [$C2\cdots O2 = 3.166$ (6) Å, $C=O\cdots C = 75.1$ (3)°, $O=C\cdots O = 104.8$ (3)°] (Fig. 3). The contact observed differs from the ideal motif-II type interaction (Sahariah & Sarma, 2019) with $O2$ lying over the adjacent pyrrolone ring (Fig. 4).

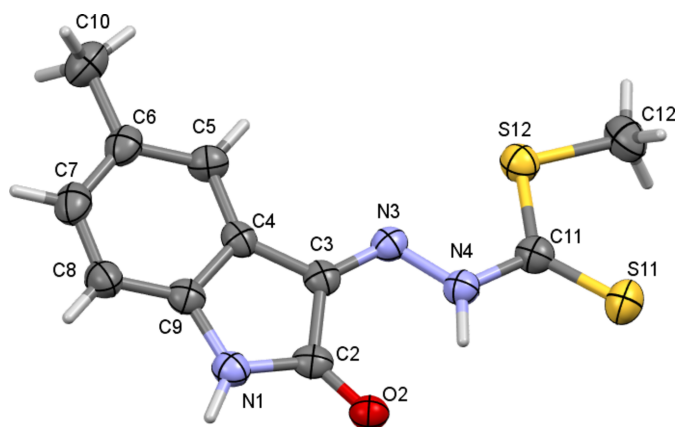


Figure 1

The molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level.

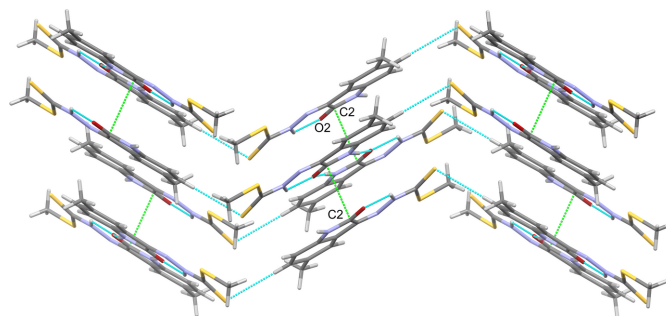


Figure 3

View showing the stacking of the corrugated sheets supported by reciprocal carbonyl-carbonyl interactions (green).

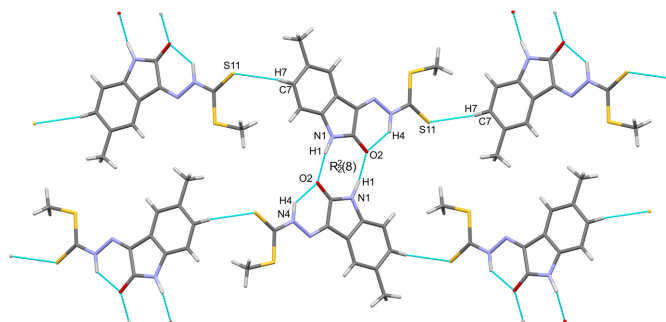


Figure 2

View of the $N-H\cdots O$ and $C-H\cdots S$ hydrogen bonds generating $R_2^2(8)$ dimers (centre) and $C(10)$ chains (left to right), which combine to form corrugated (102) sheets.

Synthesis and crystallization

The dithiocarbazate precursor (SMDTC) was prepared by the literature method (Das & Livingstone, 1976). The title compound was prepared by adding 5-methylisatin (1.61 g, 10.0 mmol, 1.0 eq) dissolved in hot ethanol (20 ml) to a solution of SMDTC (1.22 g, 10.0 mmol, 1.0 eq) in hot ethanol (35 ml). The mixture was heated (80°C) with continuous stirring for 15 min and later allowed to stand for 20 min at room temperature until a precipitate formed, which was then filtered and dried over silica gel, yielding orange needles of the title compound on recrystallization from ethanol solution (yield: 2.12 g, 80%). m.p. 236–237°C; 1H NMR (400 MHz, d_6 -DMSO) δ : (p.p.m): 2.31 (s, 3H), 2.62 (s, 3H), 6.84 (d, $J = 7.96$ Hz, 1H), 7.22 (d, $J = 7.96$ Hz, 1H), 7.36 (s, 1H), 11.27 (s, 1H), 14.00 (s, 1H); HRMS m/z (ESI⁺), found: $[M+H]^+$ 266.0417, $C_{11}H_{12}N_3OS_2$ requires $[M+H]^+$ 266.0422.

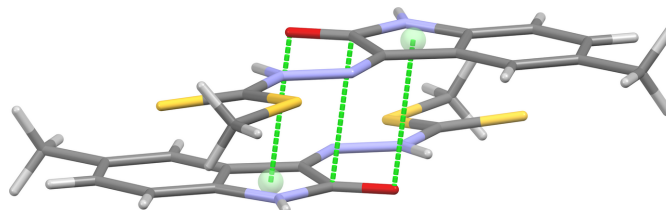


Figure 4

Offset geometry of the carbonyl-carbonyl interaction showing how $O2$ is positioned over the adjacent pyrrolone ring.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The structure was refined as a two-component twin with component 2 rotated by 2.05° around [001] (reciprocal) or [105] (direct), and a refined twin fraction of 0.128 (6).

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Table 2

Experimental details.

Crystal data	
Chemical formula	C ₁₁ H ₁₁ N ₃ OS ₂
<i>M_r</i>	265.35
Crystal system, space group	Monoclinic, <i>P</i> ₂ ₁ / <i>c</i>
Temperature (K)	125
<i>a</i> , <i>b</i> , <i>c</i> (Å)	4.9897 (4), 21.8014 (19), 11.3394 (9)
β (°)	92.995 (8)
<i>V</i> (Å ³)	1231.83 (18)
<i>Z</i>	4
Radiation type	Cu <i>K</i> α
μ (mm ⁻¹)	3.82
Crystal size (mm)	0.23 × 0.01 × 0.01
Data collection	
Diffractometer	Rigaku XtaLAB P200K
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2023)
<i>T</i> _{min} , <i>T</i> _{max}	0.631, 1.000
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	23143, 2554, 1548
<i>R</i> _{int}	0.171
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.630
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.079, 0.185, 1.09
No. of reflections	2554
No. of parameters	165
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.46, -0.63

Computer programs: *CrysAlis PRO* (Rigaku OD, 2023), *SHELXT* (Sheldrick, 2015a), *SHELXL2019/3* (Sheldrick, 2015b), *Mercury* (Macrae *et al.*, 2020), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2024). **9**, x240967 [https://doi.org/10.1107/S2414314624009672]

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Crystal data

$C_{11}H_{11}N_3OS_2$	$F(000) = 552$
$M_r = 265.35$	$D_x = 1.431 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation, $\lambda = 1.54184 \text{ \AA}$
$a = 4.9897 (4) \text{ \AA}$	Cell parameters from 2965 reflections
$b = 21.8014 (19) \text{ \AA}$	$\theta = 4.0\text{--}68.3^\circ$
$c = 11.3394 (9) \text{ \AA}$	$\mu = 3.82 \text{ mm}^{-1}$
$\beta = 92.995 (8)^\circ$	$T = 125 \text{ K}$
$V = 1231.83 (18) \text{ \AA}^3$	Needle, orange
$Z = 4$	$0.23 \times 0.01 \times 0.01 \text{ mm}$

Data collection

Rigaku XtaLAB P200K diffractometer	$T_{\min} = 0.631$, $T_{\max} = 1.000$
Radiation source: Rotating Anode, Rigaku MM-007HF	23143 measured reflections
Rigaku Osmic Confocal Optical System monochromator	2554 independent reflections
Detector resolution: $5.8140 \text{ pixels mm}^{-1}$ shutterless scans	1548 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2023)	$R_{\text{int}} = 0.171$
	$\theta_{\max} = 76.3^\circ$, $\theta_{\min} = 4.1^\circ$
	$h = -6 \rightarrow 6$
	$k = -27 \rightarrow 27$
	$l = 0 \rightarrow 14$

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.079$	$w = 1/[\sigma^2(F_o^2) + 4.5988P]$
$wR(F^2) = 0.185$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{\max} < 0.001$
2554 reflections	$\Delta\rho_{\max} = 0.46 \text{ e \AA}^{-3}$
165 parameters	$\Delta\rho_{\min} = -0.63 \text{ e \AA}^{-3}$
2 restraints	
Primary atom site location: dual	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refined as a 2-component twin using an HKLF5 file generated by TWINROTAT running in PLATON (Spek, 2009), with twin law $[-1\ 0\ 0\ 0\ -1\ 0\ 0.237\ 0\ 1]$. N—H hydrogen atoms located from F_{map} and refined isotropically with appropriate distance restraints.

The N-bound H atoms were located in a difference map and refined isotropically with a distance restraint. The C-bound H atoms were located geometrically (phenyl C—H = 0.95 Å, methyl C—H = 0.98 Å) and refined as riding atoms. The constraint $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{phenyl C})$ or $1.5U_{\text{eq}}(\text{methyl C})$ was applied in all cases.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S11	0.1241 (3)	0.27752 (7)	−0.01332 (14)	0.0469 (4)
S12	−0.0419 (3)	0.32382 (7)	0.22526 (13)	0.0413 (4)
O2	0.7445 (7)	0.43673 (16)	0.0099 (3)	0.0370 (9)
N1	0.8229 (9)	0.5243 (2)	0.1228 (4)	0.0368 (11)
H1	0.962 (11)	0.542 (3)	0.075 (6)	0.09 (3)*
N3	0.3151 (9)	0.4171 (2)	0.1850 (4)	0.0333 (10)
N4	0.3199 (9)	0.3741 (2)	0.0983 (4)	0.0348 (10)
H4	0.440 (12)	0.378 (3)	0.033 (5)	0.09 (3)*
C2	0.6980 (10)	0.4710 (2)	0.0933 (5)	0.0332 (12)
C3	0.4865 (10)	0.4614 (2)	0.1812 (5)	0.0325 (12)
C4	0.5034 (10)	0.5136 (2)	0.2617 (5)	0.0330 (12)
C5	0.3648 (11)	0.5306 (2)	0.3595 (5)	0.0364 (12)
H5	0.227148	0.505107	0.387426	0.044*
C6	0.4315 (12)	0.5858 (3)	0.4162 (5)	0.0410 (14)
C7	0.6350 (12)	0.6224 (3)	0.3727 (6)	0.0460 (15)
H7	0.678915	0.659976	0.411573	0.055*
C8	0.7741 (12)	0.6058 (3)	0.2752 (5)	0.0430 (14)
H8	0.909675	0.631488	0.246180	0.052*
C9	0.7089 (11)	0.5509 (2)	0.2222 (5)	0.0354 (12)
C10	0.2876 (13)	0.6062 (3)	0.5235 (5)	0.0503 (16)
H10A	0.195041	0.645094	0.506230	0.075*
H10B	0.418146	0.611821	0.590187	0.075*
H10C	0.156207	0.574984	0.543505	0.075*
C11	0.1427 (11)	0.3261 (3)	0.0983 (5)	0.0363 (12)
C12	−0.2434 (12)	0.2564 (3)	0.1973 (6)	0.0517 (16)
H12A	−0.344567	0.260750	0.121366	0.078*
H12B	−0.368701	0.251475	0.260409	0.078*
H12C	−0.126802	0.220314	0.195053	0.078*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S11	0.0550 (9)	0.0417 (8)	0.0435 (8)	0.0003 (7)	−0.0028 (7)	−0.0055 (7)
S12	0.0400 (8)	0.0386 (8)	0.0453 (8)	−0.0014 (6)	0.0031 (6)	0.0030 (7)
O2	0.035 (2)	0.038 (2)	0.037 (2)	0.0033 (17)	0.0029 (17)	0.0032 (17)
N1	0.033 (2)	0.035 (2)	0.043 (3)	0.002 (2)	0.002 (2)	0.003 (2)
N3	0.034 (2)	0.033 (2)	0.033 (2)	0.004 (2)	0.0005 (19)	0.0010 (19)
N4	0.035 (2)	0.034 (2)	0.036 (3)	0.001 (2)	0.002 (2)	0.001 (2)
C2	0.031 (3)	0.035 (3)	0.034 (3)	0.008 (2)	0.000 (2)	0.009 (2)

C3	0.031 (3)	0.031 (3)	0.035 (3)	0.005 (2)	-0.004 (2)	0.005 (2)
C4	0.030 (3)	0.031 (3)	0.037 (3)	0.001 (2)	-0.004 (2)	0.006 (2)
C5	0.039 (3)	0.038 (3)	0.033 (3)	0.003 (2)	0.004 (2)	0.006 (2)
C6	0.044 (3)	0.034 (3)	0.045 (3)	0.009 (3)	-0.004 (3)	-0.003 (3)
C7	0.044 (3)	0.039 (3)	0.055 (4)	0.008 (3)	-0.009 (3)	-0.008 (3)
C8	0.037 (3)	0.037 (3)	0.055 (4)	-0.001 (3)	0.004 (3)	-0.002 (3)
C9	0.032 (3)	0.037 (3)	0.036 (3)	0.005 (2)	-0.003 (2)	0.004 (2)
C10	0.063 (4)	0.045 (3)	0.043 (3)	0.010 (3)	0.001 (3)	-0.005 (3)
C11	0.037 (3)	0.034 (3)	0.038 (3)	0.003 (2)	0.001 (2)	0.006 (2)
C12	0.045 (4)	0.036 (3)	0.074 (5)	-0.002 (3)	-0.001 (3)	0.010 (3)

Geometric parameters (Å, °)

S11—C11	1.649 (6)	C5—H5	0.9500
S12—C11	1.750 (6)	C5—C6	1.396 (8)
S12—C12	1.799 (6)	C6—C7	1.402 (8)
O2—C2	1.237 (6)	C6—C10	1.511 (8)
N1—H1	0.98 (2)	C7—H7	0.9500
N1—C2	1.354 (7)	C7—C8	1.384 (8)
N1—C9	1.412 (7)	C8—H8	0.9500
N3—N4	1.360 (6)	C8—C9	1.372 (8)
N3—C3	1.292 (7)	C10—H10A	0.9800
N4—H4	0.98 (2)	C10—H10B	0.9800
N4—C11	1.370 (7)	C10—H10C	0.9800
C2—C3	1.503 (7)	C12—H12A	0.9800
C3—C4	1.460 (7)	C12—H12B	0.9800
C4—C5	1.387 (7)	C12—H12C	0.9800
C4—C9	1.400 (7)		
C11—S12—C12	101.1 (3)	C8—C7—C6	122.3 (6)
C2—N1—H1	122 (5)	C8—C7—H7	118.8
C2—N1—C9	110.5 (4)	C7—C8—H8	121.3
C9—N1—H1	128 (5)	C9—C8—C7	117.4 (5)
C3—N3—N4	117.0 (4)	C9—C8—H8	121.3
N3—N4—H4	121 (4)	C4—C9—N1	110.5 (5)
N3—N4—C11	119.3 (4)	C8—C9—N1	127.7 (5)
C11—N4—H4	119 (4)	C8—C9—C4	121.8 (5)
O2—C2—N1	127.3 (5)	C6—C10—H10A	109.5
O2—C2—C3	126.1 (5)	C6—C10—H10B	109.5
N1—C2—C3	106.6 (5)	C6—C10—H10C	109.5
N3—C3—C2	128.0 (5)	H10A—C10—H10B	109.5
N3—C3—C4	125.4 (5)	H10A—C10—H10C	109.5
C4—C3—C2	106.6 (4)	H10B—C10—H10C	109.5
C5—C4—C3	133.9 (5)	S11—C11—S12	127.0 (3)
C5—C4—C9	120.4 (5)	N4—C11—S11	120.0 (4)
C9—C4—C3	105.8 (5)	N4—C11—S12	112.9 (4)
C4—C5—H5	120.6	S12—C12—H12A	109.5
C4—C5—C6	118.7 (5)	S12—C12—H12B	109.5

C6—C5—H5	120.6	S12—C12—H12C	109.5
C5—C6—C7	119.3 (5)	H12A—C12—H12B	109.5
C5—C6—C10	120.8 (5)	H12A—C12—H12C	109.5
C7—C6—C10	119.9 (5)	H12B—C12—H12C	109.5
C6—C7—H7	118.8		
O2—C2—C3—N3	-1.0 (8)	C3—C4—C9—N1	-0.8 (6)
O2—C2—C3—C4	-179.2 (5)	C3—C4—C9—C8	177.6 (5)
N1—C2—C3—N3	178.2 (5)	C4—C5—C6—C7	0.2 (8)
N1—C2—C3—C4	0.1 (5)	C4—C5—C6—C10	-179.7 (5)
N3—N4—C11—S11	173.7 (4)	C5—C4—C9—N1	179.3 (5)
N3—N4—C11—S12	-7.1 (6)	C5—C4—C9—C8	-2.3 (8)
N3—C3—C4—C5	2.1 (9)	C5—C6—C7—C8	-0.2 (9)
N3—C3—C4—C9	-177.7 (5)	C6—C7—C8—C9	-1.0 (9)
N4—N3—C3—C2	-1.5 (7)	C7—C8—C9—N1	-179.7 (5)
N4—N3—C3—C4	176.3 (5)	C7—C8—C9—C4	2.2 (8)
C2—N1—C9—C4	0.9 (6)	C9—N1—C2—O2	178.6 (5)
C2—N1—C9—C8	-177.3 (5)	C9—N1—C2—C3	-0.6 (5)
C2—C3—C4—C5	-179.7 (5)	C9—C4—C5—C6	1.0 (8)
C2—C3—C4—C9	0.5 (5)	C10—C6—C7—C8	179.7 (5)
C3—N3—N4—C11	179.9 (5)	C12—S12—C11—S11	0.1 (5)
C3—C4—C5—C6	-178.8 (5)	C12—S12—C11—N4	-179.0 (4)

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>
N4—H4 \cdots O2	0.98 (2)	2.01 (6)	2.754 (6)	130 (6)
N1—H1 \cdots O2 ⁱ	0.98 (2)	1.85 (2)	2.825 (6)	171 (7)

Symmetry code: (i) $-x+2, -y+1, -z$.