Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5-(3-Nitrobenzyl)-1,3,4-thiadiazol-2-amine

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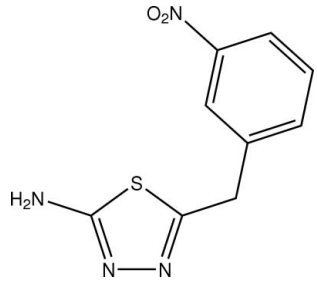
Received 17 November 2009; accepted 19 November 2009

Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.086; data-to-parameter ratio = 14.9.

In the title molecule, $C_9H_8N_4O_2S$, the dihedral angle between the thiadiazole and benzene rings is 73.92 (8)° and the thiadiazole group S atom is orientated towards the benzene ring, the central S—C—C—C torsion angle being 45.44 (18)°. In the crystal, supramolecular tapes mediated by N—H···N hydrogen bonds and comprising alternating eight-membered $\{\cdots HNCN\}_2$ and 10-membered $\{\cdots HNH\cdots NN\}_2$ synthons are formed along [010]. The tapes are consolidated into a three-dimensional network by a combination of C—H···O, C—H···S and C—H···π interactions

Related literature

For background to the biological interest of 1,3,4-thiadiazoles, see: Thomasco *et al.* (2003); Oruç *et al.* (2004); Moise *et al.* (2009); Amir *et al.* (2009). For the development of anti-trypanosomal compounds, see: Carvalho *et al.* (2004); Boechat *et al.* (2006); Boechat *et al.* (2008); Carvalho *et al.* (2008); Poorrajab *et al.* (2009) Riente *et al.* (2009). For the synthesis, see: Turner *et al.* (1988).



Experimental

Crystal data

$C_9H_8N_4O_2S$
M_r = 236.26
Triclinic, $P\overline{1}$
a = 5.0878 (2) Å
b = 5.6213 (3) Å
c = 17.8035 (9) Å
α = 80.980 (3)°
β = 85.677 (3)°
γ = 79.855 (3)°
V = 494.42 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 120 K
0.38 × 0.20 × 0.09 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.639, T_{max} = 0.746
9074 measured reflections
2256 independent reflections
1973 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.086
S = 1.05
2256 reflections
151 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H1n···N2^{i}	0.88	2.25	3.0828 (19)	157
N3—H2n···N1^{ii}	0.88	2.12	3.003 (2)	175
C3—H3a···N2^{iii}	0.99	2.60	3.552 (2)	162
C3—H3b···S1^{iv}	0.99	2.85	3.6687 (17)	141
C7—H7···O2^{v}	0.95	2.53	3.355 (2)	145
C9—H9···O1^{vi}	0.95	2.51	3.446 (2)	168
C5—H5···Cg^{iii}	0.95	2.86	3.7708 (17)	160

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+2, -y+2, -z+1$; (iii) $x-1, y, z$; (iv) $x, y+1, z$; (v) $-x, -y+1, -z+2$; (vi) $x+1, y+1, z$. Cg is the centroid of the S1/N1/N2/C1/C2 ring.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; 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: *publCIF* (Westrip, 2009).

The use of the EPSRC X-ray crystallographic service at the University of Southampton, England and the valuable assistance of the staff there is gratefully acknowledged. JLW acknowledges support from CAPES (Brazil).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2958).

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supporting information

Acta Cryst. (2009). E**65**, o3200–o3201 [doi:10.1107/S1600536809049654]

5-(3-Nitrobenzyl)-1,3,4-thiadiazol-2-amine

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S1. Comment

1,3,4-Thiadiazoles have attracted much attention due to their biological activities (Thomasco *et al.*, 2003; Oruç *et al.*, 2004; Moise *et al.*, 2009; Amir *et al.*, 2009), with particular attention being paid to the anti-trypanosomal activities of Megazol, and related compounds (Carvalho *et al.*, 2004, 2008; Riente *et al.*, 2009: Poorrajab *et al.*, 2009). In continuation of our interests in 1,3,4-thiadiazoles (Boechat *et al.*, 2006, 2008; Carvalho *et al.*, 2004, 2008), we now report the structure of the title compound, (I), obtained by modification of a general procedure (Turner *et al.*, 1988).

In the molecular structure of (I) atom S1 is orientated towards the benzene ring, Fig. 1. The dihedral angle between the thiadiazole (r.m.s. deviation = 0.005 Å) and benzene (r.m.s. deviation = 0.004 Å) rings of 73.92 (8) ° indicates a twist between planes as seen in the S1–C2–C3–C4 torsion angle of 45.44 (18) °. The nitro group is effectively co-planar with the benzene ring to which it is attached as seen in the O1–N4–C6–C5 torsion angle of 6.3 (2) °.

The crystal packing is dominated by N—H···N hydrogen bonds. Each of the amine-H atoms connects to a centrosymmetrically related molecule leading to eight-membered $\{\cdots HNCN\}_2$ and 10-membered $\{\cdots HNH\cdots NN\}_2$ synthons. Each synthon is planar and alternate in a supramolecular tape orientated along [010], Table 1 and Fig. 2. Chains are consolidated into a 3-D network by a combination of C—H···O, C—H···S and C—H···π interactions, Table 1 and Fig. 3.

S2. Experimental

A finely ground mixture of 2-nitrophenylacetic acid (0.49 g, 2.7 mmol) and thiosemicarbazide (0.25 g, 2.7 mmol) was added in portions over 0.5 h to polyphosphoric acid (5 g) at 353 K. The reaction mixture was maintained at 353 K for 5 h and cooled, water/ice was added, and the mixture was finally basified with NaOH 30% (aq.). The solids isolated by filtration were washed with water and air-dried to give (I), which was recrystallized from EtOH, m.p. 471–473 K; yield 72%. The sample used in the structure determination was obtained after a further recrystallization from EtOH. ^{1}H NMR (d_6-DMSO) δ: 4.47 (s, 2H, CH_2), 7.05 (s, 2H, NH_2), 7.55 (m, 2H, H4 and H5), 7.72 (m, 1H, H6), 8.03 (d, 1H, J = 8.0 Hz) p.p.m. ^{13}C NMR (d_6-DMSO) δ: 32.8, 124.7, 128.6, 132.0, 132.6, 133.8, 148.5, 155.1, 168.7 p.p.m.

S3. Refinement

The C-bound H atoms were geometrically placed with C—H = 0.95–0.99 Å, and refined as riding with U_{iso}(H) = 1.2U_{eq}(C). The N-bound H atoms were located from a difference map and included in the model with N–H = 0.880±0.001 Å, and with U_{iso}(H) = 1.2U_{eq}(N).

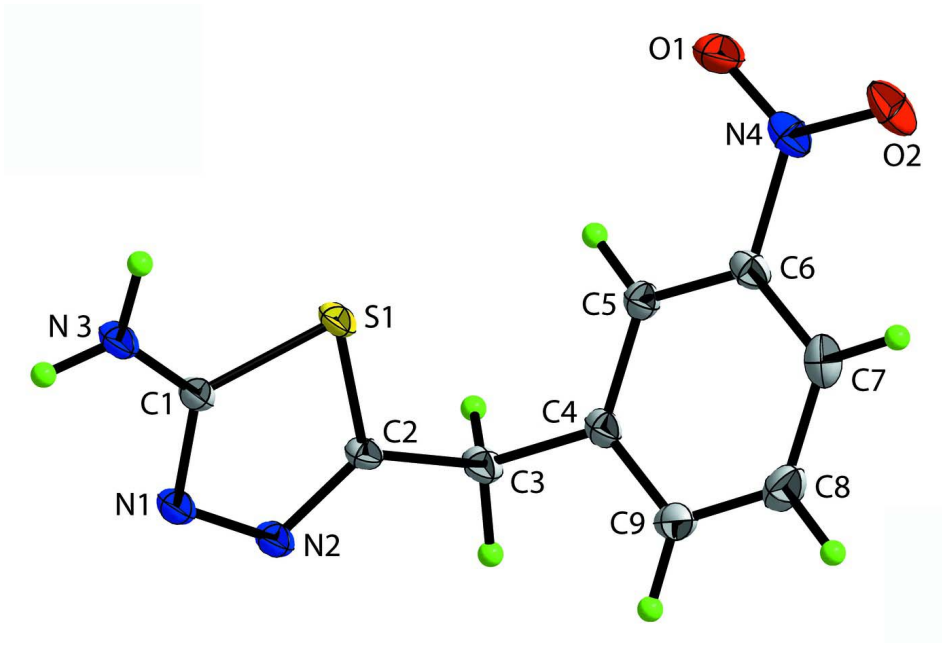

Figure 1

Molecular structure of (I) showing atom-labelling scheme and displacement ellipsoids at the 50% probability level.

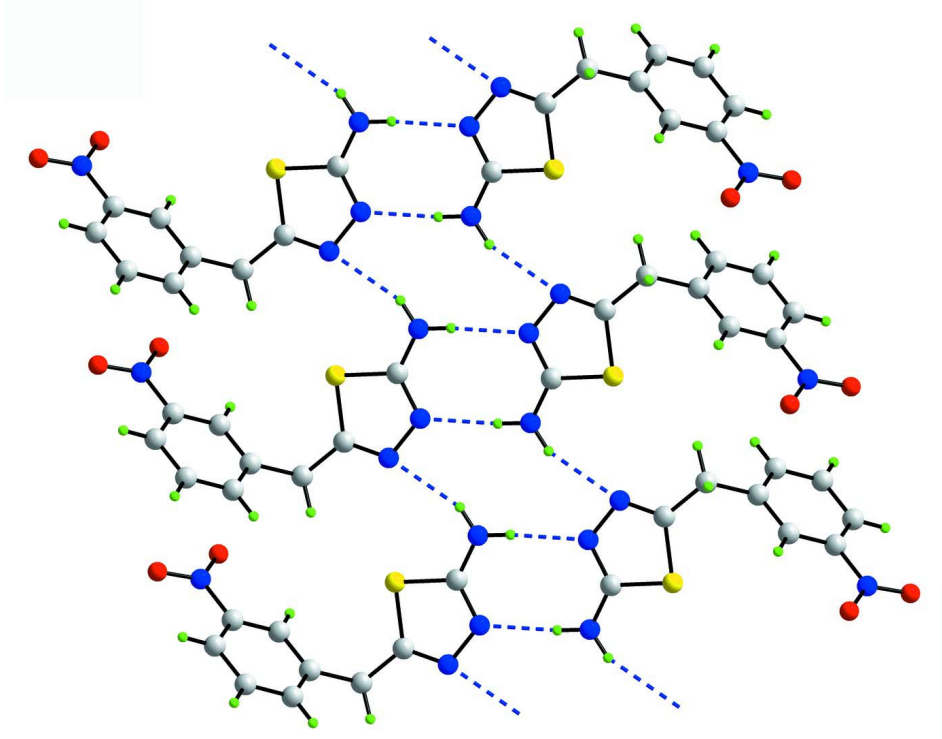

Figure 2

Supramolecular chain along [010] in (I) mediated by N–H···N hydrogen bonds (blue dashed lines). Colour code: S, yellow; O, red; N, blue; C, grey; and H, green.

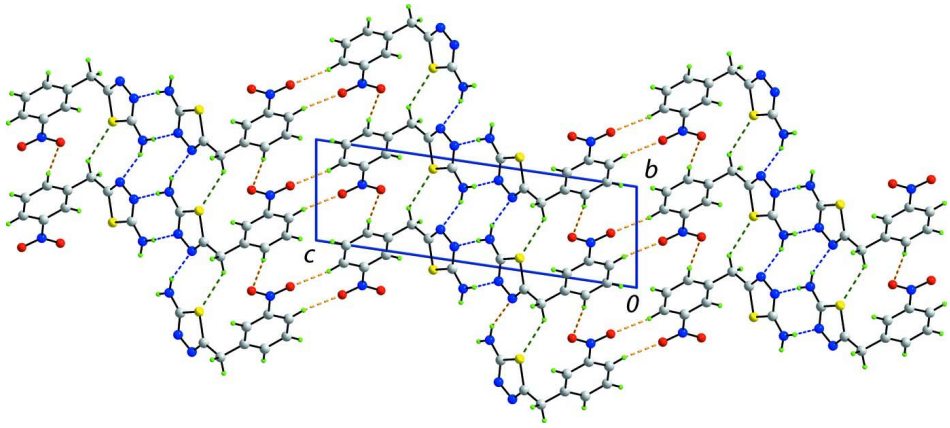

Figure 3

Unit-cell contents for (I) viewed in projection down the *a* axis. The N–H···N (blue), C—H···O (orange) and C—H···S (green) contacts are shown as dashed lines. Colour code: S, yellow; O, red; N, blue; C, grey; and H, green.

5-(3-Nitrobenzyl)-1,3,4-thiadiazol-2-amine

Crystal data

$C_9H_8N_4O_2S$
$M_r = 236.26$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.0878\ (2)$ Å
$b = 5.6213\ (3)$ Å
$c = 17.8035\ (9)$ Å
$\alpha = 80.980\ (3)°$
$\beta = 85.677\ (3)°$
$\gamma = 79.855\ (3)°$
$V = 494.42\ (4)$ Å^3
$Z = 2$
$F(000) = 244$
$D_x = 1.587$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 11753 reflections
$\theta = 2.9–27.5°$
$\mu = 0.32$ mm^{-1}
$T = 120$ K
Block, colourless
0.38 × 0.20 × 0.09 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Radiation source: Enraf Nonius FR591 rotating anode
10 cm confocal mirrors monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.639$, $T_{max} = 0.746$
9074 measured reflections
2256 independent reflections
1973 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.5°$
$h = -6\rightarrow5$
$k = -7\rightarrow7$
$l = -23\rightarrow23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.086$
$S = 1.05$
2256 reflections
151 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2 + 0.3167P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.39352 (8)	0.87897 (7)	0.63466 (2)	0.01803 (12)
O1	−0.3420 (3)	0.5966 (2)	0.79836 (7)	0.0282 (3)
O2	−0.2766 (3)	0.4981 (2)	0.91883 (7)	0.0326 (3)
N1	0.7365 (3)	1.1393 (2)	0.56903 (8)	0.0187 (3)
N2	0.5591 (3)	1.2890 (2)	0.61221 (8)	0.0185 (3)
N3	0.8153 (3)	0.7356 (2)	0.54139 (8)	0.0198 (3)
H1N	0.7552	0.5959	0.5485	0.030*
H2N	0.9445	0.7652	0.5073	0.030*
N4	−0.2396 (3)	0.6204 (2)	0.85639 (8)	0.0218 (3)
C1	0.6754 (3)	0.9177 (3)	0.57569 (9)	0.0160 (3)
C2	0.3731 (3)	1.1810 (3)	0.64921 (9)	0.0161 (3)
C3	0.1583 (3)	1.2978 (3)	0.70123 (9)	0.0189 (3)
H3A	−0.0131	1.3369	0.6754	0.023*
H3B	0.2049	1.4528	0.7116	0.023*
C4	0.1235 (3)	1.1329 (3)	0.77600 (9)	0.0167 (3)
C5	−0.0430 (3)	0.9582 (3)	0.78225 (9)	0.0164 (3)
H5	−0.1411	0.9442	0.7403	0.020*
C6	−0.0634 (3)	0.8046 (3)	0.85083 (9)	0.0180 (3)
C7	0.0726 (3)	0.8188 (3)	0.91408 (10)	0.0231 (4)
H7	0.0545	0.7117	0.9604	0.028*
C8	0.2360 (3)	0.9947 (3)	0.90746 (10)	0.0249 (4)
H8	0.3309	1.0096	0.9500	0.030*
C9	0.2626 (3)	1.1498 (3)	0.83935 (10)	0.0208 (3)
H9	0.3766	1.2684	0.8358	0.025*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0196 (2)	0.0135 (2)	0.0218 (2)	−0.00748 (15)	0.00547 (15)	−0.00271 (14)
O1	0.0321 (7)	0.0250 (6)	0.0306 (7)	−0.0141 (5)	−0.0028 (5)	−0.0022 (5)
O2	0.0328 (7)	0.0306 (7)	0.0307 (7)	−0.0112 (6)	0.0028 (6)	0.0113 (5)
N1	0.0184 (7)	0.0156 (6)	0.0228 (7)	−0.0061 (5)	0.0044 (5)	−0.0039 (5)
N2	0.0186 (7)	0.0152 (6)	0.0225 (7)	−0.0061 (5)	0.0034 (5)	−0.0036 (5)
N3	0.0206 (7)	0.0140 (6)	0.0252 (8)	−0.0067 (5)	0.0064 (5)	−0.0036 (5)
N4	0.0193 (7)	0.0170 (7)	0.0271 (8)	−0.0029 (5)	0.0029 (6)	0.0012 (6)
C1	0.0156 (7)	0.0165 (7)	0.0162 (8)	−0.0058 (6)	−0.0008 (6)	0.0001 (6)

C2	0.0188 (7)	0.0130 (7)	0.0174 (8)	−0.0060 (6)	−0.0006 (6)	−0.0014 (6)
C3	0.0214 (8)	0.0131 (7)	0.0225 (8)	−0.0052 (6)	0.0035 (6)	−0.0024 (6)
C4	0.0143 (7)	0.0145 (7)	0.0210 (8)	−0.0018 (6)	0.0046 (6)	−0.0049 (6)
C5	0.0156 (7)	0.0163 (7)	0.0170 (8)	−0.0020 (6)	0.0006 (6)	−0.0033 (6)
C6	0.0150 (7)	0.0156 (7)	0.0226 (8)	−0.0024 (6)	0.0025 (6)	−0.0020 (6)
C7	0.0226 (8)	0.0262 (9)	0.0174 (8)	0.0002 (7)	0.0019 (6)	−0.0001 (7)
C8	0.0228 (9)	0.0325 (9)	0.0209 (9)	−0.0032 (7)	−0.0041 (7)	−0.0085 (7)
C9	0.0173 (8)	0.0220 (8)	0.0254 (9)	−0.0052 (6)	0.0017 (6)	−0.0096 (7)

Geometric parameters (Å, º)

S1—C1	1.7373 (16)	C3—H3A	0.9900
S1—C2	1.7412 (15)	C3—H3B	0.9900
O1—N4	1.2271 (19)	C4—C5	1.393 (2)
O2—N4	1.2321 (18)	C4—C9	1.400 (2)
N1—C1	1.321 (2)	C5—C6	1.389 (2)
N1—N2	1.3949 (19)	C5—H5	0.9500
N2—C2	1.297 (2)	C6—C7	1.385 (2)
N3—C1	1.342 (2)	C7—C8	1.386 (2)
N3—H1N	0.8800	C7—H7	0.9500
N3—H2N	0.8799	C8—C9	1.391 (2)
N4—C6	1.472 (2)	C8—H8	0.9500
C2—C3	1.506 (2)	C9—H9	0.9500
C3—C4	1.516 (2)		
C1—S1—C2	87.36 (7)	H3A—C3—H3B	107.9
C1—N1—N2	111.82 (13)	C5—C4—C9	118.89 (15)
C2—N2—N1	113.45 (12)	C5—C4—C3	120.45 (14)
C1—N3—H1N	117.3	C9—C4—C3	120.64 (14)
C1—N3—H2N	119.9	C6—C5—C4	118.95 (14)
H1N—N3—H2N	122.0	C6—C5—H5	120.5
O1—N4—O2	123.37 (14)	C4—C5—H5	120.5
O1—N4—C6	118.11 (13)	C7—C6—C5	122.94 (15)
O2—N4—C6	118.52 (14)	C7—C6—N4	118.81 (14)
N1—C1—N3	124.39 (14)	C5—C6—N4	118.25 (14)
N1—C1—S1	113.68 (12)	C6—C7—C8	117.65 (15)
N3—C1—S1	121.93 (11)	C6—C7—H7	121.2
N2—C2—C3	124.72 (13)	C8—C7—H7	121.2
N2—C2—S1	113.68 (12)	C9—C8—C7	120.82 (15)
C3—C2—S1	121.59 (11)	C9—C8—H8	119.6
C2—C3—C4	112.03 (13)	C7—C8—H8	119.6
C2—C3—H3A	109.2	C8—C9—C4	120.74 (15)
C4—C3—H3A	109.2	C8—C9—H9	119.6
C2—C3—H3B	109.2	C4—C9—H9	119.6
C4—C3—H3B	109.2		
C1—N1—N2—C2	−0.19 (19)	C3—C4—C5—C6	177.85 (14)
N2—N1—C1—N3	−178.79 (14)	C4—C5—C6—C7	0.8 (2)

N2—N1—C1—S1	0.65 (17)	C4—C5—C6—N4	−179.81 (13)
C2—S1—C1—N1	−0.70 (12)	O1—N4—C6—C7	−174.26 (14)
C2—S1—C1—N3	178.76 (14)	O2—N4—C6—C7	5.7 (2)
N1—N2—C2—C3	178.85 (14)	O1—N4—C6—C5	6.3 (2)
N1—N2—C2—S1	−0.36 (17)	O2—N4—C6—C5	−173.78 (14)
C1—S1—C2—N2	0.59 (12)	C5—C6—C7—C8	−0.2 (2)
C1—S1—C2—C3	−178.64 (14)	N4—C6—C7—C8	−179.63 (15)
N2—C2—C3—C4	−133.70 (16)	C6—C7—C8—C9	−0.4 (3)
S1—C2—C3—C4	45.44 (18)	C7—C8—C9—C4	0.5 (3)
C2—C3—C4—C5	−85.79 (18)	C5—C4—C9—C8	0.1 (2)
C2—C3—C4—C9	92.73 (17)	C3—C4—C9—C8	−178.44 (15)
C9—C4—C5—C6	−0.7 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H1n···N2^{i}	0.88	2.25	3.0828 (19)	157
N3—H2n···N1^{ii}	0.88	2.12	3.003 (2)	175
C3—H3a···N2^{iii}	0.99	2.60	3.552 (2)	162
C3—H3b···S1^{iv}	0.99	2.85	3.6687 (17)	141
C7—H7···O2^{v}	0.95	2.53	3.355 (2)	145
C9—H9···O1^{vi}	0.95	2.51	3.446 (2)	168
C5—H5···*Cg*^{iii}	0.95	2.86	3.7708 (17)	160

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