Crystal structure of 4-(benzo[*d*]thiazol-2-yl)-1,2-dimethyl-1*H*-pyrazol-3(2*H*)-one

Heba A. Elboshi,[a] Rasha A. Azzam,[a] Galal H. Elgemeie[a] and Peter G. Jones[b]*

[a]Chemistry Department, Faculty of Science, Helwan University, Cairo, Egypt, and [b]Institut für Anorganische und Analytische Chemie, Technische Universität Braunschweig, Hagenring 30, D-38106 Braunschweig, Germany. *Correspondence e-mail: p.jones@tu-braunschweig.de

In the title compound, $C_{12}H_{11}N_3OS$, the interplanar angle between the pyrazole and benzothiazole rings is 3.31 (7)°. In the three-dimensional molecular packing, the carbonyl oxygen acts as acceptor to four C—H donors (with one H···O as short as 2.25 Å), while one methyl hydrogen is part of the three-centre system H···(S, O). A double layer structure parallel to ($\overline{1}01$) can be recognized as a subsection of the packing.

1. Chemical context

Many natural heterocyclic compounds and pharmaceuticals involve benzothiazole moieties and derivatives thereof, which are among the most significant heterocyclic compounds utilized in medicinal chemistry (Bonde *et al.*, 2015). In the search for novel and significant therapeutic drugs, benzothiazoles have a wide range of established pharmacological properties (Wang *et al.*, 2009), and their derivatives include several structural variants (Rana *et al.*, 2008). The application of benzothiazole derivatives in current research and related discoveries is a well-appreciated and quickly growing area of medicinal chemistry (Abdallah *et al.*, 2023). As an example, several drugs based on benzothiazole derivatives have been widely utilized in clinical practice to treat a variety of disorders, with a marked therapeutic efficacy (Huang *et al.*, 2009).

In the course of our studies, intended to develop syntheses of benzothiazole-based heterocycles for use as pharmaceuticals and pigments (Ahmed *et al.*, 2022, 2023), a variety of 2-pyrimidyl-, 2-pyridyl- and 2-thienyl-benzothiazole compounds with encouraging cytotoxic action have recently been synthesized and their biological activity reported (Azzam *et al.*, 2017, 2019, 2022).
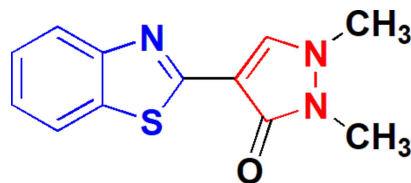
In line with these findings and our prior research (Metwally *et al.*, 2022*a*,*b*), the aim of the current investigation was to design and create benzothiazolyl-pyrazole hybrids. The reaction of 2-benzothiazolyl acetohydrazide **1** with *N*,*N*-dimethylformamide dimethyl acetal **2** at room temperature led to the synthesis of the unexpected benzothiazole-2-pyrazole derivative **3** in good yield (Fig. 1). The mechanism for the formation of **3** is currently under investigation. In order to
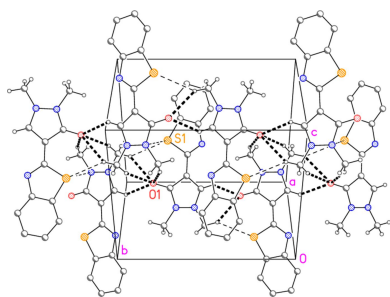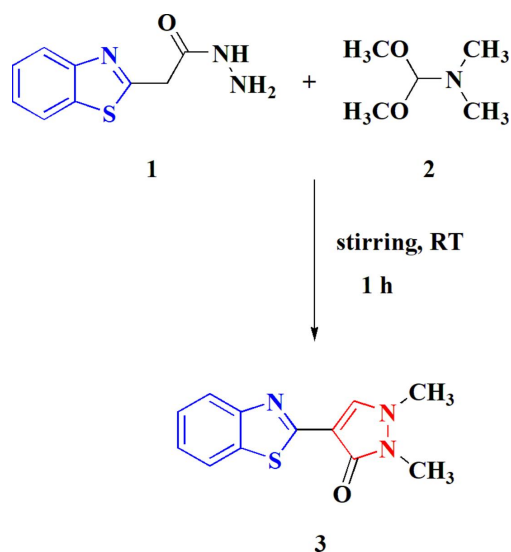
Figure 1
The synthesis of the title compound **3**.

establish the structure of the product unambiguously, its crystal structure was determined and is reported here.

2. Structural commentary

The structure of compound **3** is shown in Fig. 2, with selected molecular dimensions in Table 1. These may be regarded as normal, within the constraints of linked five-membered rings that necessarily lead to narrow angles within the rings and wide exocyclic angles [up to 127.48 (11)° for C10—C8—C2]. The molecule is essentially planar (except for the methyl hydrogens); the least-squares plane through all non-H atoms has an r.m.s.d. of only 0.037 Å. If the ring systems are regarded separately, the pyrazole and benzothiazole rings have r.m.s.d. values of 0.006 and 0.017 Å, respectively, and an interplanar angle of 3.31 (7)°. The coplanarity leads to a short intramolecular contact S1···O1 = 2.9797 (10) Å.

3. Supramolecular features

The molecular packing involves five short contacts, four C—H···O1 and one C—H···S1, that are acceptably linear and may be regarded as 'weak' hydrogen bonds (Table 2). The
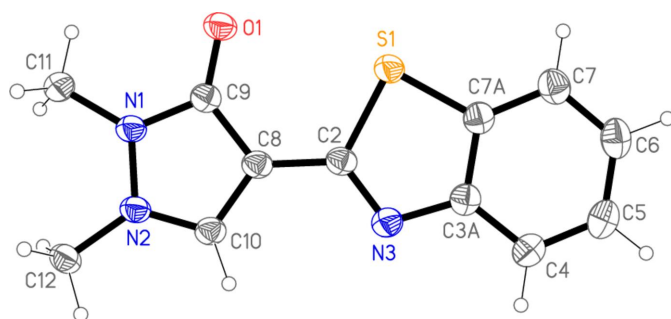
Figure 2
The structure of compound **3** in the crystal. Ellipsoids correspond to 50% probability levels.

Table 1
Selected geometric parameters (Å, °).

S1—C7A	1.7374 (13)	N2—C10	1.3326 (16)
S1—C2	1.7673 (12)	N3—C2	1.3051 (16)
O1—C9	1.2468 (15)	N3—C3A	1.3879 (16)
N1—N2	1.3766 (14)	C2—C8	1.4348 (17)
N1—C9	1.3772 (16)	C3A—C7A	1.4058 (18)
C7A—S1—C2	88.85 (6)	C7—C7A—S1	128.77 (11)
N2—N1—C9	109.59 (10)	C3A—C7A—S1	109.37 (9)
C10—N2—N1	108.87 (10)	C10—C8—C2	127.48 (11)
C2—N3—C3A	110.45 (11)	C10—C8—C9	107.06 (11)
N3—C2—C8	124.55 (11)	C2—C8—C9	125.46 (11)
N3—C2—S1	115.65 (9)	O1—C9—N1	123.88 (11)
C8—C2—S1	119.80 (9)	O1—C9—C8	130.92 (12)
N3—C3A—C4	125.04 (12)	N1—C9—C8	105.19 (10)
N3—C3A—C7A	115.66 (11)	N2—C10—C8	109.28 (11)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···O1^i	0.95	2.38	3.2055 (15)	145
C11—H11A···O1^{ii}	0.98	2.51	3.4368 (16)	158
C12—H12B···S1^i	0.98	2.86	3.7142 (13)	146
C12—H12B···O1^i	0.98	2.60	3.4696 (16)	148
C12—H12C···O1^{ii}	0.98	2.25	3.1966 (16)	163

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

donor atom H12B is part of a three-centre system with acceptors O1 and S1. The contact H12C···O1 is remarkably short at 2.25 Å. Additionally, there is a short contact S1···N1($x, \frac{3}{2} - y, \frac{1}{2} + z$) = 3.4078 (11) Å. A section of the packing is shown in Fig. 3; a ribbon parallel to the b axis and its antiparallel counterpart are shown, which form a double layer parallel to ($\bar{1}$01). However, the molecules are further linked parallel to the view direction to give a three-dimensional pattern. There are no *Cent–Cent* contacts shorter than 3.75 Å and no H···*Cent* contacts shorter than 2.99 Å (*Cent* = ring centroids).
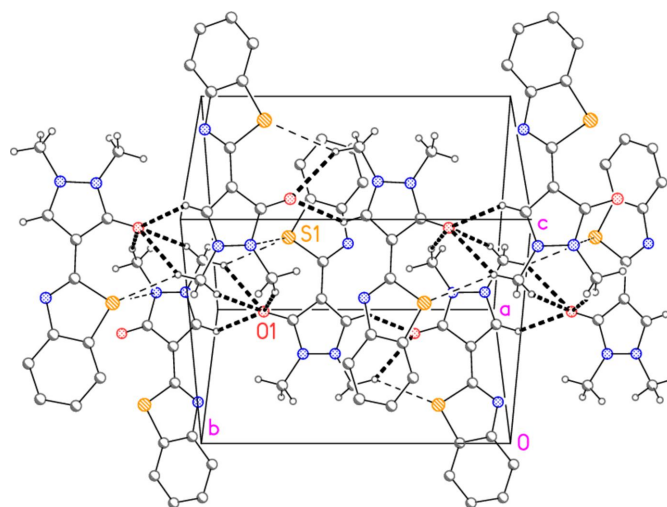
Figure 3
A section of the three-dimensional packing of compound **3**: two anti-parallel ribbons viewed perpendicular to ($\bar{1}$01). Contacts to O1 are shown as thick dashed lines and those to S1 as thin dashed lines. Hydrogen atoms not involved in hydrogen bonding are omitted. The atom labels indicate the asymmetric unit.

Table 3
Experimental details.

Crystal data
Chemical formula	$C_{12}H_{11}N_3OS$
M_r	245.30
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	8.78308 (12), 11.66215 (16), 11.00169 (15)
β (°)	97.9460 (12)
V (Å^3)	1116.08 (3)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.47
Crystal size (mm)	$0.15 \times 0.10 \times 0.03$

Data collection
Diffractometer	XtaLAB Synergy
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.731, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	46018, 2367, 2280
R_{int}	0.037
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.634

Refinement
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.081, 1.07
No. of reflections	2367
No. of parameters	156
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, −0.36

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019/3* (Sheldrick, 2015*b*) and *XP* (Bruker, 1998).

4. Database survey

The search employed the routine ConQuest (Bruno *et al.*, 2002), part of Version 2023.3.0 of the Cambridge Structural Database (Groom *et al.*, 2016).

A search for other structures containing a linked pyrazolone/benzothiazole unit as in **3** led to three hits: AZUPIV, with 1-Me, 2-Ph and 5-Me substituents on the pyrazolone ring (Chakib *et al.*, 2011), VABFIP (1-allyl, 2-Ph, 5-Me; Chakib *et al.*, 2010*a*) and VABFOV (1-propynyl, 2-Ph, 5-Me; Chakib *et al.*, 2010*b*). The interplanar angles in these compounds are 6.1 (1), 7.9 (2) and 4.7 (1)°, respectively.

5. Synthesis and crystallization

A mixture of 2-benzothiazolyl acetohydrazide **1** (0.01 mol) and *N,N*-dimethylformamide dimethyl acetal **2** (0.02 mol) was stirred at room temperature for 1 h. The excess acetal was distilled off under reduced pressure; the solid product was washed with a mixture of petroleum ether and diethyl ether (1:1) and then crystallized from ethanol.

Yellow solid; yield 85%; m.p. 414 K; IR (KBr, cm^{-1}): ν 3068 (aromatic CH), 2930 (methyl CH), 1620 (C=O), 1598 (C=N); ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.80 (*s*, 3H, CH$_3$), 4.01 (*s*, 3H, CH$_3$), 7.34 (*t*, *J* = 7.2 Hz, 1H, benzothiazole H), 7.46 (*t*, *J* = 7.2 Hz, 1H, benzothiazole H), 7.89 (*d*, *J* = 7.6 Hz, 1H, benzothiazole H), 8.03 (*d*, *J* = 8.0 Hz, 1H, benzothiazole H), 8.35 (*s*, 1H, pyrazolone H). Analysis calculated for $C_{12}H_{11}N_3OS$ (245.30): C 58.76, H 4.52, N 17.13, S 13.07. Found C 58.66, H 4.40, N 17.08, S 13.14%.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The methyl groups were included as idealized rigid groups (C—H 0.98 Å, H—C—H 109.5°) allowed to rotate but not tip (command 'AFIX 137'). Other hydrogen atoms were included using a riding model starting from calculated positions (C—H = 0.95 Å). The U_{iso}(H) values were fixed at $1.5 \times U_{eq}$ of the parent carbon atoms for the methyl group and $1.2 \times U_{eq}$ for other hydrogens. One reflection clearly in error ($F_o^2 \gg F_c^2$) was omitted from the refinement.

References

Abdallah, A. E. M., Elgemeie, G. H. & Jones, P. G. (2023). *Acta Cryst.* E**79**, 441–445.
Ahmed, E. A., Elgemeie, G. H. & Ahmed, K. A. (2022). *Pigm. Resin Technol.* **51**, 1–5.
Ahmed, E. A., Elgemeie, G. H. & Azzam, R. A. (2023). *Synth. Commun.* **53**, 386–401.
Azzam, R. A., Elgemeie, G. H., Elsayed, R. E., Gad, N. M. & Jones, P. G. (2022). *Acta Cryst.* E**78**, 369–372.
Azzam, R. A., Elgemeie, G. H., Elsayed, R. E. & Jones, P. G. (2017). *Acta Cryst.* E**73**, 1820–1822.
Azzam, R. A., Elgemeie, G. H., Osman, R. R. & Jones, P. G. (2019). *Acta Cryst.* E**75**, 367–371.
Bonde, C., Vedala, D. & Bonde, S. (2015). *J. Pharm. Res.* **9**, 573–580.
Bruker (1998). *XP*. Bruker Analytical X–Ray Instruments, Madison, Wisconsin, USA.
Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* B**58**, 389–397.
Chakib, I., Zerzouf, A., Rodi, Y. K., Essassi, E. M. & Ng, S. W. (2011). *Acta Cryst.* E**67**, o2700.
Chakib, I., Zerzouf, A., Zouihri, H., Essassi, E. M. & Ng, S. W. (2010*a*). *Acta Cryst.* E**66**, o2842.
Chakib, I., Zerzouf, A., Zouihri, H., Essassi, E. M. & Ng, S. W. (2010*b*). *Acta Cryst.* E**66**, o2843.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Huang, Q., Mao, J., Wan, B., Wang, Y., Brun, R., Franzblau, S. G. & Kozikowski, A. P. (2009). *J. Med. Chem.* **52**, 6757–6767.
Metwally, N. H., Elgemeie, G. H. & Fahmy, F. G. (2022*b*). *Egypt. J. Chem.* **65**, 679–686.
Metwally, N. H., Elgemeie, G. H. & Jones, P. G. (2022*a*). *Acta Cryst.* E**78**, 445–448.
Rana, A., Siddiqui, N., Khan, S. A., Ehtaishamul Haque, S. & Bhat, M. A. (2008). *Eur. J. Med. Chem.* **43**, 1114–1122.
Rigaku OD (2021). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Wang, X., Sarris, K., Kage, K., Zhang, D., Brown, S. P., Kolasa, T., Surowy, C., El Kouhen, O. F., Muchmore, S. W., Brioni, J. D. & Stewart, A. O. (2009). *J. Med. Chem.* **52**, 170–180.

supporting information

Crystal structure of 4-(benzo[*d*]thiazol-2-yl)-1,2-dimethyl-1*H*-pyrazol-3(2*H*)-one

Heba A. Elboshi, Rasha A. Azzam, Galal H. Elgemeie and Peter G. Jones

Computing details

4-(Benzo[*d*]thiazol-2-yl)-1,2-dimethyl-1*H*-pyrazol-3(2*H*)-one

Crystal data

$C_{12}H_{11}N_3OS$	$F(000) = 512$
$M_r = 245.30$	$D_x = 1.460$ Mg m^{-3}
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
$a = 8.78308$ (12) Å	Cell parameters from 32695 reflections
$b = 11.66215$ (16) Å	$\theta = 5.1–77.4°$
$c = 11.00169$ (15) Å	$\mu = 2.47$ mm^{-1}
$\beta = 97.9460$ (12)°	$T = 100$ K
$V = 1116.08$ (3) Å^3	Plate, pale yellow
$Z = 4$	$0.15 \times 0.10 \times 0.03$ mm

Data collection

XtaLAB Synergy diffractometer	$T_{min} = 0.731$, $T_{max} = 1.000$
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source	46018 measured reflections
	2367 independent reflections
Mirror monochromator	2280 reflections with $I > 2\sigma(I)$
Detector resolution: 10.0000 pixels mm^{-1}	$R_{int} = 0.037$
ω scans	$\theta_{max} = 77.6°$, $\theta_{min} = 5.1°$
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2021)	$h = -11 \rightarrow 11$
	$k = -14 \rightarrow 14$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.030$	H-atom parameters constrained
$wR(F^2) = 0.081$	$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 0.4017P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	
2367 reflections	$(\Delta/\sigma)_{max} = 0.001$
156 parameters	$\Delta\rho_{max} = 0.28$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.36$ e Å^{-3}
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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.63680 (4)	0.71933 (2)	0.56971 (3)	0.02849 (11)
O1	0.40109 (11)	0.79924 (7)	0.36636 (8)	0.0311 (2)
N1	0.33946 (12)	0.67380 (9)	0.20375 (9)	0.0266 (2)
N2	0.39212 (12)	0.56914 (8)	0.16939 (9)	0.0268 (2)
N3	0.73240 (12)	0.52608 (9)	0.48701 (10)	0.0288 (2)
C2	0.63324 (14)	0.60863 (10)	0.45966 (11)	0.0259 (2)
C3A	0.82145 (14)	0.54730 (11)	0.59907 (12)	0.0286 (3)
C4	0.94097 (16)	0.47710 (12)	0.65366 (13)	0.0350 (3)
H4	0.964387	0.407342	0.615676	0.042*
C5	1.02447 (16)	0.51076 (13)	0.76368 (13)	0.0382 (3)
H5	1.106443	0.463964	0.800905	0.046*
C6	0.98995 (16)	0.61274 (13)	0.82092 (13)	0.0378 (3)
H6	1.049479	0.634461	0.896126	0.045*
C7	0.87033 (16)	0.68266 (12)	0.76977 (12)	0.0339 (3)
H7	0.845688	0.751223	0.809420	0.041*
C7A	0.78751 (14)	0.64905 (11)	0.65836 (11)	0.0284 (3)
C8	0.52570 (14)	0.61387 (10)	0.34907 (11)	0.0258 (2)
C9	0.42066 (14)	0.70641 (10)	0.31446 (11)	0.0258 (2)
C10	0.50225 (14)	0.53273 (10)	0.25637 (11)	0.0267 (3)
H10	0.556198	0.462239	0.255040	0.032*
C11	0.22779 (15)	0.74119 (11)	0.12468 (12)	0.0313 (3)
H11A	0.260232	0.747813	0.043243	0.047*
H11B	0.220412	0.817829	0.159925	0.047*
H11C	0.127222	0.703488	0.117398	0.047*
C12	0.32435 (15)	0.51086 (11)	0.05843 (12)	0.0301 (3)
H12A	0.214516	0.498538	0.061218	0.045*
H12B	0.375258	0.436717	0.052279	0.045*
H12C	0.337515	0.557948	−0.013158	0.045*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.03690 (19)	0.02172 (17)	0.02606 (17)	0.00157 (11)	0.00148 (12)	−0.00057 (10)
O1	0.0411 (5)	0.0228 (4)	0.0290 (4)	0.0033 (4)	0.0038 (4)	−0.0025 (3)
N1	0.0317 (5)	0.0205 (5)	0.0273 (5)	0.0015 (4)	0.0028 (4)	−0.0008 (4)
N2	0.0334 (5)	0.0198 (5)	0.0267 (5)	0.0006 (4)	0.0030 (4)	−0.0013 (4)
N3	0.0314 (5)	0.0253 (5)	0.0295 (5)	0.0014 (4)	0.0038 (4)	0.0007 (4)
C2	0.0308 (6)	0.0210 (5)	0.0265 (6)	−0.0019 (4)	0.0062 (5)	0.0007 (4)
C3A	0.0287 (6)	0.0278 (6)	0.0294 (6)	−0.0021 (5)	0.0044 (5)	0.0023 (5)

C4	0.0338 (6)	0.0336 (7)	0.0371 (7)	0.0045 (5)	0.0033 (5)	0.0025 (5)
C5	0.0315 (7)	0.0431 (8)	0.0386 (7)	0.0022 (6)	−0.0002 (5)	0.0073 (6)
C6	0.0355 (7)	0.0437 (8)	0.0321 (7)	−0.0076 (6)	−0.0025 (5)	0.0034 (6)
C7	0.0380 (7)	0.0318 (7)	0.0312 (6)	−0.0065 (5)	0.0025 (5)	0.0005 (5)
C7A	0.0309 (6)	0.0258 (6)	0.0286 (6)	−0.0034 (5)	0.0046 (5)	0.0037 (5)
C8	0.0316 (6)	0.0204 (5)	0.0258 (6)	−0.0008 (4)	0.0051 (5)	0.0010 (4)
C9	0.0305 (6)	0.0228 (6)	0.0247 (6)	−0.0013 (4)	0.0054 (5)	0.0015 (4)
C10	0.0324 (6)	0.0206 (6)	0.0273 (6)	0.0003 (5)	0.0045 (5)	0.0017 (5)
C11	0.0353 (7)	0.0270 (6)	0.0303 (6)	0.0049 (5)	0.0000 (5)	−0.0002 (5)
C12	0.0374 (7)	0.0239 (6)	0.0281 (6)	−0.0029 (5)	0.0014 (5)	−0.0023 (5)

Geometric parameters (Å, º)

S1—C7A	1.7374 (13)	C5—C6	1.398 (2)
S1—C2	1.7673 (12)	C5—H5	0.9500
O1—C9	1.2468 (15)	C6—C7	1.386 (2)
N1—N2	1.3766 (14)	C6—H6	0.9500
N1—C9	1.3772 (16)	C7—C7A	1.3923 (18)
N1—C11	1.4493 (16)	C7—H7	0.9500
N2—C10	1.3326 (16)	C8—C10	1.3856 (17)
N2—C12	1.4511 (15)	C8—C9	1.4365 (17)
N3—C2	1.3051 (16)	C10—H10	0.9500
N3—C3A	1.3879 (16)	C11—H11A	0.9800
C2—C8	1.4348 (17)	C11—H11B	0.9800
C3A—C4	1.3995 (18)	C11—H11C	0.9800
C3A—C7A	1.4058 (18)	C12—H12A	0.9800
C4—C5	1.383 (2)	C12—H12B	0.9800
C4—H4	0.9500	C12—H12C	0.9800
C7A—S1—C2	88.85 (6)	C7A—C7—H7	121.1
N2—N1—C9	109.59 (10)	C7—C7A—C3A	121.85 (12)
N2—N1—C11	122.76 (10)	C7—C7A—S1	128.77 (11)
C9—N1—C11	127.29 (10)	C3A—C7A—S1	109.37 (9)
C10—N2—N1	108.87 (10)	C10—C8—C2	127.48 (11)
C10—N2—C12	128.87 (10)	C10—C8—C9	107.06 (11)
N1—N2—C12	122.15 (10)	C2—C8—C9	125.46 (11)
C2—N3—C3A	110.45 (11)	O1—C9—N1	123.88 (11)
N3—C2—C8	124.55 (11)	O1—C9—C8	130.92 (12)
N3—C2—S1	115.65 (9)	N1—C9—C8	105.19 (10)
C8—C2—S1	119.80 (9)	N2—C10—C8	109.28 (11)
N3—C3A—C4	125.04 (12)	N2—C10—H10	125.4
N3—C3A—C7A	115.66 (11)	C8—C10—H10	125.4
C4—C3A—C7A	119.29 (12)	N1—C11—H11A	109.5
C5—C4—C3A	119.03 (13)	N1—C11—H11B	109.5
C5—C4—H4	120.5	H11A—C11—H11B	109.5
C3A—C4—H4	120.5	N1—C11—H11C	109.5
C4—C5—C6	120.93 (13)	H11A—C11—H11C	109.5
C4—C5—H5	119.5	H11B—C11—H11C	109.5

C6—C5—H5	119.5	N2—C12—H12A	109.5
C7—C6—C5	121.11 (13)	N2—C12—H12B	109.5
C7—C6—H6	119.4	H12A—C12—H12B	109.5
C5—C6—H6	119.4	N2—C12—H12C	109.5
C6—C7—C7A	117.78 (13)	H12A—C12—H12C	109.5
C6—C7—H7	121.1	H12B—C12—H12C	109.5
C9—N1—N2—C10	1.41 (13)	C4—C3A—C7A—S1	179.30 (10)
C11—N1—N2—C10	174.94 (11)	C2—S1—C7A—C7	177.82 (13)
C9—N1—N2—C12	177.72 (11)	C2—S1—C7A—C3A	−0.88 (9)
C11—N1—N2—C12	−8.75 (17)	N3—C2—C8—C10	3.3 (2)
C3A—N3—C2—C8	178.92 (11)	S1—C2—C8—C10	−176.73 (10)
C3A—N3—C2—S1	−1.06 (13)	N3—C2—C8—C9	−176.88 (11)
C7A—S1—C2—N3	1.17 (10)	S1—C2—C8—C9	3.10 (17)
C7A—S1—C2—C8	−178.81 (10)	N2—N1—C9—O1	177.75 (11)
C2—N3—C3A—C4	−178.36 (12)	C11—N1—C9—O1	4.6 (2)
C2—N3—C3A—C7A	0.34 (15)	N2—N1—C9—C8	−1.34 (13)
N3—C3A—C4—C5	177.54 (13)	C11—N1—C9—C8	−174.50 (11)
C7A—C3A—C4—C5	−1.12 (19)	C10—C8—C9—O1	−178.19 (13)
C3A—C4—C5—C6	0.6 (2)	C2—C8—C9—O1	1.9 (2)
C4—C5—C6—C7	0.5 (2)	C10—C8—C9—N1	0.80 (13)
C5—C6—C7—C7A	−1.2 (2)	C2—C8—C9—N1	−179.06 (11)
C6—C7—C7A—C3A	0.65 (19)	N1—N2—C10—C8	−0.86 (13)
C6—C7—C7A—S1	−177.91 (10)	C12—N2—C10—C8	−176.86 (12)
N3—C3A—C7A—C7	−178.29 (11)	C2—C8—C10—N2	179.88 (12)
C4—C3A—C7A—C7	0.49 (19)	C9—C8—C10—N2	0.03 (14)
N3—C3A—C7A—S1	0.52 (14)		

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···O1^i	0.95	2.38	3.2055 (15)	145
C11—H11*A*···O1^{ii}	0.98	2.51	3.4368 (16)	158
C12—H12*B*···S1^i	0.98	2.86	3.7142 (13)	146
C12—H12*B*···O1^i	0.98	2.60	3.4696 (16)	148
C12—H12*C*···O1^{ii}	0.98	2.25	3.1966 (16)	163

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