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ISSN 2414-3146

5-[(4-Bromophenyl)diazenyl]-2-{2-[1-(1*H*-indol-3-yl)ethylidene]hydrazinyl}-4-methylthiazole dimethylformamide hemisolvate

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Received 26 September 2018
Accepted 28 September 2018

Edited by J. Simpson, University of Otago, New Zealand

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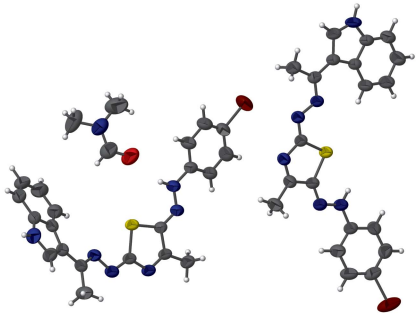
Keywords: crystal structure; indole; thiazole; hydrogen bonds.

CCDC reference: 1870513

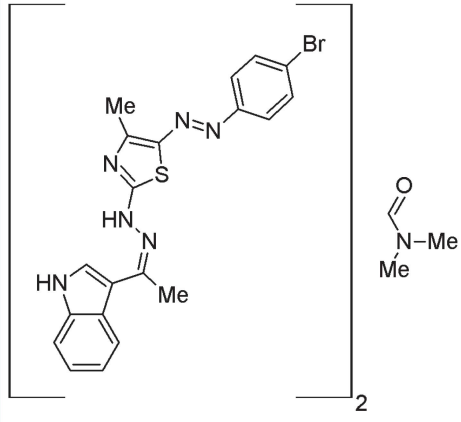
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $2C_{20}H_{17}BrN_6S\cdot C_3H_7NO$, comprises two molecules of the thiazole derivative and one molecule of dimethylformamide (DMF) solvent. The twist angles between the planes through the bromophenyl, methylthiazolyl and indolyl groups are 10.1 (1) and 44.2 (1)°, respectively, for one molecule and 11.3 (1) and 1.6 (1)° for the other. In the crystal, N—H···N hydrogen bonds link four of the main molecules into tetramers. N—H···O bonds involving the DMF solvent molecule also occur.

3D view



Chemical scheme



Structure description

Heterocycles containing both thiazole and indole moieties have various biological activities (Gu *et al.*, 1999; Guggilapu *et al.*, 2017; Tantak *et al.*, 2017; Vaddula *et al.*, 2016). The crystal structure reported here was obtained as part of a study of this class of compounds.

The asymmetric unit of the title compound comprises two molecules of the thiazole $C_{20}H_{17}BrN_6S$, and one molecule of dimethylformamide (DMF) solvent (Fig. 1). The twist angles between the planes through the bromophenyl, methylthiazolyl and indolyl groups are 10.1 (1)° and 44.2 (1)° respectively for one molecule (C1–C20) and 11.3 (1)° and 1.6 (1)° for the other (C21–C40). N—H···N hydrogen-bonding contacts form rings of

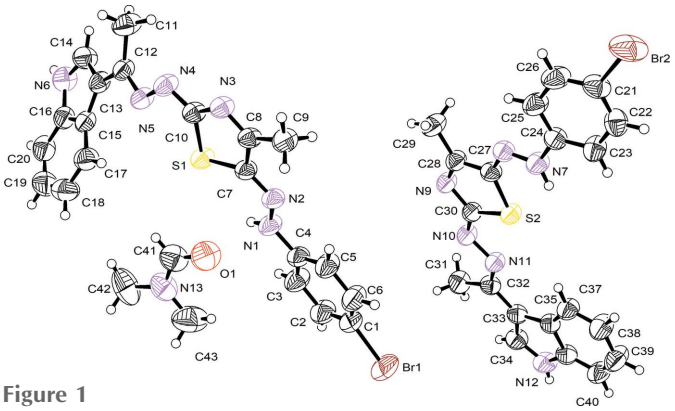


Figure 1
An *ORTEP* representation of the asymmetric unit showing 50% probability ellipsoids.

four molecules within the crystal (Table 1, Fig. 2) with two of the molecules also forming N—H···O hydrogen bonds with neighbouring DMF solvent molecules.

Synthesis and crystallization

The title compound was synthesized by the reaction of 2-[1-(1*H*-indol-3-yl)ethylidene]hydrazinecarbothioamide and *N*′-(4-bromophenyl)-2-oxopropanehydrazonoyl chloride in refluxing ethanol (4 h) containing triethylamine as a base. Crystallization of the crude product using dimethylformamide as solvent gave colourless crystals (65%), m.p. 260°C (lit m.p. 260–261°C; Abdel-Gawad *et al.*, 2010).

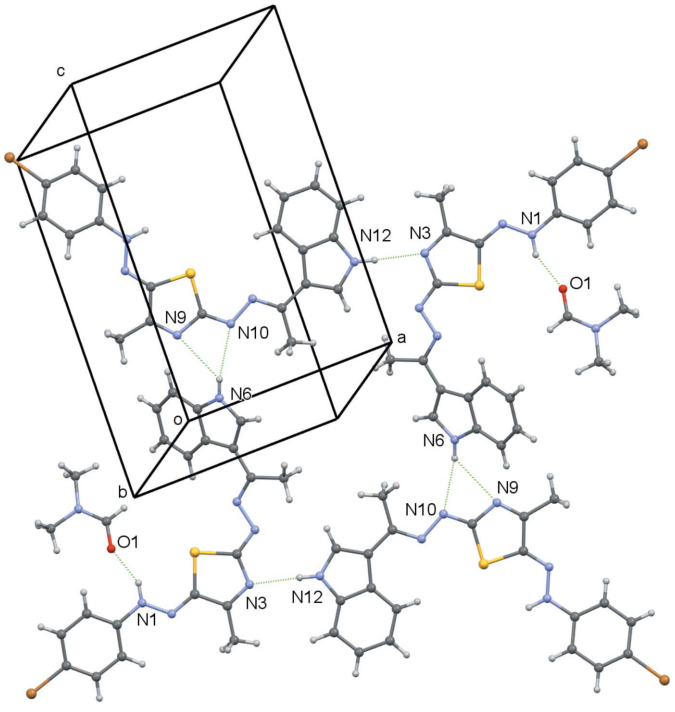


Figure 2
A segment of the crystal structure showing hydrogen-bonding contacts as dotted lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.86	2.08	2.782 (4)	138
N6—H6*A*···N9^{i}	0.86	2.62	3.292 (4)	136
N6—H6*A*···N10^{i}	0.86	2.42	3.234 (4)	159
N12—H12···N3^{ii}	0.86	2.15	3.011 (4)	177

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$2C_{20}H_{17}BrN_6S\cdot C_3H_7NO$
M_r	979.83
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, *b*, *c* (Å)	9.9957 (6), 14.5325 (9), 15.8353 (10)
α, β, γ (°)	81.671 (5), 81.344 (5), 80.469 (5)
V (Å^3)	2225.7 (2)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	1.97
Crystal size (mm)	0.25 × 0.09 × 0.04
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.827, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19885, 10602, 5116
R_{int}	0.036
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.701
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.056, 0.145, 1.01
No. of reflections	10602
No. of parameters	556
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.49, −0.57

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

MHA thanks King Abdulaziz City for Science and Technology (KACST), Saudi Arabia for financial support (award No. 020–0180).

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full crystallographic data

IUCrData (2018). **3**, x181378 [https://doi.org/10.1107/S2414314618013780]

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Crystal data

$2C_{20}H_{17}BrN_6S·C_3H_7NO$
M_r = 979.83
Triclinic, $P\overline{1}$
a = 9.9957 (6) Å
b = 14.5325 (9) Å
c = 15.8353 (10) Å
α = 81.671 (5)°
β = 81.344 (5)°
γ = 80.469 (5)°
V = 2225.7 (2) Å^3
Z = 2
$F(000)$ = 1000
D_x = 1.462 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3549 reflections
θ = 3.3–24.0°
μ = 1.97 mm^{-1}
T = 293 K
Needle, colourless
0.25 × 0.09 × 0.04 mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas diffractometer
ω scans
Absorption correction: gaussian (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.827, T_{max} = 1.000
19885 measured reflections
10602 independent reflections
5116 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 29.9°, θ_{min} = 1.3°
h = −12→12
k = −18→17
l = −20→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.145
S = 1.01
10602 reflections
556 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2 + 0.5647P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

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}
C1	0.3683 (4)	0.4890 (3)	0.2966 (3)	0.0661 (11)
C2	0.3605 (4)	0.5387 (3)	0.2167 (3)	0.0725 (12)
H2	0.439015	0.542822	0.177384	0.087*
C3	0.2340 (4)	0.5828 (3)	0.1951 (3)	0.0690 (12)
H3	0.227696	0.616794	0.141065	0.083*
C4	0.1170 (3)	0.5764 (3)	0.2536 (2)	0.0553 (10)
C5	0.1270 (4)	0.5278 (3)	0.3346 (2)	0.0686 (12)
H5	0.049302	0.524021	0.374718	0.082*
C6	0.2539 (4)	0.4849 (3)	0.3554 (3)	0.0755 (13)
H6	0.261508	0.452795	0.410069	0.091*
C7	−0.2388 (3)	0.6543 (3)	0.2642 (2)	0.0503 (9)
C8	−0.3603 (3)	0.6609 (3)	0.3284 (2)	0.0500 (9)
C9	−0.3516 (4)	0.6225 (3)	0.4198 (2)	0.0662 (11)
H9A	−0.296376	0.657467	0.443928	0.099*
H9B	−0.310921	0.557619	0.423143	0.099*
H9C	−0.441742	0.627509	0.451411	0.099*
C10	−0.4547 (3)	0.7334 (3)	0.2135 (2)	0.0503 (9)
C11	−0.7037 (4)	0.9302 (3)	0.0909 (3)	0.0775 (13)
H11A	−0.787420	0.911240	0.081728	0.116*
H11B	−0.702207	0.994822	0.067657	0.116*
H11C	−0.697737	0.922945	0.151532	0.116*
C12	−0.5837 (3)	0.8696 (3)	0.0466 (2)	0.0532 (9)
C13	−0.5446 (3)	0.8901 (3)	−0.0446 (2)	0.0527 (9)
C14	−0.5892 (4)	0.9712 (3)	−0.0958 (2)	0.0653 (11)
H14	−0.649707	1.021779	−0.076243	0.078*
C15	−0.4560 (3)	0.8309 (3)	−0.1020 (2)	0.0529 (9)
C16	−0.4509 (4)	0.8814 (3)	−0.1848 (2)	0.0582 (10)
C17	−0.3895 (4)	0.7384 (3)	−0.0925 (3)	0.0678 (11)
H17	−0.389359	0.703829	−0.038236	0.081*
C18	−0.3240 (4)	0.6987 (3)	−0.1647 (3)	0.0839 (14)
H18	−0.281517	0.636563	−0.159192	0.101*
C19	−0.3210 (4)	0.7514 (4)	−0.2458 (3)	0.0817 (14)
H19	−0.275533	0.723225	−0.293336	0.098*
C20	−0.3824 (4)	0.8428 (4)	−0.2583 (3)	0.0717 (12)
H20	−0.378876	0.877400	−0.312612	0.086*
C21	0.0369 (4)	0.8433 (3)	0.8874 (2)	0.0685 (12)
C22	0.1724 (4)	0.8075 (3)	0.8889 (3)	0.0677 (11)
H22	0.205456	0.785496	0.941102	0.081*
C23	0.2595 (4)	0.8043 (3)	0.8127 (2)	0.0627 (11)

H23	0.351116	0.778949	0.813263	0.075*
C24	0.2104 (4)	0.8386 (3)	0.7357 (2)	0.0562 (10)
C25	0.0725 (4)	0.8708 (3)	0.7344 (3)	0.0693 (12)
H25	0.038463	0.891244	0.682330	0.083*
C26	−0.0152 (4)	0.8725 (3)	0.8116 (3)	0.0752 (13)
H26	−0.108272	0.893379	0.811442	0.090*
C27	0.3534 (3)	0.8933 (3)	0.5193 (2)	0.0514 (9)
C28	0.3153 (3)	0.9414 (3)	0.4369 (2)	0.0540 (9)
C29	0.1725 (4)	0.9861 (3)	0.4279 (3)	0.0703 (12)
H29A	0.147110	1.035898	0.463550	0.105*
H29B	0.111992	0.939995	0.445346	0.105*
H29C	0.166113	1.011312	0.368891	0.105*
C30	0.5383 (3)	0.9026 (3)	0.3979 (2)	0.0514 (9)
C31	0.8812 (4)	0.8946 (3)	0.2322 (2)	0.0685 (12)
H31A	0.843492	0.855589	0.200746	0.103*
H31B	0.974539	0.898512	0.208218	0.103*
H31C	0.829083	0.956467	0.228339	0.103*
C32	0.8760 (4)	0.8529 (3)	0.3249 (2)	0.0523 (9)
C33	1.0005 (3)	0.8060 (3)	0.3569 (2)	0.0526 (9)
C34	1.1291 (4)	0.7972 (3)	0.3090 (2)	0.0624 (11)
H34	1.147138	0.821149	0.251346	0.075*
C35	1.0228 (3)	0.7596 (3)	0.4419 (2)	0.0507 (9)
C36	1.1629 (3)	0.7248 (3)	0.4387 (2)	0.0571 (10)
C37	0.9387 (4)	0.7430 (3)	0.5204 (2)	0.0646 (11)
H37	0.845420	0.765264	0.525577	0.077*
C38	0.9978 (4)	0.6929 (3)	0.5895 (3)	0.0821 (15)
H38	0.943053	0.681269	0.641737	0.099*
C39	1.1368 (4)	0.6592 (4)	0.5834 (3)	0.0864 (15)
H39	1.172934	0.625797	0.631515	0.104*
C40	1.2216 (4)	0.6739 (3)	0.5084 (3)	0.0726 (12)
H40	1.314643	0.650980	0.504184	0.087*
C41	0.0191 (5)	0.6113 (3)	−0.0223 (3)	0.0853 (14)
H41	−0.068023	0.636238	−0.035812	0.102*
C42	0.0817 (7)	0.5992 (4)	−0.1745 (3)	0.119 (2)
H42A	−0.012251	0.626721	−0.175802	0.178*
H42B	0.096583	0.539015	−0.195353	0.178*
H42C	0.139772	0.639613	−0.210323	0.178*
C43	0.2499 (6)	0.5465 (4)	−0.0693 (4)	0.127 (2)
H43A	0.311572	0.591228	−0.090221	0.191*
H43B	0.278569	0.491202	−0.097807	0.191*
H43C	0.250381	0.529812	−0.008373	0.191*
N1	−0.0093 (3)	0.6186 (2)	0.22832 (19)	0.0587 (8)
H1	−0.015244	0.643112	0.175984	0.070*
N2	−0.1210 (3)	0.6202 (2)	0.28697 (18)	0.0538 (8)
N3	−0.4736 (3)	0.7028 (2)	0.30121 (17)	0.0531 (8)
N4	−0.5533 (3)	0.7801 (2)	0.17471 (18)	0.0578 (8)
N5	−0.5105 (3)	0.7997 (2)	0.08630 (18)	0.0556 (8)
N6	−0.5323 (3)	0.9668 (2)	−0.1789 (2)	0.0667 (9)

H6A	−0.545184	1.010379	−0.220975	0.080*
N7	0.3037 (3)	0.8407 (2)	0.66017 (18)	0.0615 (9)
H7	0.386501	0.813022	0.661312	0.074*
N8	0.2636 (3)	0.8859 (2)	0.58613 (19)	0.0547 (8)
N9	0.4131 (3)	0.9447 (2)	0.37360 (18)	0.0552 (8)
N10	0.6473 (3)	0.9013 (2)	0.34273 (18)	0.0553 (8)
N11	0.7640 (3)	0.8559 (2)	0.37912 (17)	0.0543 (8)
N12	1.2240 (3)	0.7495 (2)	0.3570 (2)	0.0676 (9)
H12	1.309808	0.736557	0.339169	0.081*
N13	0.1136 (4)	0.5873 (3)	−0.0864 (2)	0.0866 (12)
O1	0.0371 (4)	0.6034 (3)	0.0529 (2)	0.1044 (12)
S1	−0.28472 (9)	0.70423 (7)	0.16186 (5)	0.0551 (3)
S2	0.53169 (9)	0.85338 (7)	0.50777 (6)	0.0563 (3)
Br1	0.53923 (5)	0.42261 (4)	0.32500 (4)	0.0973 (2)
Br2	−0.07975 (6)	0.84842 (4)	0.99418 (3)	0.1142 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.044 (2)	0.079 (3)	0.075 (3)	0.004 (2)	−0.0138 (19)	−0.018 (2)
C2	0.046 (2)	0.094 (3)	0.073 (3)	−0.002 (2)	−0.0002 (19)	−0.013 (2)
C3	0.048 (2)	0.089 (3)	0.061 (2)	0.000 (2)	−0.0017 (18)	0.003 (2)
C4	0.043 (2)	0.066 (3)	0.054 (2)	0.0027 (18)	−0.0023 (16)	−0.0114 (18)
C5	0.049 (2)	0.098 (3)	0.053 (2)	0.001 (2)	−0.0032 (17)	−0.005 (2)
C6	0.062 (3)	0.095 (3)	0.065 (3)	0.002 (2)	−0.016 (2)	−0.002 (2)
C7	0.045 (2)	0.057 (2)	0.045 (2)	0.0013 (17)	−0.0023 (15)	−0.0073 (16)
C8	0.046 (2)	0.055 (2)	0.042 (2)	0.0010 (17)	0.0028 (15)	−0.0020 (16)
C9	0.062 (2)	0.085 (3)	0.042 (2)	0.007 (2)	−0.0015 (17)	−0.0022 (19)
C10	0.0437 (19)	0.058 (2)	0.044 (2)	−0.0044 (17)	0.0026 (15)	−0.0010 (16)
C11	0.063 (3)	0.092 (3)	0.060 (3)	0.015 (2)	0.0027 (19)	0.006 (2)
C12	0.046 (2)	0.063 (3)	0.048 (2)	−0.0009 (18)	−0.0086 (16)	−0.0009 (18)
C13	0.050 (2)	0.062 (3)	0.042 (2)	−0.0020 (18)	−0.0095 (15)	0.0040 (17)
C14	0.071 (3)	0.070 (3)	0.049 (2)	0.002 (2)	−0.0030 (19)	−0.0037 (19)
C15	0.0446 (19)	0.064 (3)	0.048 (2)	−0.0047 (18)	−0.0088 (15)	−0.0014 (18)
C16	0.051 (2)	0.076 (3)	0.048 (2)	−0.010 (2)	−0.0048 (17)	−0.0084 (19)
C17	0.062 (2)	0.074 (3)	0.064 (3)	0.000 (2)	−0.006 (2)	−0.009 (2)
C18	0.075 (3)	0.084 (3)	0.087 (4)	0.008 (3)	−0.002 (2)	−0.023 (3)
C19	0.064 (3)	0.111 (4)	0.069 (3)	−0.010 (3)	0.010 (2)	−0.033 (3)
C20	0.061 (2)	0.102 (4)	0.053 (3)	−0.019 (3)	−0.0021 (19)	−0.012 (2)
C21	0.075 (3)	0.067 (3)	0.052 (2)	−0.004 (2)	0.014 (2)	−0.003 (2)
C22	0.073 (3)	0.078 (3)	0.052 (2)	−0.018 (2)	−0.006 (2)	−0.004 (2)
C23	0.048 (2)	0.085 (3)	0.054 (2)	−0.017 (2)	−0.0049 (17)	0.000 (2)
C24	0.050 (2)	0.067 (3)	0.048 (2)	−0.0084 (19)	0.0041 (16)	−0.0063 (18)
C25	0.055 (2)	0.084 (3)	0.058 (2)	0.007 (2)	−0.0014 (18)	0.001 (2)
C26	0.055 (2)	0.088 (3)	0.066 (3)	0.008 (2)	0.010 (2)	0.002 (2)
C27	0.0433 (19)	0.059 (2)	0.049 (2)	−0.0037 (17)	0.0014 (15)	−0.0069 (17)
C28	0.045 (2)	0.062 (3)	0.054 (2)	−0.0048 (18)	−0.0076 (17)	−0.0051 (18)
C29	0.047 (2)	0.085 (3)	0.072 (3)	0.000 (2)	−0.0087 (19)	0.003 (2)

C30	0.047 (2)	0.061 (2)	0.042 (2)	−0.0024 (18)	−0.0027 (15)	−0.0036 (17)
C31	0.059 (2)	0.091 (3)	0.050 (2)	−0.012 (2)	0.0064 (17)	−0.002 (2)
C32	0.050 (2)	0.056 (2)	0.048 (2)	−0.0083 (17)	0.0035 (16)	−0.0056 (17)
C33	0.0415 (19)	0.063 (3)	0.051 (2)	−0.0071 (17)	0.0041 (15)	−0.0095 (18)
C34	0.050 (2)	0.077 (3)	0.054 (2)	−0.007 (2)	0.0087 (18)	−0.007 (2)
C35	0.0411 (19)	0.062 (2)	0.048 (2)	−0.0073 (17)	0.0018 (15)	−0.0093 (17)
C36	0.042 (2)	0.070 (3)	0.056 (2)	−0.0045 (18)	0.0043 (17)	−0.0122 (19)
C37	0.044 (2)	0.088 (3)	0.055 (2)	0.002 (2)	0.0014 (17)	−0.005 (2)
C38	0.054 (2)	0.127 (4)	0.053 (3)	0.002 (3)	0.0039 (19)	0.002 (2)
C39	0.057 (3)	0.122 (4)	0.070 (3)	0.008 (3)	−0.013 (2)	0.004 (3)
C40	0.046 (2)	0.094 (3)	0.072 (3)	0.007 (2)	−0.007 (2)	−0.012 (2)
C41	0.099 (4)	0.082 (3)	0.069 (3)	−0.011 (3)	0.001 (3)	−0.005 (3)
C42	0.177 (6)	0.129 (5)	0.061 (3)	−0.060 (4)	−0.002 (3)	−0.019 (3)
C43	0.117 (5)	0.124 (5)	0.121 (5)	0.018 (4)	0.016 (4)	−0.023 (4)
N1	0.0427 (17)	0.076 (2)	0.0501 (18)	0.0044 (15)	−0.0012 (13)	−0.0040 (15)
N2	0.0424 (17)	0.063 (2)	0.0523 (18)	0.0013 (15)	−0.0014 (13)	−0.0090 (14)
N3	0.0461 (17)	0.064 (2)	0.0405 (17)	0.0002 (15)	0.0037 (12)	0.0017 (14)
N4	0.0459 (17)	0.072 (2)	0.0462 (18)	0.0031 (16)	−0.0017 (13)	0.0045 (15)
N5	0.0464 (16)	0.069 (2)	0.0433 (17)	0.0012 (15)	−0.0023 (13)	0.0034 (14)
N6	0.078 (2)	0.067 (2)	0.048 (2)	−0.0081 (19)	−0.0084 (16)	0.0102 (15)
N7	0.0465 (17)	0.082 (2)	0.0475 (19)	−0.0003 (16)	0.0031 (13)	−0.0008 (16)
N8	0.0475 (17)	0.064 (2)	0.0500 (19)	−0.0058 (15)	0.0004 (14)	−0.0064 (15)
N9	0.0444 (17)	0.070 (2)	0.0475 (18)	−0.0042 (15)	−0.0061 (13)	0.0009 (15)
N10	0.0461 (17)	0.071 (2)	0.0439 (17)	−0.0053 (15)	−0.0013 (13)	0.0015 (14)
N11	0.0433 (16)	0.072 (2)	0.0419 (16)	−0.0020 (15)	0.0003 (13)	−0.0008 (14)
N12	0.0408 (17)	0.088 (3)	0.065 (2)	−0.0022 (17)	0.0134 (15)	−0.0103 (18)
N13	0.105 (3)	0.092 (3)	0.060 (2)	−0.019 (2)	0.004 (2)	−0.011 (2)
O1	0.112 (3)	0.133 (3)	0.055 (2)	0.007 (2)	−0.0013 (17)	−0.0048 (19)
S1	0.0430 (5)	0.0724 (7)	0.0417 (5)	0.0009 (4)	0.0030 (4)	0.0005 (4)
S2	0.0450 (5)	0.0737 (7)	0.0425 (5)	0.0020 (5)	−0.0005 (4)	0.0007 (4)
Br1	0.0541 (3)	0.1219 (5)	0.1132 (4)	0.0158 (3)	−0.0292 (3)	−0.0197 (3)
Br2	0.1249 (5)	0.1113 (5)	0.0695 (3)	0.0243 (4)	0.0413 (3)	0.0070 (3)

Geometric parameters (Å, º)

C1—C6	1.365 (6)	C25—H25	0.9300
C1—C2	1.369 (6)	C26—H26	0.9300
C1—Br1	1.901 (3)	C27—N8	1.284 (4)
C2—C3	1.387 (5)	C27—C28	1.461 (5)
C2—H2	0.9300	C27—S2	1.771 (3)
C3—C4	1.384 (5)	C28—N9	1.292 (4)
C3—H3	0.9300	C28—C29	1.485 (5)
C4—C5	1.382 (5)	C29—H29A	0.9600
C4—N1	1.398 (4)	C29—H29B	0.9600
C5—C6	1.382 (5)	C29—H29C	0.9600
C5—H5	0.9300	C30—N10	1.290 (4)
C6—H6	0.9300	C30—N9	1.382 (4)
C7—N2	1.283 (4)	C30—S2	1.778 (3)

C7—C8	1.461 (4)	C31—C32	1.501 (5)
C7—S1	1.771 (3)	C31—H31A	0.9600
C8—N3	1.297 (4)	C31—H31B	0.9600
C8—C9	1.484 (5)	C31—H31C	0.9600
C9—H9A	0.9600	C32—N11	1.303 (4)
C9—H9B	0.9600	C32—C33	1.443 (5)
C9—H9C	0.9600	C33—C34	1.387 (5)
C10—N4	1.284 (4)	C33—C35	1.447 (5)
C10—N3	1.390 (4)	C34—N12	1.344 (5)
C10—S1	1.783 (3)	C34—H34	0.9300
C11—C12	1.510 (5)	C35—C36	1.404 (5)
C11—H11A	0.9600	C35—C37	1.406 (5)
C11—H11B	0.9600	C36—N12	1.370 (5)
C11—H11C	0.9600	C36—C40	1.388 (5)
C12—N5	1.292 (4)	C37—C38	1.378 (5)
C12—C13	1.441 (5)	C37—H37	0.9300
C13—C14	1.379 (5)	C38—C39	1.389 (5)
C13—C15	1.442 (5)	C38—H38	0.9300
C14—N6	1.358 (5)	C39—C40	1.363 (6)
C14—H14	0.9300	C39—H39	0.9300
C15—C17	1.396 (5)	C40—H40	0.9300
C15—C16	1.405 (5)	C41—O1	1.217 (5)
C16—N6	1.373 (5)	C41—N13	1.321 (6)
C16—C20	1.400 (5)	C41—H41	0.9300
C17—C18	1.382 (6)	C42—N13	1.458 (6)
C17—H17	0.9300	C42—H42A	0.9600
C18—C19	1.397 (6)	C42—H42B	0.9600
C18—H18	0.9300	C42—H42C	0.9600
C19—C20	1.367 (6)	C43—N13	1.442 (6)
C19—H19	0.9300	C43—H43A	0.9600
C20—H20	0.9300	C43—H43B	0.9600
C21—C26	1.363 (6)	C43—H43C	0.9600
C21—C22	1.370 (6)	N1—N2	1.340 (4)
C21—Br2	1.908 (4)	N1—H1	0.8600
C22—C23	1.380 (5)	N4—N5	1.403 (4)
C22—H22	0.9300	N6—H6A	0.8600
C23—C24	1.378 (5)	N7—N8	1.341 (4)
C23—H23	0.9300	N7—H7	0.8600
C24—C25	1.382 (5)	N10—N11	1.401 (4)
C24—N7	1.401 (4)	N12—H12	0.8600
C25—C26	1.394 (5)		

C6—C1—C2	120.7 (3)	C28—C27—S2	109.2 (2)
C6—C1—Br1	119.6 (3)	N9—C28—C27	116.2 (3)
C2—C1—Br1	119.7 (3)	N9—C28—C29	122.4 (3)
C1—C2—C3	119.1 (4)	C27—C28—C29	121.3 (3)
C1—C2—H2	120.4	C28—C29—H29A	109.5
C3—C2—H2	120.4	C28—C29—H29B	109.5

C4—C3—C2	120.4 (4)	H29A—C29—H29B	109.5
C4—C3—H3	119.8	C28—C29—H29C	109.5
C2—C3—H3	119.8	H29A—C29—H29C	109.5
C5—C4—C3	119.7 (3)	H29B—C29—H29C	109.5
C5—C4—N1	121.5 (3)	N10—C30—N9	120.3 (3)
C3—C4—N1	118.8 (3)	N10—C30—S2	125.4 (3)
C4—C5—C6	119.1 (4)	N9—C30—S2	114.4 (2)
C4—C5—H5	120.4	C32—C31—H31A	109.5
C6—C5—H5	120.4	C32—C31—H31B	109.5
C1—C6—C5	120.8 (4)	H31A—C31—H31B	109.5
C1—C6—H6	119.6	C32—C31—H31C	109.5
C5—C6—H6	119.6	H31A—C31—H31C	109.5
N2—C7—C8	120.3 (3)	H31B—C31—H31C	109.5
N2—C7—S1	130.1 (3)	N11—C32—C33	117.2 (3)
C8—C7—S1	109.5 (2)	N11—C32—C31	123.7 (3)
N3—C8—C7	116.5 (3)	C33—C32—C31	119.1 (3)
N3—C8—C9	122.6 (3)	C34—C33—C32	125.2 (3)
C7—C8—C9	120.8 (3)	C34—C33—C35	104.9 (3)
C8—C9—H9A	109.5	C32—C33—C35	130.0 (3)
C8—C9—H9B	109.5	N12—C34—C33	110.9 (3)
H9A—C9—H9B	109.5	N12—C34—H34	124.6
C8—C9—H9C	109.5	C33—C34—H34	124.6
H9A—C9—H9C	109.5	C36—C35—C37	117.9 (3)
H9B—C9—H9C	109.5	C36—C35—C33	107.1 (3)
N4—C10—N3	121.4 (3)	C37—C35—C33	135.0 (3)
N4—C10—S1	123.9 (3)	N12—C36—C40	128.8 (3)
N3—C10—S1	114.7 (2)	N12—C36—C35	107.7 (3)
C12—C11—H11A	109.5	C40—C36—C35	123.4 (3)
C12—C11—H11B	109.5	C38—C37—C35	118.4 (3)
H11A—C11—H11B	109.5	C38—C37—H37	120.8
C12—C11—H11C	109.5	C35—C37—H37	120.8
H11A—C11—H11C	109.5	C37—C38—C39	121.8 (4)
H11B—C11—H11C	109.5	C37—C38—H38	119.1
N5—C12—C13	116.7 (3)	C39—C38—H38	119.1
N5—C12—C11	123.7 (3)	C40—C39—C38	121.6 (4)
C13—C12—C11	119.6 (3)	C40—C39—H39	119.2
C14—C13—C12	126.1 (3)	C38—C39—H39	119.2
C14—C13—C15	105.7 (3)	C39—C40—C36	116.9 (3)
C12—C13—C15	128.2 (3)	C39—C40—H40	121.5
N6—C14—C13	110.4 (3)	C36—C40—H40	121.5
N6—C14—H14	124.8	O1—C41—N13	125.2 (5)
C13—C14—H14	124.8	O1—C41—H41	117.4
C17—C15—C16	118.6 (3)	N13—C41—H41	117.4
C17—C15—C13	134.2 (3)	N13—C42—H42A	109.5
C16—C15—C13	106.9 (3)	N13—C42—H42B	109.5
N6—C16—C20	129.0 (4)	H42A—C42—H42B	109.5
N6—C16—C15	107.9 (3)	N13—C42—H42C	109.5
C20—C16—C15	122.9 (4)	H42A—C42—H42C	109.5

C18—C17—C15	119.2 (4)	H42B—C42—H42C	109.5
C18—C17—H17	120.4	N13—C43—H43A	109.5
C15—C17—H17	120.4	N13—C43—H43B	109.5
C17—C18—C19	120.4 (4)	H43A—C43—H43B	109.5
C17—C18—H18	119.8	N13—C43—H43C	109.5
C19—C18—H18	119.8	H43A—C43—H43C	109.5
C20—C19—C18	122.6 (4)	H43B—C43—H43C	109.5
C20—C19—H19	118.7	N2—N1—C4	118.9 (3)
C18—C19—H19	118.7	N2—N1—H1	120.5
C19—C20—C16	116.3 (4)	C4—N1—H1	120.5
C19—C20—H20	121.8	C7—N2—N1	119.9 (3)
C16—C20—H20	121.8	C8—N3—C10	111.6 (3)
C26—C21—C22	121.3 (4)	C10—N4—N5	110.8 (3)
C26—C21—Br2	120.2 (3)	C12—N5—N4	115.3 (3)
C22—C21—Br2	118.4 (3)	C14—N6—C16	109.1 (3)
C21—C22—C23	119.6 (4)	C14—N6—H6A	125.5
C21—C22—H22	120.2	C16—N6—H6A	125.5
C23—C22—H22	120.2	N8—N7—C24	119.9 (3)
C24—C23—C22	119.9 (4)	N8—N7—H7	120.1
C24—C23—H23	120.1	C24—N7—H7	120.1
C22—C23—H23	120.1	C27—N8—N7	118.7 (3)
C23—C24—C25	120.0 (3)	C28—N9—C30	112.3 (3)
C23—C24—N7	118.3 (3)	C30—N10—N11	112.1 (3)
C25—C24—N7	121.7 (3)	C32—N11—N10	113.7 (3)
C24—C25—C26	119.7 (4)	C34—N12—C36	109.4 (3)
C24—C25—H25	120.2	C34—N12—H12	125.3
C26—C25—H25	120.2	C36—N12—H12	125.3
C21—C26—C25	119.3 (4)	C41—N13—C43	120.0 (4)
C21—C26—H26	120.4	C41—N13—C42	121.1 (5)
C25—C26—H26	120.4	C43—N13—C42	118.9 (4)
N8—C27—C28	121.0 (3)	C7—S1—C10	87.65 (16)
N8—C27—S2	129.7 (3)	C27—S2—C30	87.89 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.86	2.08	2.782 (4)	138
N6—H6*A*···N9^{i}	0.86	2.62	3.292 (4)	136
N6—H6*A*···N10^{i}	0.86	2.42	3.234 (4)	159
N12—H12···N3^{ii}	0.86	2.15	3.011 (4)	177

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