IUCrData

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N′-[5-Acetyl-3-(4-bromophenyl)-2,3-dihydro-1,3,4-thiadiazol-2-ylidene]-5-(1*H*-indol-3-yl)-1-phenyl-1*H*-pyrazole-3-carbohydrazide dimethylformamide monosolvate

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Keywords: crystal structure; thiadiazole; pyrazole; hydrogen bonds.

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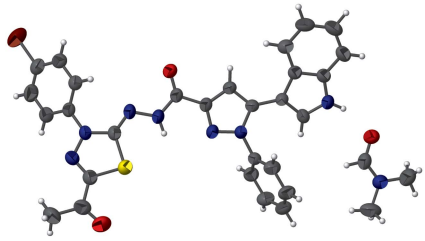
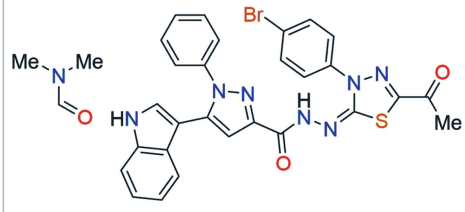
Structural data: full structural data are available from iucrdata.iucr.org

The main molecule of the title dimethylformamide monosolvate, $C_{28}H_{20}BrN_7O_2S\cdot C_3H_7NO$, comprises bromophenyl (*A*), thiadiazolyl (*B*), pyrazolyl (*C*), phenyl (*D*) and indolyl (*E*) ring systems with twist angles between the planes through neigbouring rings *A*/*B*, *B*/*C*, *C*/*D* and *C*/*E* of 33.7 (1), 14.8 (1), 60.7 (2) and 20.9 (1)°, respectively. In the crystal, the molecules are related by *c*-glide symmetry to form columns parallel to [001] which are linked by intermolecular N—H···O, C—H···O and C—H···Br contacts.

3D view



Chemical scheme



Structure description

1*H*-Pyrazole-3-carbohydrazides have been used in the synthesis of anti-nociceptive, anti-inflammatory and antipyretic agents (Malvar *et al.*, 2014). In addition, 1,3,4-thiadiazoles have different biological activities and can be used as anticancer, diuretic, antibacterial, antifungal, antitubercular and leishmanicidal agents (Dawood & Farghaly, 2017; Li *et al.*, 2013; Lv *et al.*, 2018; Serban *et al.*, 2018).

In the main molecule of the title compound (Fig. 1), the angles between planes of the bromophenyl (*A*), thiadiazolyl (*B*), pyrazolyl (*C*), phenyl (*D*) and indolyl (*E*) rings *A*/*B*, *B*/*C*, *C*/*D* and *C*/*E* are 33.7 (1), 14.8 (1), 60.7 (2) and 20.9 (1)° respectively. The molecules

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···O3^{i}	0.96	2.64	3.390 (7)	135
C16—H16···O2^{ii}	0.93	2.33	3.243 (6)	167
C30—H30B···O2^{iii}	0.96	2.59	3.409 (7)	144
C30—H30C···Br1^{ii}	0.96	3.09	3.851 (8)	137
N7—H7A···O3	0.86	1.96	2.778 (5)	158

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

are related by *c*-glide symmetry to form columns parallel to [001] which are linked by intermolecular N—H···O, C—H···O and C—H···Br contacts (Table 1, Fig. 2).

Synthesis and crystallization

The title compound was synthesized from a coupling reaction of potassium 2-(5-(1*H*-indol-3-yl)-1-phenyl-1*H*-pyrazole-3-carbonyl)hydrazinecarbodithioate and *N*′-(4-bromophenyl)-2-oxopropanehydrazonoyl chloride in boiling ethanol for 2 h. The solid obtained was collected by filtration, washed with ethanol, dried and recrystallized from dimethylformamide to give pale-yellow crystals, m.p. 207–209°C.

Refinement

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

Funding information

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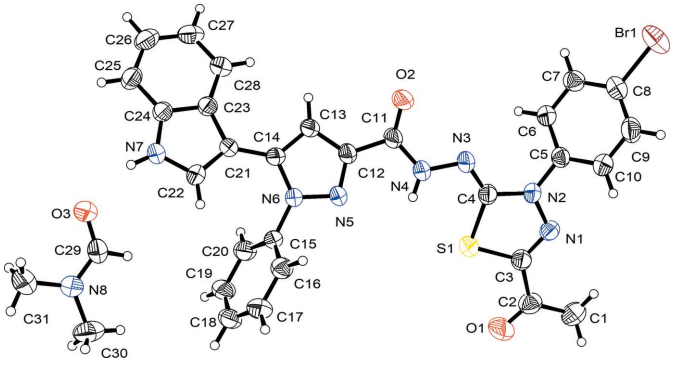

Figure 1
An *ORTEP* representation of the asymmetric unit showing 50% probability ellipsoids.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{28}H_{20}BrN_7O_2S\cdot C_3H_7NO$
M_r	671.57
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	296
a, b, c (Å)	22.5145 (11), 18.1416 (10), 7.5928 (4)
V (Å^3)	3101.3 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.44
Crystal size (mm)	0.43 × 0.08 × 0.07
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.603, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	32233, 7649, 4668
R_{int}	0.040
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.698
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.117, 1.05
No. of reflections	7649
No. of parameters	400
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.47
Absolute structure	Flack x determined using 1670 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.010 (4)

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

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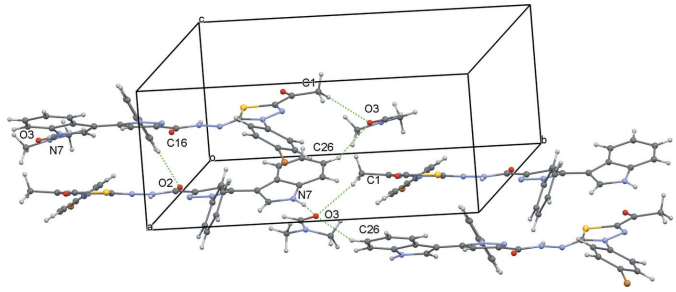

Figure 2
A segment of the crystal structure showing intermolecular contacts as dotted lines.

full crystallographic data

IUCrData (2019). **4**, x190248 [https://doi.org/10.1107/S2414314619002487]

N′-[5-Acetyl-3-(4-bromophenyl)-2,3-dihydro-1,3,4-thiadiazol-2-ylidene]-5-(1*H*-indol-3-yl)-1-phenyl-1*H*-pyrazole-3-carbohydrazide dimethylformamide monosolvate

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_N_′-[5-Acetyl-3-(4-bromophenyl)-2,3-dihydro-1,3,4-thiadiazol-2-ylidene]-5-(1*H*-indol-3-yl)-1-phenyl-1*H*-pyrazole-3-carbohydrazide dimethylformamide monosolvate

Crystal data

$C_{28}H_{20}BrN_7O_2S·C_3H_7NO$
M_r = 671.57
Orthorhombic, $Pna2_1$
a = 22.5145 (11) Å
b = 18.1416 (10) Å
c = 7.5928 (4) Å
V = 3101.3 (3) Å^3
Z = 4
F(000) = 1376
D_x = 1.438 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7129 reflections
θ = 3.6–23.5°
μ = 1.44 mm^{-1}
T = 296 K
Needle, yellow
0.43 × 0.08 × 0.07 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} = 0.603, T_{max} = 1.000
32233 measured reflections
7649 independent reflections
4668 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 29.7°, θ_{min} = 2.9°
h = −30→29
k = −25→23
l = −9→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.117
S = 1.05
7649 reflections
400 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.5275P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}
Absolute structure: Flack x determined using 1670 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.010 (4)

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. All hydrogen atoms were placed in calculated positions and refined using a riding model. Bond distances for sp^2 C—H and N—H H atoms were set to 0.93 Å and 0.83 Å respectively and their U(iso) set to 1.2 times the U_{eq}(C/N). Methyl C—H distances were set to 0.96 Å and their U(iso) to 1.5 times the U_{eq}(C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3897 (3)	0.4221 (3)	0.6408 (8)	0.0837 (16)
H1A	0.356302	0.444067	0.582081	0.126*
H1B	0.425815	0.440213	0.589650	0.126*
H1C	0.388585	0.434567	0.763603	0.126*
C2	0.3870 (2)	0.3406 (3)	0.6206 (7)	0.0667 (13)
C3	0.4422 (2)	0.2995 (2)	0.5881 (6)	0.0547 (10)
C4	0.51645 (19)	0.2049 (2)	0.5342 (5)	0.0500 (10)
C5	0.59448 (19)	0.3031 (2)	0.4890 (6)	0.0484 (9)
C6	0.64365 (19)	0.2629 (2)	0.5380 (6)	0.0541 (10)
H6	0.638893	0.219197	0.600438	0.065*
C7	0.7001 (2)	0.2871 (3)	0.4948 (6)	0.0577 (11)
H7	0.733372	0.260064	0.527992	0.069*
C8	0.7062 (2)	0.3522 (3)	0.4013 (6)	0.0602 (12)
C9	0.6574 (2)	0.3925 (3)	0.3560 (8)	0.0701 (14)
H9	0.662173	0.436579	0.295034	0.084*
C10	0.6013 (2)	0.3688 (3)	0.3995 (6)	0.0622 (12)
H10	0.568268	0.396719	0.368931	0.075*
C11	0.55267 (19)	0.0189 (2)	0.5084 (6)	0.0541 (10)
C12	0.51441 (18)	−0.0475 (2)	0.5128 (6)	0.0513 (10)
C13	0.53273 (19)	−0.1208 (2)	0.5265 (6)	0.0517 (10)
H13	0.571539	−0.137875	0.536277	0.062*
C14	0.48203 (17)	−0.1626 (2)	0.5226 (6)	0.0472 (9)
C15	0.37354 (17)	−0.1260 (2)	0.4977 (6)	0.0466 (9)
C16	0.34397 (19)	−0.1040 (2)	0.3485 (7)	0.0576 (11)
H16	0.363863	−0.078225	0.260606	0.069*
C17	0.2842 (2)	−0.1206 (3)	0.3301 (9)	0.0651 (11)
H17	0.263868	−0.105882	0.229427	0.078*
C18	0.2550 (2)	−0.1586 (3)	0.4596 (7)	0.0640 (12)
H18	0.215127	−0.170651	0.445588	0.077*
C19	0.28450 (19)	−0.1790 (3)	0.6101 (7)	0.0673 (13)
H19	0.264293	−0.203851	0.698854	0.081*
C20	0.3442 (2)	−0.1626 (3)	0.6306 (6)	0.0615 (12)
H20	0.364259	−0.176217	0.732770	0.074*
C21	0.47552 (17)	−0.2425 (2)	0.5177 (5)	0.0440 (9)
C22	0.4284 (2)	−0.2829 (2)	0.4545 (6)	0.0523 (10)
H22	0.393088	−0.262786	0.412896	0.063*

C23	0.52041 (18)	−0.2960 (2)	0.5668 (5)	0.0469 (9)
C24	0.49597 (19)	−0.3659 (2)	0.5303 (6)	0.0508 (10)
C25	0.5267 (2)	−0.4314 (3)	0.5657 (7)	0.0657 (13)
H25	0.509703	−0.477101	0.541998	0.079*
C26	0.5828 (2)	−0.4261 (3)	0.6366 (7)	0.0716 (14)
H26	0.604382	−0.468623	0.660842	0.086*
C27	0.6073 (2)	−0.3574 (3)	0.6719 (7)	0.0698 (14)
H27	0.645174	−0.354899	0.720389	0.084*
C28	0.5772 (2)	−0.2927 (3)	0.6375 (6)	0.0568 (11)
H28	0.594717	−0.247368	0.661414	0.068*
C29	0.2960 (2)	−0.4028 (3)	0.3714 (7)	0.0662 (14)
H29	0.299482	−0.353383	0.402596	0.079*
C30	0.1916 (2)	−0.3787 (3)	0.3324 (11)	0.0904 (17)
H30A	0.203331	−0.330110	0.368477	0.136*
H30B	0.163074	−0.397962	0.414266	0.136*
H30C	0.174254	−0.376465	0.217055	0.136*
C31	0.2340 (3)	−0.5018 (3)	0.2780 (10)	0.096 (2)
H31A	0.260659	−0.514233	0.183886	0.143*
H31B	0.193745	−0.508224	0.239159	0.143*
H31C	0.241467	−0.533296	0.377059	0.143*
N1	0.49317 (16)	0.32977 (19)	0.5631 (5)	0.0532 (9)
N2	0.53610 (15)	0.27826 (18)	0.5312 (5)	0.0492 (8)
N3	0.55051 (16)	0.15014 (19)	0.5048 (5)	0.0582 (9)
N4	0.52156 (17)	0.08241 (19)	0.5083 (6)	0.0643 (10)
H4	0.483382	0.081022	0.510462	0.077*
N5	0.45573 (15)	−0.04195 (19)	0.5049 (5)	0.0549 (9)
N6	0.43603 (15)	−0.11289 (17)	0.5122 (5)	0.0499 (8)
N7	0.44049 (16)	−0.35617 (19)	0.4611 (5)	0.0548 (9)
H7A	0.417057	−0.390819	0.427196	0.066*
N8	0.24315 (16)	−0.4262 (2)	0.3285 (6)	0.0628 (9)
O1	0.34070 (16)	0.3057 (2)	0.6310 (7)	0.0971 (13)
O2	0.60639 (14)	0.01563 (17)	0.5076 (5)	0.0746 (10)
O3	0.34165 (15)	−0.4403 (2)	0.3744 (5)	0.0779 (11)
S1	0.43969 (5)	0.20386 (6)	0.57886 (17)	0.0612 (3)
Br1	0.78288 (3)	0.38447 (4)	0.33102 (11)	0.0965 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.080 (4)	0.065 (3)	0.106 (4)	0.017 (3)	0.007 (3)	−0.008 (3)
C2	0.062 (3)	0.068 (3)	0.070 (3)	0.011 (3)	0.008 (2)	0.000 (2)
C3	0.056 (3)	0.052 (2)	0.056 (2)	0.000 (2)	−0.001 (2)	0.000 (2)
C4	0.053 (2)	0.044 (2)	0.053 (2)	−0.003 (2)	−0.002 (2)	0.0010 (19)
C5	0.050 (2)	0.043 (2)	0.052 (2)	−0.0047 (19)	0.0000 (19)	−0.0032 (18)
C6	0.053 (2)	0.048 (2)	0.062 (3)	−0.003 (2)	−0.002 (2)	0.0023 (19)
C7	0.053 (2)	0.059 (3)	0.062 (3)	−0.001 (2)	−0.002 (2)	−0.006 (2)
C8	0.059 (3)	0.062 (3)	0.060 (3)	−0.014 (2)	0.005 (2)	−0.003 (2)
C9	0.075 (3)	0.060 (3)	0.075 (3)	−0.014 (3)	−0.002 (3)	0.016 (2)

C10	0.062 (3)	0.052 (3)	0.073 (3)	−0.001 (2)	−0.003 (2)	0.012 (2)
C11	0.048 (2)	0.043 (2)	0.071 (3)	−0.0050 (19)	0.005 (2)	−0.013 (2)
C12	0.047 (2)	0.043 (2)	0.064 (2)	−0.0058 (18)	0.002 (2)	−0.0079 (19)
C13	0.039 (2)	0.047 (2)	0.070 (3)	−0.0007 (18)	0.003 (2)	−0.008 (2)
C14	0.039 (2)	0.046 (2)	0.057 (2)	0.0027 (18)	−0.0003 (19)	−0.0037 (19)
C15	0.040 (2)	0.042 (2)	0.058 (2)	0.0022 (17)	0.0017 (19)	−0.0025 (18)
C16	0.053 (2)	0.060 (3)	0.060 (3)	0.000 (2)	0.003 (2)	0.004 (2)
C17	0.050 (2)	0.081 (3)	0.065 (3)	0.003 (2)	−0.010 (2)	0.001 (3)
C18	0.043 (2)	0.071 (3)	0.078 (3)	−0.002 (2)	−0.002 (2)	−0.009 (3)
C19	0.044 (3)	0.075 (3)	0.083 (4)	−0.002 (2)	0.011 (2)	0.012 (3)
C20	0.050 (3)	0.069 (3)	0.066 (3)	0.003 (2)	0.002 (2)	0.012 (2)
C21	0.039 (2)	0.043 (2)	0.050 (2)	−0.0021 (17)	0.0006 (17)	−0.0002 (17)
C22	0.053 (3)	0.040 (2)	0.064 (3)	0.0024 (19)	−0.002 (2)	−0.0015 (19)
C23	0.045 (2)	0.048 (2)	0.048 (2)	0.0000 (18)	0.0043 (19)	0.0015 (19)
C24	0.048 (2)	0.047 (2)	0.058 (3)	0.0019 (19)	0.009 (2)	0.0057 (19)
C25	0.067 (3)	0.048 (2)	0.083 (3)	0.008 (2)	0.012 (3)	0.007 (2)
C26	0.069 (3)	0.064 (3)	0.082 (3)	0.022 (3)	0.011 (3)	0.011 (3)
C27	0.048 (3)	0.087 (4)	0.074 (3)	0.014 (3)	0.000 (2)	0.011 (3)
C28	0.047 (2)	0.063 (3)	0.060 (3)	0.000 (2)	0.002 (2)	0.000 (2)
C29	0.066 (3)	0.052 (3)	0.081 (4)	−0.010 (2)	0.000 (3)	−0.005 (2)
C30	0.060 (3)	0.106 (4)	0.105 (4)	0.026 (3)	0.008 (4)	0.008 (4)
C31	0.069 (3)	0.081 (4)	0.137 (6)	−0.013 (3)	−0.010 (4)	−0.021 (4)
N1	0.054 (2)	0.0465 (19)	0.060 (2)	0.0050 (17)	−0.0029 (18)	−0.0008 (17)
N2	0.051 (2)	0.0384 (17)	0.058 (2)	−0.0025 (16)	−0.0022 (17)	0.0003 (15)
N3	0.054 (2)	0.0400 (19)	0.081 (3)	−0.0071 (17)	0.0012 (19)	−0.0058 (18)
N4	0.047 (2)	0.0410 (19)	0.105 (3)	−0.0072 (17)	−0.001 (2)	−0.004 (2)
N5	0.0439 (19)	0.0415 (18)	0.079 (2)	−0.0070 (16)	0.0025 (18)	−0.0021 (17)
N6	0.0412 (19)	0.0385 (18)	0.070 (2)	−0.0014 (14)	−0.0009 (17)	0.0003 (16)
N7	0.048 (2)	0.043 (2)	0.074 (2)	−0.0066 (16)	0.0012 (18)	−0.0019 (17)
N8	0.050 (2)	0.061 (2)	0.077 (2)	0.0010 (18)	0.001 (2)	0.000 (2)
O1	0.056 (2)	0.092 (3)	0.143 (4)	−0.001 (2)	0.027 (2)	−0.005 (2)
O2	0.0462 (18)	0.0546 (18)	0.123 (3)	−0.0040 (15)	0.0031 (19)	−0.0244 (19)
O3	0.0514 (19)	0.066 (2)	0.116 (3)	0.0022 (17)	−0.0122 (19)	−0.0135 (19)
S1	0.0511 (6)	0.0541 (6)	0.0784 (7)	−0.0046 (5)	0.0081 (6)	0.0059 (6)
Br1	0.0713 (4)	0.1188 (5)	0.0994 (4)	−0.0342 (3)	0.0136 (4)	0.0080 (4)

Geometric parameters (Å, º)

C1—C2	1.487 (7)	C17—H17	0.9300
C1—H1A	0.9600	C18—C19	1.372 (7)
C1—H1B	0.9600	C18—H18	0.9300
C1—H1C	0.9600	C19—C20	1.386 (6)
C2—O1	1.222 (6)	C19—H19	0.9300
C2—C3	1.471 (6)	C20—H20	0.9300
C3—N1	1.286 (5)	C21—C22	1.376 (6)
C3—S1	1.738 (4)	C21—C23	1.449 (6)
C4—N3	1.274 (5)	C22—N7	1.357 (5)
C4—N2	1.403 (5)	C22—H22	0.9300

C4—S1	1.761 (4)	C23—C28	1.387 (6)
C5—C6	1.377 (6)	C23—C24	1.410 (6)
C5—C10	1.380 (6)	C24—N7	1.367 (5)
C5—N2	1.426 (5)	C24—C25	1.402 (6)
C6—C7	1.384 (6)	C25—C26	1.377 (7)
C6—H6	0.9300	C25—H25	0.9300
C7—C8	1.385 (7)	C26—C27	1.389 (7)
C7—H7	0.9300	C26—H26	0.9300
C8—C9	1.364 (7)	C27—C28	1.381 (7)
C8—Br1	1.898 (5)	C27—H27	0.9300
C9—C10	1.375 (7)	C28—H28	0.9300
C9—H9	0.9300	C29—O3	1.234 (6)
C10—H10	0.9300	C29—N8	1.304 (6)
C11—O2	1.211 (5)	C29—H29	0.9300
C11—N4	1.348 (5)	C30—N8	1.446 (6)
C11—C12	1.482 (6)	C30—H30A	0.9600
C12—N5	1.326 (5)	C30—H30B	0.9600
C12—C13	1.397 (6)	C30—H30C	0.9600
C13—C14	1.370 (5)	C31—N8	1.438 (7)
C13—H13	0.9300	C31—H31A	0.9600
C14—N6	1.375 (5)	C31—H31B	0.9600
C14—C21	1.458 (5)	C31—H31C	0.9600
C15—C16	1.373 (6)	N1—N2	1.366 (5)
C15—C20	1.377 (6)	N3—N4	1.391 (5)
C15—N6	1.431 (5)	N4—H4	0.8600
C16—C17	1.386 (6)	N5—N6	1.362 (5)
C16—H16	0.9300	N7—H7A	0.8600
C17—C18	1.369 (8)		

C2—C1—H1A	109.5	C15—C20—H20	120.5
C2—C1—H1B	109.5	C19—C20—H20	120.5
H1A—C1—H1B	109.5	C22—C21—C23	105.7 (3)
C2—C1—H1C	109.5	C22—C21—C14	128.0 (4)
H1A—C1—H1C	109.5	C23—C21—C14	126.1 (3)
H1B—C1—H1C	109.5	N7—C22—C21	110.7 (4)
O1—C2—C3	118.0 (4)	N7—C22—H22	124.6
O1—C2—C1	122.9 (5)	C21—C22—H22	124.6
C3—C2—C1	119.1 (5)	C28—C23—C24	118.3 (4)
N1—C3—C2	124.3 (4)	C28—C23—C21	135.5 (4)
N1—C3—S1	116.7 (3)	C24—C23—C21	106.2 (4)
C2—C3—S1	119.0 (4)	N7—C24—C25	129.3 (4)
N3—C4—N2	123.2 (4)	N7—C24—C23	108.4 (4)
N3—C4—S1	128.0 (3)	C25—C24—C23	122.2 (4)
N2—C4—S1	108.8 (3)	C26—C25—C24	117.9 (5)
C6—C5—C10	120.0 (4)	C26—C25—H25	121.0
C6—C5—N2	120.8 (4)	C24—C25—H25	121.0
C10—C5—N2	119.1 (4)	C25—C26—C27	120.2 (5)
C5—C6—C7	120.4 (4)	C25—C26—H26	119.9

C5—C6—H6	119.8	C27—C26—H26	119.9
C7—C6—H6	119.8	C28—C27—C26	122.1 (5)
C6—C7—C8	118.9 (4)	C28—C27—H27	119.0
C6—C7—H7	120.5	C26—C27—H27	119.0
C8—C7—H7	120.5	C27—C28—C23	119.3 (4)
C9—C8—C7	120.4 (4)	C27—C28—H28	120.4
C9—C8—Br1	119.7 (4)	C23—C28—H28	120.4
C7—C8—Br1	119.8 (4)	O3—C29—N8	125.7 (5)
C8—C9—C10	120.8 (5)	O3—C29—H29	117.1
C8—C9—H9	119.6	N8—C29—H29	117.1
C10—C9—H9	119.6	N8—C30—H30A	109.5
C9—C10—C5	119.4 (5)	N8—C30—H30B	109.5
C9—C10—H10	120.3	H30A—C30—H30B	109.5
C5—C10—H10	120.3	N8—C30—H30C	109.5
O2—C11—N4	124.1 (4)	H30A—C30—H30C	109.5
O2—C11—C12	122.7 (4)	H30B—C30—H30C	109.5
N4—C11—C12	113.1 (4)	N8—C31—H31A	109.5
N5—C12—C13	111.7 (4)	N8—C31—H31B	109.5
N5—C12—C11	121.1 (4)	H31A—C31—H31B	109.5
C13—C12—C11	127.2 (4)	N8—C31—H31C	109.5
C14—C13—C12	106.2 (4)	H31A—C31—H31C	109.5
C14—C13—H13	126.9	H31B—C31—H31C	109.5
C12—C13—H13	126.9	C3—N1—N2	111.4 (3)
C13—C14—N6	105.4 (3)	N1—N2—C4	115.0 (3)
C13—C14—C21	129.4 (4)	N1—N2—C5	118.4 (3)
N6—C14—C21	125.1 (3)	C4—N2—C5	126.5 (4)
C16—C15—C20	120.9 (4)	C4—N3—N4	113.8 (4)
C16—C15—N6	119.5 (4)	C11—N4—N3	120.7 (4)
C20—C15—N6	119.6 (4)	C11—N4—H4	119.6
C15—C16—C17	119.4 (5)	N3—N4—H4	119.6
C15—C16—H16	120.3	C12—N5—N6	104.5 (3)
C17—C16—H16	120.3	N5—N6—C14	112.1 (3)
C18—C17—C16	120.2 (5)	N5—N6—C15	118.3 (3)
C18—C17—H17	119.9	C14—N6—C15	129.5 (3)
C16—C17—H17	119.9	C22—N7—C24	108.9 (4)
C17—C18—C19	120.1 (4)	C22—N7—H7A	125.6
C17—C18—H18	120.0	C24—N7—H7A	125.6
C19—C18—H18	120.0	C29—N8—C31	120.6 (4)
C18—C19—C20	120.4 (4)	C29—N8—C30	122.1 (5)
C18—C19—H19	119.8	C31—N8—C30	117.3 (4)
C20—C19—H19	119.8	C3—S1—C4	88.0 (2)
C15—C20—C19	119.0 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···O3^{i}	0.96	2.64	3.390 (7)	135
C16—H16···O2^{ii}	0.93	2.33	3.243 (6)	167

C30—H30*B*···O2^{iii}	0.96	2.59	3.409 (7)	144
C30—H30*C*···Br1^{ii}	0.96	3.09	3.851 (8)	137
N7—H7*A*···O3	0.86	1.96	2.778 (5)	158

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