IUCrData

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N′-[5-Acetyl-3-(4-chlorophenyl)-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; indole; hydrogen bonds.

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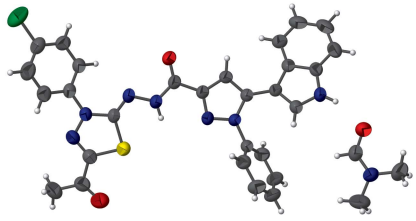
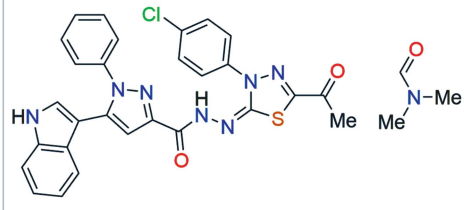
Structural data: full structural data are available from iucrdata.iucr.org

In the title solvate, $C_{28}H_{20}ClN_7O_2S\cdot C_3H_7NO$, the main molecule consists of chlorophenyl (*A*), thiadiazolyl (*B*), pyrazolyl (*C*), phenyl (*D*) and indolyl (*E*) rings, with twist angles between neighbouring rings *A*/*B*, *B*/*C*, *C*/*D* and *D*/*E* of 32.6 (1), 14.8 (1), 60.8 (1) and 20.1 (1)°, respectively. The dimethylformamide solvent molecule accepts an N—H···O hydrogen bond from the indole group. In the extended structure, molecules related by 2_1 screw axes are stacked in the [001] direction to form columns linked by weak C—H···O interactions.

3D view



Chemical scheme



Structure description

1,3,4-Thiadiazoles have various biological properties including anticancer, diuretic, antibacterial and antifungal activities (Dawood & Farghaly, 2017; Li *et al.*, 2013; Lv *et al.*, 2018; Matysiak 2015; Serban *et al.*, 2018). As part of our work in this area, we now describe the structure of the title compound.

The asymmetric unit consists of the one molecule of $C_{28}H_{20}ClN_7O_2S$ and a molecule of dimethylformamide solvent (Fig. 1). The main molecule features chlorophenyl (*A*), thiadiazolyl (*B*), pyrazolyl (*C*), phenyl (*D*) and indolyl (*E*) rings. The twist angles between the planes through the neighbouring ring pairs *A*/*B*, *B*/*C*, *C*/*D* and *D*/*E* are

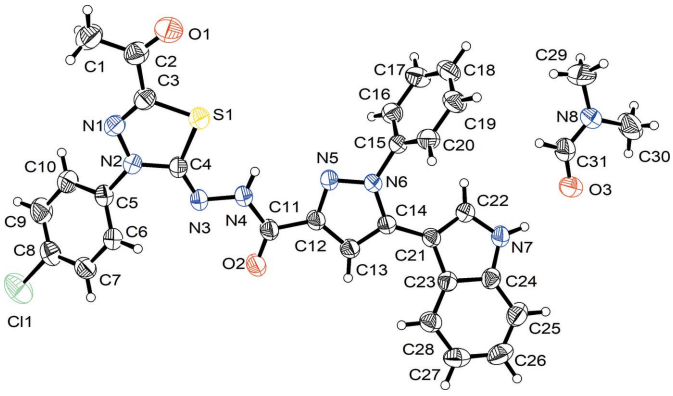


Figure 1
The molecular structure of the title compound showing 50% displacement ellipsoids.

32.6 (1), 14.8 (1), 60.8 (1) and 20.1 (1)°, respectively. The dimethylformamide solvent accepts an N—H···O hydrogen bond from the indole group. In the extended structure (Fig. 2), molecules related by a 2_1 screw axes are stacked in the [001] direction to form columns linked by weak C—H···O interactions (Table 1, Fig. 3).

Synthesis and crystallization

The title compound was synthesized as previously reported (Abdel-Gawad *et al.*, 2010) from the reaction of potassium 2-(5-(1*H*-indol-3-yl)-1-phenyl-1*H*-pyrazole-3-carbonyl)hydrazinecarbodithioate and *N*′-(4-chlorophenyl)-2-oxopropanehydrazonoyl chloride in ethanol under reflux for 2 h. The solid produced was collected by filtration, washed with ethanol,

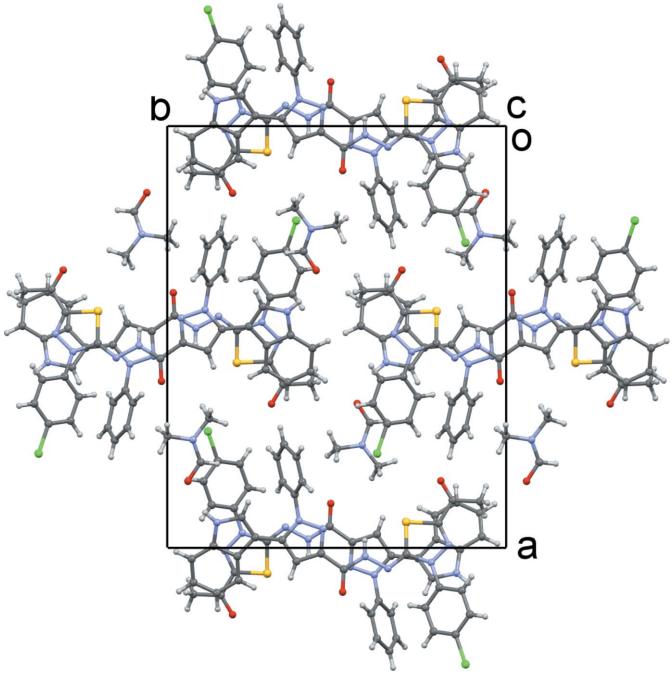


Figure 2
The crystal structure viewed down the *c*-axis direction.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N7—H7*A*···O3	0.86	1.96	2.784 (4)	159
C16—H16···O2^{i}	0.93	2.34	3.258 (5)	168

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{28}H_{20}ClN_7O_2S\cdot C_3H_7NO$
M_r	627.11
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	293
a, *b*, *c* (Å)	22.6215 (9), 18.1779 (7), 7.5064 (4)
V (Å^3)	3086.7 (2)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	0.24
Crystal size (mm)	0.55 × 0.07 × 0.03
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.680, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28180, 7744, 4455
R_{int}	0.044
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.702
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.045, 0.120, 1.01
No. of reflections	7744
No. of parameters	400
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.15, −0.22
Absolute structure	Flack *x* determined using 1442 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)
Absolute structure parameter	0.00 (3)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

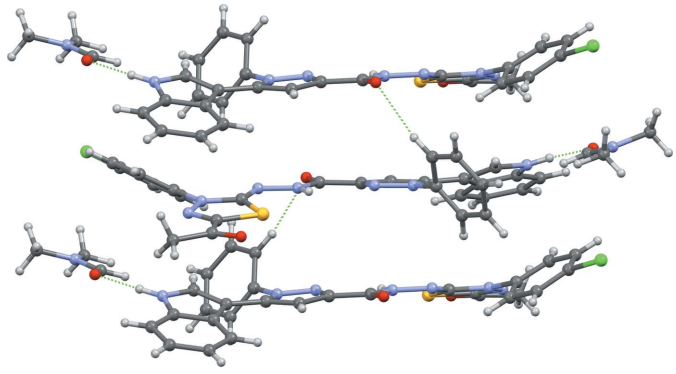


Figure 3
A segment of the crystal structure showing C—H···O contacts as dotted lines.

dried and recrystallized from dimethylformamide solution to give pale-yellow needles (m.p. 257–258°C; Abdel-Gawad *et al.*, 2010).

Refinement

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

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full crystallographic data

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N′-[5-Acetyl-3-(4-chlorophenyl)-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-chlorophenyl)-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

$C_{28}H_{20}ClN_7O_2S·C_3H_7NO$
M_r = 627.11
Orthorhombic, $Pna2_1$
a = 22.6215 (9) Å
b = 18.1779 (7) Å
c = 7.5064 (4) Å
V = 3086.7 (2) Å^3
Z = 4
F(000) = 1304
D_x = 1.349 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6090 reflections
θ = 3.2–23.1°
μ = 0.24 mm^{-1}
T = 293 K
Needle, yellow
0.55 × 0.07 × 0.03 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} = 0.680, T_{max} = 1.000
28180 measured reflections
7744 independent reflections
4455 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 29.9°, θ_{min} = 2.9°
h = −31→30
k = −18→25
l = −10→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.120
S = 1.01
7744 reflections
400 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0542P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack x determined using 1442 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)
Absolute structure parameter: 0.00 (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	0.1098 (2)	0.9233 (2)	0.8123 (8)	0.0857 (14)
H1A	0.145169	0.940879	0.868732	0.129*
H1B	0.076119	0.936566	0.883041	0.129*
H1C	0.106292	0.944924	0.696124	0.129*
C2	0.11270 (18)	0.8422 (2)	0.7952 (6)	0.0675 (11)
C3	0.05800 (16)	0.80099 (18)	0.7611 (6)	0.0567 (9)
C4	−0.01539 (14)	0.70568 (16)	0.7047 (5)	0.0488 (9)
C5	−0.09404 (14)	0.80336 (16)	0.6647 (5)	0.0506 (8)
C6	−0.14215 (14)	0.76154 (18)	0.7133 (5)	0.0555 (9)
H6	−0.136790	0.717086	0.772523	0.067*
C7	−0.19860 (15)	0.7862 (2)	0.6735 (6)	0.0619 (9)
H7	−0.231393	0.758786	0.708078	0.074*
C8	−0.20590 (17)	0.8511 (2)	0.5830 (6)	0.0679 (11)
C9	−0.15788 (19)	0.8933 (2)	0.5380 (7)	0.0776 (12)
H9	−0.163285	0.938020	0.479824	0.093*
C10	−0.10161 (18)	0.86951 (19)	0.5790 (6)	0.0673 (11)
H10	−0.068979	0.898050	0.548954	0.081*
C11	−0.05112 (14)	0.52085 (17)	0.6746 (5)	0.0539 (9)
C12	−0.01367 (13)	0.45389 (16)	0.6807 (5)	0.0516 (8)
C13	−0.03199 (13)	0.38113 (16)	0.6942 (5)	0.0506 (8)
H13	−0.070676	0.364216	0.703290	0.061*
C14	0.01868 (13)	0.33909 (16)	0.6913 (5)	0.0474 (8)
C15	0.12696 (13)	0.37600 (16)	0.6697 (5)	0.0483 (8)
C16	0.15622 (15)	0.39812 (19)	0.5195 (6)	0.0589 (9)
H16	0.136554	0.423826	0.430246	0.071*
C17	0.21581 (15)	0.3814 (2)	0.5029 (7)	0.0690 (11)
H17	0.236128	0.395727	0.400895	0.083*
C18	0.24476 (16)	0.3447 (2)	0.6329 (6)	0.0676 (11)
H18	0.284610	0.333469	0.619426	0.081*
C19	0.21521 (15)	0.3240 (2)	0.7853 (6)	0.0692 (11)
H19	0.235245	0.299127	0.875178	0.083*
C20	0.15557 (15)	0.34016 (19)	0.8050 (6)	0.0604 (10)
H20	0.135437	0.326888	0.908124	0.073*
C21	0.02495 (12)	0.25928 (16)	0.6900 (5)	0.0463 (8)
C22	0.07209 (14)	0.21870 (17)	0.6302 (5)	0.0525 (9)
H22	0.107494	0.238530	0.589491	0.063*
C23	−0.02010 (13)	0.20643 (16)	0.7389 (5)	0.0484 (8)
C24	0.00442 (14)	0.13629 (16)	0.7063 (5)	0.0522 (9)
C25	−0.02642 (17)	0.07159 (19)	0.7409 (7)	0.0699 (11)

H25	−0.009464	0.025957	0.717960	0.084*
C26	−0.08222 (19)	0.0768 (2)	0.8095 (7)	0.0757 (12)
H26	−0.103566	0.034306	0.834845	0.091*
C27	−0.10718 (17)	0.1456 (2)	0.8414 (6)	0.0709 (11)
H27	−0.145400	0.148244	0.886560	0.085*
C28	−0.07684 (15)	0.2098 (2)	0.8079 (5)	0.0583 (9)
H28	−0.094320	0.255062	0.831386	0.070*
C29	0.30679 (19)	0.1233 (3)	0.5200 (10)	0.1075 (18)
H29A	0.294325	0.171195	0.558395	0.161*
H29B	0.324845	0.126931	0.404556	0.161*
H29C	0.334853	0.103758	0.603447	0.161*
C30	0.26488 (19)	0.0004 (3)	0.4550 (8)	0.106 (2)
H30A	0.227503	−0.020796	0.422718	0.158*
H30B	0.281905	−0.027261	0.551141	0.158*
H30C	0.290980	−0.000871	0.354204	0.158*
C31	0.20302 (18)	0.0981 (2)	0.5531 (6)	0.0693 (11)
H31	0.199260	0.146797	0.589274	0.083*
N1	0.00705 (12)	0.83077 (14)	0.7353 (5)	0.0554 (7)
N2	−0.03511 (11)	0.77894 (13)	0.7037 (4)	0.0511 (7)
N3	−0.04906 (11)	0.65123 (14)	0.6751 (5)	0.0562 (8)
N4	−0.02058 (12)	0.58393 (13)	0.6786 (5)	0.0620 (8)
H4	0.017390	0.582558	0.683465	0.074*
N5	0.04496 (11)	0.45956 (13)	0.6727 (5)	0.0551 (7)
N6	0.06430 (10)	0.38905 (13)	0.6820 (4)	0.0502 (7)
N7	0.06004 (12)	0.14612 (14)	0.6385 (4)	0.0562 (8)
H7A	0.083603	0.111452	0.606301	0.067*
N8	0.25628 (13)	0.07514 (17)	0.5102 (5)	0.0706 (10)
O1	0.15870 (13)	0.80757 (17)	0.8054 (6)	0.0978 (11)
O2	−0.10500 (10)	0.51750 (12)	0.6691 (4)	0.0731 (8)
O3	0.15779 (12)	0.06068 (14)	0.5494 (5)	0.0809 (9)
S1	0.06085 (4)	0.70530 (5)	0.75099 (16)	0.0626 (3)
Cl1	−0.27630 (6)	0.88036 (9)	0.5237 (2)	0.1127 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.091 (3)	0.069 (3)	0.097 (4)	−0.017 (2)	−0.002 (3)	−0.007 (3)
C2	0.066 (2)	0.066 (2)	0.070 (3)	−0.008 (2)	−0.007 (2)	0.003 (2)
C3	0.062 (2)	0.0550 (18)	0.054 (2)	−0.0037 (17)	0.0004 (18)	0.0022 (19)
C4	0.0536 (18)	0.0422 (16)	0.051 (2)	0.0056 (14)	0.0022 (17)	0.0007 (15)
C5	0.0565 (19)	0.0464 (17)	0.049 (2)	0.0062 (16)	0.0009 (17)	−0.0025 (16)
C6	0.0573 (19)	0.0480 (17)	0.061 (3)	0.0035 (16)	0.0011 (18)	−0.0015 (17)
C7	0.0540 (18)	0.066 (2)	0.066 (3)	0.0041 (17)	0.0029 (19)	−0.009 (2)
C8	0.066 (2)	0.070 (2)	0.068 (3)	0.019 (2)	−0.003 (2)	0.002 (2)
C9	0.083 (3)	0.069 (2)	0.081 (3)	0.019 (2)	−0.002 (3)	0.023 (2)
C10	0.070 (2)	0.055 (2)	0.077 (3)	0.0043 (18)	0.005 (2)	0.013 (2)
C11	0.0506 (19)	0.0477 (18)	0.064 (2)	0.0057 (15)	−0.0025 (18)	−0.0093 (17)
C12	0.0461 (16)	0.0459 (16)	0.063 (2)	0.0030 (14)	−0.0017 (17)	−0.0093 (17)

C13	0.0431 (16)	0.0480 (17)	0.061 (2)	−0.0013 (14)	−0.0033 (17)	−0.0078 (17)
C14	0.0445 (16)	0.0442 (15)	0.054 (2)	0.0010 (13)	−0.0008 (16)	−0.0017 (16)
C15	0.0417 (15)	0.0418 (15)	0.061 (2)	−0.0003 (13)	0.0001 (17)	−0.0044 (16)
C16	0.0539 (19)	0.060 (2)	0.063 (3)	−0.0006 (17)	−0.0038 (19)	0.0059 (19)
C17	0.051 (2)	0.089 (3)	0.067 (3)	−0.001 (2)	0.008 (2)	0.005 (2)
C18	0.0440 (18)	0.078 (2)	0.081 (3)	0.0052 (19)	−0.001 (2)	−0.007 (2)
C19	0.048 (2)	0.081 (3)	0.079 (3)	0.0056 (18)	−0.008 (2)	0.011 (2)
C20	0.0514 (19)	0.066 (2)	0.063 (3)	−0.0034 (17)	−0.0002 (18)	0.010 (2)
C21	0.0416 (16)	0.0460 (15)	0.051 (2)	0.0016 (13)	−0.0033 (15)	−0.0019 (16)
C22	0.0491 (18)	0.0454 (17)	0.063 (3)	−0.0002 (15)	0.0010 (17)	−0.0017 (17)
C23	0.0470 (17)	0.0493 (16)	0.049 (2)	0.0000 (14)	−0.0082 (16)	−0.0009 (16)
C24	0.0543 (18)	0.0475 (17)	0.055 (2)	−0.0001 (15)	−0.0093 (17)	0.0039 (16)
C25	0.073 (2)	0.0526 (19)	0.084 (3)	−0.0070 (18)	−0.019 (2)	0.008 (2)
C26	0.070 (3)	0.073 (3)	0.084 (3)	−0.028 (2)	−0.013 (2)	0.016 (2)
C27	0.052 (2)	0.089 (3)	0.072 (3)	−0.017 (2)	−0.001 (2)	0.009 (2)
C28	0.0503 (19)	0.066 (2)	0.059 (3)	−0.0007 (17)	−0.0022 (17)	0.0027 (19)
C29	0.062 (2)	0.110 (4)	0.150 (5)	−0.022 (3)	−0.017 (3)	0.012 (4)
C30	0.076 (3)	0.087 (3)	0.153 (6)	0.021 (3)	0.011 (3)	−0.030 (3)
C31	0.067 (2)	0.056 (2)	0.085 (3)	0.007 (2)	0.000 (2)	−0.006 (2)
N1	0.0591 (17)	0.0492 (14)	0.058 (2)	−0.0060 (14)	0.0017 (16)	−0.0008 (15)
N2	0.0511 (15)	0.0422 (13)	0.060 (2)	0.0003 (12)	0.0016 (14)	0.0018 (13)
N3	0.0516 (15)	0.0432 (14)	0.074 (2)	0.0075 (13)	0.0011 (15)	−0.0041 (15)
N4	0.0475 (15)	0.0443 (15)	0.094 (3)	0.0061 (12)	−0.0014 (17)	−0.0041 (16)
N5	0.0467 (14)	0.0418 (13)	0.077 (2)	0.0045 (12)	−0.0045 (15)	−0.0022 (15)
N6	0.0384 (13)	0.0430 (14)	0.069 (2)	0.0023 (11)	0.0006 (14)	−0.0020 (14)
N7	0.0544 (16)	0.0423 (15)	0.072 (2)	0.0048 (12)	−0.0022 (15)	−0.0033 (14)
N8	0.0493 (17)	0.067 (2)	0.096 (3)	0.0039 (15)	−0.0039 (18)	0.0025 (19)
O1	0.0677 (17)	0.092 (2)	0.134 (3)	−0.0053 (16)	−0.0293 (19)	0.000 (2)
O2	0.0492 (14)	0.0555 (13)	0.115 (2)	0.0061 (11)	−0.0040 (15)	−0.0209 (15)
O3	0.0562 (14)	0.0685 (16)	0.118 (3)	−0.0029 (13)	0.0097 (16)	−0.0074 (17)
S1	0.0539 (5)	0.0542 (5)	0.0796 (7)	0.0026 (4)	−0.0076 (5)	0.0075 (5)
Cl1	0.0803 (7)	0.1358 (11)	0.1221 (12)	0.0411 (8)	−0.0190 (8)	0.0142 (10)

Geometric parameters (Å, º)

C1—C2	1.481 (5)	C17—H17	0.9300
C1—H1A	0.9600	C18—C19	1.378 (6)
C1—H1B	0.9600	C18—H18	0.9300
C1—H1C	0.9600	C19—C20	1.389 (5)
C2—O1	1.218 (5)	C19—H19	0.9300
C2—C3	1.469 (5)	C20—H20	0.9300
C3—N1	1.288 (4)	C21—C22	1.372 (4)
C3—S1	1.742 (3)	C21—C23	1.448 (4)
C4—N3	1.268 (4)	C22—N7	1.349 (4)
C4—N2	1.404 (4)	C22—H22	0.9300
C4—S1	1.759 (3)	C23—C28	1.385 (5)
C5—C10	1.374 (5)	C23—C24	1.412 (4)
C5—C6	1.377 (5)	C24—N7	1.369 (4)

C5—N2	1.435 (4)	C24—C25	1.392 (5)
C6—C7	1.386 (5)	C25—C26	1.366 (6)
C6—H6	0.9300	C25—H25	0.9300
C7—C8	1.372 (6)	C26—C27	1.393 (6)
C7—H7	0.9300	C26—H26	0.9300
C8—C9	1.373 (6)	C27—C28	1.377 (5)
C8—Cl1	1.737 (4)	C27—H27	0.9300
C9—C10	1.380 (6)	C28—H28	0.9300
C9—H9	0.9300	C29—N8	1.441 (5)
C10—H10	0.9300	C29—H29A	0.9600
C11—O2	1.221 (4)	C29—H29B	0.9600
C11—N4	1.339 (4)	C29—H29C	0.9600
C11—C12	1.484 (4)	C30—N8	1.434 (6)
C12—N5	1.331 (4)	C30—H30A	0.9600
C12—C13	1.390 (4)	C30—H30B	0.9600
C13—C14	1.378 (4)	C30—H30C	0.9600
C13—H13	0.9300	C31—O3	1.229 (5)
C14—N6	1.376 (4)	C31—N8	1.315 (5)
C14—C21	1.458 (4)	C31—H31	0.9300
C15—C16	1.368 (5)	N1—N2	1.361 (4)
C15—C20	1.369 (5)	N3—N4	1.383 (4)
C15—N6	1.440 (4)	N4—H4	0.8600
C16—C17	1.387 (5)	N5—N6	1.356 (4)
C16—H16	0.9300	N7—H7A	0.8600
C17—C18	1.351 (6)		

C2—C1—H1A	109.5	C15—C20—H20	120.6
C2—C1—H1B	109.5	C19—C20—H20	120.6
H1A—C1—H1B	109.5	C22—C21—C23	105.9 (3)
C2—C1—H1C	109.5	C22—C21—C14	127.8 (3)
H1A—C1—H1C	109.5	C23—C21—C14	126.2 (3)
H1B—C1—H1C	109.5	N7—C22—C21	110.7 (3)
O1—C2—C3	117.9 (3)	N7—C22—H22	124.6
O1—C2—C1	123.1 (4)	C21—C22—H22	124.6
C3—C2—C1	119.0 (4)	C28—C23—C24	117.9 (3)
N1—C3—C2	124.5 (3)	C28—C23—C21	135.9 (3)
N1—C3—S1	116.5 (3)	C24—C23—C21	106.2 (3)
C2—C3—S1	119.0 (3)	N7—C24—C25	129.8 (3)
N3—C4—N2	123.3 (3)	N7—C24—C23	107.9 (3)
N3—C4—S1	128.3 (2)	C25—C24—C23	122.3 (3)
N2—C4—S1	108.4 (2)	C26—C25—C24	118.4 (4)
C10—C5—C6	120.6 (3)	C26—C25—H25	120.8
C10—C5—N2	118.8 (3)	C24—C25—H25	120.8
C6—C5—N2	120.6 (3)	C25—C26—C27	120.1 (4)
C5—C6—C7	119.5 (3)	C25—C26—H26	120.0
C5—C6—H6	120.2	C27—C26—H26	120.0
C7—C6—H6	120.2	C28—C27—C26	121.8 (4)
C8—C7—C6	119.7 (4)	C28—C27—H27	119.1

C8—C7—H7	120.1	C26—C27—H27	119.1
C6—C7—H7	120.1	C27—C28—C23	119.5 (3)
C7—C8—C9	120.5 (4)	C27—C28—H28	120.2
C7—C8—Cl1	120.1 (3)	C23—C28—H28	120.2
C9—C8—Cl1	119.4 (3)	N8—C29—H29A	109.5
C8—C9—C10	119.9 (4)	N8—C29—H29B	109.5
C8—C9—H9	120.0	H29A—C29—H29B	109.5
C10—C9—H9	120.0	N8—C29—H29C	109.5
C5—C10—C9	119.6 (4)	H29A—C29—H29C	109.5
C5—C10—H10	120.2	H29B—C29—H29C	109.5
C9—C10—H10	120.2	N8—C30—H30A	109.5
O2—C11—N4	124.0 (3)	N8—C30—H30B	109.5
O2—C11—C12	122.0 (3)	H30A—C30—H30B	109.5
N4—C11—C12	114.0 (3)	N8—C30—H30C	109.5
N5—C12—C13	112.0 (3)	H30A—C30—H30C	109.5
N5—C12—C11	120.3 (3)	H30B—C30—H30C	109.5
C13—C12—C11	127.8 (3)	O3—C31—N8	125.6 (4)
C14—C13—C12	106.2 (3)	O3—C31—H31	117.2
C14—C13—H13	126.9	N8—C31—H31	117.2
C12—C13—H13	126.9	C3—N1—N2	111.2 (3)
N6—C14—C13	105.0 (2)	N1—N2—C4	115.6 (3)
N6—C14—C21	125.7 (3)	N1—N2—C5	118.2 (2)
C13—C14—C21	129.3 (3)	C4—N2—C5	126.1 (3)
C16—C15—C20	121.5 (3)	C4—N3—N4	114.0 (3)
C16—C15—N6	118.7 (3)	C11—N4—N3	121.1 (3)
C20—C15—N6	119.8 (3)	C11—N4—H4	119.4
C15—C16—C17	118.7 (4)	N3—N4—H4	119.4
C15—C16—H16	120.7	C12—N5—N6	104.2 (2)
C17—C16—H16	120.7	N5—N6—C14	112.6 (2)
C18—C17—C16	120.9 (4)	N5—N6—C15	118.0 (2)
C18—C17—H17	119.5	C14—N6—C15	129.2 (2)
C16—C17—H17	119.5	C22—N7—C24	109.3 (3)
C17—C18—C19	120.0 (3)	C22—N7—H7A	125.3
C17—C18—H18	120.0	C24—N7—H7A	125.3
C19—C18—H18	120.0	C31—N8—C30	119.7 (3)
C18—C19—C20	120.1 (4)	C31—N8—C29	121.4 (4)
C18—C19—H19	119.9	C30—N8—C29	118.9 (3)
C20—C19—H19	119.9	C3—S1—C4	88.20 (16)
C15—C20—C19	118.8 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N7—H7*A*···O3	0.86	1.96	2.784 (4)	159
C16—H16···O2^{i}	0.93	2.34	3.258 (5)	168

Symmetry code: (i) −*x*, −*y*+1, *z*−1/2.