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ISSN 2414-3146

5-Benzoyl-2-(5-bromo-1*H*-indol-3-yl)-4-(4-nitrophenyl)-1*H*-pyrrole-3-carbonitrile dimethyl sulfoxide monosolvate

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Received 28 December 2015
Accepted 11 April 2016

Edited by P. C. Healy, Griffith University, Australia

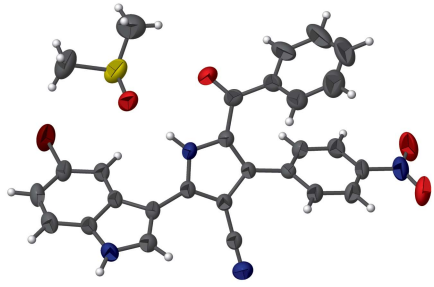
Keywords: crystal structure; indole; 1*H*-indolylpyrrole derivative; hydrogen bonding.

CCDC reference: 1473319

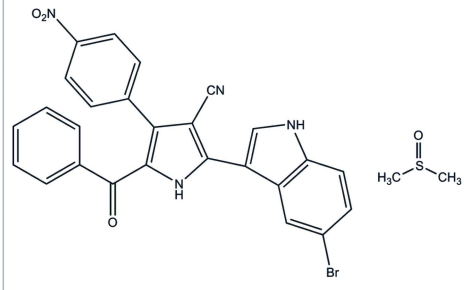
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{26}H_{15}BrN_4O_3\cdot C_2H_6OS$, contains five rings. The indole unit is essentially planar [maximum deviation = 0.0067 (1) Å for the N atom]. The central pyrrole ring makes dihedral angles of 44.1 (2) and 51.3 (2)° with the pendant indole ring system and the nitrobenzene ring, respectively. The benzene ring is inclined with the central pyrrole ring by 51.9 (3)°. In the crystal, N—H···O hydrogen-bonding interactions between aromatic-H-atom donors and sulfoxide-O-atom acceptors result in the formation of inversion dimers with an $R_4^2(16)$ ring motif. The molecules are further linked into chains running along the *c* axis by N—H···O, C—H···O and C—H···N hydrogen bonds.

3D view



Chemical scheme



Structure description

Indole derivatives are known to exhibit activities such as antitumour (Andreani *et al.*, 2001); antiviral (Kolocouris *et al.*, 1994) and anti-hepatitis C virus (Andreev *et al.*, 2015). Indoles have attracted much attention because of their wide variety of applications especially in medicinal field. Indole derivatives are used as bioactive drugs (Stevenson *et al.*, 2000) and they exhibit anti-allergic, central nervous system depressant and muscle relaxant properties (Harris & Uhle 1960; Ho *et al.*, 1986). The title compound was prepared as part of our ongoing research to synthesize and evaluate the biological activities of structural analogues of 1*H*-indolylpyrrole derivatives (Kamalraja *et al.*, 2014) and we report herein on its crystal structure.

The title compound contain 5-bromo-3-methyl-1*H*-indole connected to the 5-benzoyl-4-(4-nitrophenyl)-1*H*-pyrrole-3-carbonitrile system and a dimethyl sulfoxide solvent molecule (Fig. 1). The indole unit (N3/C19—C26) is essentially planar [maximum

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O4^{i}	0.86	2.02	2.842 (5)	161
C4—H4···N4^{ii}	0.93	2.62	3.485 (8)	155
C28—H28*C*···O1^{iii}	0.96	2.48	3.245 (9)	137
N2—H2···O4	0.86	2.03	2.876 (4)	166
C28—H28*A*···O3	0.96	2.57	3.289 (8)	132

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

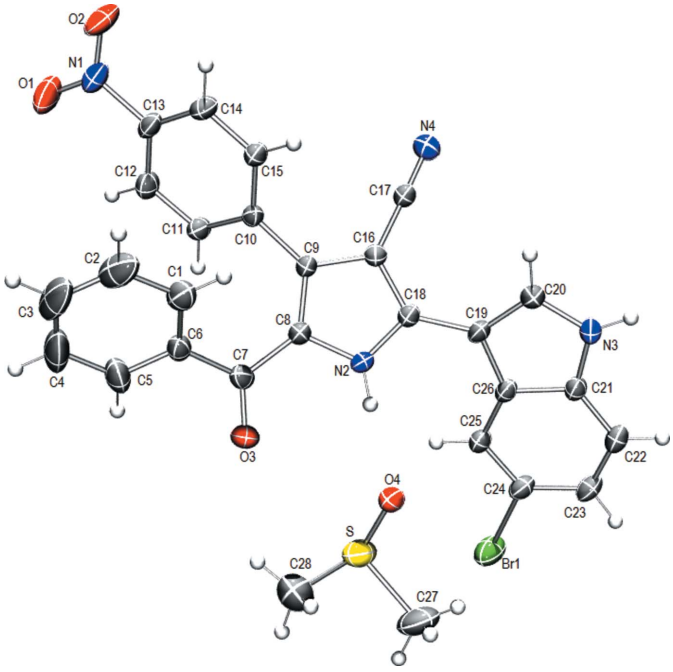


Figure 1
A view of the title compound with the atom-numbering scheme and displacement ellipsoids are drawn at 30% probability level.

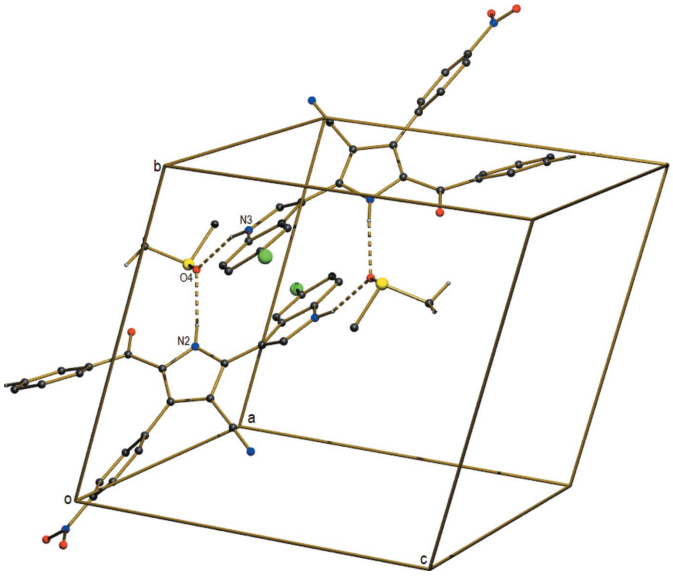


Figure 2
N—H···O interactions (dotted lines) generating an $R_4^2(16)$ ring motif.

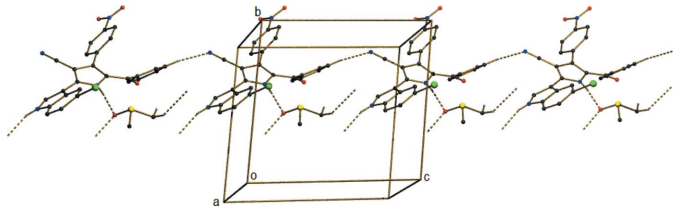


Figure 3
A partial packing view, showing hydrogen-bonded chain structure running along the *c* axis.

deviation = 0.0067 (1) Å for the N atom]. In the 2-(5-bromo-1*H*-indole-3-yl)-1*H*-pyrrole-3-carbonitrile portion, the central pyrrole ring and the pendent indole ring system make a dihedral angle of 44.1 (2)°; the torsion angles C16—C18—C19—C20 and N2—C18—C19—C26 for the link between them are 43.5 (7) and 38.6 (6)°, respectively]. The nitrobenzene and phenyl rings are inclined with the central pyrrole ring by 51.3 (2)° and 51.9 (3)°, respectively. Atoms N4 and C17 of the carbonitrile substituent deviate from the pyrrole ring plane by 0.197 (2) and 0.109 (1) Å, respectively, similar to the corresponding values in 2-amino-4-(2-naphthyl)thiophene-3-carbonitrile [0.194 (2) and 0.101 (3) Å, respectively; Çoruh *et al.*, 2005]. A similar structure, 4-(2-azido-phenyl)-5-benzoyl-2-(1*H*-indol-3-yl)-1*H*-pyrrole-3-carbonitrile is reported by Vimala *et al.* (2015).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{15}BrN_4O_3\cdot C_2H_6OS$
M_r	589.46
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, *b*, *c* (Å)	10.1721 (3), 11.2475 (3), 12.0154 (4)
α, β, γ (°)	79.638 (2), 82.454 (2), 82.371 (2)
V (Å^3)	1332.14 (7)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.66
Crystal size (mm)	0.21 × 0.19 × 0.18
Data collection	
Diffractometer	Bruker *SMART* APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.712, 0.741
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24122, 4694, 3272
R_{int}	0.037
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.059, 0.186, 1.04
No. of reflections	4694
No. of parameters	344
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.93, −0.66

Computer programs: *APEX2* (Bruker, 2008), *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

The crystal structure features a C—H···π interaction in addition to N—H···O, C—H···O and C—H···N hydrogen-bonding interactions (Table 1). The N—H···O hydrogen-bonding interactions between aromatic H-atom donors and sulfoxide-O-atom acceptors result in an $R_4^2(16)$ ring motif, as shown in Fig. 2. The molecules are further linked into chains running along [001] direction (Fig. 3).

Synthesis and crystallization

For the synthesis, see: Kamalraja *et al.* (2014). To a stirred mixture of 4-nitrobenzaldehyde 1 (1.0 mmol), 3-(5-bromo-1*H*-indol-3-yl)-3-oxopropanenitrile 2 (1.0 mmol) and phenacylazide 3 (1.0 mmol) in H_2O (3 ml), piperidine (0.25 mmol) was added at 80°C. The turbid solution slowly turned into a clear solution, followed by the formation of solid after 0.5 h. After completion of the reaction as indicated by TLC, the solid was filtered and washed with PE–EtOAc mixture (1:1 ratio, *v*/*v*, 5 ml). The compound was recrystallized by slow evaporation of an EtOH solution at room temperature to yield yellow block-shaped crystals. The yield of the isolated product was 90%.

Refinement

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

Acknowledgements

The authors thank Dr Babu Varghese, SAIF, IIT, Chennai, India, for the data collection.

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full crystallographic data

IUCrData (2016). **1**, x160597 [doi:10.1107/S2414314616005976]

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Crystal data

$C_{26}H_{15}BrN_4O_3\cdot C_2H_6OS$
M_r = 589.46
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 10.1721 (3) Å
b = 11.2475 (3) Å
c = 12.0154 (4) Å
α = 79.638 (2)°
β = 82.454 (2)°
γ = 82.371 (2)°
V = 1332.14 (7) Å^3
Z = 2
$F(000)$ = 600
D_x = 1.470 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3272 reflections
θ = 2.3–25.0°
μ = 1.66 mm^{-1}
T = 293 K
Block, yellow
0.21 × 0.19 × 0.18 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.712, T_{max} = 0.741
24122 measured reflections
4694 independent reflections
3272 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −12→12
k = −13→13
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.186
S = 1.04
4694 reflections
344 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.P)^2 + 1.7603P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.93 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0085 (18)

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. 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 $F^2 > 2\text{sigma}(F^2)$ 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}
Br1	0.49737 (5)	0.66722 (5)	0.13859 (6)	0.0800 (3)
S	0.78523 (17)	0.57068 (14)	0.37985 (14)	0.0802 (5)
N1	1.4544 (5)	1.2779 (4)	0.2474 (4)	0.0639 (11)
N2	1.0331 (3)	0.7630 (3)	0.1857 (3)	0.0427 (8)
H2	0.9831	0.7082	0.2188	0.051*
N3	1.0226 (4)	0.6139 (3)	−0.1434 (3)	0.0475 (9)
H3	1.0515	0.5781	−0.2008	0.057*
N4	1.2224 (4)	1.0041 (4)	−0.1418 (3)	0.0591 (10)
O1	1.4065 (5)	1.3381 (4)	0.3185 (4)	0.0938 (14)
O2	1.5640 (4)	1.2893 (4)	0.1934 (4)	0.0864 (12)
O3	0.9785 (4)	0.7663 (3)	0.4168 (3)	0.0694 (10)
O4	0.9070 (3)	0.5529 (3)	0.2988 (3)	0.0615 (9)
C1	1.3124 (5)	0.8293 (5)	0.3937 (4)	0.0628 (13)
H1	1.3422	0.8005	0.3259	0.075*
C2	1.4022 (7)	0.8582 (6)	0.4588 (6)	0.095 (2)
H2A	1.4933	0.8478	0.4355	0.114*
C3	1.3562 (10)	0.9028 (7)	0.5590 (7)	0.113 (3)
H3A	1.4164	0.9250	0.6014	0.135*
C4	1.2255 (11)	0.9141 (7)	0.5950 (6)	0.108 (3)
H4	1.1956	0.9428	0.6629	0.130*
C5	1.1354 (7)	0.8837 (5)	0.5322 (4)	0.0733 (16)
H5	1.0450	0.8902	0.5584	0.088*
C6	1.1786 (5)	0.8436 (4)	0.4307 (4)	0.0489 (11)
C7	1.0757 (5)	0.8122 (4)	0.3660 (3)	0.0468 (10)
C8	1.0946 (4)	0.8329 (4)	0.2412 (3)	0.0411 (9)
C9	1.1633 (4)	0.9123 (3)	0.1602 (3)	0.0371 (9)
C10	1.2376 (4)	1.0098 (3)	0.1792 (3)	0.0371 (9)
C11	1.1791 (4)	1.0927 (4)	0.2482 (4)	0.0447 (10)
H11	1.0904	1.0899	0.2787	0.054*
C12	1.2497 (5)	1.1790 (4)	0.2724 (4)	0.0512 (11)
H12	1.2106	1.2328	0.3209	0.061*
C13	1.3789 (5)	1.1843 (4)	0.2239 (4)	0.0488 (11)
C14	1.4384 (4)	1.1073 (4)	0.1515 (4)	0.0542 (12)
H14	1.5251	1.1141	0.1174	0.065*
C15	1.3672 (4)	1.0191 (4)	0.1300 (4)	0.0469 (10)

H15	1.4070	0.9654	0.0818	0.056*
C16	1.1427 (4)	0.8859 (4)	0.0530 (3)	0.0381 (9)
C17	1.1864 (4)	0.9507 (4)	−0.0557 (4)	0.0416 (9)
C18	1.0622 (4)	0.7921 (3)	0.0716 (3)	0.0388 (9)
C19	1.0173 (4)	0.7268 (4)	−0.0071 (3)	0.0419 (9)
C20	1.0932 (4)	0.6838 (4)	−0.0978 (4)	0.0477 (10)
H20	1.1801	0.7002	−0.1241	0.057*
C21	0.8990 (4)	0.6092 (3)	−0.0842 (3)	0.0404 (9)
C22	0.7946 (5)	0.5478 (4)	−0.0975 (4)	0.0499 (11)
H22	0.8037	0.4975	−0.1522	0.060*
C23	0.6783 (5)	0.5625 (4)	−0.0288 (4)	0.0531 (11)
H23	0.6070	0.5215	−0.0359	0.064*
C24	0.6658 (4)	0.6400 (4)	0.0532 (4)	0.0508 (11)
C25	0.7696 (4)	0.6980 (4)	0.0706 (4)	0.0440 (10)
H25	0.7599	0.7473	0.1262	0.053*
C26	0.8895 (4)	0.6812 (3)	0.0028 (3)	0.0391 (9)
C27	0.6901 (7)	0.4510 (7)	0.3716 (7)	0.109 (2)
H27A	0.6612	0.4623	0.2972	0.163*
H27B	0.6136	0.4520	0.4277	0.163*
H27C	0.7442	0.3743	0.3856	0.163*
C28	0.8199 (9)	0.5262 (8)	0.5162 (6)	0.112 (2)
H28A	0.8722	0.5827	0.5358	0.168*
H28B	0.8689	0.4466	0.5240	0.168*
H28C	0.7380	0.5239	0.5660	0.168*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0520 (4)	0.0853 (5)	0.1107 (6)	−0.0224 (3)	0.0108 (3)	−0.0413 (4)
S	0.0833 (10)	0.0708 (9)	0.0873 (11)	−0.0297 (8)	0.0217 (8)	−0.0221 (8)
N1	0.067 (3)	0.058 (3)	0.077 (3)	−0.020 (2)	−0.022 (2)	−0.017 (2)
N2	0.047 (2)	0.0433 (19)	0.0414 (19)	−0.0205 (15)	−0.0028 (15)	−0.0062 (15)
N3	0.052 (2)	0.053 (2)	0.042 (2)	−0.0118 (17)	−0.0029 (17)	−0.0191 (16)
N4	0.070 (3)	0.061 (2)	0.047 (2)	−0.019 (2)	0.002 (2)	−0.0079 (19)
O1	0.094 (3)	0.094 (3)	0.114 (3)	−0.028 (2)	−0.013 (3)	−0.060 (3)
O2	0.067 (3)	0.085 (3)	0.121 (3)	−0.038 (2)	−0.017 (2)	−0.026 (2)
O3	0.077 (2)	0.086 (2)	0.0494 (19)	−0.043 (2)	0.0096 (17)	−0.0105 (17)
O4	0.076 (2)	0.0576 (19)	0.0553 (19)	−0.0289 (17)	0.0117 (17)	−0.0198 (15)
C1	0.071 (3)	0.065 (3)	0.054 (3)	−0.016 (3)	−0.016 (3)	−0.001 (2)
C2	0.092 (5)	0.098 (5)	0.098 (5)	−0.037 (4)	−0.047 (4)	0.022 (4)
C3	0.151 (8)	0.111 (6)	0.095 (6)	−0.057 (6)	−0.080 (6)	0.013 (4)
C4	0.183 (9)	0.097 (5)	0.063 (4)	−0.040 (6)	−0.048 (5)	−0.017 (3)
C5	0.107 (5)	0.073 (4)	0.043 (3)	−0.012 (3)	−0.014 (3)	−0.014 (2)
C6	0.067 (3)	0.042 (2)	0.040 (2)	−0.014 (2)	−0.008 (2)	−0.0062 (18)
C7	0.058 (3)	0.041 (2)	0.042 (2)	−0.011 (2)	0.005 (2)	−0.0112 (18)
C8	0.046 (2)	0.043 (2)	0.038 (2)	−0.0145 (18)	−0.0021 (18)	−0.0089 (17)
C9	0.038 (2)	0.041 (2)	0.036 (2)	−0.0107 (17)	−0.0035 (17)	−0.0111 (16)
C10	0.044 (2)	0.038 (2)	0.032 (2)	−0.0122 (17)	−0.0060 (17)	−0.0037 (16)

C11	0.042 (2)	0.046 (2)	0.049 (2)	−0.0124 (18)	0.0027 (18)	−0.0144 (19)
C12	0.060 (3)	0.044 (2)	0.054 (3)	−0.008 (2)	−0.008 (2)	−0.017 (2)
C13	0.052 (3)	0.048 (2)	0.053 (3)	−0.020 (2)	−0.016 (2)	−0.008 (2)
C14	0.040 (2)	0.063 (3)	0.064 (3)	−0.020 (2)	0.000 (2)	−0.016 (2)
C15	0.045 (2)	0.052 (2)	0.049 (2)	−0.0155 (19)	0.0021 (19)	−0.019 (2)
C16	0.034 (2)	0.045 (2)	0.038 (2)	−0.0084 (17)	−0.0005 (16)	−0.0110 (17)
C17	0.043 (2)	0.041 (2)	0.044 (2)	−0.0109 (18)	−0.0043 (19)	−0.0113 (19)
C18	0.039 (2)	0.039 (2)	0.041 (2)	−0.0092 (17)	−0.0037 (17)	−0.0108 (17)
C19	0.047 (2)	0.038 (2)	0.045 (2)	−0.0165 (18)	−0.0060 (18)	−0.0084 (17)
C20	0.048 (2)	0.054 (3)	0.045 (2)	−0.015 (2)	−0.001 (2)	−0.0125 (19)
C21	0.047 (2)	0.036 (2)	0.041 (2)	−0.0082 (18)	−0.0084 (19)	−0.0080 (17)
C22	0.056 (3)	0.043 (2)	0.057 (3)	−0.008 (2)	−0.015 (2)	−0.016 (2)
C23	0.045 (3)	0.049 (3)	0.072 (3)	−0.014 (2)	−0.016 (2)	−0.016 (2)
C24	0.048 (3)	0.046 (2)	0.063 (3)	−0.016 (2)	−0.006 (2)	−0.012 (2)
C25	0.048 (2)	0.039 (2)	0.048 (2)	−0.0117 (18)	−0.004 (2)	−0.0129 (18)
C26	0.046 (2)	0.033 (2)	0.041 (2)	−0.0109 (17)	−0.0111 (18)	−0.0047 (16)
C27	0.102 (5)	0.107 (5)	0.124 (6)	−0.063 (4)	−0.004 (4)	−0.001 (4)
C28	0.139 (7)	0.119 (6)	0.081 (5)	−0.034 (5)	0.004 (4)	−0.021 (4)

Geometric parameters (Å, º)

C1—C2	1.382 (8)	C18—C19	1.447 (5)
C1—H1	0.9300	C19—C20	1.374 (6)
C2—C3	1.388 (11)	C20—H20	0.9300
C2—H2A	0.9300	C21—C22	1.382 (6)
C3—H3A	0.9300	C22—H22	0.9300
C4—C3	1.340 (12)	C23—C22	1.359 (6)
C4—H4	0.9300	C23—C24	1.412 (6)
C5—C4	1.372 (9)	C23—H23	0.9300
C5—H5	0.9300	C25—C24	1.369 (6)
C6—C1	1.373 (7)	C25—C26	1.386 (6)
C6—C5	1.375 (7)	C25—H25	0.9300
C7—O3	1.216 (5)	C26—C21	1.419 (5)
C7—C6	1.495 (6)	C26—C19	1.443 (5)
C8—C7	1.466 (6)	S—C27	1.782 (6)
C9—C8	1.382 (5)	C27—H27A	0.9600
C9—C16	1.421 (5)	C27—H27B	0.9600
C10—C15	1.382 (6)	C27—H27C	0.9600
C10—C11	1.383 (6)	S—O4	1.486 (4)
C10—C9	1.477 (5)	S—C28	1.693 (7)
C11—C12	1.373 (6)	C28—H28A	0.9600
C11—H11	0.9300	C28—H28B	0.9600
C12—H12	0.9300	C28—H28C	0.9600
C13—C12	1.370 (6)	N1—O1	1.199 (6)
C13—C14	1.367 (6)	N1—O2	1.225 (6)
C14—H14	0.9300	N2—C18	1.354 (5)
C13—N1	1.468 (6)	N2—C8	1.373 (5)
C15—C14	1.380 (6)	N2—H2	0.8600

C15—H15	0.9300	N3—C20	1.357 (5)
C17—N4	1.141 (5)	N3—C21	1.363 (5)
C17—C16	1.423 (6)	N3—H3	0.8600
C18—C16	1.389 (5)	Br1—C24	1.896 (5)
C18—N2—C8	110.7 (3)	C13—C12—H12	120.6
C18—N2—H2	124.7	C11—C12—H12	120.6
C8—N2—H2	124.7	O3—C7—C8	120.1 (4)
C15—C10—C11	118.7 (4)	O3—C7—C6	120.1 (4)
C15—C10—C9	120.9 (4)	C8—C7—C6	119.8 (4)
C11—C10—C9	120.4 (4)	C1—C6—C5	120.2 (5)
C8—C9—C16	106.1 (3)	C1—C6—C7	122.2 (4)
C8—C9—C10	127.7 (3)	C5—C6—C7	117.6 (5)
C16—C9—C10	126.2 (3)	C25—C24—C23	122.3 (4)
C24—C25—C26	118.0 (4)	C25—C24—Br1	119.4 (3)
C24—C25—H25	121.0	C23—C24—Br1	118.3 (3)
C26—C25—H25	121.0	C18—C16—C9	108.4 (3)
C14—C15—C10	120.8 (4)	C18—C16—C17	125.1 (3)
C14—C15—H15	119.6	C9—C16—C17	126.3 (3)
C10—C15—H15	119.6	N3—C20—C19	110.0 (4)
C20—N3—C21	109.5 (3)	N3—C20—H20	125.0
C20—N3—H3	125.2	C19—C20—H20	125.0
C21—N3—H3	125.2	C23—C22—C21	118.6 (4)
C25—C26—C21	119.4 (4)	C23—C22—H22	120.7
C25—C26—C19	134.7 (4)	C21—C22—H22	120.7
C21—C26—C19	105.8 (4)	C4—C5—C6	120.1 (7)
N4—C17—C16	178.7 (4)	C4—C5—H5	119.9
C12—C11—C10	121.0 (4)	C6—C5—H5	119.9
C12—C11—H11	119.5	C6—C1—C2	119.1 (6)
C10—C11—H11	119.5	C6—C1—H1	120.5
C14—C13—C12	121.9 (4)	C2—C1—H1	120.5
C14—C13—N1	118.9 (4)	C3—C4—C5	120.4 (7)
C12—C13—N1	119.2 (4)	C3—C4—H4	119.8
C22—C23—C24	120.0 (4)	C5—C4—H4	119.8
C22—C23—H23	120.0	C1—C2—C3	119.8 (7)
C24—C23—H23	120.0	C1—C2—H2A	120.1
C13—C14—C15	118.8 (4)	C3—C2—H2A	120.1
C13—C14—H14	120.6	C4—C3—C2	120.4 (6)
C15—C14—H14	120.6	C4—C3—H3A	119.8
N2—C8—C9	108.1 (3)	C2—C3—H3A	119.8
N2—C8—C7	118.1 (3)	O4—S—C28	110.9 (3)
C9—C8—C7	133.8 (4)	O4—S—C27	104.9 (3)
N2—C18—C16	106.8 (3)	C28—S—C27	98.1 (4)
N2—C18—C19	122.1 (3)	S—C28—H28A	109.5
C16—C18—C19	131.1 (4)	S—C28—H28B	109.5
C20—C19—C26	106.5 (3)	H28A—C28—H28B	109.5
C20—C19—C18	126.5 (4)	S—C28—H28C	109.5
C26—C19—C18	126.6 (4)	H28A—C28—H28C	109.5

N3—C21—C22	130.4 (4)	H28B—C28—H28C	109.5
N3—C21—C26	108.1 (3)	S—C27—H27A	109.5
C22—C21—C26	121.5 (4)	S—C27—H27B	109.5
O1—N1—O2	123.6 (4)	H27A—C27—H27B	109.5
O1—N1—C13	118.7 (5)	S—C27—H27C	109.5
O2—N1—C13	117.7 (4)	H27A—C27—H27C	109.5
C13—C12—C11	118.8 (4)	H27B—C27—H27C	109.5

C15—C10—C9—C8	129.3 (5)	C12—C13—N1—O2	−172.1 (4)
C11—C10—C9—C8	−49.7 (6)	C14—C13—C12—C11	0.7 (7)
C15—C10—C9—C16	−54.2 (6)	N1—C13—C12—C11	178.8 (4)
C11—C10—C9—C16	126.7 (4)	C10—C11—C12—C13	2.1 (7)
C11—C10—C15—C14	1.7 (6)	N2—C8—C7—O3	−23.4 (6)
C9—C10—C15—C14	−177.4 (4)	C9—C8—C7—O3	155.8 (5)
C24—C25—C26—C21	2.5 (6)	N2—C8—C7—C6	154.5 (4)
C24—C25—C26—C19	178.4 (4)	C9—C8—C7—C6	−26.3 (7)
C15—C10—C11—C12	−3.2 (6)	O3—C7—C6—C1	142.4 (5)
C9—C10—C11—C12	175.8 (4)	C8—C7—C6—C1	−35.4 (6)
C12—C13—C14—C15	−2.2 (7)	O3—C7—C6—C5	−35.1 (6)
N1—C13—C14—C15	179.7 (4)	C8—C7—C6—C5	147.0 (4)
C10—C15—C14—C13	1.0 (7)	C26—C25—C24—C23	1.4 (7)
C18—N2—C8—C9	1.5 (5)	C26—C25—C24—Br1	−176.7 (3)
C18—N2—C8—C7	−179.1 (4)	C22—C23—C24—C25	−3.0 (7)
C16—C9—C8—N2	−1.0 (5)	C22—C23—C24—Br1	175.2 (3)
C10—C9—C8—N2	176.0 (4)	N2—C18—C16—C9	0.7 (5)
C16—C9—C8—C7	179.7 (5)	C19—C18—C16—C9	−176.3 (4)
C10—C9—C8—C7	−3.3 (8)	N2—C18—C16—C17	−174.3 (4)
C8—N2—C18—C16	−1.4 (5)	C19—C18—C16—C17	8.7 (7)
C8—N2—C18—C19	175.9 (4)	C8—C9—C16—C18	0.2 (5)
C25—C26—C19—C20	−175.0 (4)	C10—C9—C16—C18	−176.9 (4)
C21—C26—C19—C20	1.3 (4)	C8—C9—C16—C17	175.1 (4)
C25—C26—C19—C18	12.0 (7)	C10—C9—C16—C17	−2.0 (7)
C21—C26—C19—C18	−171.7 (4)	C21—N3—C20—C19	0.0 (5)
N2—C18—C19—C20	−133.1 (5)	C26—C19—C20—N3	−0.9 (5)
C16—C18—C19—C20	43.5 (7)	C18—C19—C20—N3	172.2 (4)
N2—C18—C19—C26	38.6 (6)	C24—C23—C22—C21	0.5 (7)
C16—C18—C19—C26	−144.8 (5)	N3—C21—C22—C23	−177.4 (4)
C20—N3—C21—C22	−178.4 (4)	C26—C21—C22—C23	3.4 (6)
C20—N3—C21—C26	0.8 (5)	C1—C6—C5—C4	2.6 (8)
C25—C26—C21—N3	175.7 (4)	C7—C6—C5—C4	−179.9 (5)
C19—C26—C21—N3	−1.3 (4)	C5—C6—C1—C2	−1.4 (7)
C25—C26—C21—C22	−5.0 (6)	C7—C6—C1—C2	−178.9 (5)
C19—C26—C21—C22	178.0 (4)	C6—C5—C4—C3	−1.3 (10)
C14—C13—N1—O1	−173.5 (5)	C6—C1—C2—C3	−1.0 (9)
C12—C13—N1—O1	8.4 (7)	C5—C4—C3—C2	−1.1 (12)
C14—C13—N1—O2	6.0 (7)	C1—C2—C3—C4	2.3 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O4^{i}	0.86	2.02	2.842 (5)	161
C4—H4···N4^{ii}	0.93	2.62	3.485 (8)	155
C28—H28*C*···O1^{iii}	0.96	2.48	3.245 (9)	137
N2—H2···O4	0.86	2.03	2.876 (4)	166
C28—H28*A*···O3	0.96	2.57	3.289 (8)	132

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