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2-(5-Bromo-1*H*-indol-3-yl)-4-(4-bromophenyl)-5-(4-chlorobenzoyl)-1*H*-pyrrole-3-carbonitrile dimethyl sulfoxide monosolvate

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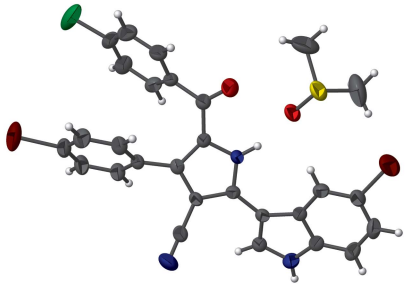
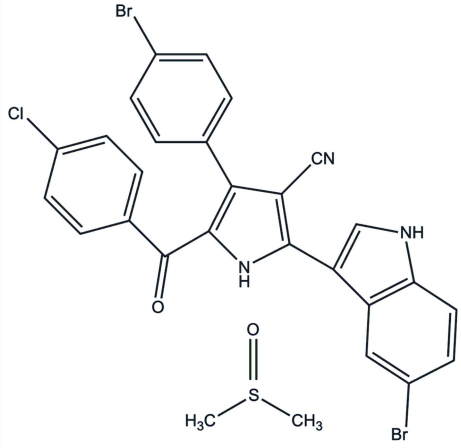
Structural data: full structural data are available from iucrdata.iucr.org

In the title solvated compound, $C_{26}H_{14}Br_2ClN_3O\cdot C_2H_6OS$, the indole ring is inclined to the central pyrrole ring by 25.7 (2)°. The chlorobenzene ring and the bromobenzene rings subtend dihedral angles of 56.5 (2) and 53.4 (2)°, respectively, with the central pyrrole ring. In the crystal, molecules are bridged by N—H···O hydrogen bonds, involving the dimethyl sulfoxide solvent molecule, forming chains along [010]. There are no other significant intermolecular interactions present.

3D view



Chemical scheme



Structure description

Indole structures are considered to be privileged structural motifs due to their ability to bind many receptors within the body (Fuwa & Sasaki, 2009). Several indole derivatives are in clinical use, such as *sunitinib* as a tyrosine kinase inhibitor (Oudard *et al.*, 2011) or *delavirdine* as a non-nucleoside reverse transcriptase inhibitor (Beale, 2011). Indole derivatives are known to exhibit biological activities such as anti-proliferative (Parrino *et al.*, 2015), potential mushroom tyrosinase inhibition (Ferro *et al.*, 2015), anti-inflammatory (Chen *et al.*, 2015) and anti-tumor (Ma *et al.*, 2015). As part of our studies of indole derivatives, we have synthesized the title compound and report herein on its crystal structure.

In the title compound, Fig. 1, the indole ring system is twisted away from the central pyrrole ring by 25.7 (2)°. The C16—C17—N3 bond angle of 178.3 (5)° indicates the linear character of the cyano group, a feature observed in carbonitrile compounds. In the benzene ring of the indole ring system, the endocyclic angle at C26 is contracted to 117.8 (4)°, while the angle at C21 is expanded to 122.6 (4)°. This would appear to be a real

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.86	2.08	2.812 (4)	143
N2—H2···O2^{i}	0.86	1.96	2.813 (4)	170

Symmetry code: (i) $-x+\frac{5}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

effect caused by the fusion of the pyrrole ring with the benzene ring resulting in an angular distortion. The chlorobenzene (C1–C6) and bromobenzene (C10–C15) rings subtend dihedral angles of 56.5 (2)° and 53.4 (2)°, respectively, with the central pyrrole ring.

In the crystal, molecules are bridged by N—H···O hydrogen bonds involving the dimethyl sulfoxide solvent molecule, forming chains along [010], see Table 1 and Fig. 2. There are no other significant intermolecular interactions present.

Synthesis and crystallization

To a stirred mixture of 4-bromobenzaldehyde 1 (1.0 mmol), 3-(5-bromo-1*H*-indol-3-yl)-3-oxopropanenitrile 2 (1.0 mmol) and 4-chlorophenacylazide 3 (1.0 mmol) in H_2O (3 ml), piperidine (0.25 mmol) was added at 353 K. The turbid solution slowly turned into a clear solution, followed by the formation of a solid after 30 min. After completion of the reaction, as indicated by TLC, the solid was filtered and washed with a PE–EtOAc mixture (1:1 ratio, *v*/*v*, 5 ml) to give the title compound (yield 91%), which was recrystallized from EtOH solution to give yellow crystals on slow evaporation of the solvent.

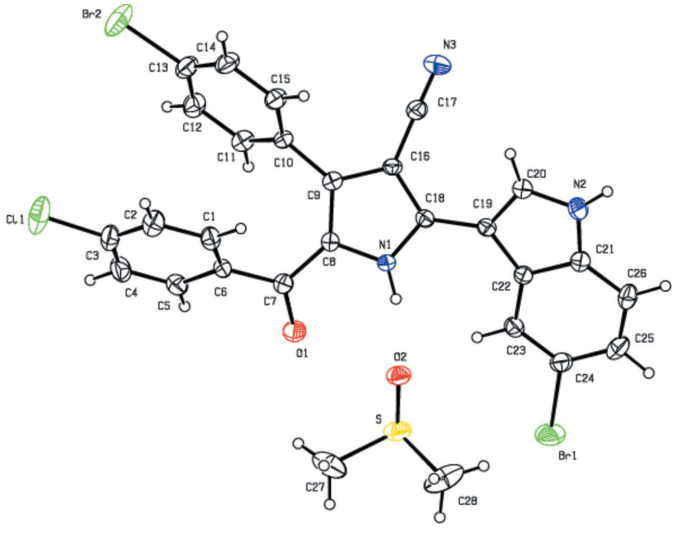


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{14}Br_2ClN_3O\cdot C_2H_6OS$
M_r	657.80
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	12.4962 (12), 12.8055 (10), 17.6834 (17)
β (°)	92.820 (3)
V (Å^3)	2826.3 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.07
Crystal size (mm)	0.20 × 0.19 × 0.17
Data collection	
Diffractometer	Bruker SMART APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.547, 0.594
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29776, 4972, 3236
R_{int}	0.054
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.070, 0.107, 1.15
No. of reflections	4972
No. of parameters	334
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.59, −0.40

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

Refinement

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

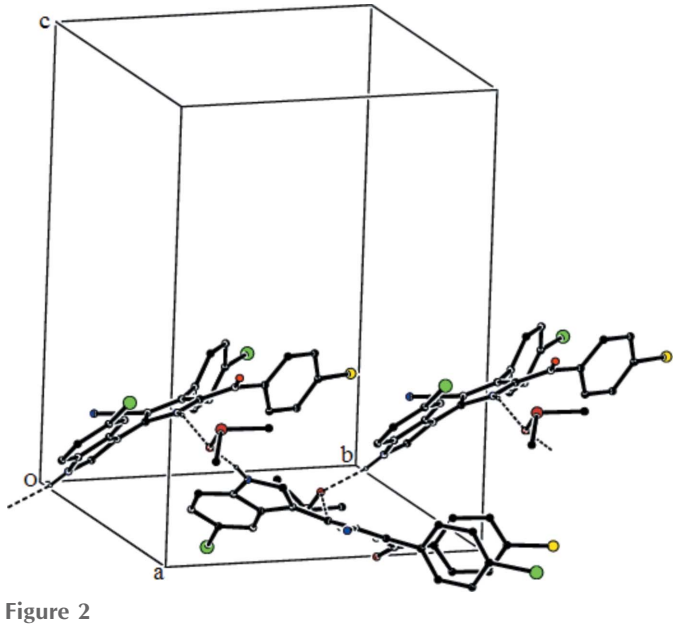


Figure 2
A view along the *b* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines (see Table 1), and for clarity C-bound H atoms have been omitted.

Acknowledgements

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full crystallographic data

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2-(5-Bromo-1*H*-indol-3-yl)-4-(4-bromophenyl)-5-(4-chlorobenzoyl)-1*H*-pyrrole-3-carbonitrile dimethyl sulfoxide monosolvate

Crystal data

$C_{26}H_{14}Br_2ClN_3O\cdot C_2H_6OS$
M_r = 657.80
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 12.4962 (12) Å
b = 12.8055 (10) Å
c = 17.6834 (17) Å
β = 92.820 (3)°
V = 2826.3 (4) Å^3
Z = 4
$F(000)$ = 1312
D_x = 1.546 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3236 reflections
θ = 2.0–25.0°
μ = 3.07 mm^{-1}
T = 293 K
Block, yellow
0.20 × 0.19 × 0.17 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} = 0.547, T_{max} = 0.594
29776 measured reflections
4972 independent reflections
3236 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 25.0°, θ_{min} = 2.0°
h = −14→14
k = −15→15
l = −20→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.107
S = 1.15
4972 reflections
334 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
$w = 1/[\sigma^2(F_o^2) + (0.0239P)^2 + 4.3884P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 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.

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}
C1	1.3650 (3)	0.7573 (3)	0.1460 (3)	0.0423 (12)
H1A	1.3715	0.7143	0.1883	0.051*
C2	1.4030 (4)	0.8589 (4)	0.1498 (3)	0.0499 (13)
H2A	1.4345	0.8849	0.1947	0.060*
C3	1.3936 (4)	0.9203 (4)	0.0868 (4)	0.0529 (14)
C4	1.3434 (4)	0.8858 (4)	0.0210 (3)	0.0563 (15)
H4	1.3355	0.9299	−0.0207	0.068*
C5	1.3050 (4)	0.7857 (4)	0.0172 (3)	0.0486 (13)
H5	1.2702	0.7618	−0.0272	0.058*
C6	1.3176 (3)	0.7199 (3)	0.0791 (3)	0.0368 (11)
C7	1.2789 (3)	0.6105 (3)	0.0726 (3)	0.0389 (11)
C8	1.3422 (3)	0.5262 (3)	0.1073 (2)	0.0320 (10)
C9	1.4510 (3)	0.5131 (3)	0.1266 (2)	0.0310 (10)
C10	1.5384 (3)	0.5894 (3)	0.1181 (2)	0.0323 (10)
C11	1.5531 (3)	0.6405 (3)	0.0511 (3)	0.0412 (11)
H11	1.5110	0.6223	0.0083	0.049*
C12	1.6288 (4)	0.7183 (4)	0.0458 (3)	0.0486 (13)
H12	1.6379	0.7524	0.0001	0.058*
C13	1.6907 (4)	0.7445 (4)	0.1096 (3)	0.0490 (13)
C14	1.6812 (3)	0.6930 (4)	0.1768 (3)	0.0487 (13)
H14	1.7249	0.7103	0.2190	0.058*
C15	1.6052 (3)	0.6148 (3)	0.1807 (3)	0.0421 (12)
H15	1.5988	0.5786	0.2259	0.050*
C16	1.4618 (3)	0.4099 (3)	0.1543 (2)	0.0305 (10)
C17	1.5598 (4)	0.3568 (4)	0.1722 (3)	0.0414 (12)
C18	1.3605 (3)	0.3633 (3)	0.1538 (2)	0.0297 (10)
C19	1.3286 (3)	0.2625 (3)	0.1812 (2)	0.0317 (10)
C20	1.3851 (3)	0.2061 (3)	0.2357 (2)	0.0370 (11)
H20	1.4483	0.2282	0.2607	0.044*
C21	1.2458 (3)	0.1067 (3)	0.2000 (2)	0.0346 (11)
C22	1.2373 (3)	0.1996 (3)	0.1580 (2)	0.0307 (10)
C23	1.1506 (3)	0.2111 (3)	0.1054 (2)	0.0370 (11)
H23	1.1429	0.2713	0.0761	0.044*
C24	1.0777 (3)	0.1317 (4)	0.0981 (3)	0.0440 (12)
C25	1.0879 (4)	0.0392 (4)	0.1398 (3)	0.0504 (13)

H25	1.0367	−0.0132	0.1330	0.060*
C26	1.1730 (4)	0.0255 (3)	0.1906 (3)	0.0447 (12)
H26	1.1817	−0.0363	0.2179	0.054*
C27	0.9319 (5)	0.5805 (5)	0.0966 (4)	0.088 (2)
H27A	0.9815	0.6227	0.0702	0.132*
H27B	0.9244	0.6082	0.1465	0.132*
H27C	0.8635	0.5808	0.0694	0.132*
C28	0.8771 (5)	0.3945 (6)	0.1528 (4)	0.108 (3)
H28A	0.8918	0.3218	0.1613	0.162*
H28B	0.8107	0.4019	0.1235	0.162*
H28C	0.8718	0.4293	0.2005	0.162*
N1	1.2906 (3)	0.4344 (2)	0.12369 (19)	0.0323 (9)
H1	1.2231	0.4237	0.1158	0.039*
N2	1.3361 (3)	0.1139 (3)	0.2479 (2)	0.0415 (10)
H2	1.3576	0.0674	0.2803	0.050*
N3	1.6377 (3)	0.3126 (3)	0.1851 (3)	0.0713 (14)
O1	1.1943 (3)	0.5897 (3)	0.0367 (2)	0.0657 (11)
O2	1.0750 (2)	0.4536 (2)	0.16015 (17)	0.0458 (8)
Cl1	1.44831 (14)	1.04501 (10)	0.09004 (10)	0.0869 (6)
Br1	0.95687 (4)	0.14674 (5)	0.03007 (4)	0.0779 (2)
Br2	1.79124 (5)	0.85467 (5)	0.10269 (4)	0.0916 (3)
S	0.98089 (9)	0.45031 (11)	0.10350 (8)	0.0537 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.047 (3)	0.035 (3)	0.046 (3)	0.004 (2)	0.015 (2)	0.004 (2)
C2	0.057 (3)	0.040 (3)	0.054 (3)	−0.002 (3)	0.022 (3)	−0.013 (3)
C3	0.052 (3)	0.029 (3)	0.081 (4)	0.002 (2)	0.037 (3)	0.000 (3)
C4	0.057 (3)	0.045 (3)	0.068 (4)	0.008 (3)	0.016 (3)	0.023 (3)
C5	0.040 (3)	0.046 (3)	0.059 (4)	0.005 (2)	0.001 (2)	0.013 (3)
C6	0.031 (2)	0.030 (2)	0.050 (3)	0.003 (2)	0.005 (2)	0.008 (2)
C7	0.035 (3)	0.038 (3)	0.044 (3)	−0.001 (2)	0.003 (2)	0.007 (2)
C8	0.032 (2)	0.029 (2)	0.035 (3)	−0.0015 (19)	0.001 (2)	0.002 (2)
C9	0.030 (2)	0.035 (3)	0.028 (3)	−0.0016 (19)	0.003 (2)	−0.004 (2)
C10	0.027 (2)	0.034 (2)	0.037 (3)	−0.0016 (19)	0.005 (2)	0.002 (2)
C11	0.038 (3)	0.046 (3)	0.040 (3)	−0.004 (2)	0.004 (2)	−0.005 (3)
C12	0.050 (3)	0.051 (3)	0.046 (3)	−0.005 (3)	0.017 (3)	0.008 (3)
C13	0.038 (3)	0.045 (3)	0.065 (4)	−0.010 (2)	0.012 (3)	−0.005 (3)
C14	0.039 (3)	0.055 (3)	0.052 (4)	−0.013 (2)	−0.006 (2)	−0.001 (3)
C15	0.038 (3)	0.048 (3)	0.040 (3)	−0.007 (2)	−0.001 (2)	0.006 (2)
C16	0.024 (2)	0.034 (2)	0.034 (3)	0.0017 (19)	0.0025 (19)	0.000 (2)
C17	0.033 (3)	0.045 (3)	0.047 (3)	−0.003 (2)	0.003 (2)	0.011 (2)
C18	0.030 (2)	0.029 (2)	0.030 (3)	0.003 (2)	−0.0008 (19)	−0.002 (2)
C19	0.028 (2)	0.030 (2)	0.038 (3)	0.0032 (19)	0.003 (2)	−0.002 (2)
C20	0.034 (3)	0.036 (3)	0.041 (3)	0.000 (2)	0.000 (2)	0.002 (2)
C21	0.036 (3)	0.034 (3)	0.035 (3)	0.001 (2)	0.011 (2)	−0.003 (2)
C22	0.029 (2)	0.030 (2)	0.033 (3)	0.0021 (19)	0.007 (2)	−0.002 (2)

C23	0.037 (3)	0.033 (3)	0.041 (3)	0.005 (2)	0.001 (2)	0.000 (2)
C24	0.032 (3)	0.042 (3)	0.057 (3)	0.000 (2)	0.002 (2)	−0.008 (3)
C25	0.044 (3)	0.047 (3)	0.060 (4)	−0.017 (2)	0.006 (3)	−0.009 (3)
C26	0.053 (3)	0.037 (3)	0.045 (3)	−0.008 (2)	0.014 (3)	0.004 (2)
C27	0.074 (4)	0.091 (5)	0.097 (5)	0.037 (4)	−0.022 (4)	−0.006 (4)
C28	0.060 (4)	0.153 (7)	0.112 (6)	−0.043 (4)	0.013 (4)	−0.005 (5)
N1	0.0240 (18)	0.030 (2)	0.042 (2)	−0.0013 (16)	−0.0044 (16)	0.0012 (17)
N2	0.045 (2)	0.040 (2)	0.039 (2)	0.0005 (18)	−0.0018 (19)	0.0119 (18)
N3	0.035 (3)	0.071 (3)	0.108 (4)	0.011 (2)	0.000 (3)	0.019 (3)
O1	0.047 (2)	0.055 (2)	0.092 (3)	−0.0101 (17)	−0.034 (2)	0.021 (2)
O2	0.0327 (17)	0.0505 (19)	0.053 (2)	−0.0011 (14)	−0.0076 (15)	−0.0094 (16)
Cl1	0.1126 (13)	0.0388 (8)	0.1155 (14)	−0.0208 (8)	0.0667 (11)	−0.0138 (8)
Br1	0.0487 (3)	0.0751 (4)	0.1063 (5)	−0.0023 (3)	−0.0312 (3)	−0.0132 (4)
Br2	0.0821 (5)	0.0819 (5)	0.1114 (6)	−0.0496 (4)	0.0096 (4)	0.0078 (4)
S	0.0351 (7)	0.0641 (9)	0.0608 (9)	−0.0025 (6)	−0.0066 (6)	−0.0133 (7)

Geometric parameters (Å, º)

C1—C6	1.383 (6)	C16—C17	1.423 (6)
C1—C2	1.386 (6)	C17—N3	1.139 (5)
C1—H1A	0.9300	C18—N1	1.352 (5)
C2—C3	1.365 (7)	C18—C19	1.443 (6)
C2—H2A	0.9300	C19—C20	1.371 (5)
C3—C4	1.367 (7)	C19—C22	1.440 (5)
C3—Cl1	1.737 (5)	C20—N2	1.353 (5)
C4—C5	1.370 (6)	C20—H20	0.9300
C4—H4	0.9300	C21—N2	1.380 (5)
C5—C6	1.384 (6)	C21—C26	1.386 (6)
C5—H5	0.9300	C21—C22	1.405 (6)
C6—C7	1.485 (6)	C22—C23	1.400 (5)
C7—O1	1.235 (5)	C23—C24	1.368 (6)
C7—C8	1.456 (6)	C23—H23	0.9300
C8—N1	1.379 (5)	C24—C25	1.397 (6)
C8—C9	1.395 (5)	C24—Br1	1.893 (4)
C9—C16	1.414 (6)	C25—C26	1.370 (6)
C9—C10	1.479 (6)	C25—H25	0.9300
C10—C11	1.373 (6)	C26—H26	0.9300
C10—C15	1.392 (6)	C27—S	1.777 (6)
C11—C12	1.381 (6)	C27—H27A	0.9600
C11—H11	0.9300	C27—H27B	0.9600
C12—C13	1.377 (6)	C27—H27C	0.9600
C12—H12	0.9300	C28—S	1.750 (6)
C13—C14	1.368 (6)	C28—H28A	0.9600
C13—Br2	1.898 (4)	C28—H28B	0.9600
C14—C15	1.384 (6)	C28—H28C	0.9600
C14—H14	0.9300	N1—H1	0.8600
C15—H15	0.9300	N2—H2	0.8600
C16—C18	1.399 (5)	O2—S	1.508 (3)

C6—C1—C2	119.9 (4)	N1—C18—C16	106.4 (3)
C6—C1—H1A	120.0	N1—C18—C19	123.5 (4)
C2—C1—H1A	120.0	C16—C18—C19	130.1 (4)
C3—C2—C1	119.0 (5)	C20—C19—C22	106.3 (4)
C3—C2—H2A	120.5	C20—C19—C18	124.5 (4)
C1—C2—H2A	120.5	C22—C19—C18	129.3 (4)
C2—C3—C4	121.8 (4)	N2—C20—C19	110.5 (4)
C2—C3—Cl1	119.0 (5)	N2—C20—H20	124.7
C4—C3—Cl1	119.2 (4)	C19—C20—H20	124.7
C3—C4—C5	119.3 (5)	N2—C21—C26	129.5 (4)
C3—C4—H4	120.3	N2—C21—C22	107.9 (4)
C5—C4—H4	120.3	C26—C21—C22	122.6 (4)
C4—C5—C6	120.3 (5)	C23—C22—C21	118.5 (4)
C4—C5—H5	119.8	C23—C22—C19	135.0 (4)
C6—C5—H5	119.8	C21—C22—C19	106.5 (3)
C1—C6—C5	119.5 (4)	C24—C23—C22	118.3 (4)
C1—C6—C7	121.2 (4)	C24—C23—H23	120.9
C5—C6—C7	119.3 (4)	C22—C23—H23	120.9
O1—C7—C8	119.4 (4)	C23—C24—C25	122.5 (4)
O1—C7—C6	120.7 (4)	C23—C24—Br1	119.4 (4)
C8—C7—C6	119.9 (4)	C25—C24—Br1	118.1 (3)
N1—C8—C9	107.8 (3)	C26—C25—C24	120.1 (4)
N1—C8—C7	118.1 (4)	C26—C25—H25	119.9
C9—C8—C7	134.0 (4)	C24—C25—H25	119.9
C8—C9—C16	105.8 (3)	C25—C26—C21	117.8 (4)
C8—C9—C10	127.7 (4)	C25—C26—H26	121.1
C16—C9—C10	126.4 (4)	C21—C26—H26	121.1
C11—C10—C15	118.3 (4)	S—C27—H27A	109.5
C11—C10—C9	122.2 (4)	S—C27—H27B	109.5
C15—C10—C9	119.4 (4)	H27A—C27—H27B	109.5
C10—C11—C12	121.6 (4)	S—C27—H27C	109.5
C10—C11—H11	119.2	H27A—C27—H27C	109.5
C12—C11—H11	119.2	H27B—C27—H27C	109.5
C13—C12—C11	118.6 (5)	S—C28—H28A	109.5
C13—C12—H12	120.7	S—C28—H28B	109.5
C11—C12—H12	120.7	H28A—C28—H28B	109.5
C14—C13—C12	121.7 (4)	S—C28—H28C	109.5
C14—C13—Br2	120.0 (4)	H28A—C28—H28C	109.5
C12—C13—Br2	118.3 (4)	H28B—C28—H28C	109.5
C13—C14—C15	118.8 (4)	C18—N1—C8	111.0 (3)
C13—C14—H14	120.6	C18—N1—H1	124.5
C15—C14—H14	120.6	C8—N1—H1	124.5
C14—C15—C10	121.0 (4)	C20—N2—C21	108.9 (3)
C14—C15—H15	119.5	C20—N2—H2	125.6
C10—C15—H15	119.5	C21—N2—H2	125.6
C18—C16—C9	109.0 (3)	O2—S—C28	104.7 (3)
C18—C16—C17	124.5 (4)	O2—S—C27	105.9 (2)

C9—C16—C17	126.2 (4)	C28—S—C27	99.0 (3)
N3—C17—C16	178.3 (5)		
C6—C1—C2—C3	−0.6 (7)	C8—C9—C16—C17	171.9 (4)
C1—C2—C3—C4	3.0 (7)	C10—C9—C16—C17	−6.5 (7)
C1—C2—C3—Cl1	−176.2 (3)	C18—C16—C17—N3	59 (18)
C2—C3—C4—C5	−2.4 (8)	C9—C16—C17—N3	−114 (18)
Cl1—C3—C4—C5	176.7 (4)	C9—C16—C18—N1	2.5 (5)
C3—C4—C5—C6	−0.5 (7)	C17—C16—C18—N1	−171.4 (4)
C2—C1—C6—C5	−2.3 (7)	C9—C16—C18—C19	−175.2 (4)
C2—C1—C6—C7	178.3 (4)	C17—C16—C18—C19	11.0 (7)
C4—C5—C6—C1	2.8 (7)	N1—C18—C19—C20	−154.1 (4)
C4—C5—C6—C7	−177.7 (4)	C16—C18—C19—C20	23.2 (7)
C1—C6—C7—O1	140.8 (5)	N1—C18—C19—C22	27.7 (7)
C5—C6—C7—O1	−38.6 (7)	C16—C18—C19—C22	−155.0 (4)
C1—C6—C7—C8	−40.5 (6)	C22—C19—C20—N2	−0.1 (5)
C5—C6—C7—C8	140.0 (4)	C18—C19—C20—N2	−178.6 (4)
O1—C7—C8—N1	−23.6 (7)	N2—C21—C22—C23	−179.5 (4)
C6—C7—C8—N1	157.8 (4)	C26—C21—C22—C23	1.1 (6)
O1—C7—C8—C9	152.9 (5)	N2—C21—C22—C19	1.6 (5)
C6—C7—C8—C9	−25.8 (8)	C26—C21—C22—C19	−177.8 (4)
N1—C8—C9—C16	0.5 (5)	C20—C19—C22—C23	−179.5 (5)
C7—C8—C9—C16	−176.2 (5)	C18—C19—C22—C23	−1.1 (8)
N1—C8—C9—C10	178.9 (4)	C20—C19—C22—C21	−1.0 (5)
C7—C8—C9—C10	2.1 (8)	C18—C19—C22—C21	177.5 (4)
C8—C9—C10—C11	−50.7 (6)	C21—C22—C23—C24	0.7 (6)
C16—C9—C10—C11	127.4 (5)	C19—C22—C23—C24	179.2 (5)
C8—C9—C10—C15	126.0 (5)	C22—C23—C24—C25	−1.4 (7)
C16—C9—C10—C15	−56.0 (6)	C22—C23—C24—Br1	177.8 (3)
C15—C10—C11—C12	−2.7 (7)	C23—C24—C25—C26	0.3 (7)
C9—C10—C11—C12	174.0 (4)	Br1—C24—C25—C26	−178.9 (4)
C10—C11—C12—C13	0.1 (7)	C24—C25—C26—C21	1.5 (7)
C11—C12—C13—C14	2.2 (7)	N2—C21—C26—C25	178.5 (4)
C11—C12—C13—Br2	−177.9 (3)	C22—C21—C26—C25	−2.2 (7)
C12—C13—C14—C15	−1.8 (7)	C16—C18—N1—C8	−2.2 (5)
Br2—C13—C14—C15	178.3 (3)	C19—C18—N1—C8	175.7 (4)
C13—C14—C15—C10	−0.9 (7)	C9—C8—N1—C18	1.1 (5)
C11—C10—C15—C14	3.1 (7)	C7—C8—N1—C18	178.4 (4)
C9—C10—C15—C14	−173.7 (4)	C19—C20—N2—C21	1.1 (5)
C8—C9—C16—C18	−1.8 (5)	C26—C21—N2—C20	177.6 (4)
C10—C9—C16—C18	179.8 (4)	C22—C21—N2—C20	−1.7 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.86	2.08	2.812 (4)	143

N2—H2···O2^{i}	0.86	1.96	2.813 (4)	170

Symmetry code: (i) $-x+5/2$, $y-1/2$, $-z+1/2$.