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5-Benzoyl-2-(5-bromo-1*H*-indol-3-yl)-4-(4-methoxyphenyl)-1*H*-pyrrole-3-carbonitrile

G. Vimala,[a] J. Kamal Raja,[b] P. T. Perumal[b] and A. SubbiahPandi[a]*

[a]Department of Physics, Presidency College (Autonomous), Chennai 600 005, India, and [b]Organic Chemistry, CSIR–Central Leather Research Institute, Adyar, Chennai 600 020, India. *Correspondence e-mail: aspandian59@gmail.com

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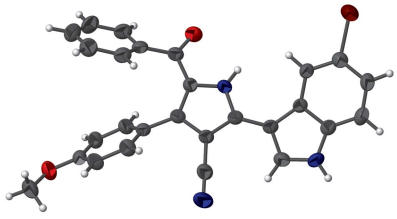
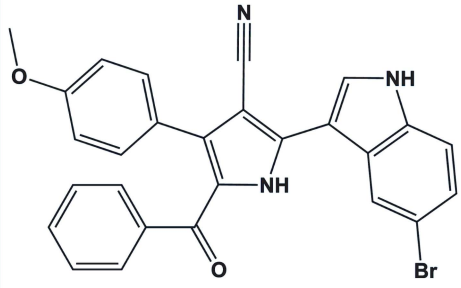
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{27}H_{18}BrN_3O$, the indole and central pyrrole ring systems are inclined to one another by 13.15 (15)°. The carbonitrile group is almost coplanar with its attached pyrrole ring, the C≡N bond making a dihedral angle of 1.9 (2)° with the ring plane. The 4-methoxybenzene ring and the benzoyl ring are inclined to the central pyrrole ring by 55.1 (2) and 51.5 (2)°, respectively. The dihedral angle between these two benzene rings is 37.68 (17)°. In the crystal, molecules are linked by pairs of N—H···N hydrogen bonds, forming inversion dimers with an $R_2^2(16)$ ring motif. The dimers are linked by offset π–π interactions [intercentroid distance = 3.614 (2) Å], which leads to the formation of chains propagating in the [010] direction.

3D view



Chemical scheme



Structure description

Indole-containing compounds are best known for their medicinal properties in the pharmaceutical industry. Today, analogues based on indole are significant players in a diverse array of markets such as dyes, plastics, agriculture, vitamin supplements, over-the-counter drugs, flavour enhancers and perfumery (Barden, 2011). Indole derivatives exhibit antibacterial, antifungal (Singh *et al.* 2000), antitumor (Andreani *et al.*, 2001), antihepatitis B virus (Chai *et al.*, 2006) and anti-inflammatory (Rodriguez *et al.*, 1985) activities. They are also used as bioactive drugs (Stevenson *et al.*, 2000) and exhibit high aldose reductase inhibitory (Rajeswaran *et al.*, 1999) and antimicrobial activities (Amal Raj *et al.*, 2003). Against this background, we synthesized the title compound and report herein on its crystal structure.

The molecular structure of the title indole derivative is illustrated in Fig. 1. The central pyrrole ring is substituted with an indole ring, a 4-methoxybenzene ring and a benzoyl group. The indole and central pyrrole rings are inclined to one another by 13.1 (2)°. The carbonitrile group is almost coplanar with its attached pyrrole ring, as indicated by the

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N3^{i}	0.86	2.21	2.916 (4)	140

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

dihedral angle of 1.9 (2)° between the C11≡N3 bond and the ring plane. The central pyrrole ring makes dihedral angles of 55.1 (2) and 51.5 (2)° with the 4-methoxybenzene ring and the benzoyl ring, respectively. The dihedral angle between these two benzene rings is 37.68 (17)°. The molecular dimensions in the title compound are in agreement with those reported for closely related compounds (Vimala *et al.*, 2015; Inglebert *et al.*, 2013).

In the crystal, molecules are linked by pairs of N_i—H···N_c (i = indole and c = carbonitrile) classical hydrogen bonds, forming inversion dimers with $R_2^2(16)$ loops (Table 1 and Fig. 2). The molecules are also linked *via* slipped parallel π–π interactions, forming chains propagating along the *b*-axis direction [*Cg*2···*Cg*3^{i} = 3.614 (2) Å; inter-planar distance = 3.535 (1) Å, slippage = 0.525 Å; *Cg*2 and *Cg*3 are the centroids of the N2/C9/C10/C12/C19 and C2–C7 rings; symmetry code: (i) $-x+1, -y, -z+1$].

Synthesis and crystallization

To a stirred mixture of 4-methoxybenzaldehyde (1.0 mmol), 3-(5-bromo-1*H*-indol-3-yl)-3-oxopropanenitrile (1.0 mmol) and phenacylazide (1.0 mmol) in water (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 1.5 h. After completion of the reaction, as indicated by TLC, the solid was filtered and washed with a petroleum ether-EtOAc mixture (1:1 ratio, *v*/*v*, 5 ml) to give title compound. It was recrystallized from ethanol by using slow evaporation, giving yellow block-like crystals (yield 85%).

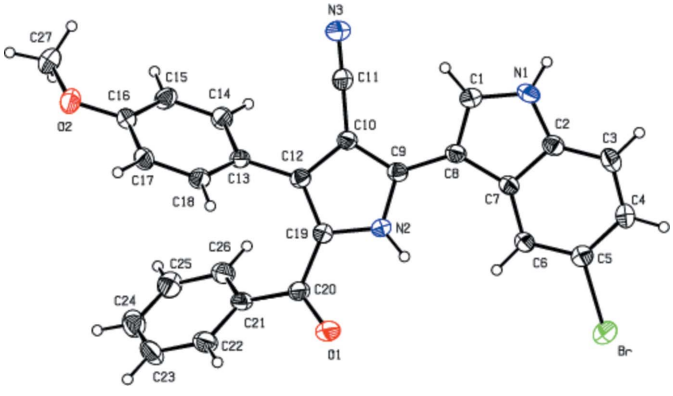


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

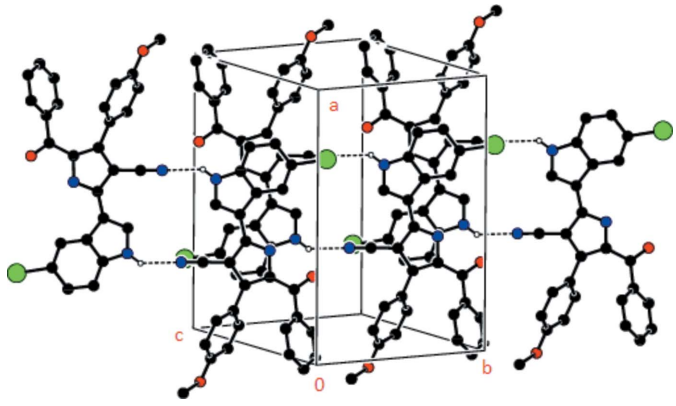


Figure 2
The crystal packing of the title compound, viewed along the normal to (011). Hydrogen bonds are shown as dashed lines (see Table 1) and C-bound H atoms have been omitted for clarity.

Refinement

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

Acknowledgements

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{27}H_{18}BrN_3O_2$
M_r	496.35
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	14.6503 (6), 9.6974 (3), 15.2946 (7)
β (°)	93.284 (2)
V (Å^3)	2169.33 (15)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.93
Crystal size (mm)	0.24 × 0.22 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.636, 0.680
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26857, 3823, 2582
R_{int}	0.047
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.139, 0.78
No. of reflections	3823
No. of parameters	298
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.55

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

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full crystallographic data

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G. Vimala, J. Kamal Raja, P. T. Perumal and A. SubbiahPandi

5-Benzoyl-2-(5-bromo-1*H*-indol-3-yl)-4-(4-methoxyphenyl)-1*H*-pyrrole-3-carbonitrile

Crystal data

$C_{27}H_{18}BrN_3O_2$
M_r = 496.35
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 14.6503 (6) Å
b = 9.6974 (3) Å
c = 15.2946 (7) Å
β = 93.284 (2)°
V = 2169.33 (15) Å^3
Z = 4
$F(000)$ = 1008
D_x = 1.520 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2582 reflections
θ = 1.9–25.0°
μ = 1.93 mm^{-1}
T = 293 K
Block, yellow
0.24 × 0.22 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.636, T_{max} = 0.680
26857 measured reflections
3823 independent reflections
2582 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 25.0°, θ_{min} = 1.9°
h = −17→17
k = −11→11
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.139
S = 0.78
3823 reflections
298 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
$w = 1/[\sigma^2(F_o^2) + (0.1132P)^2 + 1.1029P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 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}
Br	0.30324 (3)	−0.25826 (4)	0.72049 (3)	0.0638 (2)
O2	1.10059 (16)	0.3663 (2)	0.55850 (18)	0.0562 (7)
N1	0.3744 (2)	0.2552 (2)	0.5243 (2)	0.0454 (7)
H1	0.3391	0.3156	0.4989	0.055*
N2	0.63376 (17)	0.0077 (2)	0.62556 (17)	0.0380 (6)
H2	0.6021	−0.0643	0.6364	0.046*
O1	0.73519 (18)	−0.2198 (2)	0.66235 (19)	0.0591 (7)
C6	0.4113 (2)	−0.0522 (3)	0.6453 (2)	0.0382 (7)
H6	0.4609	−0.1028	0.6683	0.046*
C13	0.8450 (2)	0.2048 (3)	0.6045 (2)	0.0341 (7)
C7	0.4242 (2)	0.0693 (3)	0.5988 (2)	0.0345 (7)
C2	0.3459 (2)	0.1408 (3)	0.5665 (2)	0.0393 (8)
C17	0.9914 (2)	0.1932 (3)	0.5422 (2)	0.0442 (8)
H17	1.0320	0.1457	0.5087	0.053*
C9	0.5976 (2)	0.1268 (3)	0.5936 (2)	0.0354 (7)
C18	0.9077 (2)	0.1372 (3)	0.5559 (2)	0.0409 (8)
H18	0.8927	0.0515	0.5318	0.049*
C21	0.8702 (2)	−0.0997 (3)	0.7049 (2)	0.0408 (8)
N3	0.6659 (2)	0.4599 (3)	0.5252 (3)	0.0697 (10)
C4	0.2471 (2)	−0.0223 (4)	0.6240 (2)	0.0451 (8)
H4	0.1886	−0.0547	0.6331	0.054*
C10	0.6715 (2)	0.2150 (3)	0.5857 (2)	0.0360 (7)
C20	0.7756 (2)	−0.1084 (3)	0.6680 (2)	0.0406 (8)
C12	0.7530 (2)	0.1458 (3)	0.6133 (2)	0.0353 (7)
C15	0.9552 (2)	0.3886 (3)	0.6267 (2)	0.0444 (8)
H15	0.9710	0.4735	0.6515	0.053*
C14	0.8703 (2)	0.3318 (3)	0.6391 (2)	0.0437 (8)
H14	0.8292	0.3803	0.6716	0.052*
C19	0.7273 (2)	0.0155 (3)	0.6386 (2)	0.0372 (7)
C5	0.3234 (2)	−0.0953 (3)	0.6562 (2)	0.0422 (8)
C16	1.0161 (2)	0.3191 (3)	0.5777 (2)	0.0406 (8)
C3	0.2583 (2)	0.0967 (4)	0.5790 (2)	0.0464 (9)
H3	0.2080	0.1472	0.5572	0.056*
C22	0.9322 (3)	−0.2039 (4)	0.6870 (2)	0.0512 (9)
H22	0.9132	−0.2779	0.6518	0.061*

C26	0.8999 (2)	0.0074 (3)	0.7592 (2)	0.0464 (8)
H26	0.8597	0.0776	0.7724	0.056*
C1	0.4662 (3)	0.2596 (3)	0.5283 (2)	0.0441 (9)
H1A	0.5008	0.3284	0.5038	0.053*
C8	0.5016 (2)	0.1482 (3)	0.5737 (2)	0.0368 (7)
C25	0.9885 (3)	0.0102 (4)	0.7935 (3)	0.0573 (10)
H25	1.0076	0.0816	0.8309	0.069*
C24	1.0489 (3)	−0.0906 (5)	0.7736 (3)	0.0643 (11)
H24	1.1093	−0.0861	0.7958	0.077*
C11	0.6677 (2)	0.3509 (3)	0.5522 (2)	0.0456 (8)
C27	1.1307 (3)	0.4935 (4)	0.5947 (3)	0.0597 (10)
H27A	1.1907	0.5138	0.5760	0.090*
H27B	1.1326	0.4879	0.6574	0.090*
H27C	1.0892	0.5652	0.5752	0.090*
C23	1.0206 (3)	−0.1980 (4)	0.7209 (3)	0.0630 (11)
H23	1.0616	−0.2673	0.7080	0.076*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.0542 (3)	0.0555 (3)	0.0818 (4)	−0.01062 (17)	0.0039 (2)	0.02027 (19)
O2	0.0395 (14)	0.0513 (14)	0.0787 (18)	−0.0067 (11)	0.0114 (13)	−0.0024 (13)
N1	0.0445 (18)	0.0371 (15)	0.0539 (18)	0.0096 (12)	−0.0047 (14)	0.0085 (12)
N2	0.0366 (15)	0.0292 (13)	0.0484 (17)	−0.0014 (11)	0.0045 (12)	0.0051 (11)
O1	0.0560 (17)	0.0371 (13)	0.083 (2)	−0.0042 (12)	−0.0047 (14)	0.0106 (12)
C6	0.0348 (18)	0.0372 (17)	0.042 (2)	0.0037 (14)	−0.0001 (14)	0.0013 (14)
C13	0.0371 (18)	0.0303 (15)	0.0353 (18)	0.0019 (13)	0.0035 (14)	0.0028 (13)
C7	0.0352 (17)	0.0335 (16)	0.0349 (18)	0.0049 (13)	0.0030 (13)	−0.0003 (13)
C2	0.042 (2)	0.0361 (17)	0.0397 (19)	0.0036 (14)	−0.0005 (15)	−0.0030 (14)
C17	0.0365 (19)	0.0405 (18)	0.057 (2)	0.0061 (15)	0.0120 (16)	−0.0051 (16)
C9	0.0394 (18)	0.0328 (16)	0.0346 (18)	0.0045 (14)	0.0074 (14)	−0.0004 (13)
C18	0.042 (2)	0.0319 (16)	0.049 (2)	0.0008 (14)	0.0069 (16)	−0.0046 (14)
C21	0.044 (2)	0.0342 (17)	0.044 (2)	0.0043 (14)	0.0062 (15)	0.0113 (15)
N3	0.059 (2)	0.0448 (19)	0.107 (3)	0.0062 (15)	0.020 (2)	0.0261 (18)
C4	0.0330 (19)	0.054 (2)	0.048 (2)	0.0005 (15)	0.0032 (15)	−0.0014 (16)
C10	0.0372 (18)	0.0324 (15)	0.0390 (19)	0.0033 (13)	0.0076 (14)	0.0031 (13)
C20	0.044 (2)	0.0326 (17)	0.045 (2)	0.0013 (15)	0.0078 (16)	0.0032 (14)
C12	0.0395 (18)	0.0317 (15)	0.0352 (18)	0.0004 (13)	0.0068 (14)	−0.0010 (13)
C15	0.048 (2)	0.0341 (17)	0.052 (2)	−0.0073 (15)	0.0062 (16)	−0.0064 (15)
C14	0.043 (2)	0.0388 (18)	0.051 (2)	0.0026 (15)	0.0121 (16)	−0.0063 (15)
C19	0.0353 (18)	0.0347 (16)	0.042 (2)	0.0007 (13)	0.0036 (14)	0.0016 (13)
C5	0.044 (2)	0.0406 (18)	0.042 (2)	−0.0012 (15)	0.0031 (15)	−0.0001 (14)
C16	0.0329 (18)	0.0396 (18)	0.049 (2)	0.0024 (14)	0.0003 (15)	0.0053 (15)
C3	0.0358 (19)	0.052 (2)	0.051 (2)	0.0076 (16)	−0.0049 (16)	−0.0040 (17)
C22	0.056 (2)	0.0422 (19)	0.056 (2)	0.0091 (17)	0.0079 (19)	0.0051 (16)
C26	0.050 (2)	0.0430 (18)	0.047 (2)	0.0057 (16)	0.0055 (17)	0.0042 (15)
C1	0.046 (2)	0.0381 (19)	0.048 (2)	−0.0013 (15)	0.0048 (17)	0.0071 (15)
C8	0.0403 (19)	0.0304 (15)	0.0398 (19)	0.0042 (13)	0.0041 (14)	0.0013 (13)

C25	0.056 (3)	0.066 (2)	0.049 (2)	−0.006 (2)	−0.0010 (19)	0.0026 (19)
C24	0.047 (2)	0.087 (3)	0.059 (3)	0.004 (2)	−0.0001 (19)	0.021 (2)
C11	0.040 (2)	0.043 (2)	0.056 (2)	0.0024 (15)	0.0120 (16)	0.0042 (16)
C27	0.049 (2)	0.055 (2)	0.076 (3)	−0.0152 (18)	0.004 (2)	0.0027 (19)
C23	0.047 (2)	0.065 (2)	0.078 (3)	0.023 (2)	0.008 (2)	0.013 (2)

Geometric parameters (Å, º)

Br—C5	1.893 (3)	N3—C11	1.134 (4)
O2—C16	1.368 (4)	C4—C3	1.358 (5)
O2—C27	1.411 (4)	C4—C5	1.390 (5)
N1—C1	1.343 (5)	C4—H4	0.9300
N1—C2	1.361 (4)	C10—C12	1.412 (4)
N1—H1	0.8600	C10—C11	1.415 (4)
N2—C9	1.350 (4)	C20—C19	1.452 (4)
N2—C19	1.376 (4)	C12—C19	1.380 (4)
N2—H2	0.8600	C15—C16	1.374 (5)
O1—C20	1.233 (4)	C15—C14	1.383 (4)
C6—C5	1.373 (4)	C15—H15	0.9300
C6—C7	1.394 (4)	C14—H14	0.9300
C6—H6	0.9300	C3—H3	0.9300
C13—C18	1.380 (4)	C22—C23	1.369 (5)
C13—C14	1.383 (4)	C22—H22	0.9300
C13—C12	1.477 (4)	C26—C25	1.373 (5)
C7—C2	1.406 (4)	C26—H26	0.9300
C7—C8	1.438 (4)	C1—C8	1.369 (4)
C2—C3	1.376 (5)	C1—H1A	0.9300
C17—C18	1.368 (4)	C25—C24	1.364 (6)
C17—C16	1.376 (5)	C25—H25	0.9300
C17—H17	0.9300	C24—C23	1.367 (6)
C9—C10	1.391 (4)	C24—H24	0.9300
C9—C8	1.437 (4)	C27—H27A	0.9600
C18—H18	0.9300	C27—H27B	0.9600
C21—C26	1.384 (5)	C27—H27C	0.9600
C21—C22	1.395 (5)	C23—H23	0.9300
C21—C20	1.469 (5)		
C16—O2—C27	118.3 (3)	C14—C15—H15	120.1
C1—N1—C2	109.8 (3)	C15—C14—C13	121.7 (3)
C1—N1—H1	125.1	C15—C14—H14	119.1
C2—N1—H1	125.1	C13—C14—H14	119.1
C9—N2—C19	111.9 (3)	N2—C19—C12	107.1 (3)
C9—N2—H2	124.1	N2—C19—C20	117.6 (3)
C19—N2—H2	124.1	C12—C19—C20	135.1 (3)
C5—C6—C7	118.4 (3)	C6—C5—C4	122.9 (3)
C5—C6—H6	120.8	C6—C5—Br	119.5 (2)
C7—C6—H6	120.8	C4—C5—Br	117.6 (3)
C18—C13—C14	117.2 (3)	O2—C16—C15	125.2 (3)

C18—C13—C12	120.2 (3)	O2—C16—C17	115.7 (3)
C14—C13—C12	122.4 (3)	C15—C16—C17	119.1 (3)
C6—C7—C2	117.7 (3)	C4—C3—C2	118.4 (3)
C6—C7—C8	135.9 (3)	C4—C3—H3	120.8
C2—C7—C8	106.4 (3)	C2—C3—H3	120.8
N1—C2—C3	129.3 (3)	C23—C22—C21	120.5 (4)
N1—C2—C7	107.6 (3)	C23—C22—H22	119.7
C3—C2—C7	123.1 (3)	C21—C22—H22	119.7
C18—C17—C16	120.7 (3)	C25—C26—C21	120.1 (3)
C18—C17—H17	119.7	C25—C26—H26	119.9
C16—C17—H17	119.7	C21—C26—H26	119.9
N2—C9—C10	105.4 (3)	N1—C1—C8	110.3 (3)
N2—C9—C8	124.0 (3)	N1—C1—H1A	124.8
C10—C9—C8	130.6 (3)	C8—C1—H1A	124.8
C17—C18—C13	121.6 (3)	C1—C8—C9	124.0 (3)
C17—C18—H18	119.2	C1—C8—C7	105.9 (3)
C13—C18—H18	119.2	C9—C8—C7	130.0 (3)
C26—C21—C22	118.4 (3)	C24—C25—C26	120.7 (4)
C26—C21—C20	122.0 (3)	C24—C25—H25	119.6
C22—C21—C20	119.6 (3)	C26—C25—H25	119.6
C3—C4—C5	119.6 (3)	C25—C24—C23	120.0 (4)
C3—C4—H4	120.2	C25—C24—H24	120.0
C5—C4—H4	120.2	C23—C24—H24	120.0
C9—C10—C12	109.3 (3)	N3—C11—C10	179.0 (4)
C9—C10—C11	126.1 (3)	O2—C27—H27A	109.5
C12—C10—C11	124.5 (3)	O2—C27—H27B	109.5
O1—C20—C19	118.7 (3)	H27A—C27—H27B	109.5
O1—C20—C21	121.1 (3)	O2—C27—H27C	109.5
C19—C20—C21	120.2 (3)	H27A—C27—H27C	109.5
C19—C12—C10	106.2 (3)	H27B—C27—H27C	109.5
C19—C12—C13	130.1 (3)	C24—C23—C22	120.2 (4)
C10—C12—C13	123.3 (3)	C24—C23—H23	119.9
C16—C15—C14	119.7 (3)	C22—C23—H23	119.9
C16—C15—H15	120.1		

C5—C6—C7—C2	0.5 (4)	O1—C20—C19—N2	15.1 (5)
C5—C6—C7—C8	179.6 (3)	C21—C20—C19—N2	−164.1 (3)
C1—N1—C2—C3	179.3 (3)	O1—C20—C19—C12	−159.6 (4)
C1—N1—C2—C7	0.0 (4)	C21—C20—C19—C12	21.3 (6)
C6—C7—C2—N1	179.6 (3)	C7—C6—C5—C4	−0.8 (5)
C8—C7—C2—N1	0.3 (3)	C7—C6—C5—Br	−179.0 (2)
C6—C7—C2—C3	0.2 (5)	C3—C4—C5—C6	0.4 (5)
C8—C7—C2—C3	−179.1 (3)	C3—C4—C5—Br	178.7 (3)
C19—N2—C9—C10	0.1 (4)	C27—O2—C16—C15	3.1 (5)
C19—N2—C9—C8	180.0 (3)	C27—O2—C16—C17	−178.5 (3)
C16—C17—C18—C13	0.7 (5)	C14—C15—C16—O2	177.8 (3)
C14—C13—C18—C17	−0.1 (5)	C14—C15—C16—C17	−0.4 (5)
C12—C13—C18—C17	176.0 (3)	C18—C17—C16—O2	−178.8 (3)

N2—C9—C10—C12	0.3 (3)	C18—C17—C16—C15	−0.4 (5)
C8—C9—C10—C12	−179.6 (3)	C5—C4—C3—C2	0.3 (5)
N2—C9—C10—C11	177.9 (3)	N1—C2—C3—C4	−179.9 (3)
C8—C9—C10—C11	−2.0 (6)	C7—C2—C3—C4	−0.7 (5)
C26—C21—C20—O1	−140.4 (3)	C26—C21—C22—C23	−1.6 (5)
C22—C21—C20—O1	37.9 (5)	C20—C21—C22—C23	−179.9 (3)
C26—C21—C20—C19	38.7 (5)	C22—C21—C26—C25	0.5 (5)
C22—C21—C20—C19	−143.0 (3)	C20—C21—C26—C25	178.8 (3)
C9—C10—C12—C19	−0.6 (4)	C2—N1—C1—C8	−0.3 (4)
C11—C10—C12—C19	−178.2 (3)	N1—C1—C8—C9	−176.5 (3)
C9—C10—C12—C13	173.3 (3)	N1—C1—C8—C7	0.4 (4)
C11—C10—C12—C13	−4.3 (5)	N2—C9—C8—C1	−168.9 (3)
C18—C13—C12—C19	51.9 (5)	C10—C9—C8—C1	11.0 (5)
C14—C13—C12—C19	−132.2 (4)	N2—C9—C8—C7	15.1 (5)
C18—C13—C12—C10	−120.4 (3)	C10—C9—C8—C7	−165.0 (3)
C14—C13—C12—C10	55.5 (4)	C6—C7—C8—C1	−179.6 (4)
C16—C15—C14—C13	1.0 (5)	C2—C7—C8—C1	−0.4 (3)
C18—C13—C14—C15	−0.8 (5)	C6—C7—C8—C9	−3.0 (6)
C12—C13—C14—C15	−176.8 (3)	C2—C7—C8—C9	176.2 (3)
C9—N2—C19—C12	−0.4 (4)	C21—C26—C25—C24	1.2 (6)
C9—N2—C19—C20	−176.5 (3)	C26—C25—C24—C23	−2.0 (6)
C10—C12—C19—N2	0.6 (4)	C9—C10—C11—N3	−169 (100)
C13—C12—C19—N2	−172.7 (3)	C12—C10—C11—N3	8 (24)
C10—C12—C19—C20	175.6 (4)	C25—C24—C23—C22	0.9 (6)
C13—C12—C19—C20	2.3 (6)	C21—C22—C23—C24	0.8 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N3^{i}	0.86	2.21	2.916 (4)	140

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