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# (*E*)-*N*′-(5-Bromo-2-methoxybenzylidene)-isonicotinohydrazide

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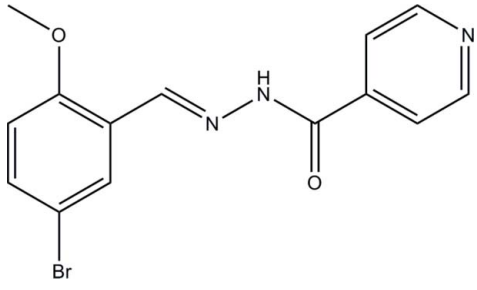
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.010 Å; $R$ factor = 0.064; $wR$ factor = 0.143; data-to-parameter ratio = 16.0.

The asymmetric unit of the title compound, $C_{14}H_{12}BrN_3O_2$, contains two independent molecules in which the dihedral angles between the benzene ring and the pyridine ring are 24.4 (6) and 23.7 (6)°. The molecules exist in a *trans* configuration with respect to the central methylidene units. In the crystal, molecules are linked through intermolecular N—H···O hydrogen bonds, forming chains along the *a* axis.

## Related literature

For the biological activity of hydrazones, see: Zhong *et al.* (2007); Raj *et al.* (2007); Jimenez-Pulido *et al.* (2008). For related structures, see: Ban (2010); Ban & Li (2008*a*,*b*); Li & Ban (2009*a*,*b*); Yehye *et al.* (2008); Fun *et al.* (2008*a*,*b*); Yang *et al.* (2008); Ejsmont *et al.* (2008); Yang (2006).




## Experimental

### Crystal data

$C_{14}H_{12}BrN_3O_2$
$M_r$ = 334.18
Monoclinic, $P2_1/c$
$a$ = 10.020 (3) Å
$b$ = 25.732 (2) Å
$c$ = 11.243 (2) Å
$\beta$ = 102.199 (3)°
$V$ = 2833.4 (10) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 2.91 mm$^{-1}$
$T$ = 298 K
0.13 × 0.10 × 0.10 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.704, $T_{max}$ = 0.760
14099 measured reflections
5922 independent reflections
2018 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.114

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.143
$S$ = 0.94
5922 reflections
369 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.43 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N5—H5···O2 | 0.90 (1) | 2.06 (2) | 2.939 (7) | 164 (6) |
| N2—H2···O4$^{i}$ | 0.90 (1) | 2.11 (2) | 2.999 (7) | 168 (6) |

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5145).

## References

Ban, H.-Y. (2010). *Acta Cryst.* E**66**, o3240.
Ban, H.-Y. & Li, C.-M. (2008*a*). *Acta Cryst.* E**64**, o2177.
Ban, H.-Y. & Li, C.-M. (2008*b*). *Acta Cryst.* E**64**, o2260.
Bruker (1998). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Ejsmont, K., Zareef, M., Arfan, M., Bashir, S. A. & Zaleski, J. (2008). *Acta Cryst.* E**64**, o1128.
Fun, H.-K., Patil, P. S., Jebas, S. R., Sujith, K. V. & Kalluraya, B. (2008*a*). *Acta Cryst.* E**64**, o1594–o1595.
Fun, H.-K., Patil, P. S., Rao, J. N., Kalluraya, B. & Chantrapromma, S. (2008*b*). *Acta Cryst.* E**64**, o1707.
Jimenez-Pulido, S. B., Linares-Ordonez, F. M., Martinez-Martos, J. M., Moreno-Carretero, M. N., Quiros-Olozabal, M. & Ramirez-Exposito, M. J. (2008). *J. Inorg. Biochem.* **102**, 1677–1683.
Li, C.-M. & Ban, H.-Y. (2009*a*). *Acta Cryst.* E**65**, o876.
Li, C.-M. & Ban, H.-Y. (2009*b*). *Acta Cryst.* E**65**, o883.
Raj, K. K. V., Narayana, B., Ashalatha, B. V., Kumari, N. S. & Sarojini, B. K. (2007). *Eur. J. Med. Chem.* **42**, 425–429.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yang, D.-S. (2006). *Acta Cryst.* E**62**, o3792–o3793.
Yang, T., Cao, G.-B., Xiang, J.-M. & Zhang, L.-H. (2008). *Acta Cryst.* E**64**, o1186.
Yehye, W. A., Rahman, N. A., Ariffin, A. & Ng, S. W. (2008). *Acta Cryst.* E**64**, o1824.
Zhong, X., Wei, H.-L., Liu, W.-S., Wang, D.-Q. & Wang, X. (2007). *Bioorg. Med. Chem. Lett.* **17**, 3774–3777.

# supporting information

*Acta Cryst.* (2011). E**67**, o1443 [doi:10.1107/S1600536811017910]

## (*E*)-*N*′-(5-Bromo-2-methoxybenzylidene)isonicotinohydrazide

**Hong-Yan Ban**

### S1. Comment

Hydrazone compounds derived from the condensation of aldehydes with hydrazides have been demonstrated to possess excellent biological activities (Zhong *et al.*, 2007; Raj *et al.*, 2007; Jimenez-Pulido *et al.*, 2008). Due to the easy synthesis of such compounds, a number of hydrazone compounds have been synthesized and structurally characterized (Yehye *et al.*, 2008; Fun *et al.*, 2008*a*,*b*; Yang *et al.*, 2008; Ejsmont *et al.*, 2008; Yang, 2006). Recently, we have reported a few such compounds (Ban, 2010; Ban & Li, 2008*a*,*b*; Li & Ban, 2009*a*,*b*). We report here the crystal structure of the title new compound.

The asymmetric unit of the title hydrazone compound, Fig. 1, contains two independent molecules. The dihedral angles between the benzene ring and the pyridine ring in each molecule are 24.4 (6) and 23.7 (6)°, respectively. The molecules exist in a *trans* configuration with respect to the central methylidene units. In the crystal structure, molecules are linked through intermolecular N—H···O hydrogen bonds (Table 1), forming chains along the *a* axis, Fig. 2.

### S2. Experimental

The title compound was prepared by refluxing 5-bromo-2-methoxybenzaldehyde (1.0 mol, 0.22 g) with isonicotinohydrazide (1.0 mol, 0.14 g) in methanol (100 ml). Excess methanol was removed from the mixture by distillation. The colourless solid product was filtered, and washed three times with methanol. Colourless block-shaped crystals of the title compound were obtained from a methanol solution of the compound by slow evaporation in air.

### S3. Refinement

Atoms H2 and H5 were located in a difference Fourier map and refined isotropically, with the N—H distances restrained to 0.90 (1) Å. The remaining H atoms were placed in calculated positions (C—H = 0.93–0.96 Å) and refined as riding with $U_{iso}$(H) = 1.2$U_{eq}$(C) and 1.5 $U_{eq}$(C7 and C21).

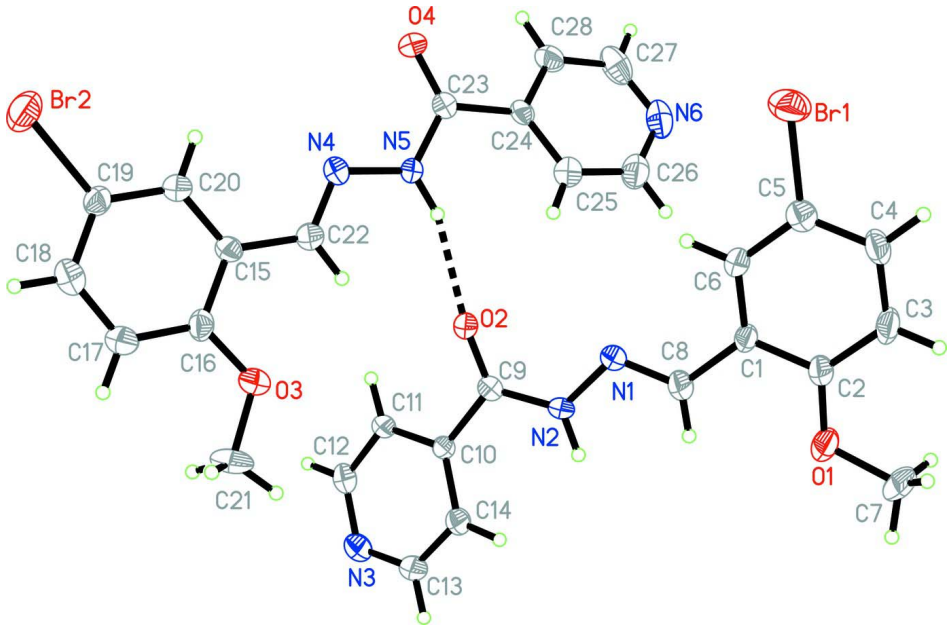


**Figure 1**

The molecular structure of the title compound, showing 30% probability displacement ellipsoids for the non-hydrogen atoms. A hydrogen bond is shown as a dashed line.

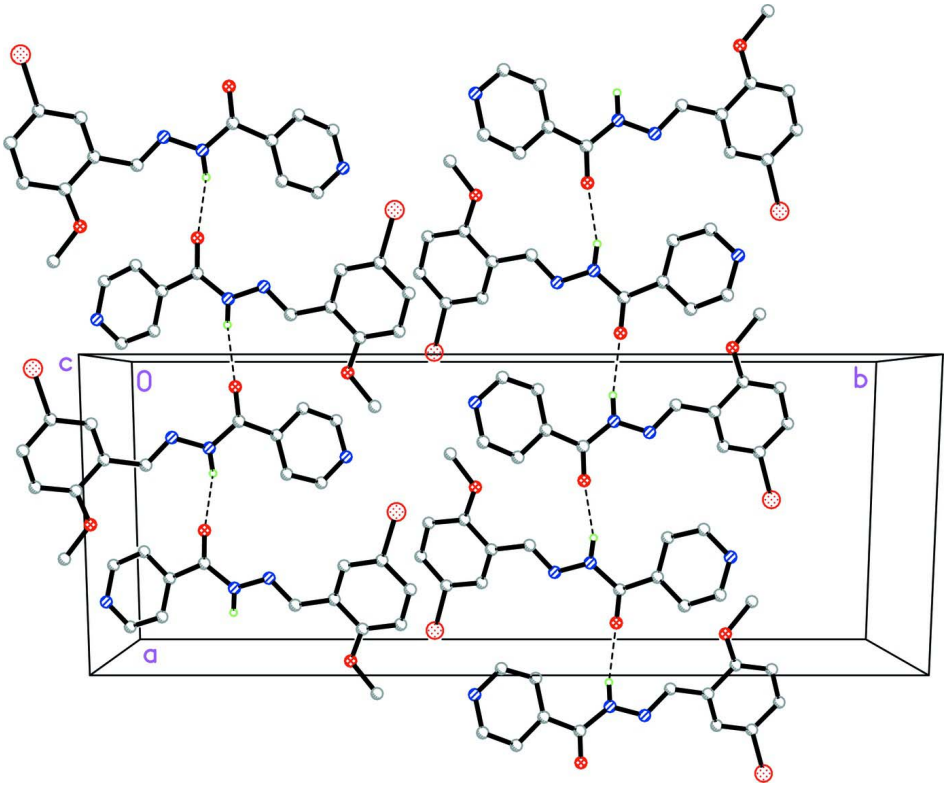


**Figure 2**

The packing diagram of the title compound, viewed along the *c* axis. Hydrogen bonds are shown as dashed lines.

**(*E*)-*N*′-(5-Bromo-2-methoxybenzylidene)isonicotinohydrazide**

*Crystal data*

$C_{14}H_{12}BrN_3O_2$
$M_r = 334.18$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.020$ (3) Å
$b = 25.732$ (2) Å
$c = 11.243$ (2) Å
$\beta = 102.199$ (3)°
$V = 2833.4$ (10) Å$^3$
$Z = 8$
$F(000) = 1344$
$D_x = 1.567$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 916 reflections
$\theta = 2.5$–$24.3°$
$\mu = 2.91$ mm$^{-1}$
$T = 298$ K
Block, colourless
0.13 × 0.10 × 0.10 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.704$, $T_{max} = 0.760$
14099 measured reflections
5922 independent reflections
2018 reflections with $I > 2\sigma(I)$
$R_{int} = 0.114$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.0°$
$h = -12 \rightarrow 12$
$k = -15 \rightarrow 32$
$l = -12 \rightarrow 14$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.143$
$S = 0.94$
5922 reflections
369 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2)]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å$^{-3}$
$\Delta\rho_{min} = -0.43$ e Å$^{-3}$

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.51353 (8) | 0.35943 (3) | 0.41403 (8) | 0.0813 (3) |
| Br2 | 0.03344 (8) | −0.09381 (3) | 0.49305 (8) | 0.0786 (3) |
| N1 | 0.7533 (5) | 0.1886 (2) | 0.2601 (5) | 0.0433 (14) |

| | | | | |
|---|---|---|---|---|
| N2 | 0.7920 (5) | 0.1410 (2) | 0.2216 (5) | 0.0483 (15) |
| N3 | 0.8554 (7) | −0.0399 (2) | 0.0738 (5) | 0.0570 (17) |
| N4 | 0.2636 (5) | 0.0667 (2) | 0.2875 (5) | 0.0469 (15) |
| N5 | 0.3008 (5) | 0.1126 (2) | 0.2381 (5) | 0.0455 (15) |
| N6 | 0.3357 (8) | 0.2873 (2) | 0.0375 (6) | 0.070 (2) |
| O1 | 1.0434 (5) | 0.29599 (17) | 0.2924 (4) | 0.0661 (14) |
| O2 | 0.5883 (5) | 0.10295 (15) | 0.2207 (4) | 0.0531 (13) |
| O3 | 0.5607 (5) | −0.03865 (16) | 0.3491 (4) | 0.0627 (14) |
| O4 | 0.0906 (5) | 0.14763 (16) | 0.2208 (5) | 0.0675 (15) |
| C1 | 0.8234 (7) | 0.2757 (2) | 0.3160 (6) | 0.0396 (17) |
| C2 | 0.9269 (8) | 0.3125 (3) | 0.3234 (6) | 0.0504 (19) |
| C3 | 0.9065 (7) | 0.3632 (3) | 0.3589 (6) | 0.056 (2) |
| H3 | 0.9754 | 0.3878 | 0.3643 | 0.068* |
| C4 | 0.7825 (8) | 0.3763 (3) | 0.3859 (6) | 0.056 (2) |
| H4 | 0.7671 | 0.4102 | 0.4087 | 0.068* |
| C5 | 0.6821 (7) | 0.3396 (3) | 0.3791 (6) | 0.0478 (19) |
| C6 | 0.7036 (7) | 0.2897 (3) | 0.3450 (6) | 0.0497 (19) |
| H6 | 0.6350 | 0.2651 | 0.3417 | 0.060* |
| C7 | 1.1577 (7) | 0.3308 (3) | 0.3069 (6) | 0.070 (2) |
| H7A | 1.1368 | 0.3586 | 0.2489 | 0.105* |
| H7B | 1.2364 | 0.3123 | 0.2936 | 0.105* |
| H7C | 1.1763 | 0.3449 | 0.3878 | 0.105* |
| C8 | 0.8473 (7) | 0.2231 (2) | 0.2755 (6) | 0.054 (2) |
| H8 | 0.9325 | 0.2146 | 0.2606 | 0.064* |
| C9 | 0.7057 (7) | 0.1007 (2) | 0.2057 (6) | 0.0432 (18) |
| C10 | 0.7624 (7) | 0.0518 (2) | 0.1629 (6) | 0.0387 (17) |
| C11 | 0.6714 (7) | 0.0151 (2) | 0.1033 (6) | 0.052 (2) |
| H11 | 0.5777 | 0.0201 | 0.0927 | 0.062* |
| C12 | 0.7233 (8) | −0.0294 (3) | 0.0596 (6) | 0.058 (2) |
| H12 | 0.6615 | −0.0534 | 0.0177 | 0.069* |
| C13 | 0.9394 (7) | −0.0048 (3) | 0.1323 (6) | 0.055 (2) |
| H13 | 1.0325 | −0.0113 | 0.1443 | 0.066* |
| C14 | 0.8989 (7) | 0.0409 (2) | 0.1769 (6) | 0.0464 (18) |
| H14 | 0.9638 | 0.0644 | 0.2165 | 0.056* |
| C15 | 0.3380 (7) | −0.0171 (2) | 0.3649 (6) | 0.0431 (18) |
| C16 | 0.4437 (7) | −0.0535 (3) | 0.3829 (6) | 0.0456 (18) |
| C17 | 0.4289 (7) | −0.1015 (3) | 0.4355 (6) | 0.055 (2) |
| H17 | 0.4998 | −0.1255 | 0.4484 | 0.066* |
| C18 | 0.3064 (8) | −0.1126 (3) | 0.4681 (6) | 0.057 (2) |
| H18 | 0.2953 | −0.1445 | 0.5040 | 0.068* |
| C19 | 0.2015 (6) | −0.0777 (3) | 0.4487 (6) | 0.0452 (18) |
| C20 | 0.2170 (7) | −0.0301 (3) | 0.3968 (6) | 0.0473 (18) |
| H20 | 0.1450 | −0.0065 | 0.3832 | 0.057* |
| C21 | 0.6772 (7) | −0.0721 (3) | 0.3758 (6) | 0.072 (2) |
| H21A | 0.6994 | −0.0793 | 0.4615 | 0.107* |
| H21B | 0.7534 | −0.0553 | 0.3525 | 0.107* |
| H21C | 0.6571 | −0.1040 | 0.3315 | 0.107* |
| C22 | 0.3574 (7) | 0.0332 (3) | 0.3104 (6) | 0.0483 (19) |

| | | | | |
|---|---|---|---|---|
| H22 | 0.4416 | 0.0407 | 0.2919 | 0.058* |
| C23 | 0.2085 (8) | 0.1511 (2) | 0.2091 (6) | 0.0479 (19) |
| C24 | 0.2575 (7) | 0.1983 (2) | 0.1524 (6) | 0.0398 (18) |
| C25 | 0.3935 (7) | 0.2111 (3) | 0.1626 (6) | 0.059 (2) |
| H25 | 0.4620 | 0.1904 | 0.2077 | 0.071* |
| C26 | 0.4257 (8) | 0.2552 (3) | 0.1049 (7) | 0.069 (2) |
| H26 | 0.5177 | 0.2632 | 0.1137 | 0.083* |
| C27 | 0.2071 (10) | 0.2744 (3) | 0.0269 (7) | 0.073 (3) |
| H27 | 0.1409 | 0.2951 | −0.0214 | 0.087* |
| C28 | 0.1643 (7) | 0.2316 (3) | 0.0838 (6) | 0.053 (2) |
| H28 | 0.0714 | 0.2253 | 0.0755 | 0.064* |
| H5 | 0.388 (2) | 0.116 (2) | 0.232 (6) | 0.080* |
| H2 | 0.880 (2) | 0.139 (3) | 0.214 (6) | 0.080* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0673 (6) | 0.0816 (6) | 0.0990 (7) | 0.0128 (5) | 0.0266 (5) | −0.0272 (6) |
| Br2 | 0.0568 (6) | 0.0881 (7) | 0.0920 (7) | −0.0143 (5) | 0.0184 (5) | 0.0230 (6) |
| N1 | 0.038 (4) | 0.035 (3) | 0.059 (4) | 0.002 (3) | 0.016 (3) | −0.003 (3) |
| N2 | 0.032 (3) | 0.034 (3) | 0.081 (4) | 0.007 (3) | 0.018 (3) | −0.001 (3) |
| N3 | 0.057 (4) | 0.039 (4) | 0.078 (5) | 0.007 (4) | 0.021 (4) | −0.002 (3) |
| N4 | 0.047 (4) | 0.032 (3) | 0.064 (4) | 0.000 (3) | 0.016 (3) | −0.002 (3) |
| N5 | 0.037 (4) | 0.030 (3) | 0.074 (4) | −0.001 (3) | 0.022 (3) | 0.007 (3) |
| N6 | 0.091 (6) | 0.044 (4) | 0.076 (5) | −0.012 (4) | 0.021 (5) | 0.000 (4) |
| O1 | 0.050 (3) | 0.054 (3) | 0.102 (4) | −0.018 (3) | 0.032 (3) | −0.016 (3) |
| O2 | 0.042 (3) | 0.033 (3) | 0.090 (4) | −0.002 (2) | 0.026 (3) | 0.000 (2) |
| O3 | 0.050 (3) | 0.049 (3) | 0.096 (4) | 0.013 (3) | 0.028 (3) | 0.011 (3) |
| O4 | 0.036 (3) | 0.045 (3) | 0.127 (5) | 0.002 (3) | 0.032 (3) | 0.003 (3) |
| C1 | 0.038 (4) | 0.034 (4) | 0.051 (5) | −0.009 (4) | 0.018 (4) | −0.004 (4) |
| C2 | 0.049 (5) | 0.035 (5) | 0.069 (6) | −0.007 (4) | 0.018 (4) | −0.012 (4) |
| C3 | 0.058 (5) | 0.040 (5) | 0.074 (6) | −0.021 (4) | 0.022 (4) | −0.002 (4) |
| C4 | 0.070 (6) | 0.033 (4) | 0.070 (6) | −0.007 (4) | 0.022 (5) | −0.015 (4) |
| C5 | 0.051 (5) | 0.047 (5) | 0.044 (5) | 0.002 (4) | 0.006 (4) | 0.001 (4) |
| C6 | 0.039 (5) | 0.039 (5) | 0.072 (6) | −0.008 (4) | 0.014 (4) | −0.008 (4) |
| C7 | 0.043 (5) | 0.078 (6) | 0.094 (6) | −0.020 (4) | 0.029 (4) | 0.000 (5) |
| C8 | 0.053 (5) | 0.034 (4) | 0.077 (6) | −0.004 (4) | 0.021 (4) | −0.011 (4) |
| C9 | 0.039 (5) | 0.033 (4) | 0.059 (5) | 0.004 (4) | 0.013 (4) | 0.003 (4) |
| C10 | 0.035 (4) | 0.031 (4) | 0.055 (5) | 0.003 (3) | 0.020 (4) | 0.007 (4) |
| C11 | 0.035 (4) | 0.030 (4) | 0.090 (6) | 0.001 (4) | 0.015 (4) | −0.004 (4) |
| C12 | 0.058 (6) | 0.033 (5) | 0.083 (6) | −0.004 (4) | 0.018 (5) | 0.000 (4) |
| C13 | 0.042 (5) | 0.043 (5) | 0.083 (6) | 0.006 (4) | 0.018 (4) | −0.003 (5) |
| C14 | 0.045 (5) | 0.033 (4) | 0.063 (5) | −0.002 (4) | 0.017 (4) | −0.009 (4) |
| C15 | 0.040 (5) | 0.033 (4) | 0.058 (5) | 0.003 (4) | 0.015 (4) | −0.008 (4) |
| C16 | 0.053 (5) | 0.034 (4) | 0.053 (5) | −0.009 (4) | 0.018 (4) | −0.005 (4) |
| C17 | 0.047 (5) | 0.050 (5) | 0.069 (6) | 0.009 (4) | 0.013 (4) | 0.000 (4) |
| C18 | 0.067 (6) | 0.042 (5) | 0.058 (5) | 0.000 (4) | 0.008 (4) | 0.003 (4) |
| C19 | 0.034 (4) | 0.045 (5) | 0.054 (5) | −0.005 (4) | 0.004 (4) | 0.006 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C20 | 0.042 (5) | 0.043 (5) | 0.059 (5) | 0.003 (4) | 0.017 (4) | 0.000 (4) |
| C21 | 0.053 (5) | 0.079 (6) | 0.085 (6) | 0.033 (5) | 0.020 (4) | −0.002 (5) |
| C22 | 0.046 (5) | 0.041 (5) | 0.063 (5) | 0.001 (4) | 0.023 (4) | 0.000 (4) |
| C23 | 0.045 (5) | 0.033 (5) | 0.069 (5) | 0.001 (4) | 0.021 (4) | 0.002 (4) |
| C24 | 0.039 (4) | 0.028 (4) | 0.052 (5) | 0.000 (4) | 0.008 (4) | −0.013 (4) |
| C25 | 0.052 (5) | 0.048 (5) | 0.078 (6) | −0.002 (4) | 0.016 (4) | 0.000 (5) |
| C26 | 0.062 (6) | 0.052 (5) | 0.092 (7) | −0.010 (5) | 0.012 (5) | 0.011 (5) |
| C27 | 0.106 (8) | 0.046 (6) | 0.063 (6) | 0.013 (5) | 0.011 (6) | 0.015 (5) |
| C28 | 0.045 (5) | 0.045 (5) | 0.066 (5) | 0.011 (4) | 0.004 (4) | 0.005 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—C5 | 1.884 (7) | C8—H8 | 0.9300 |
| Br2—C19 | 1.900 (6) | C9—C10 | 1.500 (8) |
| N1—C8 | 1.279 (7) | C10—C14 | 1.373 (8) |
| N1—N2 | 1.382 (6) | C10—C11 | 1.384 (8) |
| N2—C9 | 1.337 (8) | C11—C12 | 1.390 (8) |
| N2—H2 | 0.900 (10) | C11—H11 | 0.9300 |
| N3—C13 | 1.313 (8) | C12—H12 | 0.9300 |
| N3—C12 | 1.326 (8) | C13—C14 | 1.372 (8) |
| N4—C22 | 1.262 (7) | C13—H13 | 0.9300 |
| N4—N5 | 1.388 (6) | C14—H14 | 0.9300 |
| N5—C23 | 1.347 (8) | C15—C20 | 1.376 (8) |
| N5—H5 | 0.901 (10) | C15—C16 | 1.395 (8) |
| N6—C27 | 1.312 (9) | C15—C22 | 1.464 (8) |
| N6—C26 | 1.335 (8) | C16—C17 | 1.391 (8) |
| O1—C2 | 1.354 (8) | C17—C18 | 1.384 (9) |
| O1—C7 | 1.437 (7) | C17—H17 | 0.9300 |
| O2—C9 | 1.224 (7) | C18—C19 | 1.364 (8) |
| O3—C16 | 1.361 (7) | C18—H18 | 0.9300 |
| O3—C21 | 1.430 (7) | C19—C20 | 1.381 (8) |
| O4—C23 | 1.219 (7) | C20—H20 | 0.9300 |
| C1—C6 | 1.358 (8) | C21—H21A | 0.9600 |
| C1—C2 | 1.394 (8) | C21—H21B | 0.9600 |
| C1—C8 | 1.463 (8) | C21—H21C | 0.9600 |
| C2—C3 | 1.392 (8) | C22—H22 | 0.9300 |
| C3—C4 | 1.382 (9) | C23—C24 | 1.502 (8) |
| C3—H3 | 0.9300 | C24—C28 | 1.377 (8) |
| C4—C5 | 1.371 (8) | C24—C25 | 1.383 (8) |
| C4—H4 | 0.9300 | C25—C26 | 1.378 (9) |
| C5—C6 | 1.369 (8) | C25—H25 | 0.9300 |
| C6—H6 | 0.9300 | C26—H26 | 0.9300 |
| C7—H7A | 0.9600 | C27—C28 | 1.386 (9) |
| C7—H7B | 0.9600 | C27—H27 | 0.9300 |
| C7—H7C | 0.9600 | C28—H28 | 0.9300 |
| | | | |
| C8—N1—N2 | 114.2 (5) | N3—C13—C14 | 124.4 (7) |
| C9—N2—N1 | 120.9 (5) | N3—C13—H13 | 117.8 |

| | | | |
|---|---|---|---|
| C9—N2—H2 | 124 (4) | C14—C13—H13 | 117.8 |
| N1—N2—H2 | 115 (4) | C13—C14—C10 | 119.9 (6) |
| C13—N3—C12 | 116.0 (6) | C13—C14—H14 | 120.1 |
| C22—N4—N5 | 114.3 (6) | C10—C14—H14 | 120.1 |
| C23—N5—N4 | 119.6 (6) | C20—C15—C16 | 118.9 (6) |
| C23—N5—H5 | 122 (4) | C20—C15—C22 | 121.7 (6) |
| N4—N5—H5 | 118 (4) | C16—C15—C22 | 119.3 (6) |
| C27—N6—C26 | 115.3 (7) | O3—C16—C17 | 122.9 (6) |
| C2—O1—C7 | 119.0 (5) | O3—C16—C15 | 116.4 (6) |
| C16—O3—C21 | 119.1 (5) | C17—C16—C15 | 120.7 (7) |
| C6—C1—C2 | 119.3 (6) | C18—C17—C16 | 118.5 (7) |
| C6—C1—C8 | 122.2 (6) | C18—C17—H17 | 120.7 |
| C2—C1—C8 | 118.6 (6) | C16—C17—H17 | 120.7 |
| O1—C2—C3 | 123.7 (6) | C19—C18—C17 | 121.1 (7) |
| O1—C2—C1 | 116.3 (6) | C19—C18—H18 | 119.4 |
| C3—C2—C1 | 120.1 (7) | C17—C18—H18 | 119.4 |
| C4—C3—C2 | 119.1 (6) | C18—C19—C20 | 120.0 (6) |
| C4—C3—H3 | 120.4 | C18—C19—Br2 | 120.7 (6) |
| C2—C3—H3 | 120.4 | C20—C19—Br2 | 119.3 (5) |
| C5—C4—C3 | 120.1 (6) | C15—C20—C19 | 120.6 (6) |
| C5—C4—H4 | 120.0 | C15—C20—H20 | 119.7 |
| C3—C4—H4 | 120.0 | C19—C20—H20 | 119.7 |
| C6—C5—C4 | 120.4 (6) | O3—C21—H21A | 109.5 |
| C6—C5—Br1 | 120.9 (6) | O3—C21—H21B | 109.5 |
| C4—C5—Br1 | 118.7 (6) | H21A—C21—H21B | 109.5 |
| C1—C6—C5 | 121.1 (6) | O3—C21—H21C | 109.5 |
| C1—C6—H6 | 119.5 | H21A—C21—H21C | 109.5 |
| C5—C6—H6 | 119.5 | H21B—C21—H21C | 109.5 |
| O1—C7—H7A | 109.5 | N4—C22—C15 | 122.1 (6) |
| O1—C7—H7B | 109.5 | N4—C22—H22 | 119.0 |
| H7A—C7—H7B | 109.5 | C15—C22—H22 | 119.0 |
| O1—C7—H7C | 109.5 | O4—C23—N5 | 123.5 (6) |
| H7A—C7—H7C | 109.5 | O4—C23—C24 | 121.0 (6) |
| H7B—C7—H7C | 109.5 | N5—C23—C24 | 115.4 (6) |
| N1—C8—C1 | 121.3 (6) | C28—C24—C25 | 115.9 (6) |
| N1—C8—H8 | 119.4 | C28—C24—C23 | 119.8 (6) |
| C1—C8—H8 | 119.4 | C25—C24—C23 | 124.3 (6) |
| O2—C9—N2 | 123.9 (6) | C26—C25—C24 | 118.8 (7) |
| O2—C9—C10 | 121.6 (6) | C26—C25—H25 | 120.6 |
| N2—C9—C10 | 114.5 (6) | C24—C25—H25 | 120.6 |
| C14—C10—C11 | 117.0 (6) | N6—C26—C25 | 125.5 (8) |
| C14—C10—C9 | 124.8 (6) | N6—C26—H26 | 117.3 |
| C11—C10—C9 | 118.2 (6) | C25—C26—H26 | 117.3 |
| C10—C11—C12 | 118.4 (6) | N6—C27—C28 | 123.6 (7) |
| C10—C11—H11 | 120.8 | N6—C27—H27 | 118.2 |
| C12—C11—H11 | 120.8 | C28—C27—H27 | 118.2 |
| N3—C12—C11 | 124.3 (7) | C24—C28—C27 | 120.9 (7) |
| N3—C12—H12 | 117.9 | C24—C28—H28 | 119.5 |

| | | | |
|---|---|---|---|
| C11—C12—H12 | 117.9 | C27—C28—H28 | 119.5 |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N5—H5···O2 | 0.90 (1) | 2.06 (2) | 2.939 (7) | 164 (6) |
| N2—H2···O4$^{i}$ | 0.90 (1) | 2.11 (2) | 2.999 (7) | 168 (6) |

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