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# 2-Methoxy-*N*′-(2-methoxybenzylidene)-benzohydrazide

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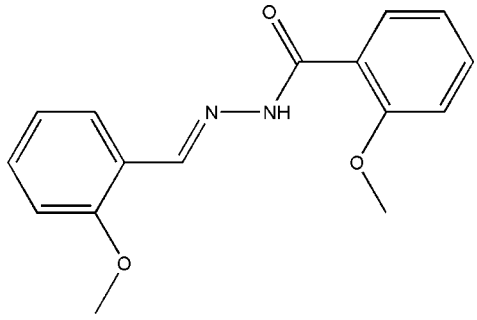
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.051; $wR$ factor = 0.095; data-to-parameter ratio = 8.4.

The title Schiff base compound, $C_{16}H_{16}N_2O_3$, was derived from the condensation of 2-methoxybenzaldehyde with 2-methoxybenzohydrazide in an ethanol solution. The dihedral angle between the two aromatic rings is 87.5 (3)°. In the crystal structure, the molecules are linked into chains running parallel to the *a* axis by intermolecular N—H···O hydrogen bonds.

## Related literature

For related literature, see: Lu *et al.* (2008*a*,*b*); Nie (2008); He (2008); Shi *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).



## Experimental

### *Crystal data*

$C_{16}H_{16}N_2O_3$
$M_r$ = 284.31
Monoclinic, $P2_1$
$a$ = 4.9998 (13) Å
$b$ = 13.475 (4) Å
$c$ = 10.824 (3) Å
$\beta$ = 93.674 (4)°
$V$ = 727.7 (4) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 298 (2) K
0.30 × 0.30 × 0.28 mm

### *Data collection*

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min}$ = 0.973, $T_{max}$ = 0.975
6081 measured reflections
1647 independent reflections
1229 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.055

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.095
$S$ = 1.11
1647 reflections
195 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2···O2$^{i}$ | 0.90 (1) | 1.99 (1) | 2.873 (3) | 167 (4) |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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: CI2648).

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# supporting information

*Acta Cryst.* (2008). E**64**, o1695 [doi:10.1107/S160053680802521X]

## 2-Methoxy-*N*′-(2-methoxybenzylidene)benzohydrazide

**Jiu-Fu Lu, Suo-Tian Min, Xiao-Hui Ji and Zhong-Hai Dang**

### S1. Comment

As part of our investigation of the crystal structures of Schiff bases derived from the condensation of aldehydes with benzohydrazides (Lu *et al.*, 2008*a*,b), we report here the crystal structure of the title new Schiff base compound.

In the title molecule (Fig. 1). the bond lengths have normal values (Allen *et al.*, 1987), and are comparable to those observed in related compounds (Nie, 2008; He, 2008; Shi *et al.*, 2007). The dihedral angle between the two aromatic rings is 87.5 (3)°, indicating that they are almost perpendicular to one another.

In the crystal structure, the molecules are linked into chains (Fig. 2) running parallel to the *a* axis by intermolecular N–H···O hydrogen bonds (Table 1).

### S2. Experimental

The title compound was prepared by the Schiff base condensation of 2-methoxybenzaldehyde (0.1 mol) and 2-methoxybenzohydrazide (0.1 mmol) in ethanol (50 ml). The excess ethanol was removed by distillation. The colorless solid obtained was filtered and washed with ethanol. Single crystals suitable for X-ray diffraction were obatined by slow evaporation of an ethanol solution at room temperature.

### S3. Refinement

The imino H atom was located in a difference map and refined with a N–H distance restraint of 0.90 (1) Å. The other H atoms were positioned geometrically (C–H = 0.93-0.96 Å) and refined using a riding model, with $U_{iso}$(H) = 1.2$U_{eq}$(C) and 1.5$U_{eq}$($C_{methyl}$). In the absence of significant anomalous scattering, Friedel pairs were merged.

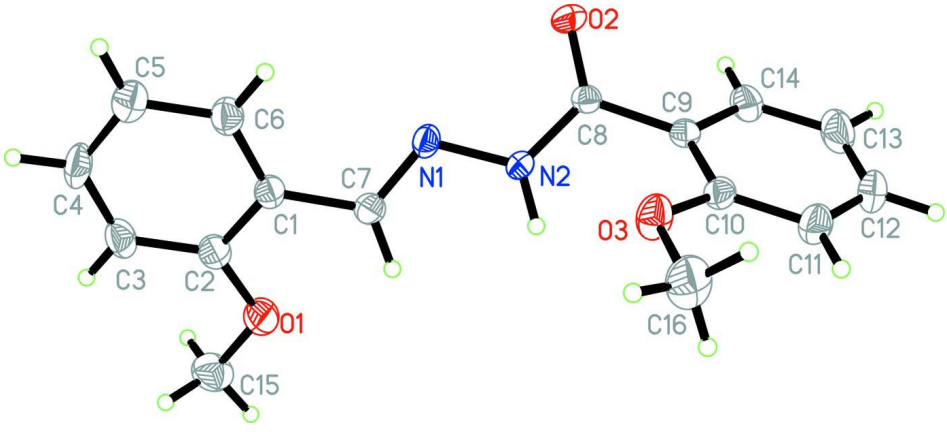


**Figure 1**

The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. Dashed lines indicate hydrogen bonds.

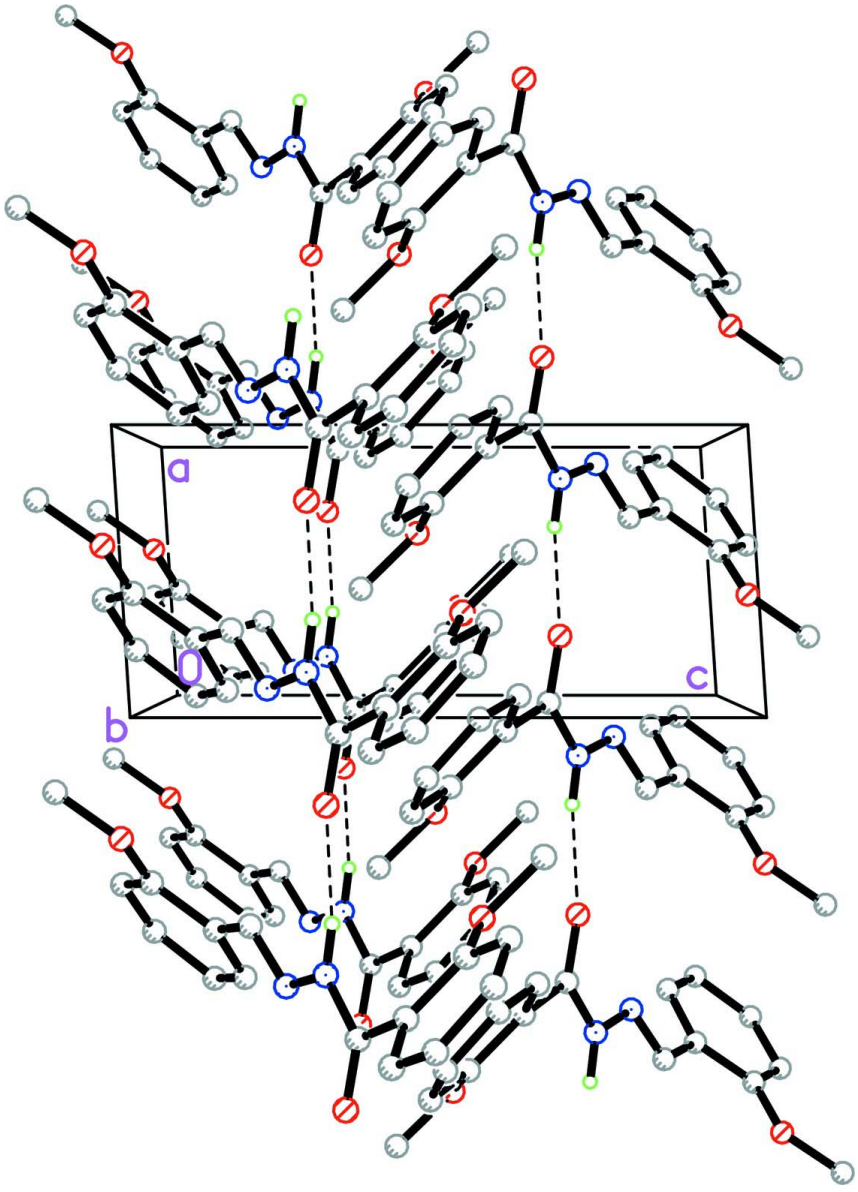


**Figure 2**

The crystal packing of the title compound, viewed along the *b* axis. Dashed lines indicate hydrogen bonds.

### 2-Methoxy-*N*′-(2-methoxybenzylidene)benzohydrazide

*Crystal data*

$C_{16}H_{16}N_2O_3$
$M_r = 284.31$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 4.9998\ (13)$ Å
$b = 13.475\ (4)$ Å
$c = 10.824\ (3)$ Å
$\beta = 93.674\ (4)°$
$V = 727.7\ (4)$ Å$^3$
$Z = 2$

$F(000) = 300$
$D_x = 1.297$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 744 reflections
$\theta = 2.5–24.0°$
$\mu = 0.09$ mm$^{-1}$
$T = 298$ K
Block, colourless
0.30 × 0.30 × 0.28 mm

*Data collection*

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min}$ = 0.973, $T_{max}$ = 0.975
6081 measured reflections
1647 independent reflections
1229 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.055
$\theta_{max}$ = 27.0°, $\theta_{min}$ = 1.9°
$h = -6 \rightarrow 6$
$k = -17 \rightarrow 16$
$l = -13 \rightarrow 13$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.095
$S$ = 1.11
1647 reflections
195 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
$w = 1/[\sigma^2(F_o^2) + (0.0297P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 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 $F^2 > 2$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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.4130 (5) | 0.5063 (2) | 1.0258 (2) | 0.0579 (8) |
| O2 | 1.2673 (4) | 0.71624 (19) | 0.6930 (2) | 0.0436 (6) |
| O3 | 0.6361 (5) | 0.7245 (2) | 0.4683 (2) | 0.0513 (6) |
| N1 | 0.8931 (5) | 0.5916 (2) | 0.7771 (2) | 0.0357 (7) |
| N2 | 0.8339 (5) | 0.67811 (19) | 0.7116 (3) | 0.0354 (7) |
| C1 | 0.7337 (7) | 0.4561 (2) | 0.8904 (3) | 0.0371 (9) |
| C2 | 0.5766 (7) | 0.4321 (3) | 0.9892 (3) | 0.0426 (9) |
| C3 | 0.6008 (7) | 0.3398 (3) | 1.0439 (3) | 0.0501 (10) |
| H3 | 0.4953 | 0.3233 | 1.1086 | 0.060* |
| C4 | 0.7794 (8) | 0.2725 (3) | 1.0032 (4) | 0.0549 (11) |
| H4 | 0.7928 | 0.2102 | 1.0400 | 0.066* |
| C5 | 0.9407 (8) | 0.2954 (3) | 0.9081 (4) | 0.0537 (10) |
| H5 | 1.0645 | 0.2498 | 0.8818 | 0.064* |
| C6 | 0.9142 (7) | 0.3876 (3) | 0.8529 (3) | 0.0455 (9) |
| H6 | 1.0216 | 0.4036 | 0.7887 | 0.055* |

| | | | | |
|---|---|---|---|---|
| C7 | 0.6996 (7) | 0.5520 (2) | 0.8295 (3) | 0.0377 (8) |
| H7 | 0.5353 | 0.5844 | 0.8291 | 0.045* |
| C8 | 1.0305 (6) | 0.7328 (2) | 0.6674 (3) | 0.0296 (7) |
| C9 | 0.9390 (6) | 0.8198 (2) | 0.5913 (3) | 0.0343 (8) |
| C10 | 0.7391 (6) | 0.8162 (3) | 0.4959 (3) | 0.0358 (8) |
| C11 | 0.6635 (7) | 0.9012 (3) | 0.4321 (3) | 0.0518 (10) |
| H11 | 0.5257 | 0.8990 | 0.3703 | 0.062* |
| C12 | 0.7913 (8) | 0.9890 (3) | 0.4597 (4) | 0.0606 (12) |
| H12 | 0.7384 | 1.0462 | 0.4168 | 0.073* |
| C13 | 0.9946 (8) | 0.9936 (3) | 0.5493 (4) | 0.0617 (12) |
| H13 | 1.0835 | 1.0533 | 0.5659 | 0.074* |
| C14 | 1.0677 (7) | 0.9096 (3) | 0.6151 (4) | 0.0478 (10) |
| H14 | 1.2059 | 0.9131 | 0.6767 | 0.057* |
| C15 | 0.2563 (8) | 0.4878 (4) | 1.1267 (4) | 0.0653 (12) |
| H15A | 0.1495 | 0.4295 | 1.1105 | 0.098* |
| H15B | 0.1410 | 0.5435 | 1.1385 | 0.098* |
| H15C | 0.3714 | 0.4778 | 1.2001 | 0.098* |
| C16 | 0.4372 (8) | 0.7167 (4) | 0.3692 (3) | 0.0712 (12) |
| H16A | 0.2821 | 0.7542 | 0.3885 | 0.107* |
| H16B | 0.3884 | 0.6483 | 0.3573 | 0.107* |
| H16C | 0.5066 | 0.7422 | 0.2949 | 0.107* |
| H2 | 0.662 (3) | 0.696 (3) | 0.696 (3) | 0.080* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0577 (16) | 0.0581 (19) | 0.0601 (19) | 0.0064 (15) | 0.0196 (15) | 0.0132 (15) |
| O2 | 0.0265 (12) | 0.0451 (14) | 0.0586 (14) | 0.0050 (12) | −0.0024 (10) | 0.0062 (13) |
| O3 | 0.0604 (15) | 0.0471 (15) | 0.0439 (13) | −0.0052 (14) | −0.0149 (11) | 0.0053 (14) |
| N1 | 0.0391 (16) | 0.0318 (15) | 0.0356 (15) | 0.0028 (13) | −0.0030 (13) | 0.0079 (13) |
| N2 | 0.0271 (14) | 0.0357 (16) | 0.0428 (16) | 0.0036 (13) | −0.0018 (13) | 0.0124 (13) |
| C1 | 0.037 (2) | 0.038 (2) | 0.0354 (19) | −0.0036 (16) | −0.0070 (16) | 0.0053 (16) |
| C2 | 0.041 (2) | 0.046 (2) | 0.040 (2) | −0.0060 (18) | −0.0050 (18) | 0.0062 (18) |
| C3 | 0.054 (2) | 0.051 (3) | 0.045 (2) | −0.011 (2) | −0.0020 (18) | 0.0176 (19) |
| C4 | 0.069 (3) | 0.035 (2) | 0.058 (3) | 0.000 (2) | −0.016 (2) | 0.018 (2) |
| C5 | 0.061 (3) | 0.043 (2) | 0.056 (3) | 0.0023 (19) | −0.001 (2) | 0.001 (2) |
| C6 | 0.049 (2) | 0.042 (2) | 0.045 (2) | −0.0021 (19) | 0.0002 (18) | 0.0085 (18) |
| C7 | 0.0336 (18) | 0.043 (2) | 0.0357 (19) | 0.0002 (16) | −0.0008 (16) | 0.0078 (16) |
| C8 | 0.0279 (17) | 0.0279 (18) | 0.0332 (16) | −0.0013 (15) | 0.0026 (13) | −0.0029 (15) |
| C9 | 0.0317 (17) | 0.0346 (19) | 0.0377 (18) | 0.0046 (15) | 0.0098 (14) | 0.0017 (16) |
| C10 | 0.0368 (19) | 0.0353 (19) | 0.0357 (19) | 0.0037 (16) | 0.0051 (15) | 0.0015 (17) |
| C11 | 0.055 (2) | 0.056 (3) | 0.044 (2) | 0.008 (2) | 0.001 (2) | 0.013 (2) |
| C12 | 0.065 (3) | 0.046 (3) | 0.071 (3) | 0.007 (2) | 0.009 (2) | 0.027 (2) |
| C13 | 0.072 (3) | 0.039 (2) | 0.076 (3) | −0.010 (2) | 0.014 (3) | 0.008 (2) |
| C14 | 0.048 (2) | 0.037 (2) | 0.058 (2) | −0.0087 (19) | 0.0060 (19) | 0.003 (2) |
| C15 | 0.060 (3) | 0.083 (3) | 0.054 (3) | −0.002 (3) | 0.012 (2) | 0.009 (2) |
| C16 | 0.077 (3) | 0.078 (3) | 0.055 (2) | −0.014 (3) | −0.023 (2) | 0.009 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C2 | 1.367 (4) | C6—H6 | 0.93 |
| O1—C15 | 1.407 (4) | C7—H7 | 0.93 |
| O2—C8 | 1.220 (3) | C8—C9 | 1.488 (4) |
| O3—C10 | 1.364 (4) | C9—C14 | 1.387 (5) |
| O3—C16 | 1.419 (4) | C9—C10 | 1.391 (4) |
| N1—C7 | 1.270 (4) | C10—C11 | 1.378 (5) |
| N1—N2 | 1.387 (3) | C11—C12 | 1.368 (5) |
| N2—C8 | 1.341 (4) | C11—H11 | 0.93 |
| N2—H2 | 0.901 (10) | C12—C13 | 1.360 (5) |
| C1—C6 | 1.370 (5) | C12—H12 | 0.93 |
| C1—C2 | 1.405 (5) | C13—C14 | 1.375 (5) |
| C1—C7 | 1.456 (4) | C13—H13 | 0.93 |
| C2—C3 | 1.380 (5) | C14—H14 | 0.93 |
| C3—C4 | 1.365 (5) | C15—H15A | 0.96 |
| C3—H3 | 0.93 | C15—H15B | 0.96 |
| C4—C5 | 1.383 (5) | C15—H15C | 0.96 |
| C4—H4 | 0.93 | C16—H16A | 0.96 |
| C5—C6 | 1.381 (5) | C16—H16B | 0.96 |
| C5—H5 | 0.93 | C16—H16C | 0.96 |
| | | | |
| C2—O1—C15 | 118.0 (3) | C14—C9—C10 | 118.1 (3) |
| C10—O3—C16 | 118.0 (3) | C14—C9—C8 | 117.5 (3) |
| C7—N1—N2 | 115.9 (3) | C10—C9—C8 | 124.3 (3) |
| C8—N2—N1 | 120.5 (2) | O3—C10—C11 | 123.8 (3) |
| C8—N2—H2 | 120 (3) | O3—C10—C9 | 115.9 (3) |
| N1—N2—H2 | 120 (3) | C11—C10—C9 | 120.3 (3) |
| C6—C1—C2 | 118.8 (3) | C12—C11—C10 | 120.0 (4) |
| C6—C1—C7 | 121.6 (3) | C12—C11—H11 | 120.0 |
| C2—C1—C7 | 119.6 (3) | C10—C11—H11 | 120.0 |
| O1—C2—C3 | 125.0 (3) | C13—C12—C11 | 120.8 (4) |
| O1—C2—C1 | 115.3 (3) | C13—C12—H12 | 119.6 |
| C3—C2—C1 | 119.7 (4) | C11—C12—H12 | 119.6 |
| C4—C3—C2 | 120.1 (4) | C12—C13—C14 | 119.6 (4) |
| C4—C3—H3 | 120.0 | C12—C13—H13 | 120.2 |
| C2—C3—H3 | 119.9 | C14—C13—H13 | 120.2 |
| C3—C4—C5 | 121.1 (3) | C13—C14—C9 | 121.2 (4) |
| C3—C4—H4 | 119.5 | C13—C14—H14 | 119.4 |
| C5—C4—H4 | 119.5 | C9—C14—H14 | 119.4 |
| C6—C5—C4 | 118.6 (4) | O1—C15—H15A | 109.5 |
| C6—C5—H5 | 120.7 | O1—C15—H15B | 109.5 |
| C4—C5—H5 | 120.7 | H15A—C15—H15B | 109.5 |
| C1—C6—C5 | 121.6 (4) | O1—C15—H15C | 109.5 |
| C1—C6—H6 | 119.2 | H15A—C15—H15C | 109.5 |
| C5—C6—H6 | 119.2 | H15B—C15—H15C | 109.5 |
| N1—C7—C1 | 120.3 (3) | O3—C16—H16A | 109.5 |
| N1—C7—H7 | 119.9 | O3—C16—H16B | 109.5 |

| | | | |
|---|---|---|---|
| C1—C7—H7 | 119.9 | H16A—C16—H16B | 109.5 |
| O2—C8—N2 | 122.8 (3) | O3—C16—H16C | 109.5 |
| O2—C8—C9 | 122.0 (3) | H16A—C16—H16C | 109.5 |
| N2—C8—C9 | 115.1 (3) | H16B—C16—H16C | 109.5 |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2···O2$^{i}$ | 0.90 (1) | 1.99 (1) | 2.873 (3) | 167 (4) |

Symmetry code: (i) *x*−1, *y*, *z*.