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# *N*′-(3-Ethoxy-2-hydroxybenzylidene)-4-hydroxy-3-methoxybenzohydrazide monohydrate

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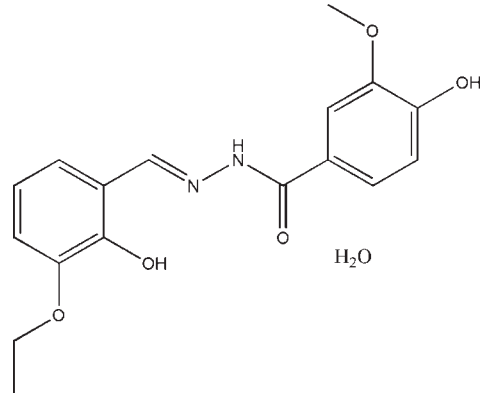
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.041; $wR$ factor = 0.111; data-to-parameter ratio = 15.1.

In the title compound, $C_{17}H_{18}N_2O_5\cdot H_2O$, the dihedral angle between the two aromatic rings is 7.86 (7)° and an intramolecular O—H···N hydrogen bond is observed. In the crystal structure, molecules are linked into a three-dimensional network by intermolecular O—H···O and N—H···O hydrogen bonds.

## Related literature

For related structures, see: Lu *et al.* (2008*a*,*b*,*c*); Abdul Alhadi *et al.* (2009); Mohd Lair *et al.* (2009); Narayana *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).




## Experimental

### *Crystal data*

$C_{17}H_{18}N_2O_5\cdot H_2O$
$M_r$ = 348.35
Monoclinic, $P2_1/n$
$a$ = 9.4063 (11) Å
$b$ = 10.0598 (12) Å
$c$ = 17.667 (2) Å
$\beta$ = 93.702 (2)°
$V$ = 1668.3 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 298 K
0.23 × 0.20 × 0.20 mm

### *Data collection*

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min}$ = 0.976, $T_{max}$ = 0.979
9554 measured reflections
3606 independent reflections
2530 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.111
$S$ = 1.05
3606 reflections
239 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···N1 | 0.82 | 1.94 | 2.6529 (16) | 144 |
| O5—H5···O6$^{i}$ | 0.82 | 1.81 | 2.6177 (17) | 170 |
| O6—H6$A$···O3$^{ii}$ | 0.84 (1) | 1.96 (1) | 2.7908 (17) | 176 (2) |
| O6—H6$B$···O1$^{iii}$ | 0.84 (1) | 2.08 (1) | 2.8714 (18) | 157 (2) |
| N2—H2···O4$^{iv}$ | 0.89 (1) | 2.54 (2) | 3.1181 (17) | 123 (2) |
| N2—H2···O5$^{iv}$ | 0.89 (1) | 2.19 (1) | 3.0496 (18) | 163 (2) |

Symmetry codes: (i) $x-1, y, z$; (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x-\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

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: CI2887).

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# supporting information

*Acta Cryst.* (2009). E**65**, o2316 [doi:10.1107/S1600536809033236]

## *N*′-(3-Ethoxy-2-hydroxybenzylidene)-4-hydroxy-3-methoxybenzohydrazide monohydrate

**Jiu-Fu Lu, Yue-Fei Bai, Suo-Tian Min, Hong-Guang Ge and Xiao-Hui Ji**

### S1. Comment

Schiff bases and their metal complexes have received much attention in recent years. As part of our investigation on crystal structures of Schiff bases derived from the condensation of aldehydes with benzohydrazides (Lu *et al.*, 2008*a*,b,c), we report herein the crystal structure of the title new Schiff base compound.

The asymmetric unit of the title compound (Fig. 1), consists of a Schiff base molecule and a water molecule of crystallization. The bond lengths have normal values (Allen *et al.*, 1987), and are comparable to those observed in similar compounds (Abdul Alhadi *et al.*, 2009; Mohd Lair *et al.*, 2009; Narayana *et al.*, 2007). The dihedral angle between the two aromatic rings is 7.86 (7)°, indicating that they are approximately coplanar. The methoxy and ethoxy groups are coplanar with the attached rings [C17—O4—C11—C10 = 4.6 (2)°, C15—O2—C3—C4 = -2.6 (2)° and C3—O2—C15—C16 = 177.98 (14)]. An intramolecular O—H···N hydrogen bond is observed (Table 1 and Fig. 1).

In the crystal structure, molecules are linked into a three-dimensional network (Fig. 2) by intermolecular O—H···O and N—H···O hydrogen bonds (Table 1).

### S2. Experimental

The title compound was prepared by the Schiff base condensation of 2-hydroxy-3-ethoxybenzaldehyde (0.1 mol) and 4-hydroxy-3-methoxybenzohydrazide (0.1 mmol) in 95% ethanol (50 ml). The excess ethanol was removed by distillation. The colourless solid obtained was filtered and washed with ethanol. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a 95% ethanol solution at room temperature.

### S3. Refinement

The imino and water H atoms were located in a difference map and refined with N-H, O-H, and H···H distance restraints of 0.90 (1), 0.85 (1) and 1.37 (2) Å, respectively. Other H atoms were positioned geometrically (C-H = 0.93-0.97 Å, O-H = 0.82 Å) and refined using a riding model, with $U_{iso}$(H) = 1.2$U_{eq}$(C) and 1.5$U_{eq}$($C_{methyl}$ and O).

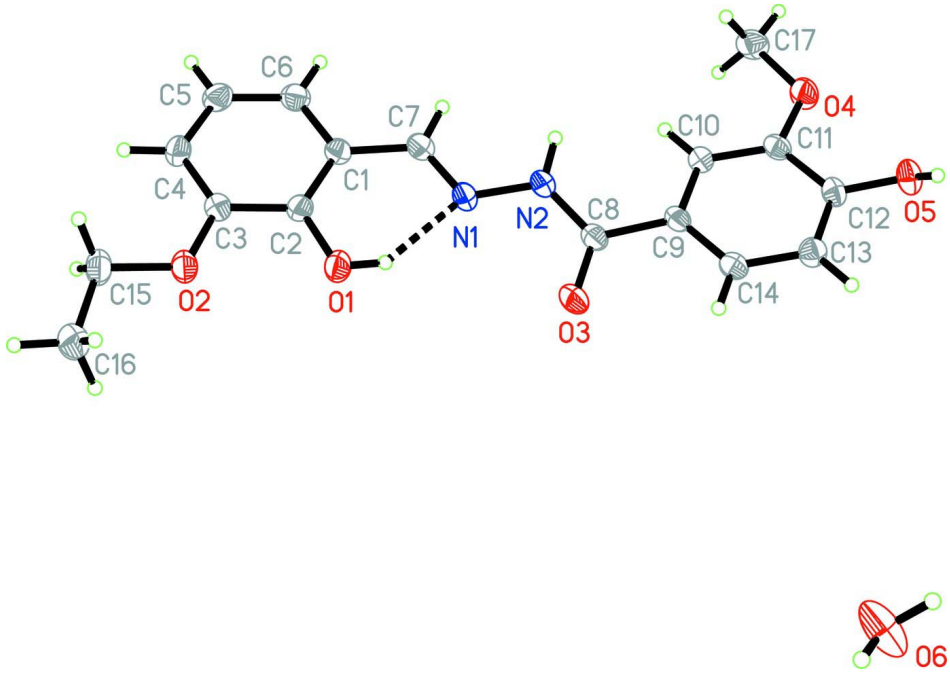


**Figure 1**

The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. The dashed line indicates a hydrogen bond.

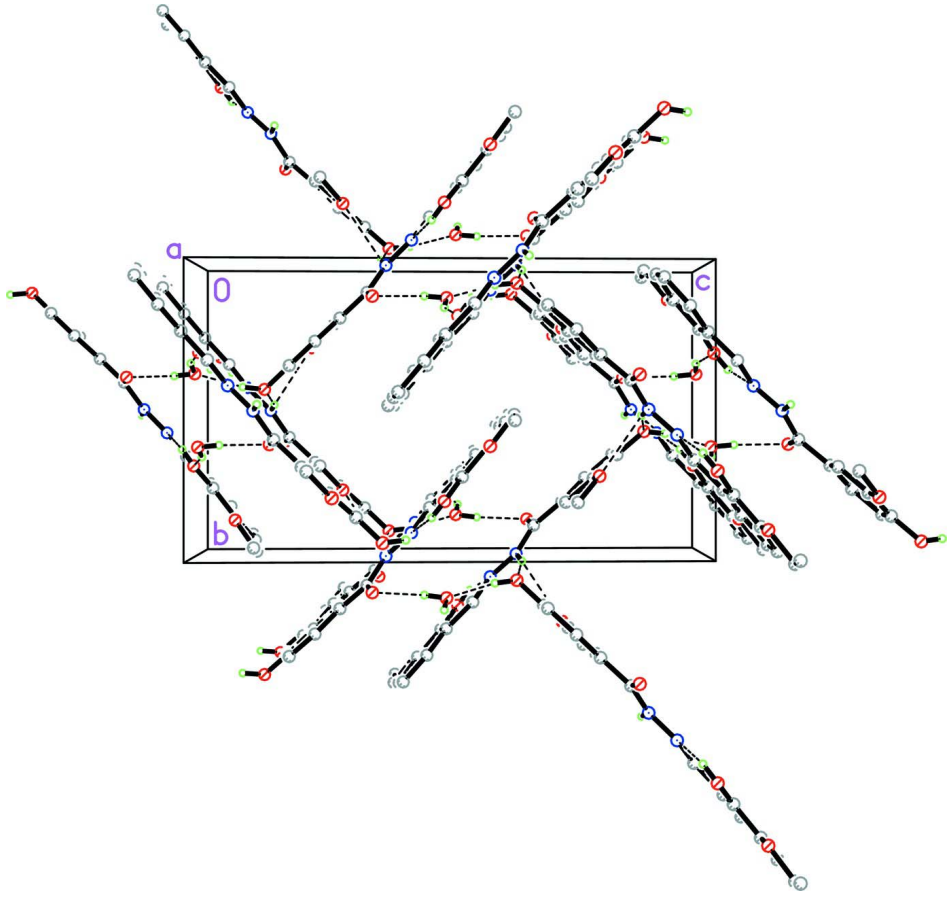


**Figure 2**

The crystal packing of the title compound, viewed along the a axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

### *N*′-(3-Ethoxy-2-hydroxybenzylidene)-4-hydroxy-3-methoxybenzohydrazide monohydrate

*Crystal data*

$C_{17}H_{18}N_2O_5 \cdot H_2O$
$M_r = 348.35$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 9.4063$ (11) Å
$b = 10.0598$ (12) Å
$c = 17.667$ (2) Å
$\beta = 93.702$ (2)°
$V = 1668.3$ (3) Å$^3$
$Z = 4$
$F(000) = 736$
$D_x = 1.387$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2358 reflections
$\theta = 2.3$–24.5°
$\mu = 0.11$ mm$^{-1}$
$T = 298$ K
Block, colourless
0.23 × 0.20 × 0.20 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)
$T_{min} = 0.976$, $T_{max} = 0.979$
9554 measured reflections
3606 independent reflections
2530 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.022
$\theta_{max}$ = 27.0°, $\theta_{min}$ = 2.3°
$h$ = −12→6
$k$ = −12→12
$l$ = −19→22

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.111
$S$ = 1.05
3606 reflections
239 parameters
4 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
$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 0.153P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.10205 (14) | 0.58113 (13) | 0.92228 (7) | 0.0430 (3) |
| N2 | 0.02746 (14) | 0.49793 (13) | 0.87165 (7) | 0.0439 (3) |
| O1 | 0.33352 (11) | 0.69470 (12) | 0.98717 (7) | 0.0540 (3) |
| H1 | 0.2897 | 0.6377 | 0.9621 | 0.081* |
| O2 | 0.44363 (11) | 0.88030 (11) | 1.07376 (6) | 0.0500 (3) |
| O3 | 0.22665 (12) | 0.38467 (12) | 0.84788 (6) | 0.0540 (3) |
| O4 | −0.35636 (11) | 0.22118 (12) | 0.71623 (6) | 0.0519 (3) |
| O5 | −0.21352 (12) | 0.07248 (12) | 0.62606 (6) | 0.0495 (3) |
| H5 | −0.1832 | 0.0803 | 0.5838 | 0.074* |
| O6 | 0.87031 (16) | 0.12628 (18) | 0.49098 (7) | 0.0831 (5) |
| C1 | 0.09270 (16) | 0.76123 (14) | 1.00984 (8) | 0.0386 (4) |
| C2 | 0.23985 (16) | 0.77422 (14) | 1.02122 (8) | 0.0381 (3) |
| C3 | 0.29798 (17) | 0.87517 (15) | 1.06851 (8) | 0.0401 (4) |
| C4 | 0.20833 (19) | 0.95870 (16) | 1.10488 (9) | 0.0461 (4) |
| H4 | 0.2463 | 1.0260 | 1.1361 | 0.055* |
| C5 | 0.06202 (19) | 0.94300 (17) | 1.09513 (9) | 0.0491 (4) |
| H5A | 0.0024 | 0.9986 | 1.1207 | 0.059* |
| C6 | 0.00461 (18) | 0.84627 (16) | 1.04808 (9) | 0.0455 (4) |
| H6 | −0.0938 | 0.8371 | 1.0415 | 0.055* |
| C7 | 0.02778 (17) | 0.66469 (15) | 0.95732 (8) | 0.0432 (4) |
| H7 | −0.0708 | 0.6636 | 0.9489 | 0.052* |

| | | | | |
|---|---|---|---|---|
| C8 | 0.09772 (16) | 0.40175 (15) | 0.83586 (8) | 0.0384 (4) |
| C9 | 0.01099 (15) | 0.31662 (14) | 0.78123 (8) | 0.0351 (3) |
| C10 | −0.13784 (16) | 0.31459 (14) | 0.77666 (8) | 0.0365 (3) |
| H10 | −0.1878 | 0.3686 | 0.8084 | 0.044* |
| C11 | −0.21102 (15) | 0.23219 (15) | 0.72488 (8) | 0.0366 (3) |
| C12 | −0.13654 (17) | 0.15245 (14) | 0.67632 (8) | 0.0377 (3) |
| C13 | 0.01011 (17) | 0.15321 (15) | 0.68193 (8) | 0.0420 (4) |
| H13 | 0.0602 | 0.0985 | 0.6506 | 0.050* |
| C14 | 0.08347 (16) | 0.23511 (15) | 0.73412 (8) | 0.0397 (4) |
| H14 | 0.1825 | 0.2351 | 0.7374 | 0.048* |
| C15 | 0.50926 (19) | 0.98456 (17) | 1.11853 (11) | 0.0572 (5) |
| H15A | 0.4796 | 0.9801 | 1.1701 | 0.069* |
| H15B | 0.4817 | 1.0705 | 1.0974 | 0.069* |
| C16 | 0.66733 (19) | 0.9667 (2) | 1.11801 (12) | 0.0642 (5) |
| H16A | 0.6931 | 0.8805 | 1.1379 | 0.096* |
| H16B | 0.7144 | 1.0340 | 1.1489 | 0.096* |
| H16C | 0.6958 | 0.9740 | 1.0670 | 0.096* |
| C17 | −0.44022 (17) | 0.30663 (19) | 0.75946 (10) | 0.0555 (5) |
| H17A | −0.4195 | 0.2898 | 0.8125 | 0.083* |
| H17B | −0.5394 | 0.2902 | 0.7466 | 0.083* |
| H17C | −0.4184 | 0.3975 | 0.7484 | 0.083* |
| H2 | −0.0640 (12) | 0.519 (2) | 0.8616 (11) | 0.080* |
| H6A | 0.8271 (18) | 0.119 (2) | 0.4483 (7) | 0.080* |
| H6B | 0.9512 (13) | 0.161 (2) | 0.4869 (11) | 0.080* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0430 (8) | 0.0417 (7) | 0.0424 (7) | −0.0028 (6) | −0.0102 (6) | −0.0046 (6) |
| N2 | 0.0378 (7) | 0.0425 (7) | 0.0495 (7) | −0.0006 (6) | −0.0130 (6) | −0.0076 (6) |
| O1 | 0.0423 (7) | 0.0555 (7) | 0.0638 (8) | 0.0032 (6) | −0.0008 (6) | −0.0259 (6) |
| O2 | 0.0426 (7) | 0.0509 (7) | 0.0560 (7) | −0.0028 (5) | −0.0007 (5) | −0.0188 (5) |
| O3 | 0.0348 (6) | 0.0661 (8) | 0.0591 (7) | 0.0020 (6) | −0.0115 (5) | −0.0130 (6) |
| O4 | 0.0321 (6) | 0.0615 (7) | 0.0616 (7) | −0.0057 (5) | −0.0012 (5) | −0.0146 (6) |
| O5 | 0.0477 (7) | 0.0577 (7) | 0.0426 (6) | −0.0144 (6) | 0.0003 (5) | −0.0110 (5) |
| O6 | 0.0632 (9) | 0.1350 (14) | 0.0491 (7) | −0.0436 (9) | −0.0107 (7) | 0.0188 (8) |
| C1 | 0.0404 (9) | 0.0381 (8) | 0.0367 (8) | 0.0013 (7) | −0.0030 (7) | 0.0019 (6) |
| C2 | 0.0421 (9) | 0.0359 (8) | 0.0360 (7) | 0.0038 (7) | 0.0012 (7) | −0.0027 (6) |
| C3 | 0.0393 (9) | 0.0415 (8) | 0.0391 (8) | 0.0004 (7) | −0.0014 (7) | −0.0028 (7) |
| C4 | 0.0549 (11) | 0.0411 (9) | 0.0420 (8) | 0.0016 (8) | −0.0001 (8) | −0.0104 (7) |
| C5 | 0.0500 (10) | 0.0490 (10) | 0.0488 (9) | 0.0113 (8) | 0.0060 (8) | −0.0058 (7) |
| C6 | 0.0416 (9) | 0.0481 (9) | 0.0465 (9) | 0.0043 (8) | 0.0008 (7) | 0.0004 (7) |
| C7 | 0.0396 (9) | 0.0448 (9) | 0.0442 (9) | 0.0001 (7) | −0.0061 (7) | 0.0000 (7) |
| C8 | 0.0367 (9) | 0.0412 (9) | 0.0362 (8) | −0.0015 (7) | −0.0055 (7) | 0.0024 (6) |
| C9 | 0.0349 (8) | 0.0366 (8) | 0.0328 (7) | −0.0019 (7) | −0.0047 (6) | 0.0039 (6) |
| C10 | 0.0364 (8) | 0.0378 (8) | 0.0350 (7) | 0.0002 (7) | −0.0006 (6) | −0.0010 (6) |
| C11 | 0.0302 (8) | 0.0400 (8) | 0.0391 (8) | −0.0041 (7) | −0.0017 (6) | 0.0048 (6) |
| C12 | 0.0408 (8) | 0.0382 (8) | 0.0334 (7) | −0.0085 (7) | −0.0024 (6) | 0.0001 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C13 | 0.0399 (9) | 0.0457 (9) | 0.0407 (8) | −0.0014 (7) | 0.0057 (7) | −0.0030 (7) |
| C14 | 0.0314 (8) | 0.0449 (9) | 0.0422 (8) | −0.0019 (7) | −0.0009 (7) | 0.0017 (7) |
| C15 | 0.0513 (11) | 0.0513 (10) | 0.0682 (11) | −0.0078 (9) | −0.0016 (9) | −0.0219 (9) |
| C16 | 0.0497 (11) | 0.0614 (12) | 0.0804 (13) | −0.0063 (9) | −0.0032 (10) | −0.0139 (10) |
| C17 | 0.0362 (9) | 0.0684 (12) | 0.0622 (11) | 0.0030 (9) | 0.0043 (8) | −0.0016 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C7 | 1.278 (2) | C5—H5A | 0.93 |
| N1—N2 | 1.3827 (17) | C6—H6 | 0.93 |
| N2—C8 | 1.352 (2) | C7—H7 | 0.93 |
| N2—H2 | 0.891 (9) | C8—C9 | 1.493 (2) |
| O1—C2 | 1.3589 (18) | C9—C14 | 1.380 (2) |
| O1—H1 | 0.82 | C9—C10 | 1.397 (2) |
| O2—C3 | 1.3681 (19) | C10—C11 | 1.384 (2) |
| O2—C15 | 1.4296 (18) | C10—H10 | 0.93 |
| O3—C8 | 1.2297 (18) | C11—C12 | 1.396 (2) |
| O4—C11 | 1.3703 (17) | C12—C13 | 1.377 (2) |
| O4—C17 | 1.422 (2) | C13—C14 | 1.387 (2) |
| O5—C12 | 1.3700 (17) | C13—H13 | 0.93 |
| O5—H5 | 0.82 | C14—H14 | 0.93 |
| O6—H6A | 0.836 (9) | C15—C16 | 1.498 (2) |
| O6—H6B | 0.844 (9) | C15—H15A | 0.97 |
| C1—C2 | 1.392 (2) | C15—H15B | 0.97 |
| C1—C6 | 1.395 (2) | C16—H16A | 0.96 |
| C1—C7 | 1.450 (2) | C16—H16B | 0.96 |
| C2—C3 | 1.403 (2) | C16—H16C | 0.96 |
| C3—C4 | 1.378 (2) | C17—H17A | 0.96 |
| C4—C5 | 1.385 (2) | C17—H17B | 0.96 |
| C4—H4 | 0.93 | C17—H17C | 0.96 |
| C5—C6 | 1.368 (2) | | |

| | | | |
|---|---|---|---|
| C7—N1—N2 | 116.17 (13) | C10—C9—C8 | 123.32 (13) |
| C8—N2—N1 | 119.54 (13) | C11—C10—C9 | 120.03 (14) |
| C8—N2—H2 | 124.6 (13) | C11—C10—H10 | 120.0 |
| N1—N2—H2 | 115.6 (13) | C9—C10—H10 | 120.0 |
| C2—O1—H1 | 109.5 | O4—C11—C10 | 124.89 (14) |
| C3—O2—C15 | 117.38 (12) | O4—C11—C12 | 114.95 (12) |
| C11—O4—C17 | 118.38 (12) | C10—C11—C12 | 120.16 (13) |
| C12—O5—H5 | 109.5 | O5—C12—C13 | 122.36 (14) |
| H6A—O6—H6B | 110.4 (17) | O5—C12—C11 | 118.08 (13) |
| C2—C1—C6 | 119.25 (14) | C13—C12—C11 | 119.53 (13) |
| C2—C1—C7 | 121.93 (14) | C12—C13—C14 | 120.30 (14) |
| C6—C1—C7 | 118.79 (14) | C12—C13—H13 | 119.8 |
| O1—C2—C1 | 123.22 (13) | C14—C13—H13 | 119.8 |
| O1—C2—C3 | 116.79 (14) | C9—C14—C13 | 120.67 (14) |
| C1—C2—C3 | 119.97 (14) | C9—C14—H14 | 119.7 |
| O2—C3—C4 | 125.84 (14) | C13—C14—H14 | 119.7 |

| | | | |
|---|---|---|---|
| O2—C3—C2 | 114.69 (13) | O2—C15—C16 | 107.56 (14) |
| C4—C3—C2 | 119.48 (15) | O2—C15—H15A | 110.2 |
| C3—C4—C5 | 120.36 (15) | C16—C15—H15A | 110.2 |
| C3—C4—H4 | 119.8 | O2—C15—H15B | 110.2 |
| C5—C4—H4 | 119.8 | C16—C15—H15B | 110.2 |
| C6—C5—C4 | 120.45 (15) | H15A—C15—H15B | 108.5 |
| C6—C5—H5A | 119.8 | C15—C16—H16A | 109.5 |
| C4—C5—H5A | 119.8 | C15—C16—H16B | 109.5 |
| C5—C6—C1 | 120.45 (16) | H16A—C16—H16B | 109.5 |
| C5—C6—H6 | 119.8 | C15—C16—H16C | 109.5 |
| C1—C6—H6 | 119.8 | H16A—C16—H16C | 109.5 |
| N1—C7—C1 | 121.97 (14) | H16B—C16—H16C | 109.5 |
| N1—C7—H7 | 119.0 | O4—C17—H17A | 109.5 |
| C1—C7—H7 | 119.0 | O4—C17—H17B | 109.5 |
| O3—C8—N2 | 121.72 (14) | H17A—C17—H17B | 109.5 |
| O3—C8—C9 | 121.55 (14) | O4—C17—H17C | 109.5 |
| N2—C8—C9 | 116.73 (13) | H17A—C17—H17C | 109.5 |
| C14—C9—C10 | 119.27 (13) | H17B—C17—H17C | 109.5 |
| C14—C9—C8 | 117.40 (13) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···N1 | 0.82 | 1.94 | 2.6529 (16) | 144 |
| O5—H5···O6$^{i}$ | 0.82 | 1.81 | 2.6177 (17) | 170 |
| O6—H6*A*···O3$^{ii}$ | 0.84 (1) | 1.96 (1) | 2.7908 (17) | 176 (2) |
| O6—H6*B*···O1$^{iii}$ | 0.84 (1) | 2.08 (1) | 2.8714 (18) | 157 (2) |
| N2—H2···O4$^{iv}$ | 0.89 (1) | 2.54 (2) | 3.1181 (17) | 123 (2) |
| N2—H2···O5$^{iv}$ | 0.89 (1) | 2.19 (1) | 3.0496 (18) | 163 (2) |

Symmetry codes: (i) $x-1, y, z$; (ii) $x+1/2, -y+1/2, z-1/2$; (iii) $-x+3/2, y-1/2, -z+3/2$; (iv) $-x-1/2, y+1/2, -z+3/2$.