Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# *N*′-(3-Ethoxy-2-hydroxybenzylidene)-3-hydroxynaphthalene-2-carbohydrazide

**Jun-Tao Lei,[a] Yan-Xia Jiang,[b] Li-Yan Tao,[c] Shan-Shan Huang[c]* and Hou-Li Zhang[c]***

[a]Department of Pharmacopedics, Jilin Medical College, Jilin 132013, People's Republic of China, [b]Department of Biochemistry, Jilin Medical College, Jilin 132013, People's Republic of China, and [c]College of Pharmacy, Dalian Medical University, Dalian 116044, People's Republic of China
Correspondence e-mail: jlcpcxb@yahoo.com.cn, houlizh@yahoo.com.cn

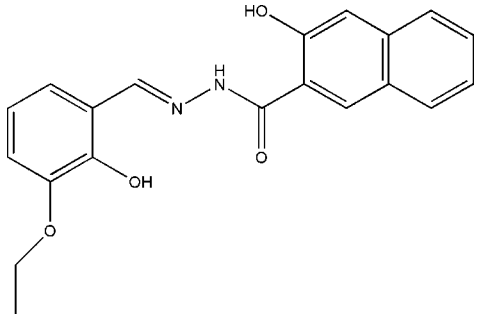
Received 15 April 2008; accepted 19 April 2008

Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.060; $wR$ factor = 0.178; data-to-parameter ratio = 14.5.

In the molecule of the title compound, $C_{20}H_{18}N_2O_4$, the dihedral angle between the benzene ring and the naphthyl ring system is 8.5 (2)°. In the crystal structure, molecules are linked through intermolecular O—H···O hydrogen bonds, forming chains running along the *b* axis.

## Related literature

For background on Schiff base compounds and their biological applications, see: Schiff (1864); Brückner *et al.* (2000); Harrop *et al.* (2003); Ren *et al.* (2002). For related structures, see: Diao (2007); Diao *et al.* (2007, 2008); Huang *et al.* (2007); Li *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).




## Experimental

### *Crystal data*

$C_{20}H_{18}N_2O_4$
$M_r$ = 350.36
Monoclinic, $C2/c$
$a$ = 28.420 (15) Å
$b$ = 6.456 (5) Å
$c$ = 18.800 (14) Å
$\beta$ = 100.658 (10)°
$V$ = 3390 (4) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 298 (2) K
0.30 × 0.27 × 0.27 mm

### *Data collection*

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.972, $T_{max}$ = 0.974
13100 measured reflections
3503 independent reflections
2183 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.057

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.178
$S$ = 1.06
3503 reflections
242 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···O2$^{i}$ | 0.82 | 1.87 | 2.661 (3) | 161 |
| O3—H3···N2 | 0.82 | 1.87 | 2.589 (3) | 146 |
| N1—H1*A*···O1 | 0.900 (10) | 1.95 (2) | 2.619 (3) | 130 (2) |

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

We thank Dr Yun-Peng Diao for assistance with the experiment and structure refinement. The project was supported financially by Jilin Medical College.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2080).

## References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Brückner, C., Rettig, S. J. & Dolphin, D. (2000). *Inorg. Chem.* **39**, 6100–6106.
Bruker (2000). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Diao, Y.-P. (2007). *Acta Cryst.* E**63**, m1453–m1454.
Diao, Y.-P., Shu, X.-H., Zhang, B.-J., Zhen, Y.-H. & Kang, T.-G. (2007). *Acta Cryst.* E**63**, m1816.
Diao, Y.-P., Zhen, Y.-H., Han, X. & Deng, S. (2008). *Acta Cryst.* E**64**, o101.
Harrop, T. C., Olmstead, M. M. & Mascharak, P. K. (2003). *Chem. Commun.* pp. 410–411.
Huang, S.-S., Zhou, Q. & Diao, Y.-P. (2007). *Acta Cryst.* E**63**, o4659.
Li, K., Huang, S.-S., Zhang, B.-J., Meng, D.-L. & Diao, Y.-P. (2007). *Acta Cryst.* E**63**, m2291.
Ren, S., Wang, R., Komatsu, K., Bonaz-Krause, P., Zyrianov, Y., McKenna, C. E., Csipke, C., Tokes, Z. A. & Lien, E. J. (2002). *J. Med. Chem.* **45**, 410–419.
Schiff, H. (1864). *Ann. Chem. Pharm.* **131**, 118–124.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2008). E**64**, o909 [doi:10.1107/S1600536808010933]

## *N*′-(3-Ethoxy-2-hydroxybenzylidene)-3-hydroxynaphthalene-2-carbohydrazide

**Jun-Tao Lei, Yan-Xia Jiang, Li-Yan Tao, Shan-Shan Huang and Hou-Li Zhang**

### S1. Comment

The compounds derived from the condensation reactions of aldehydes with primary amines are called Schiff base compounds (Schiff, 1864). Schiff base compounds and their metal complexes have attracted much interest for their wide applications, especially for their potential pharmacological and antitumor properties (Brückner *et al.*, 2000; Harrop *et al.*, 2003; Ren *et al.*, 2002). In this paper, the preparation and crystal structure of the title compound, (I), is reported.

In the structure of (I) (Fig. 1), the naphthyl ring and 2-hydroxyphenyl methylidene hydrazide moiety are nearly coplanar with the dihedral angle between the phenyl ring and the naphthyl ring is 8.5 (2) °; the torsion angles C13—C12—N2—N1 and N2—N1—C11—C1 are 3.5 (2) and 1.4 (2)°, respectively. The methoxy group is slightly twisted out of the plane of the phenyl ring with torsion angle C15—O4—C19—C20 being 13.1 (2)°. The molecules of (I) are linked through intermolecular O–H···O hydrogen bonds, forming chains running along the *b* axis. The structure is further stabilized by intramolecular interactions N1—H1A···O1 and O3—H3···N2 (Table 1). All the bond lengths are within normal ranges (Allen *et al.*, 1987) and comparable to the values observed in other similar compounds (Diao *et al.*, 2008; Diao *et al.*, 2007; Diao, 2007; Li *et al.*, 2007; Huang *et al.*, 2007).

### S2. Experimental

3-Ethoxysalicylaldehyde (0.1 mmol, 16.6 mg) and 3-hydroxynaphthalene-2-carboxylic acid hydrazide (0.1 mmol, 20.2 mg) were dissolved in a methanol solution (20 ml). The mixture was stirred at reflux for 1 h and cooled to room temperature. After keeping the solution in air for a few days, colorless block-like crystals were formed.

### S3. Refinement

H1A was located from a difference Fourier map and refined isotropically. The rest of the H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C–H distances of 0.93–0.97 Å, O–H distances of 0.82 Å, and with $U_{iso}$(H) = 1.2$U_{eq}$(C) and 1.5$U_{eq}$(O and methyl C).

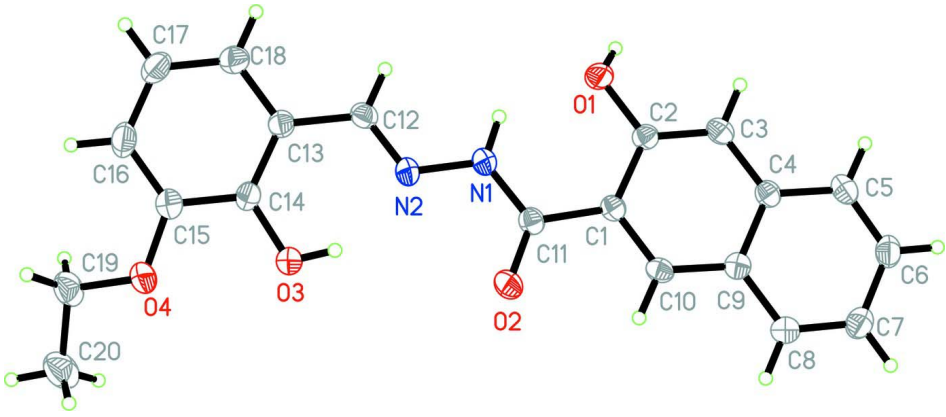



**Figure 1**

The structure of (I) with displacement parameters drawn at the 30% probability level.

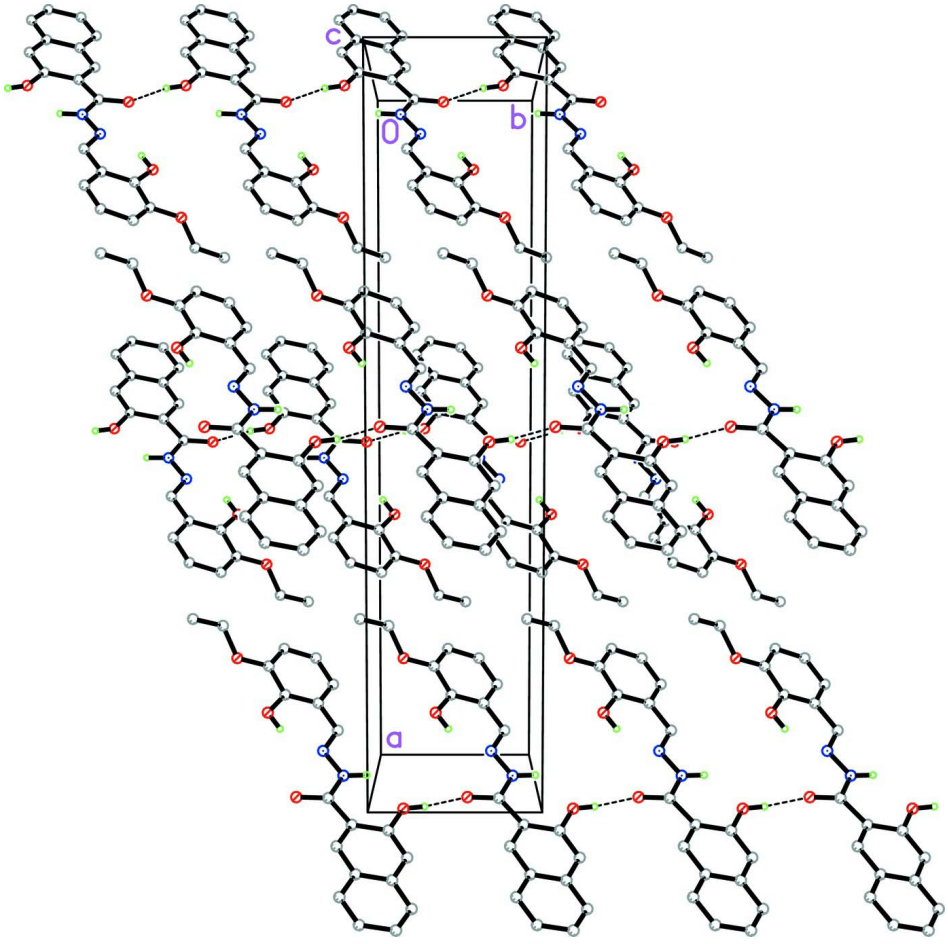



**Figure 2**

The molecular packing of (I) showing intermolecular hydrogen-bonds with dashed lines.

**N′-(3-Ethoxy-2-hydroxybenzylidene)-3-hydroxynaphthalene-2-carbohydrazide**

*Crystal data*

$C_{20}H_{18}N_2O_4$
$M_r = 350.36$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 28.420\ (15)$ Å
$b = 6.456\ (5)$ Å
$c = 18.800\ (14)$ Å
$\beta = 100.658\ (10)°$
$V = 3390\ (4)$ Å$^3$
$Z = 8$
$F(000) = 1472$
$D_x = 1.373$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1359 reflections
$\theta = 2.2–24.3°$
$\mu = 0.10$ mm$^{-1}$
$T = 298$ K
Block, colorless
0.30 × 0.27 × 0.27 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.972$, $T_{max} = 0.974$
13100 measured reflections
3503 independent reflections
2183 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 26.5°$, $\theta_{min} = 1.5°$
$h = -35\rightarrow35$
$k = -8\rightarrow8$
$l = -23\rightarrow22$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.178$
$S = 1.06$
3503 reflections
242 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + 0.1909P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å$^{-3}$
$\Delta\rho_{min} = -0.19$ e Å$^{-3}$
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0024 (6)

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 1.00934 (6) | −0.1963 (2) | 0.34159 (8) | 0.0489 (5) |
| H1 | 1.0059 | −0.3211 | 0.3470 | 0.073* |
| O2 | 0.98937 (6) | 0.4267 (2) | 0.38501 (9) | 0.0528 (5) |

| | | | | |
|---|---|---|---|---|
| O3 | 0.88269 (7) | 0.6149 (3) | 0.24267 (9) | 0.0611 (6) |
| H3 | 0.9039 | 0.5398 | 0.2644 | 0.092* |
| O4 | 0.81068 (6) | 0.8088 (3) | 0.16639 (10) | 0.0592 (5) |
| N1 | 0.96591 (7) | 0.1590 (3) | 0.31039 (10) | 0.0396 (5) |
| N2 | 0.93488 (7) | 0.2841 (3) | 0.26466 (10) | 0.0394 (5) |
| C1 | 1.02434 (7) | 0.1001 (3) | 0.41996 (11) | 0.0336 (5) |
| C2 | 1.03361 (8) | −0.1122 (3) | 0.40475 (11) | 0.0363 (5) |
| C3 | 1.06657 (8) | −0.2231 (3) | 0.45120 (13) | 0.0405 (6) |
| H3A | 1.0734 | −0.3580 | 0.4390 | 0.049* |
| C4 | 1.09062 (8) | −0.1396 (3) | 0.51714 (12) | 0.0377 (5) |
| C5 | 1.12406 (8) | −0.2534 (4) | 0.56714 (14) | 0.0467 (6) |
| H5 | 1.1314 | −0.3888 | 0.5563 | 0.056* |
| C6 | 1.14561 (9) | −0.1678 (4) | 0.63087 (14) | 0.0502 (6) |
| H6 | 1.1670 | −0.2465 | 0.6635 | 0.060* |
| C7 | 1.13609 (8) | 0.0384 (4) | 0.64834 (13) | 0.0498 (7) |
| H7 | 1.1516 | 0.0960 | 0.6917 | 0.060* |
| C8 | 1.10409 (8) | 0.1528 (4) | 0.60139 (12) | 0.0431 (6) |
| H8 | 1.0976 | 0.2882 | 0.6133 | 0.052* |
| C9 | 1.08064 (8) | 0.0685 (3) | 0.53476 (11) | 0.0364 (5) |
| C10 | 1.04759 (8) | 0.1814 (3) | 0.48433 (12) | 0.0372 (5) |
| H10 | 1.0412 | 0.3179 | 0.4952 | 0.045* |
| C11 | 0.99190 (8) | 0.2416 (3) | 0.37086 (12) | 0.0365 (5) |
| C12 | 0.91016 (8) | 0.2028 (4) | 0.20827 (12) | 0.0402 (6) |
| H12 | 0.9147 | 0.0643 | 0.1977 | 0.048* |
| C13 | 0.87471 (8) | 0.3253 (4) | 0.16007 (12) | 0.0392 (6) |
| C14 | 0.86145 (8) | 0.5211 (4) | 0.18082 (12) | 0.0426 (6) |
| C15 | 0.82336 (9) | 0.6255 (4) | 0.13816 (13) | 0.0471 (6) |
| C16 | 0.80210 (9) | 0.5426 (4) | 0.07255 (13) | 0.0562 (7) |
| H16 | 0.7776 | 0.6148 | 0.0431 | 0.067* |
| C17 | 0.81680 (9) | 0.3529 (4) | 0.04985 (14) | 0.0566 (7) |
| H17 | 0.8027 | 0.3001 | 0.0049 | 0.068* |
| C18 | 0.85201 (8) | 0.2431 (4) | 0.09359 (13) | 0.0465 (6) |
| H18 | 0.8609 | 0.1134 | 0.0791 | 0.056* |
| C19 | 0.76647 (9) | 0.9005 (4) | 0.13279 (16) | 0.0612 (8) |
| H19A | 0.7413 | 0.7971 | 0.1251 | 0.073* |
| H19B | 0.7694 | 0.9590 | 0.0863 | 0.073* |
| C20 | 0.75477 (11) | 1.0676 (4) | 0.18230 (17) | 0.0764 (9) |
| H20A | 0.7498 | 1.0067 | 0.2269 | 0.115* |
| H20B | 0.7262 | 1.1384 | 0.1597 | 0.115* |
| H20C | 0.7808 | 1.1643 | 0.1920 | 0.115* |
| H1A | 0.9661 (10) | 0.0234 (18) | 0.2992 (15) | 0.080* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0656 (11) | 0.0304 (9) | 0.0453 (10) | 0.0015 (8) | −0.0038 (8) | −0.0026 (7) |
| O2 | 0.0653 (12) | 0.0272 (9) | 0.0598 (11) | 0.0042 (8) | −0.0043 (9) | 0.0031 (8) |
| O3 | 0.0697 (13) | 0.0505 (11) | 0.0525 (11) | 0.0209 (9) | −0.0165 (9) | −0.0120 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O4 | 0.0558 (11) | 0.0509 (11) | 0.0628 (12) | 0.0186 (8) | −0.0098 (9) | −0.0038 (9) |
| N1 | 0.0435 (11) | 0.0338 (10) | 0.0395 (11) | 0.0055 (9) | 0.0022 (9) | 0.0036 (9) |
| N2 | 0.0412 (11) | 0.0362 (11) | 0.0388 (11) | 0.0058 (8) | 0.0020 (9) | 0.0052 (9) |
| C1 | 0.0351 (12) | 0.0299 (12) | 0.0364 (12) | −0.0008 (9) | 0.0082 (10) | 0.0037 (9) |
| C2 | 0.0409 (13) | 0.0313 (12) | 0.0365 (12) | −0.0030 (10) | 0.0066 (10) | 0.0005 (10) |
| C3 | 0.0442 (14) | 0.0308 (12) | 0.0473 (14) | 0.0021 (10) | 0.0105 (11) | 0.0017 (10) |
| C4 | 0.0351 (12) | 0.0369 (13) | 0.0422 (13) | 0.0013 (10) | 0.0099 (10) | 0.0020 (10) |
| C5 | 0.0451 (14) | 0.0446 (14) | 0.0514 (15) | 0.0114 (11) | 0.0114 (12) | 0.0047 (12) |
| C6 | 0.0422 (14) | 0.0616 (17) | 0.0448 (15) | 0.0093 (12) | 0.0029 (12) | 0.0051 (12) |
| C7 | 0.0435 (15) | 0.0634 (18) | 0.0410 (14) | −0.0001 (12) | 0.0041 (12) | −0.0010 (12) |
| C8 | 0.0463 (14) | 0.0407 (13) | 0.0430 (14) | −0.0013 (11) | 0.0098 (11) | −0.0030 (11) |
| C9 | 0.0369 (12) | 0.0394 (13) | 0.0342 (12) | −0.0012 (10) | 0.0099 (10) | 0.0025 (10) |
| C10 | 0.0442 (13) | 0.0275 (11) | 0.0413 (13) | −0.0002 (10) | 0.0113 (11) | 0.0009 (10) |
| C11 | 0.0379 (12) | 0.0312 (13) | 0.0407 (13) | −0.0006 (10) | 0.0077 (10) | 0.0045 (10) |
| C12 | 0.0438 (14) | 0.0388 (13) | 0.0395 (13) | 0.0073 (10) | 0.0118 (11) | −0.0009 (10) |
| C13 | 0.0394 (13) | 0.0432 (13) | 0.0357 (13) | 0.0042 (10) | 0.0086 (10) | 0.0016 (10) |
| C14 | 0.0427 (14) | 0.0478 (15) | 0.0349 (12) | 0.0048 (11) | 0.0009 (11) | 0.0013 (11) |
| C15 | 0.0449 (14) | 0.0476 (15) | 0.0469 (14) | 0.0064 (12) | 0.0032 (12) | 0.0020 (12) |
| C16 | 0.0531 (17) | 0.0645 (18) | 0.0455 (15) | 0.0097 (13) | −0.0052 (12) | 0.0103 (13) |
| C17 | 0.0573 (17) | 0.0694 (19) | 0.0389 (14) | 0.0010 (14) | −0.0023 (12) | −0.0065 (13) |
| C18 | 0.0496 (15) | 0.0490 (15) | 0.0418 (14) | 0.0010 (12) | 0.0106 (12) | −0.0036 (11) |
| C19 | 0.0419 (15) | 0.0561 (17) | 0.081 (2) | 0.0104 (12) | −0.0009 (14) | 0.0025 (15) |
| C20 | 0.0619 (19) | 0.066 (2) | 0.101 (2) | 0.0174 (15) | 0.0127 (18) | −0.0019 (18) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C2 | 1.370 (3) | C7—C8 | 1.362 (3) |
| O1—H1 | 0.8200 | C7—H7 | 0.9300 |
| O2—C11 | 1.230 (3) | C8—C9 | 1.414 (3) |
| O3—C14 | 1.350 (3) | C8—H8 | 0.9300 |
| O3—H3 | 0.8200 | C9—C10 | 1.408 (3) |
| O4—C15 | 1.372 (3) | C10—H10 | 0.9300 |
| O4—C19 | 1.426 (3) | C12—C13 | 1.457 (3) |
| N1—C11 | 1.346 (3) | C12—H12 | 0.9300 |
| N1—N2 | 1.374 (2) | C13—C14 | 1.395 (3) |
| N1—H1A | 0.900 (10) | C13—C18 | 1.401 (3) |
| N2—C12 | 1.272 (3) | C14—C15 | 1.396 (3) |
| C1—C10 | 1.371 (3) | C15—C16 | 1.377 (3) |
| C1—C2 | 1.434 (3) | C16—C17 | 1.387 (4) |
| C1—C11 | 1.490 (3) | C16—H16 | 0.9300 |
| C2—C3 | 1.360 (3) | C17—C18 | 1.369 (3) |
| C3—C4 | 1.407 (3) | C17—H17 | 0.9300 |
| C3—H3A | 0.9300 | C18—H18 | 0.9300 |
| C4—C5 | 1.413 (3) | C19—C20 | 1.501 (4) |
| C4—C9 | 1.425 (3) | C19—H19A | 0.9700 |
| C5—C6 | 1.358 (3) | C19—H19B | 0.9700 |
| C5—H5 | 0.9300 | C20—H20A | 0.9600 |
| C6—C7 | 1.409 (4) | C20—H20B | 0.9600 |

| | | | |
|---|---|---|---|
| C6—H6 | 0.9300 | C20—H20C | 0.9600 |
| | | | |
| C2—O1—H1 | 109.5 | O2—C11—N1 | 121.5 (2) |
| C14—O3—H3 | 109.5 | O2—C11—C1 | 121.1 (2) |
| C15—O4—C19 | 117.36 (19) | N1—C11—C1 | 117.43 (19) |
| C11—N1—N2 | 118.96 (19) | N2—C12—C13 | 120.4 (2) |
| C11—N1—H1A | 123.8 (18) | N2—C12—H12 | 119.8 |
| N2—N1—H1A | 117.1 (18) | C13—C12—H12 | 119.8 |
| C12—N2—N1 | 118.05 (19) | C14—C13—C18 | 119.3 (2) |
| C10—C1—C2 | 117.73 (19) | C14—C13—C12 | 120.6 (2) |
| C10—C1—C11 | 117.0 (2) | C18—C13—C12 | 120.0 (2) |
| C2—C1—C11 | 125.3 (2) | O3—C14—C13 | 123.1 (2) |
| C3—C2—O1 | 121.6 (2) | O3—C14—C15 | 117.0 (2) |
| C3—C2—C1 | 120.3 (2) | C13—C14—C15 | 119.8 (2) |
| O1—C2—C1 | 118.02 (19) | O4—C15—C16 | 125.3 (2) |
| C2—C3—C4 | 121.9 (2) | O4—C15—C14 | 115.2 (2) |
| C2—C3—H3A | 119.0 | C16—C15—C14 | 119.5 (2) |
| C4—C3—H3A | 119.0 | C15—C16—C17 | 120.8 (2) |
| C3—C4—C5 | 123.0 (2) | C15—C16—H16 | 119.6 |
| C3—C4—C9 | 118.7 (2) | C17—C16—H16 | 119.6 |
| C5—C4—C9 | 118.3 (2) | C18—C17—C16 | 120.0 (2) |
| C6—C5—C4 | 120.9 (2) | C18—C17—H17 | 120.0 |
| C6—C5—H5 | 119.6 | C16—C17—H17 | 120.0 |
| C4—C5—H5 | 119.6 | C17—C18—C13 | 120.3 (2) |
| C5—C6—C7 | 121.0 (2) | C17—C18—H18 | 119.8 |
| C5—C6—H6 | 119.5 | C13—C18—H18 | 119.8 |
| C7—C6—H6 | 119.5 | O4—C19—C20 | 107.5 (2) |
| C8—C7—C6 | 119.7 (2) | O4—C19—H19A | 110.2 |
| C8—C7—H7 | 120.2 | C20—C19—H19A | 110.2 |
| C6—C7—H7 | 120.2 | O4—C19—H19B | 110.2 |
| C7—C8—C9 | 120.9 (2) | C20—C19—H19B | 110.2 |
| C7—C8—H8 | 119.5 | H19A—C19—H19B | 108.5 |
| C9—C8—H8 | 119.5 | C19—C20—H20A | 109.5 |
| C10—C9—C8 | 122.9 (2) | C19—C20—H20B | 109.5 |
| C10—C9—C4 | 117.9 (2) | H20A—C20—H20B | 109.5 |
| C8—C9—C4 | 119.2 (2) | C19—C20—H20C | 109.5 |
| C1—C10—C9 | 123.3 (2) | H20A—C20—H20C | 109.5 |
| C1—C10—H10 | 118.4 | H20B—C20—H20C | 109.5 |
| C9—C10—H10 | 118.4 | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···O2$^{i}$ | 0.82 | 1.87 | 2.661 (3) | 161 |
| O3—H3···N2 | 0.82 | 1.87 | 2.589 (3) | 146 |
| N1—H1*A*···O1 | 0.90 (1) | 1.95 (2) | 2.619 (3) | 130 (2) |

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