Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

OPEN ACCESS

ISSN 2056-9890

# Crystal structure of (*E*)-5-diethylamino-2-({[4-(dimethylamino)phenyl]imino}-methyl)phenol

**C. Vidya Rani,[a] G. Chakkaravarthi[b]* and G. Rajagopal[a]***

[a]PG & Research Department of Chemistry, Chikkanna Government Arts College, Tiruppur 641 602, India, and [b]Department of Physics, CPCL Polytechnic College, Chennai 600 068, India. *Correspondence e-mail: chakkaravarthi_2005@yahoo.com, rajagopal18@yahoo.com

Received 15 June 2015; accepted 19 June 2015

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

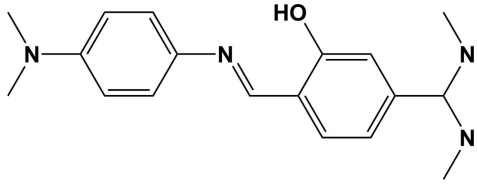
The title Schiff base compound, $C_{19}H_{25}N_3O$, is approximately planar, with a dihedral angle of 9.03 (13)° between the planes of the aromatic rings, and has an *E* conformation about the N=C bond. The molecular structure is stabilized by an intramolecular O—H···N hydrogen bond, with an *S*(6) ring motif. In the crystal, molecules are linked by C—H···$\pi$ interactions, forming sheets parallel to the *bc* plane.

**Keywords:** crystal structure; Schiff base; intramolecular O—H···N hydrogen bond; C—H···$\pi$ interactions.

**CCDC reference**: 1407678

## 1. Related literature

For biological activities of Schiff base derivatives, see: Savaliya *et al.* (2010); Xu *et al.* (2012). For the structures of similar compounds, see: Manvizhi *et al.* (2011); Thirugnanasundar *et al.* (2011).




## 2. Experimental

### 2.1. Crystal data

$C_{19}H_{25}N_3O$
$M_r$ = 311.42
Monoclinic, $P2_1$
$a$ = 8.8201 (7) Å
$b$ = 7.8850 (7) Å
$c$ = 13.0639 (10) Å
$\beta$ = 108.407 (3)°
$V$ = 862.06 (12) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 295 K
0.26 × 0.22 × 0.20 mm

### 2.2. Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.981, $T_{max}$ = 0.985
13009 measured reflections
3825 independent reflections
2438 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.159
$S$ = 1.03
3825 reflections
214 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

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

*Cg*1 and *Cg*2 are the centroids of rings C3–C8 and C10–C15, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···N2 | 0.82 | 1.85 | 2.585 (3) | 148 |
| C11—H11···*Cg*1$^{i}$ | 0.93 | 2.71 | 3.517 (3) | 145 |
| C17—H17*B*···*Cg*2$^{ii}$ | 0.96 | 2.90 | 3.743 (5) | 147 |

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

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: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* and *PLATON*.

## Acknowledgements

The authors acknowledge the SAIF, IIT, Madras, for the data collection.

Supporting information for this paper is available from the IUCr electronic archives (Reference: SU5157).

## References

Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Manvizhi, K., Chakkaravarthi, G., Anbalagan, G. & Rajagopal, G. (2011). *Acta Cryst.* E**67**, o2500.
Savaliya, M. D., Dobaria, J. G. & Purohit, D. M. (2010). *An Indian J.* **6**, 267–271.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Thirugnanasundar, A., Suresh, J., Ramu, A. & RajaGopal, G. (2011). *Acta Cryst.* E**67**, o2303.
Xu, R.-B., Zhang, N., Zhou, H.-Y., Yang, S.-P., Li, Y.-Y., Shi, D.-H., Ma, W.-X. & Xu, X.-Y. (2012). *J. Chem. Crystallogr.* **42**, 928–932.

# supporting information

*Acta Cryst.* (2015). E**71**, o503 [doi:10.1107/S2056989015011779]

# Crystal structure of (*E*)-5-diethylamino-2-({[4-(dimethylamino)phenyl]imino}-methyl)phenol

**C. Vidya Rani, G. Chakkaravarthi and G. Rajagopal**

## S1. Structural commentary

Schiff base derivatives are known to exhibit antimicrobial (Savaliya *et al.*, 2010) and antibacterial (Xu *et al.*, 2012) activities. Herein we report on the synthesis and the crystal structure of a new Schiff base compound.

The molecular structure of the title compound is illustrated in Fg. 1. The geometric parameters are comparable to those reported for similar structures (Manvizhi *et al.*, 2011; Thirugnanasundar *et al.*, 2011). The dihedral angle between the benzene rings (C3—C8) and (C10—C15) is 9.03 (13)°. The molecular structure is stabilized by an intramolecular O—H···N hydrogen bond (Table 1 and Fig. 1).

In the crystal, molecules are linked by C—H···$\pi$ interactions forming sheets parallel to the bc plane (Table 1 and Fig. 2).

## S2. Synthesis and crystallization

To an ethanol solution (10 ml) of 5-(diethylamino)-2-hydroxybenzaldehyde (96.5 mg, 0.5 mol) was added $N^1$,$N^1$-dimethylbenzene-1,4-diamine (68 mg, 0.5 mol). The mixture was stirred and 2 to 3 drops of glacial acetic acid were added. Stirring was continued for 30 mins and then the reaction mixture was refluxed for 2 h. On completion of the reaction, monitored by TLC, the mixture was allowed to cool to room temperature and the solid yellow precipitate that formed was filtered, dried, and recrystallized from DMF, giving colourless block-like crystals.

## S3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were positioned geometrically and refined using riding model: O—H = 0.82 Å, C—H = 0.93 - 0.97 Å with $U_{iso}$(H) = 1.5Ueq(O,C) for the hydroxyl and methyl H atoms and 1.2$U_{eq}$(C) for other H atoms. The components of the anisotropic displacement parameters of the atoms in bonds N3—C16, N3—C18 and N1—C2 were restrained to be equal within an effective standard deviation of 0.001 using the DELU command, and the C16—C17 bond distance was restrained to 1.54 (1) Å.

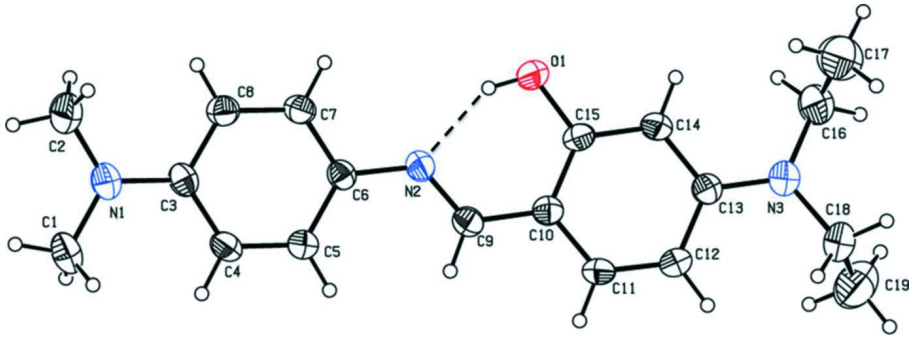



**Figure 1**

The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular O—H..N hydrogen bonds is shown as a dashd lines (see Table 1 for details).

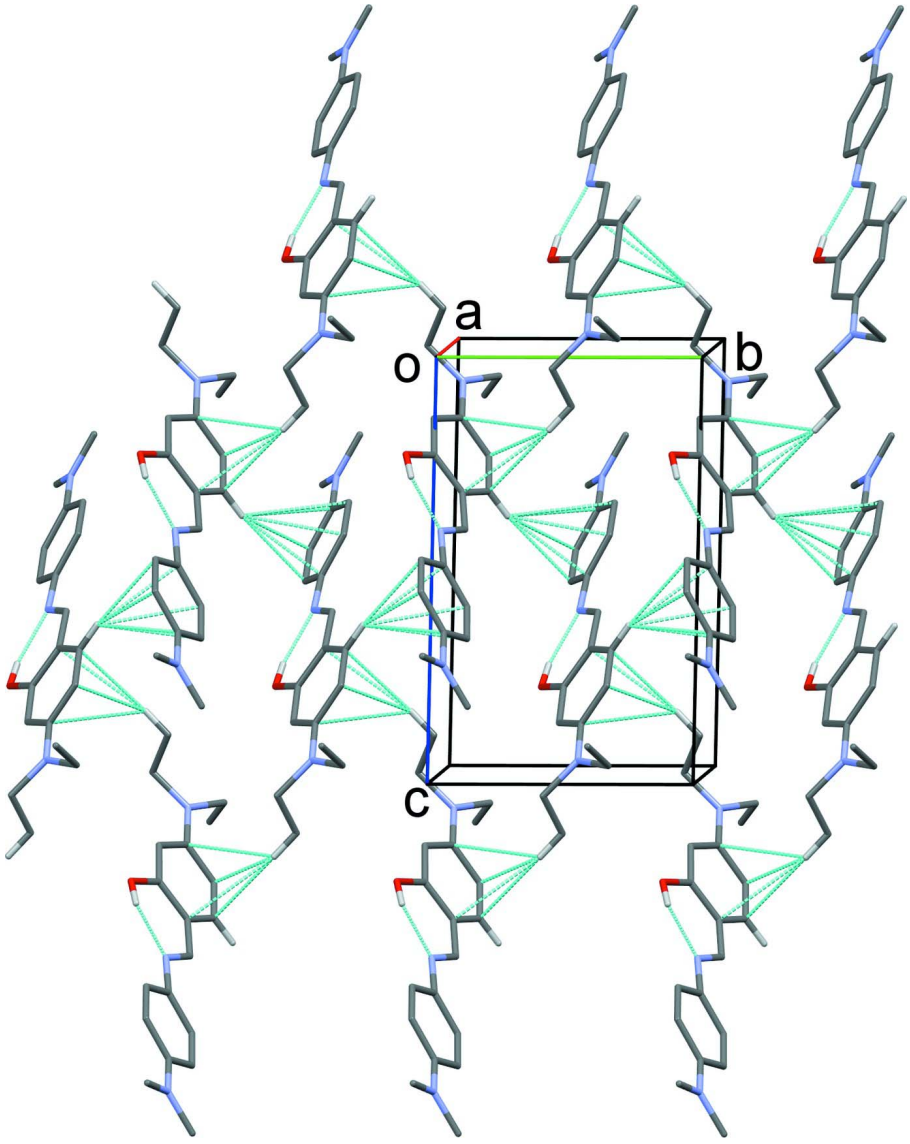



**Figure 2**

A view along the *a* axis of the crystal apcking of the title compound. The O—H..N and C-H···$\pi$ interactions are illustrated by dashed lines (see Table 1 for details).

### (*E*)-5-Diethylamino-2-({[4-(dimethylamino)phenyl]imino}methyl)phenol

*Crystal data*

$C_{19}H_{25}N_3O$
$M_r$ = 311.42
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a$ = 8.8201 (7) Å
$b$ = 7.8850 (7) Å
$c$ = 13.0639 (10) Å
$\beta$ = 108.407 (3)°
$V$ = 862.06 (12) Å$^3$
$Z$ = 2
$F(000)$ = 336
$D_x$ = 1.200 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 4428 reflections
$\theta$ = 2.4–27.2°
$\mu$ = 0.08 mm$^{-1}$
$T$ = 295 K
Block, colourless
0.26 × 0.22 × 0.20 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.981, $T_{max}$ = 0.985
13009 measured reflections
3825 independent reflections
2438 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027
$\theta_{max}$ = 27.3°, $\theta_{min}$ = 2.4°
$h$ = −11→10
$k$ = −10→10
$l$ = −16→16

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.159
$S$ = 1.03
3825 reflections
214 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.0751P)^2 + 0.1538P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.014 (4)

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.4431 (4) | 0.6814 (5) | 0.2015 (2) | 0.0780 (10) |
| H1A | 0.3484 | 0.6253 | 0.1573 | 0.117* |
| H1B | 0.5213 | 0.6840 | 0.1644 | 0.117* |
| H1C | 0.4171 | 0.7953 | 0.2159 | 0.117* |
| C2 | 0.6641 (4) | 0.5264 (6) | 0.3287 (3) | 0.0902 (12) |
| H2A | 0.7316 | 0.5867 | 0.3901 | 0.135* |
| H2B | 0.7039 | 0.5405 | 0.2688 | 0.135* |
| H2C | 0.6635 | 0.4081 | 0.3459 | 0.135* |
| C3 | 0.4220 (3) | 0.5850 (3) | 0.3736 (2) | 0.0502 (6) |
| C4 | 0.2713 (3) | 0.6598 (4) | 0.3525 (2) | 0.0547 (7) |
| H4 | 0.2275 | 0.7180 | 0.2880 | 0.066* |
| C5 | 0.1861 (3) | 0.6502 (4) | 0.42371 (19) | 0.0512 (6) |
| H5 | 0.0860 | 0.7008 | 0.4067 | 0.061* |
| C6 | 0.2487 (3) | 0.5648 (3) | 0.52175 (18) | 0.0444 (6) |
| C7 | 0.3965 (3) | 0.4922 (3) | 0.5425 (2) | 0.0508 (6) |

| | | | | |
|---|---|---|---|---|
| H7 | 0.4405 | 0.4352 | 0.6075 | 0.061* |
| C8 | 0.4820 (3) | 0.5003 (4) | 0.4715 (2) | 0.0537 (7) |
| H8 | 0.5816 | 0.4483 | 0.4889 | 0.064* |
| C9 | 0.0435 (3) | 0.6249 (4) | 0.59847 (19) | 0.0481 (6) |
| H9 | −0.0034 | 0.6975 | 0.5411 | 0.058* |
| C10 | −0.0294 (3) | 0.6066 (3) | 0.68154 (19) | 0.0462 (6) |
| C11 | −0.1669 (3) | 0.6947 (3) | 0.6784 (2) | 0.0537 (7) |
| H11 | −0.2150 | 0.7626 | 0.6188 | 0.064* |
| C12 | −0.2347 (3) | 0.6864 (4) | 0.7586 (2) | 0.0596 (8) |
| H12 | −0.3278 | 0.7467 | 0.7524 | 0.072* |
| C13 | −0.1648 (3) | 0.5871 (4) | 0.8507 (2) | 0.0528 (6) |
| C14 | −0.0279 (3) | 0.4940 (3) | 0.8547 (2) | 0.0523 (7) |
| H14 | 0.0198 | 0.4255 | 0.9141 | 0.063* |
| C15 | 0.0370 (3) | 0.5025 (3) | 0.7722 (2) | 0.0472 (6) |
| C16 | −0.1784 (4) | 0.4511 (5) | 1.0194 (3) | 0.0834 (10) |
| H16A | −0.2702 | 0.4176 | 1.0403 | 0.100* |
| H16B | −0.1393 | 0.3520 | 0.9915 | 0.100* |
| C17 | −0.0541 (5) | 0.5166 (6) | 1.1125 (3) | 0.1089 (14) |
| H17A | 0.0389 | 0.5432 | 1.0925 | 0.163* |
| H17B | −0.0274 | 0.4327 | 1.1686 | 0.163* |
| H17C | −0.0917 | 0.6173 | 1.1380 | 0.163* |
| C18 | −0.3507 (4) | 0.7080 (5) | 0.9409 (3) | 0.0835 (10) |
| H18A | −0.3375 | 0.7326 | 1.0160 | 0.100* |
| H18B | −0.3372 | 0.8131 | 0.9062 | 0.100* |
| C19 | −0.5106 (4) | 0.6420 (8) | 0.8890 (4) | 0.1178 (15) |
| H19A | −0.5223 | 0.6129 | 0.8156 | 0.177* |
| H19B | −0.5881 | 0.7267 | 0.8905 | 0.177* |
| H19C | −0.5270 | 0.5428 | 0.9268 | 0.177* |
| N1 | 0.5063 (3) | 0.5915 (4) | 0.30117 (18) | 0.0693 (7) |
| N2 | 0.1707 (2) | 0.5451 (3) | 0.60028 (16) | 0.0495 (5) |
| N3 | −0.2261 (3) | 0.5836 (4) | 0.9344 (2) | 0.0826 (9) |
| O1 | 0.1678 (2) | 0.4075 (3) | 0.77919 (17) | 0.0695 (6) |
| H1 | 0.2010 | 0.4308 | 0.7289 | 0.104* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.097 (2) | 0.090 (3) | 0.0568 (17) | −0.0042 (19) | 0.0384 (16) | 0.0063 (17) |
| C2 | 0.0743 (17) | 0.127 (3) | 0.082 (2) | 0.0100 (19) | 0.0428 (18) | 0.012 (2) |
| C3 | 0.0561 (14) | 0.0511 (15) | 0.0454 (13) | −0.0092 (13) | 0.0189 (11) | 0.0004 (12) |
| C4 | 0.0608 (16) | 0.0587 (17) | 0.0431 (13) | 0.0034 (14) | 0.0143 (12) | 0.0113 (13) |
| C5 | 0.0487 (13) | 0.0557 (16) | 0.0487 (14) | 0.0064 (12) | 0.0148 (11) | 0.0060 (13) |
| C6 | 0.0510 (14) | 0.0410 (14) | 0.0418 (13) | −0.0028 (12) | 0.0154 (11) | 0.0013 (11) |
| C7 | 0.0506 (14) | 0.0535 (16) | 0.0453 (14) | 0.0033 (13) | 0.0110 (11) | 0.0073 (12) |
| C8 | 0.0494 (14) | 0.0554 (16) | 0.0544 (16) | 0.0018 (12) | 0.0137 (12) | 0.0038 (13) |
| C9 | 0.0505 (14) | 0.0473 (15) | 0.0436 (13) | −0.0018 (13) | 0.0107 (11) | 0.0001 (11) |
| C10 | 0.0455 (13) | 0.0444 (14) | 0.0467 (13) | −0.0009 (11) | 0.0116 (10) | −0.0012 (11) |
| C11 | 0.0547 (14) | 0.0533 (16) | 0.0496 (14) | 0.0138 (12) | 0.0113 (12) | 0.0110 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C12 | 0.0529 (14) | 0.066 (2) | 0.0604 (16) | 0.0188 (13) | 0.0188 (13) | 0.0095 (14) |
| C13 | 0.0533 (14) | 0.0548 (16) | 0.0530 (14) | 0.0039 (13) | 0.0207 (11) | 0.0075 (13) |
| C14 | 0.0543 (15) | 0.0523 (16) | 0.0506 (15) | 0.0101 (13) | 0.0167 (12) | 0.0147 (13) |
| C15 | 0.0403 (12) | 0.0443 (14) | 0.0554 (15) | 0.0053 (11) | 0.0129 (11) | 0.0050 (12) |
| C16 | 0.086 (2) | 0.093 (3) | 0.081 (2) | 0.0042 (18) | 0.0414 (19) | 0.0168 (16) |
| C17 | 0.126 (3) | 0.098 (3) | 0.097 (3) | 0.010 (3) | 0.028 (3) | −0.008 (3) |
| C18 | 0.080 (2) | 0.107 (3) | 0.075 (2) | 0.0190 (17) | 0.0400 (18) | 0.0039 (19) |
| C19 | 0.094 (3) | 0.134 (4) | 0.131 (4) | 0.014 (3) | 0.043 (3) | −0.015 (3) |
| N1 | 0.0737 (14) | 0.083 (2) | 0.0611 (15) | 0.0044 (13) | 0.0357 (13) | 0.0146 (14) |
| N2 | 0.0530 (12) | 0.0515 (14) | 0.0459 (11) | 0.0007 (10) | 0.0184 (9) | 0.0030 (10) |
| N3 | 0.0769 (16) | 0.112 (2) | 0.0696 (16) | 0.0288 (15) | 0.0381 (13) | 0.0210 (15) |
| O1 | 0.0666 (12) | 0.0777 (14) | 0.0737 (14) | 0.0302 (11) | 0.0356 (10) | 0.0283 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.432 (4) | C11—C12 | 1.363 (4) |
| C1—H1A | 0.9600 | C11—H11 | 0.9300 |
| C1—H1B | 0.9600 | C12—C13 | 1.404 (4) |
| C1—H1C | 0.9600 | C12—H12 | 0.9300 |
| C2—N1 | 1.419 (4) | C13—N3 | 1.364 (3) |
| C2—H2A | 0.9600 | C13—C14 | 1.400 (3) |
| C2—H2B | 0.9600 | C14—C15 | 1.373 (4) |
| C2—H2C | 0.9600 | C14—H14 | 0.9300 |
| C3—N1 | 1.377 (3) | C15—O1 | 1.354 (3) |
| C3—C8 | 1.390 (4) | C16—C17 | 1.451 (5) |
| C3—C4 | 1.400 (4) | C16—N3 | 1.485 (4) |
| C4—C5 | 1.370 (4) | C16—H16A | 0.9700 |
| C4—H4 | 0.9300 | C16—H16B | 0.9700 |
| C5—C6 | 1.397 (3) | C17—H17A | 0.9600 |
| C5—H5 | 0.9300 | C17—H17B | 0.9600 |
| C6—C7 | 1.370 (3) | C17—H17C | 0.9600 |
| C6—N2 | 1.413 (3) | C18—C19 | 1.454 (5) |
| C7—C8 | 1.370 (4) | C18—N3 | 1.495 (4) |
| C7—H7 | 0.9300 | C18—H18A | 0.9700 |
| C8—H8 | 0.9300 | C18—H18B | 0.9700 |
| C9—N2 | 1.280 (3) | C19—H19A | 0.9600 |
| C9—C10 | 1.433 (3) | C19—H19B | 0.9600 |
| C9—H9 | 0.9300 | C19—H19C | 0.9600 |
| C10—C11 | 1.386 (3) | O1—H1 | 0.8200 |
| C10—C15 | 1.407 (3) | | |
| | | | |
| N1—C1—H1A | 109.5 | N3—C13—C14 | 121.0 (2) |
| N1—C1—H1B | 109.5 | N3—C13—C12 | 121.3 (2) |
| H1A—C1—H1B | 109.5 | C14—C13—C12 | 117.7 (2) |
| N1—C1—H1C | 109.5 | C15—C14—C13 | 120.9 (2) |
| H1A—C1—H1C | 109.5 | C15—C14—H14 | 119.5 |
| H1B—C1—H1C | 109.5 | C13—C14—H14 | 119.5 |
| N1—C2—H2A | 109.5 | O1—C15—C14 | 118.5 (2) |

| | | | |
|---|---|---|---|
| N1—C2—H2B | 109.5 | O1—C15—C10 | 119.9 (2) |
| H2A—C2—H2B | 109.5 | C14—C15—C10 | 121.6 (2) |
| N1—C2—H2C | 109.5 | C17—C16—N3 | 109.7 (3) |
| H2A—C2—H2C | 109.5 | C17—C16—H16A | 109.7 |
| H2B—C2—H2C | 109.5 | N3—C16—H16A | 109.7 |
| N1—C3—C8 | 121.2 (2) | C17—C16—H16B | 109.7 |
| N1—C3—C4 | 122.3 (2) | N3—C16—H16B | 109.7 |
| C8—C3—C4 | 116.4 (2) | H16A—C16—H16B | 108.2 |
| C5—C4—C3 | 122.2 (2) | C16—C17—H17A | 109.5 |
| C5—C4—H4 | 118.9 | C16—C17—H17B | 109.5 |
| C3—C4—H4 | 118.9 | H17A—C17—H17B | 109.5 |
| C4—C5—C6 | 120.4 (2) | C16—C17—H17C | 109.5 |
| C4—C5—H5 | 119.8 | H17A—C17—H17C | 109.5 |
| C6—C5—H5 | 119.8 | H17B—C17—H17C | 109.5 |
| C7—C6—C5 | 117.3 (2) | C19—C18—N3 | 111.1 (3) |
| C7—C6—N2 | 117.5 (2) | C19—C18—H18A | 109.4 |
| C5—C6—N2 | 125.2 (2) | N3—C18—H18A | 109.4 |
| C8—C7—C6 | 122.6 (2) | C19—C18—H18B | 109.4 |
| C8—C7—H7 | 118.7 | N3—C18—H18B | 109.4 |
| C6—C7—H7 | 118.7 | H18A—C18—H18B | 108.0 |
| C7—C8—C3 | 121.0 (2) | C18—C19—H19A | 109.5 |
| C7—C8—H8 | 119.5 | C18—C19—H19B | 109.5 |
| C3—C8—H8 | 119.5 | H19A—C19—H19B | 109.5 |
| N2—C9—C10 | 122.5 (2) | C18—C19—H19C | 109.5 |
| N2—C9—H9 | 118.8 | H19A—C19—H19C | 109.5 |
| C10—C9—H9 | 118.8 | H19B—C19—H19C | 109.5 |
| C11—C10—C15 | 116.4 (2) | C3—N1—C2 | 120.8 (2) |
| C11—C10—C9 | 121.6 (2) | C3—N1—C1 | 120.2 (2) |
| C15—C10—C9 | 121.9 (2) | C2—N1—C1 | 118.6 (2) |
| C12—C11—C10 | 123.1 (2) | C9—N2—C6 | 123.9 (2) |
| C12—C11—H11 | 118.5 | C13—N3—C16 | 121.5 (3) |
| C10—C11—H11 | 118.5 | C13—N3—C18 | 121.1 (3) |
| C11—C12—C13 | 120.3 (2) | C16—N3—C18 | 117.4 (2) |
| C11—C12—H12 | 119.8 | C15—O1—H1 | 109.5 |
| C13—C12—H12 | 119.8 | | |

| | | | |
|---|---|---|---|
| N1—C3—C4—C5 | 178.6 (3) | C13—C14—C15—C10 | 1.1 (4) |
| C8—C3—C4—C5 | −0.3 (4) | C11—C10—C15—O1 | 177.5 (3) |
| C3—C4—C5—C6 | 0.5 (4) | C9—C10—C15—O1 | −4.4 (4) |
| C4—C5—C6—C7 | −0.2 (4) | C11—C10—C15—C14 | −2.3 (4) |
| C4—C5—C6—N2 | −179.1 (3) | C9—C10—C15—C14 | 175.8 (3) |
| C5—C6—C7—C8 | −0.3 (4) | C8—C3—N1—C2 | −6.4 (5) |
| N2—C6—C7—C8 | 178.7 (2) | C4—C3—N1—C2 | 174.8 (3) |
| C6—C7—C8—C3 | 0.5 (4) | C8—C3—N1—C1 | −179.2 (3) |
| N1—C3—C8—C7 | −179.0 (3) | C4—C3—N1—C1 | 2.1 (4) |
| C4—C3—C8—C7 | −0.2 (4) | C10—C9—N2—C6 | −177.7 (2) |
| N2—C9—C10—C11 | 179.7 (2) | C7—C6—N2—C9 | 170.0 (2) |
| N2—C9—C10—C15 | 1.7 (4) | C5—C6—N2—C9 | −11.0 (4) |

| | | | |
|---|---|---|---|
| C15—C10—C11—C12 | 1.4 (4) | C14—C13—N3—C16 | −15.8 (5) |
| C9—C10—C11—C12 | −176.7 (3) | C12—C13—N3—C16 | 165.5 (3) |
| C10—C11—C12—C13 | 0.8 (4) | C14—C13—N3—C18 | 167.5 (3) |
| C11—C12—C13—N3 | 176.7 (3) | C12—C13—N3—C18 | −11.3 (5) |
| C11—C12—C13—C14 | −2.1 (4) | C17—C16—N3—C13 | 97.4 (4) |
| N3—C13—C14—C15 | −177.6 (3) | C17—C16—N3—C18 | −85.7 (4) |
| C12—C13—C14—C15 | 1.2 (4) | C19—C18—N3—C13 | 91.4 (4) |
| C13—C14—C15—O1 | −178.8 (3) | C19—C18—N3—C16 | −85.5 (4) |

*Hydrogen-bond geometry (Å, º)*

Cg1 and Cg2 are the centroids of rings C3-C8 and C10-C15, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···N2 | 0.82 | 1.85 | 2.585 (3) | 148 |
| C11—H11···*Cg*1$^{i}$ | 0.93 | 2.71 | 3.517 (3) | 145 |
| C17—H17*B*···*Cg*2$^{ii}$ | 0.96 | 2.90 | 3.743 (5) | 147 |

Symmetry codes: (i) −*x*, *y*+1/2, −*z*+1; (ii) −*x*, *y*−1/2, −*z*+2.