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# 1-(3-Hydroxypropyl)-3-phenylquinoxalin-2(1*H*)-one

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**Keywords:** crystal structure; dihydroquinoxaline; hydrogen bond; C—H···π(ring).

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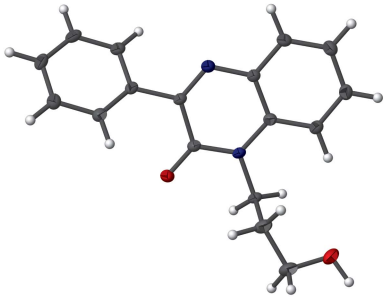
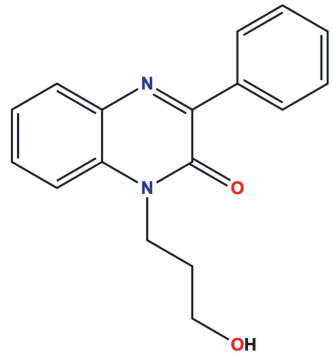
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title molecule, $C_{17}H_{16}N_2O_2$, the quinoxaline portion is slightly folded about the N···N axis with an angle of 4.27 (4)°. In the crystal, O—H···O and weak C—H···O hydrogen bonds link molecules along the *b*-axis direction. In addition, two sets of weak C—H···π(ring) interactions form a two-dimensional 'step' motif parallel to the *bc* plane.

**3D view**



**Chemical scheme**




## Structure description

Quinoxalines and their derivatives, especially the quinoxalinones, are of great importance in medicinal chemistry (Ramli & Essassi, 2015). As a continuation of our work on the synthesis of quinoxalin-2-one derivatives in order to evaluate their pharmacological activities (Ramli *et al.*, 2010*a*,*b*, 2011, 2013; Caleb *et al.*, 2016; Missioui *et al.*, 2017) we report herein the synthesis and crystal structure of the title compound.

The molecular structure of the title compound is shown in Fig. 1. The dihydroquinoxaline fragment shows a slight fold of 4.27 (4)° about the N1···N2 axis and the C9–C14 phenyl ring is inclined at 44.89 (3)° to the mean plane of the N1/N2/C1–C6 fragment. In the crystal, O—H···O and weak C—H···O hydrogen bonds form ribbons two molecules wide extending along the *b*-axis direction. Each half of the ribbon is reinforced by C3—H3···*Cg*1$^{ii}$ interactions (Table 1 and Fig. 2). The ribbons are connected into a 'step' motif running parallel to the *bc* plane by C10—H10···*Cg*2$^{iii}$ interactions (Table 1 and Figs. 2–4).

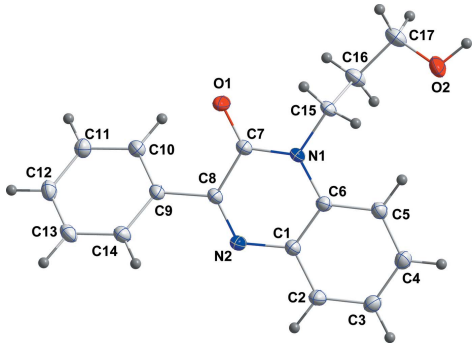



**Figure 1**
The molecular structure of the title molecule with the labelling scheme and 50% probability ellipsoids.

## Synthesis and crystallization

A solution of 1-(3-bromopropyl)-3-phenylquinoxalin-2(*1H*)-one (1 g, 2.9 mmol) methanol/water (20/5 ml) was stirred under reflex for 12 h. After completion of the reaction (monitored by TLC), the solution was concentrated and the residue was purified by column chromatography on silica gel by using a mixture (hexane/ethyl acetate 9/1). The solid product was purified by recrystallization from ethanol solution to afford colourless crystals in 20% yield.

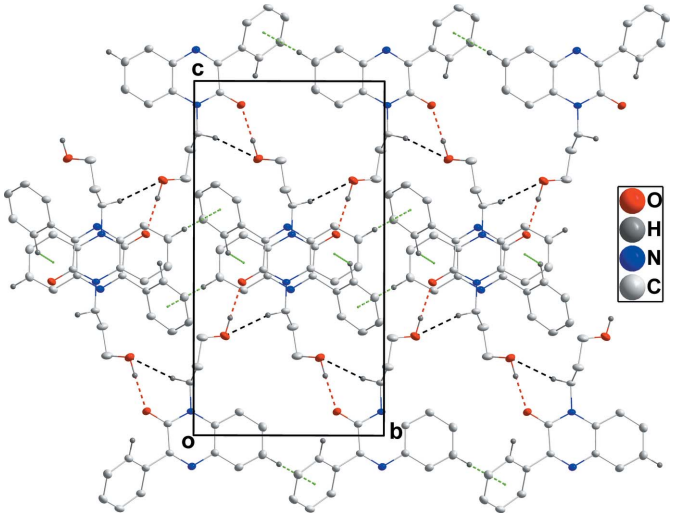



**Figure 2**
Part of the crystal structure viewed along the *a*-axis direction. The O—H···O and C—H···O hydrogen bonds are shown, respectively, by red and black dashed lines. C—H···$\pi$(ring) interactions are shown by green dashed lines.

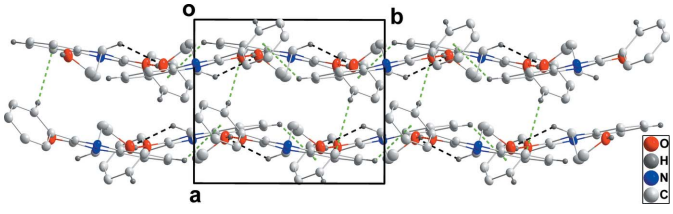



**Figure 3**
Part of the crystal structure viewed along the *c*-axis direction showing C—H···$\pi$(ring) interactions as green dashed lines. Hydrogen bonds are as depicted as in Fig. 2.

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

*Cg*1 and *Cg*2 are the centroids of the C9–C14 and C1–C6 benzene rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2*A*···O1$^{i}$ | 0.949 (15) | 1.888 (15) | 2.8345 (10) | 174.4 (14) |
| C15—H15*A*···O2$^{ii}$ | 0.969 (11) | 2.582 (12) | 3.3425 (13) | 135.5 (9) |
| C3—H3···*Cg*1$^{iii}$ | 0.953 (12) | 2.734 (12) | 3.4708 (12) | 134.8 (9) |
| C10—H10···*Cg*2$^{iv}$ | 1.003 (12) | 2.916 (13) | 3.5859 (12) | 124.9 (9) |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{17}H_{16}N_2O_2$ |
| $M_r$ | 280.32 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 120 |
| *a*, *b*, *c* (Å) | 8.1914 (14), 9.5151 (16), 17.781 (3) |
| $\beta$ (°) | 94.880 (2) |
| *V* (Å$^3$) | 1380.9 (4) |
| *Z* | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.09 |
| Crystal size (mm) | 0.36 × 0.30 × 0.24 |
| | |
| Data collection | |
| Diffractometer | Bruker SMART APEX CCD |
| Absorption correction | Multi-scan (*SADABS*; Krause *et al.*, 2015) |
| $T_{min}$, $T_{max}$ | 0.90, 0.98 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 26403, 3863, 3134 |
| $R_{int}$ | 0.033 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.696 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.046, 0.135, 1.10 |
| No. of reflections | 3863 |
| No. of parameters | 254 |
| H-atom treatment | All H-atom parameters refined |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.48, −0.25 |

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/1* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

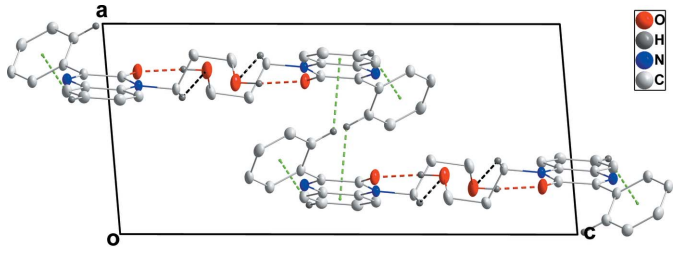



**Figure 4**
A view of portions of two chains viewed along the *b*-axis direction showing their association through C—H···$\pi$(ring) interactions. These and the hydrogen bonds are depicted as in Fig. 2.

## Acknowledgements

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# full crystallographic data

*IUCrData* (2018). **3**, x181633 [https://doi.org/10.1107/S2414314618016334]

## 1-(3-Hydroxypropyl)-3-phenylquinoxalin-2(1*H*)-one

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### 1-(3-Hydroxypropyl)-3-phenylquinoxalin-2(1*H*)-one

*Crystal data*

$C_{17}H_{16}N_2O_2$
$M_r$ = 280.32
Monoclinic, $P2_1/n$
$a$ = 8.1914 (14) Å
$b$ = 9.5151 (16) Å
$c$ = 17.781 (3) Å
$\beta$ = 94.880 (2)°
$V$ = 1380.9 (4) Å$^3$
$Z$ = 4
$F(000)$ = 592
$D_x$ = 1.348 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9996 reflections
$\theta$ = 2.3–29.5°
$\mu$ = 0.09 mm$^{-1}$
$T$ = 120 K
Block, colourless
0.36 × 0.30 × 0.24 mm

*Data collection*

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
$T_{min}$ = 0.90, $T_{max}$ = 0.98
26403 measured reflections
3863 independent reflections
3134 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033
$\theta_{max}$ = 29.7°, $\theta_{min}$ = 2.3°
$h$ = −11→11
$k$ = −13→13
$l$ = −24→24

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.135
$S$ = 1.10
3863 reflections
254 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0966P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.48 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

*Special details*

**Experimental**. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in $\omega$, colllected at $\varphi$ = 0.00, 90.00 and 180.00° and 2 sets of 800 frames, each of width 0.45° in $\varphi$, collected at $\omega$ = –30.00 and 210.00°. The scan time was 10 sec/frame.

**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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.27209 (9) | 0.74659 (7) | 0.56746 (4) | 0.02520 (19) |
| O2 | 0.22106 (10) | 0.33666 (7) | 0.78036 (4) | 0.0312 (2) |
| H2A | 0.2164 (19) | 0.3088 (16) | 0.8314 (8) | 0.048 (4)* |
| N1 | 0.20531 (9) | 0.51397 (8) | 0.56730 (4) | 0.01714 (18) |
| N2 | 0.23410 (10) | 0.50846 (8) | 0.41202 (4) | 0.01962 (19) |
| C1 | 0.19860 (11) | 0.38735 (9) | 0.45045 (5) | 0.0185 (2) |
| C2 | 0.17979 (12) | 0.26102 (9) | 0.40970 (6) | 0.0222 (2) |
| H2 | 0.1884 (17) | 0.2662 (13) | 0.3542 (8) | 0.032 (3)* |
| C3 | 0.15117 (12) | 0.13665 (10) | 0.44606 (6) | 0.0229 (2) |
| H3 | 0.1392 (14) | 0.0507 (13) | 0.4187 (6) | 0.024 (3)* |
| C4 | 0.13883 (12) | 0.13696 (10) | 0.52385 (6) | 0.0220 (2) |
| H4 | 0.1204 (15) | 0.0500 (13) | 0.5494 (7) | 0.032 (3)* |
| C5 | 0.15550 (11) | 0.25972 (9) | 0.56534 (5) | 0.0203 (2) |
| H5 | 0.1496 (15) | 0.2574 (11) | 0.6206 (8) | 0.027 (3)* |
| C6 | 0.18532 (10) | 0.38650 (9) | 0.52882 (5) | 0.01701 (19) |
| C7 | 0.24818 (11) | 0.63536 (9) | 0.53240 (5) | 0.01806 (19) |
| C8 | 0.25998 (11) | 0.62434 (9) | 0.44965 (5) | 0.01757 (19) |
| C9 | 0.30450 (11) | 0.75076 (9) | 0.40701 (5) | 0.0181 (2) |
| C10 | 0.43131 (12) | 0.83965 (10) | 0.43404 (5) | 0.0200 (2) |
| H10 | 0.4888 (16) | 0.8204 (13) | 0.4851 (7) | 0.029 (3)* |
| C11 | 0.47873 (12) | 0.95075 (10) | 0.39000 (6) | 0.0232 (2) |
| H11 | 0.5651 (15) | 1.0131 (11) | 0.4081 (6) | 0.022 (3)* |
| C12 | 0.39868 (12) | 0.97456 (10) | 0.31921 (5) | 0.0238 (2) |
| H12 | 0.4319 (17) | 1.0523 (15) | 0.2884 (8) | 0.047 (4)* |
| C13 | 0.27064 (12) | 0.88795 (10) | 0.29237 (5) | 0.0231 (2) |
| H13 | 0.2131 (16) | 0.9078 (14) | 0.2422 (8) | 0.036 (3)* |
| C14 | 0.22437 (12) | 0.77595 (10) | 0.33558 (5) | 0.0214 (2) |
| H14 | 0.1360 (15) | 0.7173 (12) | 0.3173 (7) | 0.023 (3)* |
| C15 | 0.18946 (11) | 0.51763 (10) | 0.64903 (5) | 0.0191 (2) |
| H15A | 0.1498 (14) | 0.6104 (12) | 0.6607 (6) | 0.024 (3)* |
| H15B | 0.1017 (13) | 0.4501 (11) | 0.6590 (6) | 0.017 (3)* |
| C16 | 0.35032 (12) | 0.47987 (12) | 0.69358 (5) | 0.0256 (2) |
| H16A | 0.4287 (15) | 0.5601 (13) | 0.6897 (7) | 0.031 (3)* |
| H16B | 0.4001 (16) | 0.3962 (14) | 0.6743 (7) | 0.032 (3)* |
| C17 | 0.32545 (15) | 0.45535 (12) | 0.77586 (6) | 0.0302 (2) |
| H17A | 0.2795 (15) | 0.5397 (13) | 0.8020 (7) | 0.033 (3)* |

| | | | | |
|---|---|---|---|---|
| H17B | 0.4311 (18) | 0.4404 (14) | 0.8036 (8) | 0.042 (4)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0405 (4) | 0.0198 (3) | 0.0159 (4) | −0.0061 (3) | 0.0058 (3) | −0.0034 (2) |
| O2 | 0.0500 (5) | 0.0257 (4) | 0.0187 (4) | 0.0036 (3) | 0.0068 (3) | 0.0059 (3) |
| N1 | 0.0217 (4) | 0.0188 (4) | 0.0110 (4) | −0.0012 (3) | 0.0014 (3) | 0.0001 (3) |
| N2 | 0.0249 (4) | 0.0194 (4) | 0.0147 (4) | −0.0030 (3) | 0.0021 (3) | −0.0011 (3) |
| C1 | 0.0221 (4) | 0.0185 (4) | 0.0148 (4) | −0.0021 (3) | 0.0014 (3) | 0.0001 (3) |
| C2 | 0.0284 (5) | 0.0220 (5) | 0.0165 (4) | −0.0037 (4) | 0.0031 (4) | −0.0030 (3) |
| C3 | 0.0255 (5) | 0.0196 (4) | 0.0235 (5) | −0.0037 (4) | 0.0020 (4) | −0.0026 (3) |
| C4 | 0.0225 (4) | 0.0201 (4) | 0.0232 (5) | −0.0040 (3) | 0.0009 (4) | 0.0022 (3) |
| C5 | 0.0223 (4) | 0.0218 (5) | 0.0166 (4) | −0.0028 (3) | 0.0014 (3) | 0.0020 (3) |
| C6 | 0.0176 (4) | 0.0185 (4) | 0.0149 (4) | −0.0010 (3) | 0.0006 (3) | −0.0006 (3) |
| C7 | 0.0218 (4) | 0.0190 (4) | 0.0135 (4) | −0.0009 (3) | 0.0020 (3) | −0.0006 (3) |
| C8 | 0.0213 (4) | 0.0190 (4) | 0.0125 (4) | −0.0011 (3) | 0.0020 (3) | 0.0007 (3) |
| C9 | 0.0234 (4) | 0.0174 (4) | 0.0139 (4) | 0.0000 (3) | 0.0044 (3) | 0.0005 (3) |
| C10 | 0.0232 (4) | 0.0204 (4) | 0.0164 (4) | 0.0001 (3) | 0.0013 (3) | 0.0011 (3) |
| C11 | 0.0256 (5) | 0.0215 (5) | 0.0226 (5) | −0.0031 (4) | 0.0036 (4) | 0.0016 (4) |
| C12 | 0.0301 (5) | 0.0216 (4) | 0.0205 (5) | 0.0010 (4) | 0.0071 (4) | 0.0058 (3) |
| C13 | 0.0290 (5) | 0.0269 (5) | 0.0136 (4) | 0.0036 (4) | 0.0026 (3) | 0.0028 (3) |
| C14 | 0.0255 (5) | 0.0238 (4) | 0.0150 (4) | −0.0017 (4) | 0.0021 (3) | −0.0004 (3) |
| C15 | 0.0245 (4) | 0.0222 (4) | 0.0106 (4) | −0.0016 (4) | 0.0024 (3) | 0.0002 (3) |
| C16 | 0.0249 (5) | 0.0358 (5) | 0.0157 (4) | −0.0029 (4) | −0.0011 (4) | 0.0024 (4) |
| C17 | 0.0384 (6) | 0.0358 (6) | 0.0156 (5) | −0.0003 (5) | −0.0028 (4) | 0.0019 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C7 | 1.2354 (11) | C9—C10 | 1.3930 (13) |
| O2—C17 | 1.4229 (14) | C9—C14 | 1.3998 (13) |
| O2—H2A | 0.949 (15) | C10—C11 | 1.3904 (12) |
| N1—C7 | 1.3710 (11) | C10—H10 | 1.003 (12) |
| N1—C6 | 1.3954 (11) | C11—C12 | 1.3876 (14) |
| N1—C15 | 1.4704 (11) | C11—H11 | 0.958 (12) |
| N2—C8 | 1.2977 (11) | C12—C13 | 1.3862 (14) |
| N2—C1 | 1.3832 (11) | C12—H12 | 0.973 (15) |
| C1—C2 | 1.4051 (12) | C13—C14 | 1.3854 (13) |
| C1—C6 | 1.4071 (12) | C13—H13 | 0.991 (14) |
| C2—C3 | 1.3781 (13) | C14—H14 | 0.950 (12) |
| C2—H2 | 0.996 (13) | C15—C16 | 1.5216 (14) |
| C3—C4 | 1.3954 (14) | C15—H15A | 0.969 (11) |
| C3—H3 | 0.953 (12) | C15—H15B | 0.991 (10) |
| C4—C5 | 1.3822 (13) | C16—C17 | 1.5123 (14) |
| C4—H4 | 0.962 (13) | C16—H16A | 1.003 (13) |
| C5—C6 | 1.4012 (12) | C16—H16B | 0.970 (13) |
| C5—H5 | 0.988 (13) | C17—H17A | 1.016 (12) |
| C7—C8 | 1.4865 (12) | C17—H17B | 0.969 (15) |

| | | | |
|---|---|---|---|
| C8—C9 | 1.4838 (12) | | |
| | | | |
| C17—O2—H2A | 110.4 (9) | C11—C10—H10 | 121.1 (7) |
| C7—N1—C6 | 122.30 (7) | C9—C10—H10 | 118.7 (7) |
| C7—N1—C15 | 118.36 (7) | C12—C11—C10 | 120.13 (9) |
| C6—N1—C15 | 119.25 (7) | C12—C11—H11 | 118.8 (7) |
| C8—N2—C1 | 119.03 (8) | C10—C11—H11 | 121.0 (7) |
| N2—C1—C2 | 118.46 (8) | C13—C12—C11 | 120.04 (9) |
| N2—C1—C6 | 122.09 (8) | C13—C12—H12 | 119.8 (8) |
| C2—C1—C6 | 119.43 (8) | C11—C12—H12 | 120.2 (8) |
| C3—C2—C1 | 120.55 (9) | C14—C13—C12 | 120.06 (9) |
| C3—C2—H2 | 122.4 (7) | C14—C13—H13 | 120.9 (8) |
| C1—C2—H2 | 117.0 (7) | C12—C13—H13 | 119.0 (8) |
| C2—C3—C4 | 119.52 (9) | C13—C14—C9 | 120.38 (9) |
| C2—C3—H3 | 120.8 (7) | C13—C14—H14 | 120.0 (7) |
| C4—C3—H3 | 119.7 (7) | C9—C14—H14 | 119.6 (7) |
| C5—C4—C3 | 121.25 (9) | N1—C15—C16 | 111.32 (8) |
| C5—C4—H4 | 119.1 (7) | N1—C15—H15A | 107.0 (7) |
| C3—C4—H4 | 119.6 (7) | C16—C15—H15A | 113.3 (7) |
| C4—C5—C6 | 119.56 (9) | N1—C15—H15B | 106.7 (6) |
| C4—C5—H5 | 120.1 (6) | C16—C15—H15B | 111.3 (6) |
| C6—C5—H5 | 120.4 (6) | H15A—C15—H15B | 106.9 (9) |
| N1—C6—C5 | 122.61 (8) | C17—C16—C15 | 110.98 (8) |
| N1—C6—C1 | 117.70 (7) | C17—C16—H16A | 108.8 (7) |
| C5—C6—C1 | 119.68 (8) | C15—C16—H16A | 108.4 (7) |
| O1—C7—N1 | 121.94 (8) | C17—C16—H16B | 108.1 (7) |
| O1—C7—C8 | 122.62 (8) | C15—C16—H16B | 112.4 (8) |
| N1—C7—C8 | 115.43 (7) | H16A—C16—H16B | 108.1 (10) |
| N2—C8—C9 | 117.51 (8) | O2—C17—C16 | 107.93 (9) |
| N2—C8—C7 | 123.28 (8) | O2—C17—H17A | 110.7 (7) |
| C9—C8—C7 | 119.21 (7) | C16—C17—H17A | 114.0 (7) |
| C10—C9—C14 | 119.17 (8) | O2—C17—H17B | 111.7 (8) |
| C10—C9—C8 | 121.63 (8) | C16—C17—H17B | 109.1 (8) |
| C14—C9—C8 | 119.06 (8) | H17A—C17—H17B | 103.5 (11) |
| C11—C10—C9 | 120.21 (9) | | |
| | | | |
| C8—N2—C1—C2 | −176.53 (9) | C1—N2—C8—C7 | −2.06 (14) |
| C8—N2—C1—C6 | 1.73 (13) | O1—C7—C8—N2 | −179.52 (9) |
| N2—C1—C2—C3 | 177.28 (9) | N1—C7—C8—N2 | −0.87 (13) |
| C6—C1—C2—C3 | −1.03 (14) | O1—C7—C8—C9 | 0.91 (13) |
| C1—C2—C3—C4 | 0.79 (15) | N1—C7—C8—C9 | 179.56 (8) |
| C2—C3—C4—C5 | −0.28 (15) | N2—C8—C9—C10 | −135.20 (9) |
| C3—C4—C5—C6 | 0.01 (15) | C7—C8—C9—C10 | 44.40 (12) |
| C7—N1—C6—C5 | 174.33 (8) | N2—C8—C9—C14 | 40.45 (12) |
| C15—N1—C6—C5 | −2.04 (13) | C7—C8—C9—C14 | −139.95 (9) |
| C7—N1—C6—C1 | −4.68 (13) | C14—C9—C10—C11 | −0.85 (13) |
| C15—N1—C6—C1 | 178.95 (7) | C8—C9—C10—C11 | 174.79 (8) |
| C4—C5—C6—N1 | −179.24 (8) | C9—C10—C11—C12 | 0.72 (14) |

| | | | |
|---|---|---|---|
| C4—C5—C6—C1 | −0.25 (13) | C10—C11—C12—C13 | 0.31 (14) |
| N2—C1—C6—N1 | 1.55 (13) | C11—C12—C13—C14 | −1.19 (14) |
| C2—C1—C6—N1 | 179.79 (8) | C12—C13—C14—C9 | 1.04 (14) |
| N2—C1—C6—C5 | −177.49 (9) | C10—C9—C14—C13 | −0.03 (14) |
| C2—C1—C6—C5 | 0.75 (13) | C8—C9—C14—C13 | −175.78 (8) |
| C6—N1—C7—O1 | −177.04 (8) | C7—N1—C15—C16 | −91.26 (10) |
| C15—N1—C7—O1 | −0.64 (13) | C6—N1—C15—C16 | 85.24 (10) |
| C6—N1—C7—C8 | 4.31 (12) | N1—C15—C16—C17 | −168.64 (8) |
| C15—N1—C7—C8 | −179.30 (8) | C15—C16—C17—O2 | 63.85 (11) |
| C1—N2—C8—C9 | 177.52 (8) | | |

*Hydrogen-bond geometry (Å, º)*

Cg1 and Cg2 are the centroids of the C9–C14 and C1–C6 benzene rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2*A*···O1$^{i}$ | 0.949 (15) | 1.888 (15) | 2.8345 (10) | 174.4 (14) |
| C15—H15*A*···O2$^{ii}$ | 0.969 (11) | 2.582 (12) | 3.3425 (13) | 135.5 (9) |
| C3—H3···*Cg*1$^{iii}$ | 0.953 (12) | 2.734 (12) | 3.4708 (12) | 134.8 (9) |
| C10—H10···*Cg*2$^{iv}$ | 1.003 (12) | 2.916 (13) | 3.5859 (12) | 124.9 (9) |

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