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

# 2,2′-(Quinoxaline-2,3-diyl)diphenol dimethylformamide solvate

**Zhong-Lu You**

State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian 116012, People's Republic of China
Correspondence e-mail: youzhonglu@lnnu.edu.cn

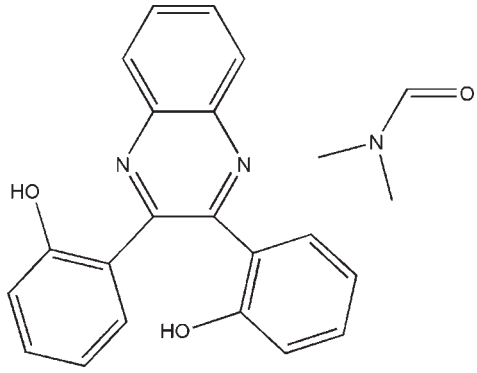
Received 14 December 2009; accepted 16 December 2009

Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.043; $wR$ factor = 0.102; data-to-parameter ratio = 16.2.

In the title compound, $C_{20}H_{14}N_2O_2\cdot C_3H_7NO$, the quinoxaline ring forms dihedral angles of 64.9 (2) and 30.9 (2)° with the two substituted benzene rings, which are themselves inclined at 58.4 (2)°. An intramolecular O—H···N hydrogen bond occurs. In the crystal, molecules are linked through intermolecular O—H···O hydrogen bonds.

## Related literature

For details of cyanide-catalysed cyclizations *via* aldimine coupling, see: Reich *et al.* (2004).




## Experimental

### Crystal data

$C_{20}H_{14}N_2O_2\cdot C_3H_7NO$
$M_r$ = 387.43
Orthorhombic, $P2_12_12_1$
$a$ = 9.759 (2) Å
$b$ = 10.672 (2) Å
$c$ = 19.049 (4) Å
$V$ = 1983.9 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 298 K
0.23 × 0.21 × 0.20 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.980, $T_{max}$ = 0.983
11593 measured reflections
4322 independent reflections
3434 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.102
$S$ = 1.05
4322 reflections
266 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2···O3$^{i}$ | 0.82 | 1.81 | 2.6172 (19) | 168 |
| O1—H1···N1 | 0.82 | 1.94 | 2.647 (2) | 144 |

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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*.

The author acknowledges Dalian University of Technology for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2713).

## References

Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Reich, B. J. E., Justice, A. K., Beckstead, B. T., Reibenspies, J. H. & Miller, S. A. (2004). *J. Org. Chem.* **69**, 1357–1359.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2010). E**66**, o395 [https://doi.org/10.1107/S1600536809054385]

## 2,2′-(Quinoxaline-2,3-diyl)diphenol dimethylformamide solvate

**Zhong-Lu You**

### S1. Comment

Reich and co-workers have reported a series of compounds with the cyanide-catalyzed cyclizations *via* aldimine coupling (Reich *et al.*, 2004), including the crystal structure of 2,2′-(quinoxaline-2,3-diyl)diphenol. In this paper, the title compound, Fig. 1, 2,2′-(quinoxaline-2,3-diyl)diphenol as the *N,N*dimethylformamide solvate is formed in an aldimine coupling reaction and its structure is reported here.

In the compound, the dimethylformamide molecule is linked to the 2,2′-(quinoxaline-2,3-diyl)diphenol molecule through an intermolecular O2—H2···O3 hydrogen bond (Table 1 and Fig. 2). The quinoxaline ring forms dihedral angles of 64.9 (2) and 30.9 (2)°, respectively, with the two substituted benzene rings C9-C14 and C15-C20. The dihedral angle between the two substituted benzene rings is 58.4 (2)°. An intramolecular O1—H1···N1 hydrogen bond (Table 1) is observed in the 2,2′-(quinoxaline-2,3-diyl)diphenol molecule.

### S2. Experimental

The compound was prepared according to a literature procedure (Reich *et al.*, 2004). Yellow block-shaped crystals suitable for X-ray structural determination were obtained by slow diffusion of diethyl ether into a *N,N*dimethylformamide solution.

### S3. Refinement

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93-0.96 Å, O—H distances of 0.82 Å, and with $U_{iso}$(H) = 1.2$U_{eq}$(C) and 1.5$U_{eq}$($C_{methyl}$ and O). In the absence of significant anomalous scattering effects, 1843 Friedel opposites were merged in the final refinement.

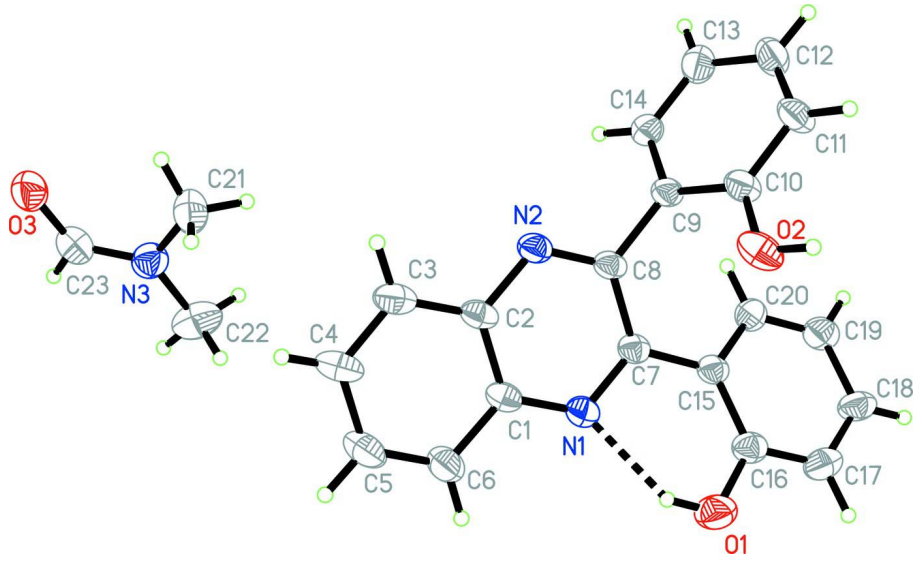



**Figure 1**

The molecular structure of the title compound with ellipsoids drawn at the 30% probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

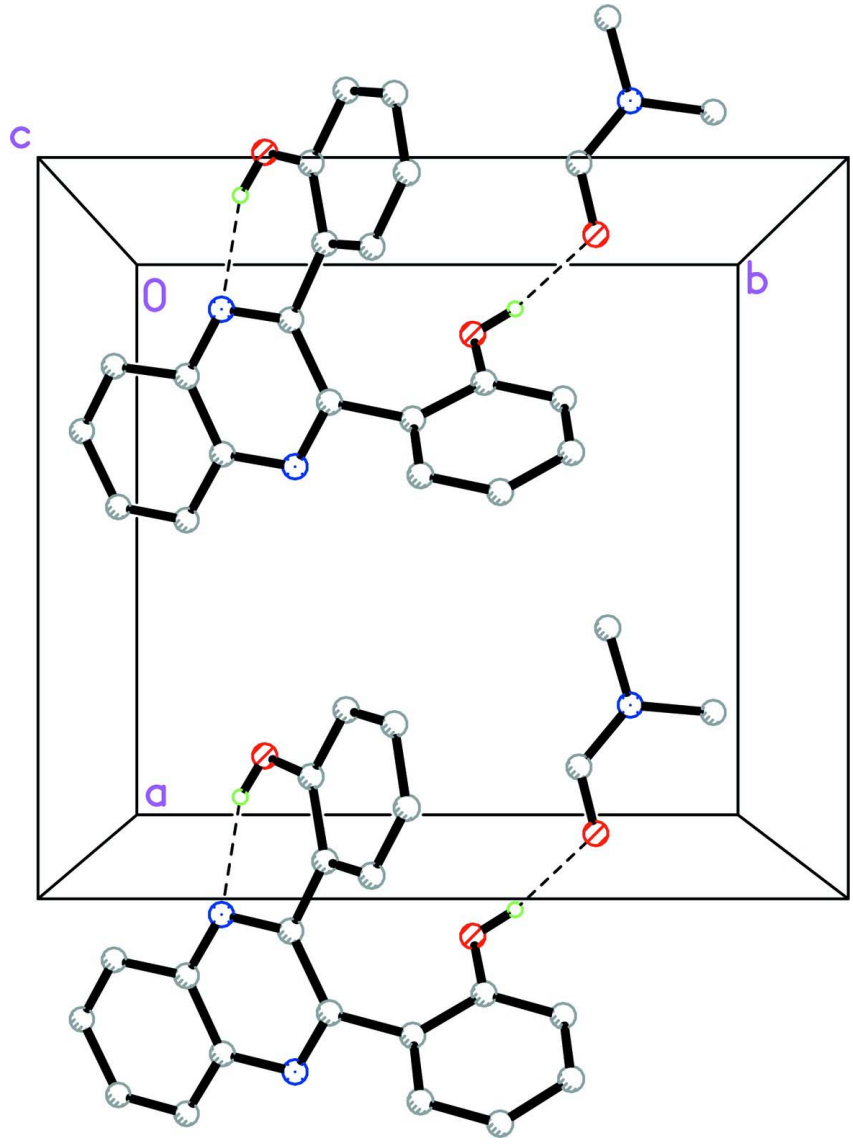



**Figure 2**

The molecular packing of the title compound, viewed along the *c* axis. Hydrogen bonds are drawn as dashed lines. Hydrogen atoms not involved in hydrogen bonding have been omitted.

## 2,2′-(Quinoxaline-2,3-diyl)diphenol dimethylformamide solvate

*Crystal data*

$C_{20}H_{14}N_2O_2·C_3H_7NO$
$M_r$ = 387.43
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a$ = 9.759 (2) Å
$b$ = 10.672 (2) Å
$c$ = 19.049 (4) Å
$V$ = 1983.9 (7) Å$^3$
$Z$ = 4

$F(000)$ = 816
$D_x$ = 1.297 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 4283 reflections
$\theta$ = 2.2–25.9°
$\mu$ = 0.09 mm$^{-1}$
$T$ = 298 K
Block, yellow
0.23 × 0.21 × 0.20 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, 2001)
$T_{min}$ = 0.980, $T_{max}$ = 0.983
11593 measured reflections
4322 independent reflections
3434 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028
$\theta_{max}$ = 27.0°, $\theta_{min}$ = 2.2°
$h$ = −12→12
$k$ = −13→10
$l$ = −24→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.102
$S$ = 1.05
4322 reflections
266 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.0554P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 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 | 0.87527 (15) | 0.67113 (14) | 0.14671 (8) | 0.0496 (3) |
| N2 | 0.61529 (14) | 0.78228 (13) | 0.14710 (8) | 0.0494 (4) |
| N3 | 0.22105 (17) | 0.28969 (17) | 0.15246 (8) | 0.0639 (4) |
| O1 | 1.13645 (14) | 0.73589 (16) | 0.15603 (8) | 0.0771 (4) |
| H1 | 1.0673 | 0.6979 | 0.1681 | 0.116* |
| O2 | 0.83600 (16) | 1.05141 (12) | 0.16631 (7) | 0.0695 (4) |
| H2 | 0.8792 | 1.1162 | 0.1731 | 0.104* |
| O3 | 0.00473 (16) | 0.23971 (15) | 0.18290 (9) | 0.0795 (5) |
| C1 | 0.76781 (19) | 0.61476 (16) | 0.18052 (9) | 0.0483 (4) |
| C2 | 0.63779 (19) | 0.66962 (16) | 0.18002 (9) | 0.0486 (4) |
| C3 | 0.5287 (2) | 0.61110 (19) | 0.21599 (11) | 0.0639 (5) |
| H3 | 0.4419 | 0.6472 | 0.2163 | 0.077* |
| C4 | 0.5521 (3) | 0.5016 (2) | 0.25004 (11) | 0.0711 (6) |
| H4 | 0.4808 | 0.4635 | 0.2744 | 0.085* |
| C5 | 0.6807 (2) | 0.4452 (2) | 0.24920 (11) | 0.0721 (6) |
| H5 | 0.6935 | 0.3691 | 0.2721 | 0.087* |

| | | | | |
|---|---|---|---|---|
| C6 | 0.7878 (2) | 0.49954 (18) | 0.21537 (11) | 0.0641 (5) |
| H6 | 0.8735 | 0.4613 | 0.2152 | 0.077* |
| C7 | 0.85364 (16) | 0.77757 (15) | 0.11304 (8) | 0.0430 (4) |
| C8 | 0.71927 (17) | 0.83557 (15) | 0.11509 (8) | 0.0433 (4) |
| C9 | 0.68921 (17) | 0.96032 (16) | 0.08390 (9) | 0.0464 (4) |
| C10 | 0.75162 (19) | 1.06703 (16) | 0.11096 (9) | 0.0528 (5) |
| C11 | 0.7215 (2) | 1.18364 (17) | 0.08143 (11) | 0.0638 (5) |
| H11 | 0.7619 | 1.2557 | 0.0994 | 0.077* |
| C12 | 0.6323 (2) | 1.1920 (2) | 0.02580 (12) | 0.0684 (6) |
| H12 | 0.6153 | 1.2697 | 0.0055 | 0.082* |
| C13 | 0.5678 (2) | 1.0874 (2) | −0.00042 (12) | 0.0676 (5) |
| H13 | 0.5062 | 1.0943 | −0.0375 | 0.081* |
| C14 | 0.59580 (18) | 0.97191 (18) | 0.02901 (11) | 0.0550 (5) |
| H14 | 0.5517 | 0.9009 | 0.0119 | 0.066* |
| C15 | 0.97327 (16) | 0.83049 (16) | 0.07577 (9) | 0.0453 (4) |
| C16 | 1.10760 (18) | 0.80861 (18) | 0.09958 (9) | 0.0529 (4) |
| C17 | 1.2185 (2) | 0.8622 (2) | 0.06566 (11) | 0.0625 (5) |
| H17 | 1.3065 | 0.8496 | 0.0830 | 0.075* |
| C18 | 1.1996 (2) | 0.9338 (2) | 0.00648 (10) | 0.0633 (5) |
| H18 | 1.2746 | 0.9701 | −0.0157 | 0.076* |
| C19 | 1.0700 (2) | 0.95219 (19) | −0.02002 (10) | 0.0615 (5) |
| H19 | 1.0576 | 0.9991 | −0.0607 | 0.074* |
| C20 | 0.95835 (19) | 0.90080 (18) | 0.01386 (9) | 0.0523 (4) |
| H20 | 0.8712 | 0.9130 | −0.0047 | 0.063* |
| C21 | 0.2074 (3) | 0.4182 (2) | 0.17613 (15) | 0.0940 (8) |
| H21A | 0.2527 | 0.4731 | 0.1436 | 0.141* |
| H21B | 0.2483 | 0.4268 | 0.2217 | 0.141* |
| H21C | 0.1120 | 0.4399 | 0.1787 | 0.141* |
| C22 | 0.3494 (2) | 0.2530 (3) | 0.11988 (14) | 0.0951 (8) |
| H22A | 0.3473 | 0.1649 | 0.1095 | 0.143* |
| H22B | 0.4238 | 0.2704 | 0.1514 | 0.143* |
| H22C | 0.3619 | 0.2993 | 0.0772 | 0.143* |
| C23 | 0.1181 (2) | 0.2123 (2) | 0.15743 (10) | 0.0660 (5) |
| H23 | 0.1303 | 0.1311 | 0.1408 | 0.079* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0505 (8) | 0.0416 (8) | 0.0568 (8) | −0.0064 (7) | −0.0007 (7) | 0.0007 (7) |
| N2 | 0.0512 (8) | 0.0368 (8) | 0.0601 (8) | −0.0058 (6) | 0.0123 (7) | −0.0042 (6) |
| N3 | 0.0591 (10) | 0.0707 (11) | 0.0620 (9) | 0.0009 (9) | 0.0025 (8) | −0.0038 (8) |
| O1 | 0.0513 (8) | 0.0915 (11) | 0.0886 (10) | −0.0128 (8) | −0.0080 (7) | 0.0264 (9) |
| O2 | 0.0955 (11) | 0.0479 (8) | 0.0652 (8) | −0.0194 (7) | −0.0054 (7) | −0.0031 (6) |
| O3 | 0.0707 (10) | 0.0683 (10) | 0.0996 (11) | −0.0145 (8) | 0.0137 (9) | −0.0173 (8) |
| C1 | 0.0572 (10) | 0.0390 (8) | 0.0486 (9) | −0.0130 (8) | 0.0007 (8) | −0.0009 (7) |
| C2 | 0.0576 (10) | 0.0378 (9) | 0.0504 (9) | −0.0130 (9) | 0.0080 (8) | −0.0041 (7) |
| C3 | 0.0657 (12) | 0.0562 (12) | 0.0697 (12) | −0.0169 (10) | 0.0190 (10) | 0.0010 (9) |
| C4 | 0.0841 (16) | 0.0620 (13) | 0.0673 (13) | −0.0310 (12) | 0.0107 (12) | 0.0086 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C5 | 0.0904 (17) | 0.0550 (13) | 0.0709 (12) | −0.0213 (12) | −0.0100 (12) | 0.0199 (10) |
| C6 | 0.0700 (12) | 0.0502 (11) | 0.0721 (12) | −0.0085 (10) | −0.0075 (11) | 0.0112 (10) |
| C7 | 0.0475 (9) | 0.0362 (8) | 0.0454 (8) | −0.0051 (7) | 0.0043 (7) | −0.0075 (7) |
| C8 | 0.0478 (8) | 0.0343 (8) | 0.0478 (8) | −0.0065 (7) | 0.0088 (8) | −0.0061 (7) |
| C9 | 0.0470 (9) | 0.0364 (8) | 0.0559 (9) | −0.0021 (7) | 0.0157 (8) | −0.0025 (7) |
| C10 | 0.0645 (11) | 0.0408 (9) | 0.0530 (10) | −0.0061 (8) | 0.0175 (9) | −0.0023 (8) |
| C11 | 0.0821 (13) | 0.0348 (9) | 0.0747 (13) | −0.0040 (10) | 0.0253 (11) | −0.0012 (9) |
| C12 | 0.0776 (14) | 0.0490 (12) | 0.0786 (14) | 0.0106 (11) | 0.0244 (12) | 0.0142 (10) |
| C13 | 0.0598 (12) | 0.0668 (14) | 0.0762 (13) | 0.0110 (11) | 0.0068 (10) | 0.0094 (11) |
| C14 | 0.0470 (10) | 0.0502 (11) | 0.0679 (11) | 0.0005 (8) | 0.0102 (9) | −0.0015 (9) |
| C15 | 0.0478 (9) | 0.0362 (9) | 0.0519 (9) | −0.0041 (7) | 0.0088 (8) | −0.0068 (7) |
| C16 | 0.0544 (10) | 0.0481 (10) | 0.0564 (10) | −0.0085 (8) | 0.0057 (8) | −0.0063 (8) |
| C17 | 0.0482 (10) | 0.0697 (13) | 0.0696 (12) | −0.0101 (10) | 0.0085 (10) | −0.0117 (10) |
| C18 | 0.0584 (12) | 0.0635 (13) | 0.0681 (12) | −0.0121 (10) | 0.0250 (10) | −0.0117 (10) |
| C19 | 0.0715 (13) | 0.0592 (12) | 0.0539 (10) | −0.0016 (10) | 0.0217 (9) | −0.0018 (9) |
| C20 | 0.0548 (10) | 0.0509 (10) | 0.0513 (10) | 0.0036 (9) | 0.0120 (8) | −0.0033 (8) |
| C21 | 0.0760 (15) | 0.0876 (18) | 0.119 (2) | −0.0221 (15) | 0.0046 (15) | −0.0334 (16) |
| C22 | 0.0715 (15) | 0.128 (2) | 0.0853 (16) | 0.0205 (16) | 0.0133 (12) | 0.0106 (16) |
| C23 | 0.0809 (15) | 0.0573 (13) | 0.0598 (12) | 0.0019 (11) | 0.0001 (11) | −0.0042 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C7 | 1.321 (2) | C9—C14 | 1.393 (3) |
| N1—C1 | 1.370 (2) | C10—C11 | 1.397 (3) |
| N2—C8 | 1.313 (2) | C11—C12 | 1.374 (3) |
| N2—C2 | 1.374 (2) | C11—H11 | 0.9300 |
| N3—C23 | 1.304 (3) | C12—C13 | 1.376 (3) |
| N3—C21 | 1.450 (3) | C12—H12 | 0.9300 |
| N3—C22 | 1.452 (3) | C13—C14 | 1.381 (3) |
| O1—C16 | 1.356 (2) | C13—H13 | 0.9300 |
| O1—H1 | 0.8200 | C14—H14 | 0.9300 |
| O2—C10 | 1.348 (2) | C15—C20 | 1.405 (2) |
| O2—H2 | 0.8200 | C15—C16 | 1.407 (3) |
| O3—C23 | 1.243 (2) | C16—C17 | 1.384 (3) |
| C1—C2 | 1.398 (3) | C17—C18 | 1.375 (3) |
| C1—C6 | 1.411 (3) | C17—H17 | 0.9300 |
| C2—C3 | 1.412 (2) | C18—C19 | 1.376 (3) |
| C3—C4 | 1.356 (3) | C18—H18 | 0.9300 |
| C3—H3 | 0.9300 | C19—C20 | 1.380 (3) |
| C4—C5 | 1.393 (3) | C19—H19 | 0.9300 |
| C4—H4 | 0.9300 | C20—H20 | 0.9300 |
| C5—C6 | 1.358 (3) | C21—H21A | 0.9600 |
| C5—H5 | 0.9300 | C21—H21B | 0.9600 |
| C6—H6 | 0.9300 | C21—H21C | 0.9600 |
| C7—C8 | 1.451 (2) | C22—H22A | 0.9600 |
| C7—C15 | 1.479 (2) | C22—H22B | 0.9600 |
| C8—C9 | 1.487 (2) | C22—H22C | 0.9600 |
| C9—C10 | 1.391 (2) | C23—H23 | 0.9300 |

| | | | |
|---|---|---|---|
| C7—N1—C1 | 118.91 (15) | C11—C12—H12 | 119.4 |
| C8—N2—C2 | 117.87 (15) | C13—C12—H12 | 119.4 |
| C23—N3—C21 | 120.37 (19) | C12—C13—C14 | 119.1 (2) |
| C23—N3—C22 | 121.7 (2) | C12—C13—H13 | 120.5 |
| C21—N3—C22 | 117.9 (2) | C14—C13—H13 | 120.5 |
| C16—O1—H1 | 109.5 | C13—C14—C9 | 120.89 (19) |
| C10—O2—H2 | 109.5 | C13—C14—H14 | 119.6 |
| N1—C1—C2 | 120.52 (15) | C9—C14—H14 | 119.6 |
| N1—C1—C6 | 119.86 (18) | C20—C15—C16 | 117.11 (15) |
| C2—C1—C6 | 119.61 (17) | C20—C15—C7 | 121.67 (15) |
| N2—C2—C1 | 120.99 (15) | C16—C15—C7 | 121.18 (15) |
| N2—C2—C3 | 119.22 (18) | O1—C16—C17 | 116.38 (17) |
| C1—C2—C3 | 119.74 (17) | O1—C16—C15 | 122.97 (16) |
| C4—C3—C2 | 119.1 (2) | C17—C16—C15 | 120.65 (17) |
| C4—C3—H3 | 120.4 | C18—C17—C16 | 120.49 (19) |
| C2—C3—H3 | 120.4 | C18—C17—H17 | 119.8 |
| C3—C4—C5 | 121.28 (19) | C16—C17—H17 | 119.8 |
| C3—C4—H4 | 119.4 | C17—C18—C19 | 120.25 (18) |
| C5—C4—H4 | 119.4 | C17—C18—H18 | 119.9 |
| C6—C5—C4 | 121.0 (2) | C19—C18—H18 | 119.9 |
| C6—C5—H5 | 119.5 | C18—C19—C20 | 119.84 (19) |
| C4—C5—H5 | 119.5 | C18—C19—H19 | 120.1 |
| C5—C6—C1 | 119.3 (2) | C20—C19—H19 | 120.1 |
| C5—C6—H6 | 120.4 | C19—C20—C15 | 121.53 (18) |
| C1—C6—H6 | 120.4 | C19—C20—H20 | 119.2 |
| N1—C7—C8 | 119.88 (14) | C15—C20—H20 | 119.2 |
| N1—C7—C15 | 115.80 (15) | N3—C21—H21A | 109.5 |
| C8—C7—C15 | 124.31 (15) | N3—C21—H21B | 109.5 |
| N2—C8—C7 | 121.74 (15) | H21A—C21—H21B | 109.5 |
| N2—C8—C9 | 114.88 (15) | N3—C21—H21C | 109.5 |
| C7—C8—C9 | 123.34 (14) | H21A—C21—H21C | 109.5 |
| C10—C9—C14 | 119.49 (17) | H21B—C21—H21C | 109.5 |
| C10—C9—C8 | 119.91 (16) | N3—C22—H22A | 109.5 |
| C14—C9—C8 | 120.57 (15) | N3—C22—H22B | 109.5 |
| O2—C10—C9 | 117.14 (15) | H22A—C22—H22B | 109.5 |
| O2—C10—C11 | 123.62 (17) | N3—C22—H22C | 109.5 |
| C9—C10—C11 | 119.22 (18) | H22A—C22—H22C | 109.5 |
| C12—C11—C10 | 120.10 (19) | H22B—C22—H22C | 109.5 |
| C12—C11—H11 | 120.0 | O3—C23—N3 | 124.4 (2) |
| C10—C11—H11 | 120.0 | O3—C23—H23 | 117.8 |
| C11—C12—C13 | 121.16 (19) | N3—C23—H23 | 117.8 |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2···O3$^{i}$ | 0.82 | 1.81 | 2.6172 (19) | 168 |

| | | | | |
|---|---|---|---|---|
| O1—H1···N1 | 0.82 | 1.94 | 2.647 (2) | 144 |

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