

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

3-[(*E*)-(Pyridin-3-ylimino)methyl]phenolM. Nawaz Tahir,<sup>a\*</sup> Akbar Ali,<sup>b</sup> M. Naveed Umar,<sup>b</sup> Ishtiaq Hussain<sup>c</sup> and Hazoor Ahmad Shad<sup>d</sup>

<sup>a</sup>Department of Physics, University of Sargodha, Sargodha, Pakistan, <sup>b</sup>Department of Chemistry, University of Malakand, Pakistan, <sup>c</sup>Department of Chemistry, University of Sargodha, Pakistan, and <sup>d</sup>Department of Chemistry, Government Post Graduate College, Gojra, Punjab, Pakistan

Correspondence e-mail: dmntahir\_uos@yahoo.com

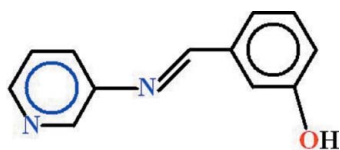
Received 1 June 2012; accepted 6 June 2012

Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.044;  $wR$  factor = 0.118; data-to-parameter ratio = 14.9.

Two independent molecules are present in the asymmetric unit of the title compound,  $\text{C}_{12}\text{H}_{10}\text{N}_2\text{O}$ , in which the 3-hydroxybenzaldehyde and the pyridin-3-amine units are almost planar [r.m.s. deviations of 0.0236 and 0.0116 Å, respectively, in one molecule and 0.0245 and 0.0162 Å, respectively, in the other] and are oriented at dihedral angles of 7.21 (7) and 14.77 (7)°. In the crystal, molecules of the same type form inversion dimers *via* pairs of  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds, forming  $R_2^2(20)$  ring motifs. There exist  $\pi-\pi$  interactions between the benzene and pyridine rings of molecules of the same type with centroid-centroid distances of 3.7127 (10) and 3.8439 (10) Å.

## Related literature

For a related structure, see: Wiebcke & Mootz (1982). For graph-set notation, see: Bernstein *et al.* (1995).



## Experimental

## Crystal data

$\text{C}_{12}\text{H}_{10}\text{N}_2\text{O}$   
 $M_r = 198.22$   
 Triclinic,  $P\bar{1}$

$a = 5.7768$  (5) Å  
 $b = 12.1450$  (11) Å  
 $c = 14.8194$  (13) Å

$\alpha = 78.207$  (4)°  
 $\beta = 89.641$  (3)°  
 $\gamma = 77.601$  (4)°  
 $V = 993.26$  (15) Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.30 \times 0.25 \times 0.20$  mm

## Data collection

Bruker Kappa APEXII CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2005)  
 $T_{\min} = 0.957$ ,  $T_{\max} = 0.966$

14798 measured reflections  
 3876 independent reflections  
 2704 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.029$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.118$   
 $S = 1.04$   
 3876 reflections

261 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.12$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.16$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1}\cdots\text{N2}^i$	0.82	2.00	2.810 (2)	172
$\text{O2}-\text{H2A}\cdots\text{N4}^{ii}$	0.82	1.99	2.8058 (12)	174

Symmetry codes: (i)  $-x + 1, -y, -z$ ; (ii)  $-x + 1, -y, -z + 1$ .

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997) and PLATON (Spek, 2009); software used to prepare material for publication: WinGX (Farrugia, 1999) and PLATON.

The authors acknowledge the provision of funds for the purchase of a diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2365).

## References

- Bernstein, J., Davis, R. E., Shimon, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.  
 Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Bruker (2007). *APEX2* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.  
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.  
 Wiebcke, M. & Mootz, D. (1982). *Acta Cryst.* **B38**, 2008–2013.

## supporting information

*Acta Cryst.* (2012). E68, o2072 [https://doi.org/10.1107/S1600536812025822]

### 3-[(*E*)-(Pyridin-3-ylimino)methyl]phenol

M. Nawaz Tahir, Akbar Ali, M. Naveed Umar, Ishtiaq Hussain and Hazoor Ahmad Shad

#### S1. Comment

In the crystal structure, (Fig. 1), of title compound, two molecules in the asymmetric unit are present, which differ slightly from each other geometrically. In one molecule, the 3-hydroxybenzaldehyde group A (C1–C7/O1) and the pyridin-3-amine moiety B (C8–C12/N1/N2) are planar with r.m.s. deviation of 0.0236 Å and 0.0116 Å, respectively. The dihedral angle between A/B is 14.78 (7)°. In second molecule, the similar groups C (C13–C19/O2) and D (C20–C24/N3/N4) are also planar with r.m.s. deviation of 0.0245 Å and 0.0162 Å, respectively and the dihedral angle between C/D is 7.21 (7)°. Both molecules are dimerized with themselves due to intermolecular H-bonding of O—H···N type (Table 1, Fig. 2) and form  $R_2^2(20)$  ring motif (Bernstein *et al.*, 1995). There exist  $\pi\cdots\pi$  interaction between  $Cg1\cdots Cg2^{iii}$  and  $Cg2\cdots Cg1^{iii}$  at a distance of 3.8439 (11) Å. Similarly, there exist  $\pi\cdots\pi$  interaction between  $Cg3\cdots Cg4^{iv}$  and  $Cg4\cdots Cg3^{iv}$  at a distance of 3.7126 (10) Å.  $Cg1$ ,  $Cg2$ ,  $Cg3$  and  $Cg4$  are the centroids of (C8–C12/N2), (C1–C6), (C20–C24/N4) and (C13–C18) rings, respectively. Symmetry codes: (iii) =  $-x, -y, -z$ ; (iv) =  $-x, -y, -z+1$ .

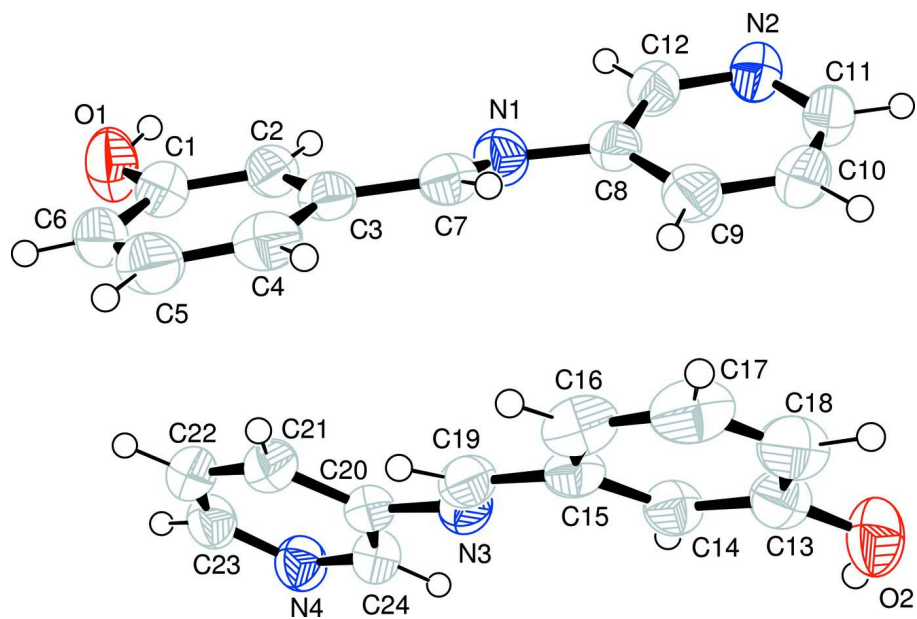
The structure of related compounds - *trans-N*-benzylidene-3-pyridinamine has been published by Wiebcke & Mootz, 1982.

#### S2. Experimental

The title compound has been synthesized as a derivative. Equimolar quantities of 3-hydroxybenzaldehyde and pyridin-3-amine were refluxed in methanol along with few drops of acetic acid as catalyst for 30 min resulting in colourless solution. The solution was kept at room temperature which afforded colourless prisms after three days.

#### S3. Refinement

The H-atoms were positioned geometrically (C—H = 0.93 Å, O—H = 0.82 Å) and refined as riding with  $U_{iso}(H) = xU_{eq}(C, O)$ , where  $x = 1.5$  for hydroxy and  $x = 1.2$  for other H-atoms.

**Figure 1**

View of the title compound with the atom numbering scheme. The displacement ellipsoids are drawn at the 50% probability level. The H atoms are shown as small circles of arbitrary radii.

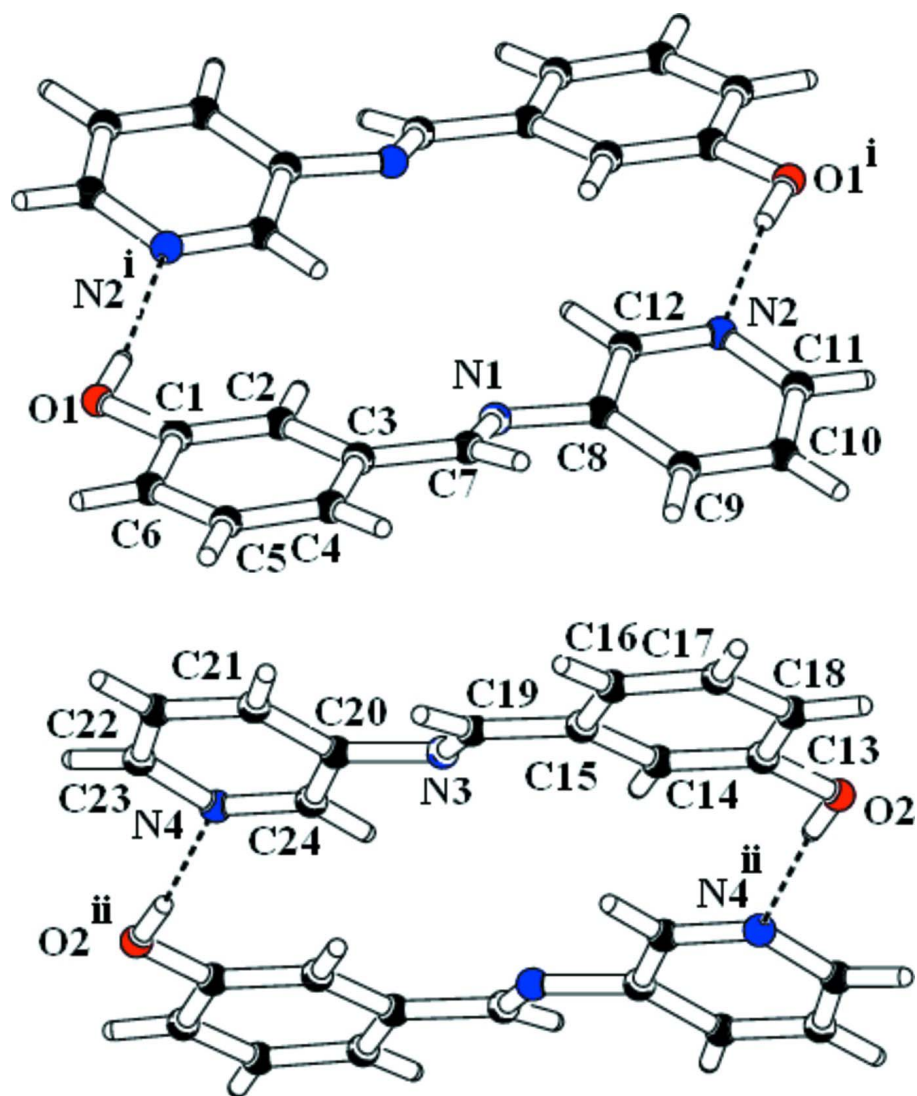


Figure 2

The partial packing which shows that molecules form dimers. Symmetry codes: (i) =  $-x+1, -y, -z$ ; (ii) =  $-x+1, -y, -z+1$ .

### 3-[(E)-(Pyridin-3-ylimino)methyl]phenol

#### Crystal data

$C_{12}H_{10}N_2O$

$M_r = 198.22$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 5.7768$  (5) Å

$b = 12.1450$  (11) Å

$c = 14.8194$  (13) Å

$\alpha = 78.207$  (4)°

$\beta = 89.641$  (3)°

$\gamma = 77.601$  (4)°

$V = 993.26$  (15) Å<sup>3</sup>

$Z = 4$

$F(000) = 416$

$D_x = 1.326$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2704 reflections

$\theta = 1.8$ – $26.0$ °

$\mu = 0.09$  mm<sup>-1</sup>

$T = 296$  K

Prism, colourless

$0.30 \times 0.25 \times 0.20$  mm

*Data collection*

Bruker Kappa APEXII CCD  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 8.00 pixels mm<sup>-1</sup>

$\omega$ -scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2005)

$T_{\min} = 0.957$ ,  $T_{\max} = 0.966$

14798 measured reflections

3876 independent reflections

2704 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 26.0^\circ$ ,  $\theta_{\min} = 1.8^\circ$

$h = -6 \rightarrow 7$

$k = -14 \rightarrow 14$

$l = -18 \rightarrow 18$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.118$

$S = 1.04$

3876 reflections

261 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

$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 0.1521P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.12 \text{ e } \text{Å}^{-3}$

$\Delta\rho_{\min} = -0.16 \text{ e } \text{Å}^{-3}$

*Special details*

**Geometry.** All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 ( $\text{Å}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.3002 (3)	-0.38329 (11)	0.13058 (10)	0.0720 (6)
N1	0.1603 (3)	0.05071 (12)	0.10067 (9)	0.0500 (5)
N2	0.4028 (3)	0.29991 (13)	0.00539 (10)	0.0566 (6)
C1	0.1241 (3)	-0.29847 (16)	0.15019 (12)	0.0525 (6)
C2	0.1340 (3)	-0.18383 (14)	0.12760 (11)	0.0470 (6)
C3	-0.0509 (3)	-0.09881 (15)	0.14672 (11)	0.0453 (6)
C4	-0.2498 (3)	-0.13042 (17)	0.18808 (12)	0.0562 (7)
C5	-0.2555 (3)	-0.24564 (19)	0.21309 (13)	0.0622 (8)
C6	-0.0716 (3)	-0.32902 (17)	0.19536 (12)	0.0603 (7)
C7	-0.0320 (3)	0.02167 (15)	0.12514 (11)	0.0478 (6)
C8	0.1768 (3)	0.16709 (14)	0.08358 (11)	0.0450 (5)
C9	0.0388 (3)	0.25436 (16)	0.12042 (12)	0.0574 (7)
C10	0.0867 (4)	0.36199 (16)	0.09900 (13)	0.0642 (7)
C11	0.2672 (3)	0.38158 (16)	0.04216 (13)	0.0609 (7)
C12	0.3563 (3)	0.19524 (15)	0.02750 (12)	0.0506 (6)
O2	-0.01543 (13)	0.39654 (6)	0.38845 (7)	0.0683 (5)

N3	0.19245 (12)	-0.03508 (6)	0.39821 (6)	0.0500 (5)
N4	0.64794 (12)	-0.29360 (6)	0.47831 (6)	0.0537 (5)
C13	-0.12229 (13)	0.31831 (6)	0.36181 (7)	0.0512 (6)
C14	-0.02002 (12)	0.20228 (6)	0.37886 (6)	0.0467 (6)
C15	-0.1372 (3)	0.12369 (15)	0.35433 (11)	0.0451 (6)
C16	-0.3621 (3)	0.16340 (18)	0.31206 (12)	0.0573 (7)
C17	-0.4595 (3)	0.28010 (19)	0.29175 (13)	0.0638 (7)
C18	-0.3421 (3)	0.35724 (17)	0.31563 (12)	0.0598 (7)
C19	-0.0232 (3)	0.00155 (15)	0.37155 (11)	0.0480 (6)
C20	0.3013 (3)	-0.15308 (14)	0.41181 (11)	0.0436 (5)
C21	0.2182 (3)	-0.23740 (15)	0.37925 (12)	0.0516 (6)
C22	0.3527 (3)	-0.34747 (15)	0.39586 (12)	0.0553 (7)
C23	0.5661 (3)	-0.37225 (15)	0.44406 (12)	0.0547 (6)
C24	0.5160 (3)	-0.18691 (15)	0.46091 (12)	0.0491 (6)
H1	0.38859	-0.35466	0.09392	0.1080*
H2	0.26668	-0.16302	0.09910	0.0564*
H4	-0.37822	-0.07438	0.19884	0.0674*
H5	-0.38665	-0.26689	0.24252	0.0747*
H6	-0.07728	-0.40633	0.21353	0.0723*
H7	-0.16522	0.07872	0.12950	0.0574*
H9	-0.08377	0.23995	0.15891	0.0689*
H10	-0.00331	0.42169	0.12306	0.0771*
H11	0.29688	0.45537	0.02849	0.0732*
H12	0.45151	0.13687	0.00348	0.0606*
H2A	0.09555	0.36277	0.42494	0.1024*
H14	0.13035	0.17617	0.40734	0.0560*
H16	-0.44634	0.11167	0.29759	0.0688*
H17	-0.60742	0.30686	0.26131	0.0765*
H18	-0.40970	0.43573	0.30089	0.0717*
H19	-0.11186	-0.05113	0.36265	0.0576*
H21	0.07331	-0.21935	0.34665	0.0620*
H22	0.29991	-0.40511	0.37463	0.0663*
H23	0.65766	-0.44690	0.45330	0.0656*
H24	0.57225	-0.13110	0.48342	0.0589*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0813 (10)	0.0476 (8)	0.0915 (11)	-0.0207 (7)	0.0199 (8)	-0.0179 (7)
N1	0.0536 (9)	0.0454 (9)	0.0502 (9)	-0.0099 (7)	0.0086 (7)	-0.0094 (7)
N2	0.0648 (9)	0.0486 (10)	0.0605 (10)	-0.0178 (8)	0.0029 (7)	-0.0147 (8)
C1	0.0600 (11)	0.0510 (11)	0.0503 (11)	-0.0189 (9)	0.0007 (8)	-0.0123 (9)
C2	0.0508 (10)	0.0507 (11)	0.0430 (10)	-0.0191 (8)	0.0057 (7)	-0.0093 (8)
C3	0.0466 (9)	0.0554 (11)	0.0358 (9)	-0.0146 (8)	-0.0006 (7)	-0.0099 (8)
C4	0.0474 (10)	0.0757 (14)	0.0498 (11)	-0.0184 (9)	0.0040 (8)	-0.0180 (10)
C5	0.0592 (12)	0.0834 (16)	0.0531 (12)	-0.0352 (11)	0.0082 (9)	-0.0145 (10)
C6	0.0728 (13)	0.0638 (13)	0.0529 (12)	-0.0372 (11)	0.0017 (9)	-0.0083 (9)
C7	0.0481 (10)	0.0534 (11)	0.0406 (10)	-0.0049 (8)	0.0003 (8)	-0.0132 (8)

C8	0.0507 (9)	0.0424 (10)	0.0400 (9)	-0.0059 (8)	-0.0024 (7)	-0.0087 (8)
C9	0.0662 (12)	0.0530 (12)	0.0500 (11)	-0.0053 (9)	0.0103 (9)	-0.0120 (9)
C10	0.0836 (14)	0.0471 (12)	0.0605 (12)	-0.0029 (10)	0.0044 (10)	-0.0198 (10)
C11	0.0778 (13)	0.0447 (11)	0.0613 (12)	-0.0143 (10)	-0.0061 (10)	-0.0120 (9)
C12	0.0550 (10)	0.0472 (11)	0.0514 (11)	-0.0103 (8)	0.0046 (8)	-0.0156 (8)
O2	0.0658 (8)	0.0451 (8)	0.0890 (10)	-0.0024 (6)	-0.0092 (7)	-0.0127 (7)
N3	0.0533 (9)	0.0449 (9)	0.0511 (9)	-0.0079 (7)	-0.0042 (7)	-0.0112 (7)
N4	0.0559 (9)	0.0460 (9)	0.0565 (9)	-0.0070 (7)	0.0029 (7)	-0.0089 (7)
C13	0.0488 (10)	0.0517 (11)	0.0492 (10)	-0.0036 (8)	0.0047 (8)	-0.0096 (8)
C14	0.0430 (9)	0.0482 (11)	0.0441 (10)	-0.0014 (8)	-0.0026 (7)	-0.0075 (8)
C15	0.0454 (9)	0.0539 (11)	0.0352 (9)	-0.0067 (8)	0.0054 (7)	-0.0121 (8)
C16	0.0438 (10)	0.0779 (14)	0.0521 (11)	-0.0082 (9)	0.0017 (8)	-0.0230 (10)
C17	0.0444 (10)	0.0849 (16)	0.0539 (12)	0.0083 (10)	-0.0056 (8)	-0.0191 (11)
C18	0.0546 (11)	0.0592 (12)	0.0540 (11)	0.0103 (9)	0.0030 (9)	-0.0092 (10)
C19	0.0526 (10)	0.0538 (11)	0.0422 (10)	-0.0158 (8)	0.0053 (8)	-0.0159 (8)
C20	0.0506 (9)	0.0428 (10)	0.0385 (9)	-0.0111 (8)	0.0044 (7)	-0.0100 (8)
C21	0.0586 (10)	0.0509 (11)	0.0470 (10)	-0.0135 (9)	-0.0027 (8)	-0.0122 (8)
C22	0.0721 (12)	0.0460 (11)	0.0512 (11)	-0.0168 (9)	0.0018 (9)	-0.0140 (9)
C23	0.0675 (12)	0.0404 (10)	0.0540 (11)	-0.0093 (9)	0.0101 (9)	-0.0075 (8)
C24	0.0526 (10)	0.0442 (10)	0.0521 (11)	-0.0122 (8)	0.0020 (8)	-0.0122 (8)

*Geometric parameters (Å, °)*

O1—C1	1.360 (2)	C6—H6	0.9300
O1—H1	0.8200	C7—H7	0.9300
O2—C13	1.3594 (11)	C9—H9	0.9300
O2—H2A	0.8200	C10—H10	0.9300
N1—C7	1.265 (2)	C11—H11	0.9300
N1—C8	1.408 (2)	C12—H12	0.9300
N2—C11	1.333 (2)	C13—C14	1.3775 (11)
N2—C12	1.331 (2)	C13—C18	1.388 (2)
N3—C20	1.4094 (19)	C14—C15	1.3870 (19)
N3—C19	1.2658 (19)	C15—C16	1.389 (3)
N4—C23	1.3374 (19)	C15—C19	1.459 (3)
N4—C24	1.330 (2)	C16—C17	1.379 (3)
C1—C6	1.390 (3)	C17—C18	1.369 (3)
C1—C2	1.377 (3)	C20—C21	1.389 (2)
C2—C3	1.389 (2)	C20—C24	1.381 (2)
C3—C4	1.388 (3)	C21—C22	1.369 (3)
C3—C7	1.460 (3)	C22—C23	1.373 (3)
C4—C5	1.380 (3)	C14—H14	0.9300
C5—C6	1.366 (3)	C16—H16	0.9300
C8—C12	1.381 (2)	C17—H17	0.9300
C8—C9	1.388 (3)	C18—H18	0.9300
C9—C10	1.368 (3)	C19—H19	0.9300
C10—C11	1.366 (3)	C21—H21	0.9300
C2—H2	0.9300	C22—H22	0.9300
C4—H4	0.9300	C23—H23	0.9300

C5—H5	0.9300	C24—H24	0.9300
C1—O1—H1	109.00	C10—C11—H11	118.00
C13—O2—H2A	109.00	C8—C12—H12	118.00
C7—N1—C8	120.93 (16)	N2—C12—H12	118.00
C11—N2—C12	116.56 (16)	O2—C13—C18	118.56 (11)
C19—N3—C20	121.28 (12)	C14—C13—C18	119.06 (11)
C23—N4—C24	116.83 (12)	O2—C13—C14	122.38 (8)
C2—C1—C6	119.03 (17)	C13—C14—C15	121.21 (10)
O1—C1—C6	118.63 (17)	C14—C15—C19	120.14 (14)
O1—C1—C2	122.33 (16)	C16—C15—C19	120.83 (17)
C1—C2—C3	121.07 (16)	C14—C15—C16	119.02 (16)
C2—C3—C7	119.93 (16)	C15—C16—C17	119.49 (18)
C2—C3—C4	119.13 (17)	C16—C17—C18	121.11 (17)
C4—C3—C7	120.93 (17)	C13—C18—C17	119.99 (17)
C3—C4—C5	119.48 (18)	N3—C19—C15	122.14 (15)
C4—C5—C6	121.09 (17)	N3—C20—C24	115.98 (14)
C1—C6—C5	120.09 (19)	C21—C20—C24	117.11 (16)
N1—C7—C3	121.91 (16)	N3—C20—C21	126.89 (15)
C9—C8—C12	117.15 (16)	C20—C21—C22	119.00 (16)
N1—C8—C12	116.06 (15)	C21—C22—C23	119.57 (17)
N1—C8—C9	126.72 (16)	N4—C23—C22	122.80 (16)
C8—C9—C10	118.67 (17)	N4—C24—C20	124.66 (16)
C9—C10—C11	119.83 (18)	C13—C14—H14	119.00
N2—C11—C10	123.09 (18)	C15—C14—H14	119.00
N2—C12—C8	124.68 (17)	C15—C16—H16	120.00
C3—C2—H2	119.00	C17—C16—H16	120.00
C1—C2—H2	119.00	C16—C17—H17	119.00
C3—C4—H4	120.00	C18—C17—H17	119.00
C5—C4—H4	120.00	C13—C18—H18	120.00
C4—C5—H5	119.00	C17—C18—H18	120.00
C6—C5—H5	119.00	N3—C19—H19	119.00
C1—C6—H6	120.00	C15—C19—H19	119.00
C5—C6—H6	120.00	C20—C21—H21	120.00
N1—C7—H7	119.00	C22—C21—H21	121.00
C3—C7—H7	119.00	C21—C22—H22	120.00
C8—C9—H9	121.00	C23—C22—H22	120.00
C10—C9—H9	121.00	N4—C23—H23	119.00
C11—C10—H10	120.00	C22—C23—H23	119.00
C9—C10—H10	120.00	N4—C24—H24	118.00
N2—C11—H11	118.00	C20—C24—H24	118.00
C8—N1—C7—C3	-177.57 (15)	C12—C8—C9—C10	0.4 (3)
C7—N1—C8—C9	25.4 (3)	C9—C8—C12—N2	-1.2 (3)
C7—N1—C8—C12	-157.68 (16)	N1—C8—C12—N2	-178.40 (16)
C12—N2—C11—C10	-0.7 (3)	C8—C9—C10—C11	0.2 (3)
C11—N2—C12—C8	1.3 (3)	C9—C10—C11—N2	0.0 (3)
C20—N3—C19—C15	-178.07 (14)	O2—C13—C14—C15	177.30 (11)



C19—N3—C20—C21	16.4 (2)	C18—C13—C14—C15	-2.84 (17)
C19—N3—C20—C24	-165.28 (15)	O2—C13—C18—C17	-176.90 (14)
C23—N4—C24—C20	1.1 (2)	C14—C13—C18—C17	3.2 (2)
C24—N4—C23—C22	-2.3 (2)	C13—C14—C15—C16	-0.2 (2)
C6—C1—C2—C3	-2.0 (3)	C13—C14—C15—C19	178.83 (12)
O1—C1—C6—C5	-177.63 (17)	C14—C15—C16—C17	2.8 (2)
O1—C1—C2—C3	178.60 (16)	C19—C15—C16—C17	-176.18 (16)
C2—C1—C6—C5	2.9 (3)	C14—C15—C19—N3	-8.8 (2)
C1—C2—C3—C4	-0.9 (3)	C16—C15—C19—N3	170.20 (15)
C1—C2—C3—C7	177.73 (16)	C15—C16—C17—C18	-2.5 (3)
C2—C3—C7—N1	-9.6 (2)	C16—C17—C18—C13	-0.6 (3)
C4—C3—C7—N1	169.05 (16)	N3—C20—C21—C22	177.27 (15)
C2—C3—C4—C5	2.9 (3)	C24—C20—C21—C22	-1.0 (2)
C7—C3—C4—C5	-175.76 (16)	N3—C20—C24—N4	-177.97 (14)
C3—C4—C5—C6	-2.0 (3)	C21—C20—C24—N4	0.5 (3)
C4—C5—C6—C1	-1.0 (3)	C20—C21—C22—C23	-0.1 (3)
N1—C8—C9—C10	177.26 (17)	C21—C22—C23—N4	1.8 (3)

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O1—H1 $\cdots$ N2 <sup>i</sup>	0.82	2.00	2.810 (2)	172
O2—H2A $\cdots$ N4 <sup>ii</sup>	0.82	1.99	2.8058 (12)	174

Symmetry codes: (i)  $-x+1, -y, -z$ ; (ii)  $-x+1, -y, -z+1$ .