Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(1*H*-Benzimidazol-1-yl)-1-phenylethanone oxime

Özden Özel Güven,[a] Taner Erdoğan,[a] Nagihan Çaylak[b] and Tuncer Hökelek[c]*

[a]Department of Chemistry, Zonguldak Karaelmas University, 67100 Zonguldak, Turkey, [b]Department of Physics, Faculty of Arts and Sciences, Sakarya University, 54187 Esentepe, Adapazarı, Turkey, and [c]Department of Physics, Hacettepe University, 06800 Beytepe, Ankara, Turkey
Correspondence e-mail: merzifon@hacettepe.edu.tr

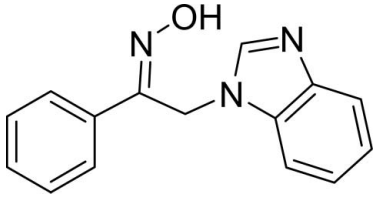
Received 9 July 2007; accepted 10 July 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.011 Å; R factor = 0.045; wR factor = 0.128; data-to-parameter ratio = 6.6.

In the molecule of the title compound, $C_{15}H_{13}N_3O$, intramolecular C—H···O hydrogen bonding causes the formation of a planar five-membered ring. The oxime unit has an E configuration. In this configuration, the oxime groups are involved as donors in intermolecular O—H···N hydrogen bonds, linking the molecules into chains elongated approximately parallel to the c axis and stacked along the b axis.

Related literature

For general background, see: Sevagapandian *et al.* (2000); Marsman *et al.* (1999); Karle *et al.* (1996); Etter *et al.* (1990); Chertanova *et al.* (1994). For related structures, see: Özel Güven *et al.* (2007); Hökelek, Batı *et al.* (2001); Hökelek, Zülfikaroğlu *et al.* (2001); Büyükgüngör *et al.* (2003); Hökelek *et al.* (2004); Hökelek *et al.* (2004*a*,*b*). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{15}H_{13}N_3O$
M_r = 251.29
Orthorhombic, $Pna2_1$
a = 9.3295 (1) Å
b = 11.2863 (2) Å
c = 12.5962 (2) Å
V = 1326.32 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 294 (2) K
0.35 × 0.25 × 0.20 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.933, T_{max} = 0.977
1252 measured reflections
1252 independent reflections
714 reflections with $I > 2\sigma(I)$
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.128
S = 1.00
1252 reflections
189 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O—H···N1^{i}	0.87 (6)	1.84 (5)	2.654 (7)	155 (6)
C8—H82···O	0.96 (6)	2.26 (6)	2.634 (9)	102 (4)

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

Table 2
Comparison of the bond lengths and angles (Å, °) in the oxime moieties of (I) with the corresponding values in the related structures (II)–(VII).

	(I)	(II)	(III)	(IV)	(V)	(VI)	(VII)
N3—O	1.383 (7)	1.403 (2)	1.423 (3)	1.4167 (10)	1.429 (4)	1.424 (2)	1.416 (3)
		1.396 (2)	1.396 (3)				1.397 (3)
N3—C9	1.300 (7)	1.281 (2)	1.290 (3)	1.2897 (12)	1.241 (6)	1.289 (2)	1.282 (3)
		1.281 (2)	1.282 (3)				1.289 (3)
C9—C10	1.491 (8)	1.477 (3)	1.489 (3)	1.5098 (13)	1.551 (7)	1.513 (2)	1.501 (4)
		1.473 (3)					1.502 (4)
C10–C9–N3	115.3 (5)	115.2 (2)	116.6 (2)	114.32 (8)	118.3 (5)	113.2 (1)	114.4 (2)
		115.0 (2)	115.0 (2)				113.4 (2)
C9—N3—O	111.4 (5)	112.4 (1)	109.4 (2)	110.66 (8)	112.2 (4)	110.6 (1)	110.7 (2)
		112.2 (1)	111.5 (2)				111.1 (2)

Notes: (II) 2,3-dimethylquinoxaline–dimethylglyoxime (1/1) (Hökelek, Batı *et al.*, 2001); (III) 1-(2,6-dimethylphenyl-amino)propane-1,2-dione dioxime (Hökelek, Zülfikaroğlu & Batı, 2001); (IV) *N*-hydroxy-2-oxo-2,*N*′-diphenylacetamidine (Büyükgüngör *et al.*, 2003); (V) *N*-(3,4-dichlorophenyl)-*N*′-hydroxy-2-oxo-2-phenylacetamidine (Hökelek *et al.*, 2004*a*); (VI) *N*-hydroxy-*N*′-(1-naphthyl)-2-phenylacetamidin-2-one (Hökelek *et al.*, 2004*b*); (VII) *N*-(3-chloro-4-methylphenyl)-*N*′-hydroxy-2-oxo-2-phenylacetamidine-2,3-dimethylquinoxaline–dimethylglyoxime (1/1) (Hökelek *et al.*, 2004*c*).

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors acknowledge the purchase of the CAD-4 diffractometer under grant DPT/TBAG1 of the Scientific and Technical Research Council of Turkey.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2293).

 doi:10.1107/S1600536807033570

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.

Büyükgüngör, O., Hökelek, T., Taş, M. & Batı, H. (2003). *Acta Cryst.* E**59**, o883–o885.

Chertanova, L., Pascard, C. & Sheremetev, A. (1994). *Acta Cryst.* B**50**, 708–716.

Enraf–Nonius (1994). *CAD-4 EXPRESS*. Enraf–Nonius, Delft, The Netherlands.

Etter, M. C., MacDonald, J. C. & Bernstein, J. (1990). *Acta Cryst.* B**46**, 256–262.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.

Hökelek, T., Batı, H., Bekdemir, Y. & Kütük, H. (2001). *Acta Cryst.* E**57**, o663–o665.

Hökelek, T., Büyükgüngör, O., Taş, M. & Batı, H. (2004*a*). *Acta Cryst.* E**60**, o109–o111.

Hökelek, T., Büyükgüngör, O., Taş, M. & Batı, H. (2004*b*). *Acta Cryst.* E**60**, o406–o408.

Hökelek, T., Taş, M. & Batı, H. (2004). *Cryst. Res. Technol.* **39**, 363–367.

Hökelek, T., Zülfikaroğlu, A. & Batı, H. (2001). *Acta Cryst.* E**57**, o1247–o1249.

Karle, I. L., Ranganathan, D. & Haridas, V. (1996). *J. Am. Chem. Soc.* **118**, 7128–7133.

Marsman, A. W., Leussing, E. D., Zwikker, J. W. & Jenneskens, L. W. (1999). *Chem. Mater.* **11**, 1484–1491.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.

Özel Güven, Ö., Erdoğan, T., Göker, H. & Yıldız, S. (2007). *Bioorg. Med. Chem. Lett.* **17**, 2233–2236.

Sevagapandian, S., Rjagopal, G., Nehru, K. & Athappan, P. (2000). *Transition Met. Chem.* **25**, 388–393.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supplementary materials

Acta Cryst. (2007). E**63**, o3463-o3464 [**doi:10.1107/S1600536807033570**]

2-(1*H*-Benzimidazol-1-yl)-1-phenylethanone oxime

Ö. Özel Güven, T. Erdogan, N. Çaylak and T. Hökelek

Comment

Oxime and dioxime derivatives are very important compounds in the chemical industry and medicine (Sevagapandian *et al.*, 2000\bbr018). The oxime (–C=N—OH) moiety is potentially ambidentate, with possibilities of coordination through nitrogen and/or oxygen atoms. It is a functional group that has not been extensively explored in crystal engineering. In the solid state, oximes are usually associated *via* O—H···N hydrogen bonds of length 2.8 Å.

Oxime groups possess stronger hydrogen-bonding capabilities than alcohols, phenols, and carboxylic acids (Marsman *et al.*, 1999\bbr015), in which intermolecular hydrogen bonding combines moderate strength and directionality (Karle *et al.*, 1996\bbr014) in linking molecules to form supramolecular structures; this has received considerable attention with respect to directional noncovalent intermolecular interactions (Etter *et al.*, 1990\bbr005).

The structures of oxime and dioxime derivatives have been the subject of much interest in our laboratory; examples are 2,3-dimethylquinoxaline-dimethyl- glyoxime (1/1), [(II) Hökelek, Batı *et al.*, 2001\bbr009], 1-(2,6-dimethylphenylamino)propane-1,2-dione dioxime, [(III) (Hökelek, Zülfikaroğlu *et al.*, 2001\bbr013), *N*-hydroxy-2-oxo-2,*N*'-diphenylacetamidine, [(IV) (Büyükgüngör *et al.*, 2003\bbr002], *N*-(3,4-dichlorophenyl)-*N*'-hydroxy-2-oxo-2-phenylacetamidine, [(V) Hökelek *et al.*, 2004\bbr012], *N*-hydroxy-*N*'-(1-naphthyl)-2-phenylacetamidin-2-one [(VI) Hökelek *et al.*, 2004*a*\bbr010] and *N*-(3-chloro-4-methylphenyl)-*N*'-hydroxy-2 -oxo-2-phenylacetamidine [(VII) Hökelek *et al.*, 2004*b*\bbr011]. The structure determination of the title molecule, (I) was carried out in order to investigate the strength of the hydrogen bonding capability of the oxime groups and to compare the geometry of the oxime moieties with the previously reported ones.

In the molecule of the title compound (Fig. 1) the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987\bbr001). The intramolecular C—H···O hydrogen bond (Table 1) causes to the formation of a five-membered planar ring A (O/N3/C8/C9/H82). The benzimidazol B (N1/N2/C7/C1—C6) and phenyl C (C10—C15) rings are, of course, planar and the dihedral angles between the rings are A/B = 89.6 (3)°, A/C = 31.4 (3) and B/C = 74.9 (2)°.

Some significant changes in the geometry of the oxime moieties are evident when the bond lengths and angles are compared with the corresponding values in compounds (II)-(VII) (Table 2). The oxime moiety has an E configuration [C10—C9—N3—O 174.9 (5)°; Chertanova *et al.*, 1994\bbr003]. In this configuration, the oxime groups are involved as donors in O—H···N intermolecular hydrogen bondings (Table 1).

In the crystal structure, the intermolecular O—H···N hydrogen bonds (Table 1) link the molecules into chains elongated approximately parallel to the *c* axis and stacked along the *b* axis (Fig. 2). The intra- and intermolecular hydrogen bonds seem to be effective in the stabilization of the crystal structure.

Experimental

The title compound was prepared from a mixture of 2-(1*H*-benzimidazol-1-yl)-1-phenylethanone (Özel Güven *et al.*, 2007\bbr017) (2.09 g, 8.84 mmol) in methanol (5 ml) and hydroxylaminehydrogensulfate (1.45 g, 8.84 mmol) in water

(3 ml), which was stirred for 24 h at room temperature. Then, methanol was evaporated and extracted with ether and the organic layer was dried and evaporated to dryness. The crude residue was purified by chromatography and recrystallized from methanol solution to obtain colorless crystals (yield; 1.44 g, 65%).

Refinement

Atoms H, H7, H81 and H82 were located in difference syntheses and refined isotropically [O—H = 0.87 (5) Å, U_{iso}(H) = 0.11 (3) Å^2; C—H = 0.93 (6)–0.96 (6) Å, U_{iso}(H) = 0.053 (17)–0.062 (19) Å^2]. The remaining H atoms were positioned geometrically, with C—H = 0.93 Å, and constrained to ride on their parent atom, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

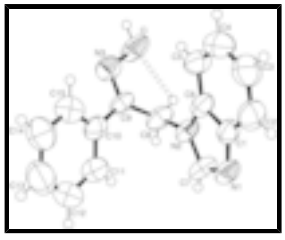


Fig. 1. The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

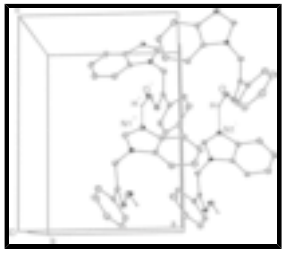


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity [symmetry codes: (') −*x*, −*y*, *z* + 1/2; (") −*x* + 1/2, *y* + 1/2, *z* + 1/2; *x* + 1/2, −*y* + 1/2, *z*].

2-(1*H*-Benzimidazol-1-yl)-1-phenylethanone oxime

Crystal data

$C_{15}H_{13}N_3O$	D_x = 1.258 Mg m^{-3}
M_r = 251.29	Melting point: 465-468 K
Orthorhombic, *Pna*2$_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2c -2n	Cell parameters from 25 reflections
a = 9.3295 (1) Å	θ = 3.6–18.8º
b = 11.2863 (2) Å	μ = 0.08 mm^{-1}
c = 12.5962 (2) Å	*T* = 294 (2) K
V = 1326.32 (3) Å^3	Block, colourless
Z = 4	0.35 × 0.25 × 0.20 mm
F_{000} = 528	

Data collection

Enraf–Nonius TurboCAD-4	R_{int} = 0.0000

diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 294(2) K

non–profiled ω scans

Absorption correction: ψ scan (North *et al.*, 1968\bbr016)

T_{min} = 0.933, T_{max} = 0.977

1252 measured reflections

1252 independent reflections

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

θ_{max} = 25.3º

θ_{min} = 2.4º

h = −11→0

k = 0→13

l = −15→0

3 standard reflections

every 120 min

intensity decay: 1%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.045

$wR(F^2)$ = 0.128

S = 1.00

1252 reflections

189 parameters

4 restraints

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

$w = 1/[\sigma^2(F_o^2) + (0.0654P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max}$ = 0.16 e Å^{-3}

$\Delta\rho_{min}$ = −0.13 e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 1997\bbr019), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.017 (5)

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O	0.3005 (7)	1.2486 (4)	0.6439 (4)	0.0909 (16)
N1	0.2400 (7)	0.8842 (4)	0.9744 (4)	0.0668 (15)

N2	0.3004 (6)	1.0208 (4)	0.8558 (4)	0.0598 (14)
N3	0.3436 (6)	1.1408 (5)	0.6026 (5)	0.0700 (15)
C1	0.1192 (7)	0.9178 (5)	0.9184 (5)	0.0589 (16)
C2	−0.0212 (9)	0.8795 (6)	0.9275 (7)	0.080 (2)
C3	−0.1197 (9)	0.9278 (7)	0.8627 (7)	0.091 (2)
C4	−0.0845 (9)	1.0144 (8)	0.7884 (7)	0.095 (3)
C5	0.0541 (8)	1.0552 (6)	0.7774 (5)	0.074 (2)
C6	0.1554 (7)	1.0039 (5)	0.8440 (5)	0.0601 (17)
C7	0.3432 (10)	0.9469 (6)	0.9337 (5)	0.0697 (19)
C8	0.3909 (10)	1.1002 (7)	0.7907 (6)	0.070 (2)
C9	0.3845 (6)	1.0686 (5)	0.6770 (5)	0.0562 (16)
C10	0.4210 (7)	0.9465 (5)	0.6408 (5)	0.0613 (17)
C11	0.5217 (9)	0.8793 (7)	0.6923 (7)	0.091 (2)
C12	0.5529 (10)	0.7643 (9)	0.6562 (8)	0.119 (3)
C13	0.4857 (11)	0.7195 (8)	0.5701 (8)	0.111 (3)
C14	0.3855 (9)	0.7856 (7)	0.5190 (7)	0.091 (2)
C15	0.3517 (7)	0.8977 (6)	0.5544 (6)	0.074 (2)
H	0.261 (7)	1.288 (5)	0.592 (4)	0.11 (3)*
H2	−0.0466	0.8220	0.9769	0.096*
H3	−0.2144	0.9026	0.8677	0.109*
H4	−0.1561	1.0455	0.7451	0.114*
H5	0.0783	1.1135	0.7285	0.089*
H7	0.437 (7)	0.951 (5)	0.959 (5)	0.062 (18)*
H11	0.5694	0.9098	0.7511	0.109*
H12	0.6204	0.7187	0.6920	0.142*
H13	0.5079	0.6439	0.5459	0.134*
H14	0.3393	0.7550	0.4596	0.109*
H15	0.2812	0.9411	0.5196	0.089*
H81	0.484 (6)	1.088 (5)	0.817 (5)	0.053 (17)*
H82	0.361 (6)	1.180 (5)	0.806 (5)	0.062 (19)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O	0.151 (5)	0.060 (3)	0.062 (3)	−0.006 (3)	−0.015 (3)	0.017 (2)
N1	0.088 (4)	0.058 (3)	0.055 (3)	−0.005 (3)	0.001 (3)	0.018 (3)
N2	0.077 (4)	0.057 (3)	0.045 (3)	−0.010 (3)	−0.005 (3)	0.014 (3)
N3	0.086 (4)	0.055 (3)	0.069 (3)	−0.010 (3)	0.000 (3)	0.012 (3)
C1	0.073 (5)	0.053 (4)	0.050 (4)	0.001 (3)	0.010 (3)	0.007 (3)
C2	0.093 (6)	0.067 (4)	0.079 (5)	−0.004 (4)	0.016 (5)	0.016 (4)
C3	0.075 (5)	0.101 (5)	0.097 (6)	−0.001 (5)	0.015 (5)	0.012 (5)
C4	0.077 (6)	0.109 (6)	0.099 (6)	0.020 (5)	−0.008 (5)	0.017 (5)
C5	0.086 (6)	0.069 (4)	0.068 (5)	0.010 (4)	−0.007 (4)	0.015 (4)
C6	0.081 (5)	0.054 (3)	0.046 (4)	−0.002 (3)	−0.001 (4)	0.007 (3)
C7	0.091 (6)	0.069 (4)	0.049 (4)	−0.010 (4)	−0.021 (4)	0.020 (4)
C8	0.080 (5)	0.071 (5)	0.059 (4)	−0.025 (4)	−0.013 (4)	0.019 (4)
C9	0.066 (4)	0.057 (4)	0.046 (3)	−0.017 (3)	−0.008 (3)	0.019 (3)
C10	0.062 (4)	0.065 (4)	0.057 (4)	−0.009 (3)	0.010 (3)	0.019 (4)

C11	0.093 (5)	0.107 (6)	0.071 (5)	0.021 (5)	−0.005 (4)	0.015 (5)
C12	0.132 (8)	0.123 (8)	0.102 (7)	0.064 (6)	0.009 (6)	0.014 (6)
C13	0.130 (8)	0.092 (6)	0.112 (8)	0.019 (6)	0.036 (7)	0.002 (6)
C14	0.095 (6)	0.077 (5)	0.100 (6)	−0.007 (4)	0.007 (5)	−0.017 (4)
C15	0.066 (5)	0.067 (4)	0.091 (5)	−0.007 (3)	−0.005 (4)	0.004 (4)

Geometric parameters (Å, °)

O—N3	1.383 (7)	C5—C6	1.389 (9)
O—H	0.87 (5)	C7—H7	0.93 (6)
N1—C7	1.300 (9)	C8—H81	0.94 (6)
N2—C6	1.375 (8)	C8—H82	0.96 (6)
N2—C7	1.348 (8)	C9—C8	1.478 (10)
N2—C8	1.479 (8)	C10—C9	1.491 (8)
N3—C9	1.300 (7)	C10—C11	1.370 (10)
C1—N1	1.383 (8)	C10—C15	1.381 (9)
C1—C2	1.384 (10)	C11—H11	0.9300
C1—C6	1.392 (8)	C11—C12	1.405 (11)
C2—C3	1.345 (11)	C12—H12	0.9300
C2—H2	0.9300	C12—C13	1.351 (13)
C3—H3	0.9300	C13—H13	0.9300
C3—C4	1.393 (11)	C14—C13	1.358 (12)
C4—H4	0.9300	C14—H14	0.9300
C5—C4	1.379 (9)	C15—C14	1.378 (9)
C5—H5	0.9300	C15—H15	0.9300
N3—O—H	107 (4)	N2—C8—H81	104 (3)
N1—C1—C2	130.1 (6)	N2—C8—H82	107 (4)
N1—C1—C6	109.7 (6)	C9—C8—N2	111.5 (5)
C7—N1—C1	104.7 (5)	C9—C8—H81	110 (4)
C6—N2—C8	125.9 (5)	C9—C8—H82	114 (4)
C7—N2—C6	106.5 (6)	H81—C8—H82	110 (5)
C7—N2—C8	127.5 (6)	N3—C9—C8	124.0 (6)
C9—N3—O	111.4 (5)	N3—C9—C10	115.3 (5)
C2—C1—C6	120.2 (6)	C8—C9—C10	120.7 (6)
C1—C2—H2	121.0	C11—C10—C15	118.2 (6)
C3—C2—C1	118.1 (7)	C11—C10—C9	121.6 (7)
C3—C2—H2	121.0	C15—C10—C9	120.2 (6)
C2—C3—C4	122.1 (8)	C10—C11—C12	120.0 (8)
C2—C3—H3	119.0	C10—C11—H11	120.0
C4—C3—H3	119.0	C12—C11—H11	120.0
C3—C4—H4	119.3	C11—C12—H12	119.7
C5—C4—C3	121.5 (8)	C13—C12—C11	120.6 (9)
C5—C4—H4	119.3	C13—C12—H12	119.7
C4—C5—C6	116.0 (7)	C12—C13—C14	119.6 (9)
C4—C5—H5	122.0	C12—C13—H13	120.2
C6—C5—H5	122.0	C14—C13—H13	120.2
N2—C6—C5	132.6 (6)	C13—C14—C15	120.5 (8)
N2—C6—C1	105.2 (5)	C13—C14—H14	119.7
C5—C6—C1	122.2 (7)	C15—C14—H14	119.7

N1—C7—N2	113.9 (7)	C10—C15—H15	119.5
N1—C7—H7	126 (4)	C14—C15—C10	121.0 (7)
N2—C7—H7	120 (4)	C14—C15—H15	119.5
C1—N1—C7—N2	0.8 (7)	C1—C2—C3—C4	−0.3 (12)
C7—N2—C6—C5	179.4 (7)	C2—C3—C4—C5	0.0 (13)
C8—N2—C6—C5	−3.6 (11)	C6—C5—C4—C3	0.6 (12)
C7—N2—C6—C1	0.0 (6)	C4—C5—C6—N2	179.8 (7)
C8—N2—C6—C1	177.0 (6)	C4—C5—C6—C1	−0.9 (10)
C6—N2—C7—N1	−0.5 (7)	N3—C9—C8—N2	121.9 (7)
C8—N2—C7—N1	−177.5 (6)	C10—C9—C8—N2	−55.9 (10)
C7—N2—C8—C9	117.9 (8)	C11—C10—C9—N3	149.8 (6)
C6—N2—C8—C9	−58.5 (10)	C11—C10—C9—C8	−32.2 (9)
O—N3—C9—C8	−3.0 (9)	C15—C10—C9—N3	−31.0 (8)
O—N3—C9—C10	174.9 (5)	C15—C10—C9—C8	147.0 (7)
C2—C1—N1—C7	179.6 (7)	C15—C10—C11—C12	0.5 (11)
C6—C1—N1—C7	−0.8 (6)	C9—C10—C11—C12	179.7 (7)
N1—C1—C2—C3	179.6 (7)	C9—C10—C15—C14	179.1 (6)
C6—C1—C2—C3	0.0 (10)	C11—C10—C15—C14	−1.7 (10)
N1—C1—C6—N2	0.5 (6)	C10—C11—C12—C13	0.9 (13)
C2—C1—C6—N2	−179.9 (6)	C11—C12—C13—C14	−1.0 (14)
N1—C1—C6—C5	−179.0 (6)	C15—C14—C13—C12	−0.1 (13)
C2—C1—C6—C5	0.6 (9)	C10—C15—C14—C13	1.6 (11)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O—H···N1^{i}	0.87 (6)	1.84 (5)	2.654 (7)	155 (6)
C8—H82···O	0.96 (6)	2.26 (6)	2.634 (9)	102 (4)

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

Comparison of the bond lengths and angles (Å, °) in the oxime moieties of (I) with the corresponding values in the related structures (II)–(VII)

	(I)	(II)	(III)	(IV)	(V)	(VI)	(VII)
N3—O	1.383 (7)	1.403 (2)	1.423 (3)	1.4167 (10)	1.429 (4)	1.424 (2)	1.416 (3)
		1.396 (2)	1.396 (3)				1.397 (3)
N3—C9	1.300 (7)	1.281 (2)	1.290 (3)	1.2897 (12)	1.241 (6)	1.289 (2)	1.282 (3)
		1.281 (2)	1.282 (3)				1.289 (3)
C9—C10	1.491 (8)	1.477 (3)	1.489 (3)	1.5098 (13)	1.551 (7)	1.513 (2)	1.501 (4)
		1.473 (3)					1.502 (4)
C10—C9—N3	115.3 (5)	115.2 (2)	116.6 (2)	114.32 (8)	118.3 (5)	113.2 (1)	114.4 (2)
		115.0 (2)	115.0 (2)				113.4 (2)
C9—N3—O	111.4 (5)	112.4 (1)	109.4 (2)	110.66 (8)	112.2 (4)	110.6 (1)	110.7 (2)
		112.2 (1)	111.5 (2)				111.1 (2)

Notes: (II) 2,3-dimethylquinoxaline–dimethylglyoxime (1/1) (Hökelek, Batı *et al.*, 2001\bbr009); (III) 1-(2,6-dimethylphenylamino)propane-1,2-dione dioxime (Hökelek, Zülfikar-oğlu *et al.*, 2001); (IV) *N*-hydroxy-2-oxo-2,*N*'-diphenylacetamidine (Büyükgüngör *et al.*, 2003\bbr002); (V) *N*-(3,4-dichlorophenyl)-*N*'-hydroxy-2-oxo-2-phenylacetamidine (Hökelek *et al.*, 2004*a*\bbr010); (VI) *N*-hydroxy-*N*'-(1-naphthyl)-2-phenylacetamidin-2-one (Hökelek *et al.*, 2004*b*\bbr011); (VII) *N*-(3-chloro-4-methylphenyl)-*N*'-hydroxy-2-oxo-2-phenylacetamidine-2,3- dimethylquinoxaline–dimethyl–glyoxime (1/1) (Hökelek *et al.*, 2004\bbr012*c*).

Fig. 1

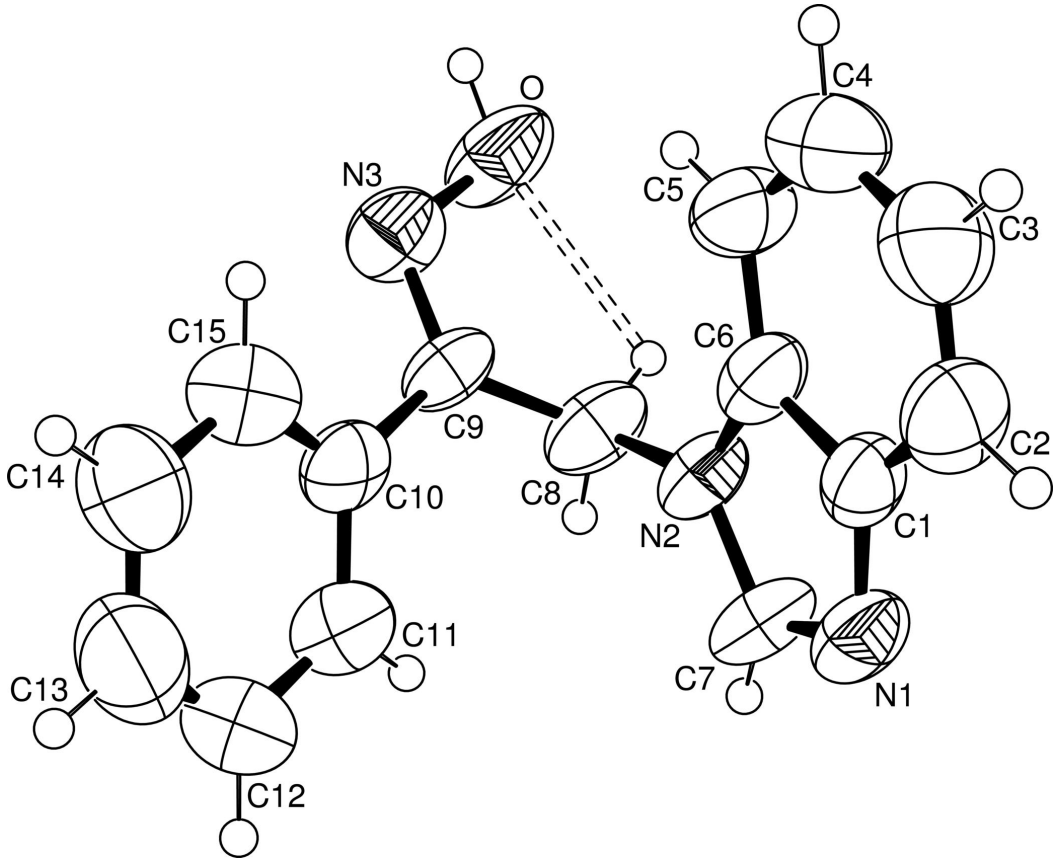


Fig. 2