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2-(1*H*-Benzimidazol-1-yl)-1-(furan-2-yl)-ethanone *O*-2,4-dichlorobenzyloxime

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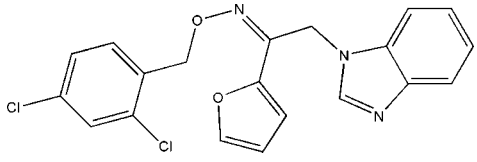
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.044; wR factor = 0.117; data-to-parameter ratio = 8.2.

In the title compound, $C_{20}H_{15}Cl_2N_3O_2$, intramolecular C—H···O hydrogen bonding causes the formation of a planar six-membered ring, which is also coplanar with the adjacent furan ring. The benzimidazole ring system is also planar and is oriented with respect to the coplanar ring system at a dihedral angle of 81.74 (10)°. The benzene ring is oriented with respect to the coplanar ring and benzimidazole ring systems at dihedral angles of 87.75 (15) and 84.24 (12)°, respectively. The oxime unit has an *E* configuration.

Related literature

For general background, see: Mann *et al.* (2001); Roth *et al.* (1997); Evans *et al.* (1996); Chen *et al.* (1993); Saito *et al.* (1993); Awouters *et al.* (1983); Brandstrom *et al.* (1985); Preston (1974); Lipshutz (1986); Coşkun *et al.* (1999); Sevagapandian *et al.* (2000); Forman (1964); Holan *et al.* (1984); Balsamo *et al.* (1990); Chertanova *et al.* (1994). For related literature, see: Hökelek, Batı *et al.* (2001); Hökelek, Zülfikaroğlu & Batı (2001); Büyükgüngör *et al.* (2003); Hökelek *et al.* (2004); Hökelek *et al.* (2004*a*,*b*); Özel Güven, Erdoğan, Çaylak & Hökelek (2007); Özel Güven, Erdoğan, Göker & Yıldız (2007); Özel Güven, Çaylak & Hökelek (2007); Sarıkavaklı *et al.* (2007). For bond length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{20}H_{15}Cl_2N_3O_2$
M_r = 400.25
Monoclinic, $P2_1$
a = 9.4407 (1) Å
b = 5.3902 (2) Å
c = 18.6522 (3) Å
β = 94.036 (10)°
V = 946.81 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 298 (2) K
0.25 × 0.20 × 0.15 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.915, T_{max} = 0.948
2117 measured reflections
1995 independent reflections
1174 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.118
S = 1.03
1995 reflections
244 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack (1983), with no Friedel pairs
Flack parameter: −0.01 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···O1	0.93	2.43	2.823 (7)	105

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

Bond/angle	(I)	(II)	(III)	(IV)	(V)	(VI)	(VII)
N1—O1	1.395 (5)	1.403 (2) 1.396 (2)	1.423 (3) 1.396 (3)	1.417 (1)	1.429 (4)	1.424 (2)	1.416 (3) 1.397 (3)
N1—C1	1.287 (6)	1.281 (2) 1.281 (2)	1.290 (3) 1.282 (3)	1.290 (1)	1.241 (6)	1.289 (2)	1.282 (3) 1.289 (3)
C1—C13	1.508 (6)	1.477 (3) 1.473 (3)	1.489 (3)	1.510 (1)	1.551 (7)	1.513 (2)	1.501 (4) 1.502 (4)
C13—C1—N1	112.0 (5)	115.2 (2) 115.0 (2)	116.6 (2) 115.0 (2)	114.3 (1)	118.3 (5)	113.2 (1)	114.4 (2) 113.4 (2)
C1—N1—O1	111.3 (4)	112.4 (1) 112.2 (1)	109.4 (2) 111.5 (2)	110.7 (1)	112.2 (4)	110.6 (1)	110.7 (2) 111.1 (2)

Notes: (II): 2,3-dimethylquinoxaline–dimethylglyoxime (1/1) (Hökelek, Batı *et al.*, 2001); (III): 1-(2,6-dimethylphenylamino)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); (VI): *N*-hydroxy-*N*′-(1-naphthyl)-2-phenylacetamidin-2-one (Hökelek *et al.*, 2004*a*); (VII): *N*-(3-chloro-4-methylphenyl)-*N*′-hydroxy-2-oxo-2-phenylacetamidine-2,3-dimethylquinoxaline–dimethylglyoxime (1/1) (Hökelek *et al.*, 2004*b*).

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2319).

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supplementary materials

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2-(1*H*-Benzimidazol-1-yl)-1-(furan-2-yl)ethanone *O*-2,4-dichlorobenzyloxime

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Comment

In recent years, the benzimidazole heterocyclic ring system has attracted considerable attention, due to its useful properties for the development of interesting new pharmaceutical compounds (Mann *et al.*, 2001). Some of the substituted benzimidazole derivatives have antitumour, antiviral, antibacterial, anti-inflammatory (Roth *et al.*, 1997; Evans *et al.*, 1996; Chen *et al.*, 1993) and therapeutic (Saito *et al.*, 1993; Awouters *et al.*, 1983; Brandstrom *et al.*, 1985) activities. On the other hand, a series of benzimidazole derivatives are useful for central nervous system disorders (Preston, 1974).

Furans, oximes and amines are very important compounds in organic chemistry. Furan is a relatively highly reactive heteroaromatic compound and is frequently used as an intermediate in organic synthesis (Lipshutz, 1986). In literature, Beckmann fragmentation reaction of *N*-aryl-*N*,*N*-diphenacylamine dioximes has been reported as a new method for the synthesis of imidazooxadiazolones which are imidazole derivatives (Coşkun *et al.*, 1999).

Oxime and dioxime derivatives are very important compounds in the chemical industry and medicine (Sevagapandian *et al.*, 2000). They have a broad pharmacological activity spectrum, encompassing antibacterial, antidepressant and antifungal activities (Forman, 1964; Holan *et al.*, 1984; Balsamo *et al.*, 1990). The oxime (–C=N—OH) moiety is potentially ambidentate, with possibilities of coordination through nitrogen and/or oxygen atoms.

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], 1-(2,6-dimethylphenylamino)propane-1,2-dione dioxime, [(III) (Hökelek, Zülfikaroğlu *et al.*, 2001), *N*-hydroxy-2-oxo-2,*N*'-diphenylacetamidine, [(IV) (Büyükgüngör *et al.*, 2003], *N*-(3,4-dichlorophenyl)-*N*'-hydroxy-2-oxo-2-phenylacetamidine, [(V) Hökelek *et al.*, 2004], *N*-hydroxy-*N*'-(1-naphthyl)-2-phenylacetamidin-2-one [(VI) Hökelek *et al.*, 2004*a*], *N*-(3-chloro-4-methylphenyl)-*N*'-hydroxy-2 -oxo-2-phenylacetamidine [(VII) Hökelek *et al.*, 2004*b*], 2-(1*H*-benzimidazol −1-yl)-1-phenylethanone oxime [(VIII) Özel Güven, Erdoğan, Çaylak & Hökelek, 2007], (1*Z*,2E)-1-(3,5-dimethyl-1*H*-pyrazole-1-yl)ethane-1,2-dione dioxime [(IX) Sarıkavaklı *et al.*, 2007] and *N*,*N*-bis[2-(2-furyl)-2-(hydroxyimino)ethyl]- aniline [(*X*) Özel Güven, Çaylak & Hökelek, 2007]. The structure determination of the title molecule, (I) was carried out in order to investigate the strength of the hydrogen bonding capability and to compare the geometry of the oxime moiety with the previously reported ones.

In the molecule of the title compound, (I), (Fig. 1) the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987). The intramolecular C—H···O hydrogen bond (Table 1) causes the formation of a planar six-membered ring B (O1/N1/C1/C9/C10/H10). The rings A (C3—C8), C (O2/C9—C12), D (N2/N3/C14/C15/C20) and E (C15—C20) are, of course, planar and rings B, C and D, E are also coplanar with dihedral angles of B/C = 0.63 (10)° and D/E = 0.77 (10)°. The coplanar ring systems containing rings B and D are oriented at a dihedral angle of 81.74 (10)°, their orientations with respect to ring A may also be given by the dihedral angles of 84.24 (12)° and 87.75 (15)°, respectively.

Some significant changes in the geometry of the oxime moiety are evident when the bond lengths and angles are compared with the corresponding values in compounds (II)-(VII) (Table 2). The oxime moiety has E configuration [C13—C1—N1—O1 176.9 (4)°; Chertanova *et al.*, 1994].

In the crystal structure, the molecules are elongated approximatelly along the [101] direction and stacked along the *b* axis (Fig. 2).

Experimental

The title compound, (I), was synthesized by the reaction of 2-(1*H*-benzimidazol −1-yl)-1-(furan-2-yl)ethanone oxime (unpublished results) obtained from 2-(1H -benzimidazol-1-yl)-1-(furan-2-yl)ethanone (Özel Güven, Erdoğan, Göker & Yıldız, 2007) with 2,4-dichlorobenzyl chloride. To a solution of 2-(1*H*-benzimidazol-1-yl)-1-(furan −2-yl)ethanone oxime (300 mg, 1.244 mmol) in DMF (3 ml) was added NaH (49 mg, 1.244 mmol) in small fractions. Then, 2,4-dichlorobenzyl chloride (243 mg, 1.244 mmol) in DMF (1.2 ml) was added dropwise. The mixture was stirred at room temperature for 3 h and the excess of hydride was decomposed with a small amount of methyl alcohol. After evaporation to dryness under reduced pressure, the crude residue was suspended with water and extracted with methylene chloride. The organic layer was dried over anhydrous sodium sulfate and then evaporated to dryness. The crude residue was purified by chromatography on a silica-gel column using chloroform and recrystallized from hexane-ethyl acetate mixture (1:3) (yield; 198.8 mg, 40%).

Refinement

H atoms were placed in calculated positions with C—H = 0.93 (aromatic) or 0.97 Å (methylene), and refined in riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

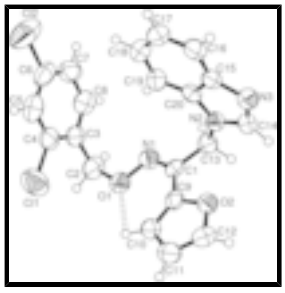

Fig. 1. The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

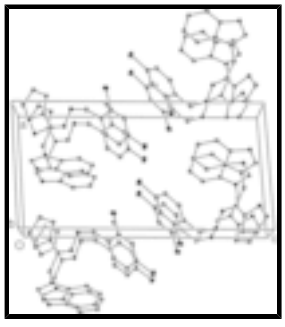

Fig. 2. A packing diagram for (I).

2-(1*H*-Benzimidazol-1-yl)-1-(furan-2-yl)ethanone *O*-2,4-dichlorobenzyloxime

Crystal data

$C_{20}H_{15}Cl_2N_3O_2$ $F_{000} = 412$

M_r = 400.25	D_x = 1.404 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 25 reflections
a = 9.4407 (1) Å	θ = 3.5–18.6º
b = 5.3902 (2) Å	μ = 0.36 mm^{-1}
c = 18.6522 (3) Å	T = 298 (2) K
β = 94.036 (10)º	Rod-shaped, colorless
V = 946.81 (4) Å^3	0.25 × 0.20 × 0.15 mm
Z = 2	

Data collection

Enraf–Nonius TurboCAD-4 diffractometer	R_{int} = 0.036
Radiation source: fine-focus sealed tube	θ_{max} = 25.7º
Monochromator: graphite	θ_{min} = 3.0º
T = 298(2) K	h = 0→11
Non–profiled ω scans	k = −6→0
Absorption correction: ψ scan (North *et al.*, 1968)	l = −22→22
T_{min} = 0.915, T_{max} = 0.948	3 standard reflections
2117 measured reflections	every 120 min
1995 independent reflections	intensity decay: 1%
1174 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.1729P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.118	$(\Delta/\sigma)_{max} < 0.001$
S = 1.03	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
1995 reflections	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
244 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), with no Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.01 (14)
Secondary atom site location: difference Fourier map	

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}
Cl1	0.63539 (17)	0.8163 (4)	0.37586 (10)	0.1067 (7)
Cl2	0.1649 (2)	0.7940 (5)	0.51681 (9)	0.1270 (9)
O1	0.4975 (3)	0.5363 (8)	0.22831 (17)	0.0662 (12)
O2	0.3559 (3)	0.9900 (8)	0.06584 (16)	0.0543 (9)
N1	0.3599 (4)	0.5022 (10)	0.1976 (2)	0.0595 (12)
N2	0.0875 (4)	0.8162 (9)	0.11909 (19)	0.0492 (10)
N3	−0.0552 (4)	1.1369 (10)	0.0901 (2)	0.0559 (11)
C1	0.3307 (5)	0.6582 (11)	0.1464 (2)	0.0453 (12)
C2	0.5134 (6)	0.3715 (12)	0.2900 (3)	0.0739 (18)
H2A	0.6132	0.3570	0.3059	0.089*
H2B	0.4785	0.2077	0.2764	0.089*
C3	0.4328 (5)	0.4690 (13)	0.3499 (3)	0.0574 (14)
C4	0.4757 (6)	0.6715 (13)	0.3905 (3)	0.0618 (15)
C5	0.3959 (7)	0.7696 (13)	0.4422 (3)	0.0733 (17)
H5	0.4274	0.9075	0.4687	0.088*
C6	0.2697 (7)	0.6603 (16)	0.4538 (3)	0.0734 (18)
C7	0.2235 (6)	0.4581 (15)	0.4166 (3)	0.0769 (18)
H7	0.1379	0.3829	0.4257	0.092*
C8	0.3069 (6)	0.3649 (12)	0.3644 (3)	0.0689 (16)
H8	0.2753	0.2259	0.3384	0.083*
C9	0.4190 (5)	0.8531 (10)	0.1216 (2)	0.0457 (12)
C10	0.5505 (5)	0.9418 (12)	0.1382 (3)	0.0545 (14)
H10	0.6154	0.8834	0.1741	0.065*
C11	0.5712 (6)	1.1388 (13)	0.0911 (3)	0.0641 (15)
H11	0.6526	1.2353	0.0895	0.077*
C12	0.4519 (6)	1.1616 (12)	0.0489 (3)	0.0599 (14)
H12	0.4369	1.2796	0.0128	0.072*
C13	0.1856 (5)	0.6136 (11)	0.1096 (2)	0.0529 (13)
H13A	0.1950	0.5892	0.0586	0.063*
H13B	0.1465	0.4625	0.1284	0.063*
C14	0.0276 (5)	0.9663 (12)	0.0671 (2)	0.0532 (13)
H14	0.0444	0.9486	0.0188	0.064*
C15	−0.0491 (5)	1.1001 (10)	0.1642 (3)	0.0484 (13)
C16	−0.1138 (5)	1.2320 (11)	0.2159 (3)	0.0604 (16)
H16	−0.1709	1.3685	0.2039	0.072*
C17	−0.0910 (5)	1.1544 (15)	0.2863 (3)	0.0703 (17)
H17	−0.1347	1.2387	0.3222	0.084*
C18	−0.0042 (6)	0.9532 (15)	0.3044 (3)	0.0697 (17)

H18	0.0087	0.9054	0.3523	0.084*
C19	0.0631 (5)	0.8225 (13)	0.2535 (2)	0.0613 (15)
H19	0.1223	0.6888	0.2657	0.074*
C20	0.0379 (5)	0.9009 (10)	0.1831 (2)	0.0477 (13)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0859 (11)	0.1158 (16)	0.1163 (12)	−0.0308 (13)	−0.0083 (9)	0.0296 (14)
Cl2	0.1575 (16)	0.148 (2)	0.0799 (11)	0.0560 (19)	0.0406 (11)	0.0051 (14)
O1	0.062 (2)	0.084 (3)	0.053 (2)	0.008 (2)	0.0046 (17)	0.013 (2)
O2	0.0514 (18)	0.059 (2)	0.0527 (18)	−0.002 (2)	0.0043 (15)	0.008 (2)
N1	0.056 (3)	0.067 (3)	0.056 (2)	0.006 (3)	0.006 (2)	−0.003 (3)
N2	0.045 (2)	0.056 (3)	0.047 (2)	−0.002 (3)	0.0030 (18)	−0.006 (2)
N3	0.051 (2)	0.064 (3)	0.053 (2)	0.003 (3)	0.0043 (19)	0.004 (3)
C1	0.051 (3)	0.048 (3)	0.038 (2)	0.002 (3)	0.011 (2)	−0.005 (3)
C2	0.079 (3)	0.080 (5)	0.063 (3)	0.031 (4)	0.001 (3)	0.017 (4)
C3	0.056 (3)	0.064 (4)	0.052 (3)	0.010 (3)	0.000 (2)	0.015 (3)
C4	0.067 (3)	0.066 (4)	0.051 (3)	0.000 (4)	−0.005 (3)	0.017 (3)
C5	0.099 (4)	0.062 (4)	0.057 (3)	0.005 (4)	−0.010 (3)	0.000 (3)
C6	0.092 (5)	0.084 (5)	0.045 (3)	0.020 (5)	0.007 (3)	0.008 (4)
C7	0.066 (3)	0.090 (5)	0.076 (4)	−0.006 (4)	0.011 (3)	0.017 (4)
C8	0.086 (4)	0.057 (4)	0.063 (3)	0.002 (4)	0.002 (3)	0.005 (3)
C9	0.048 (3)	0.049 (3)	0.040 (2)	0.006 (3)	0.004 (2)	−0.006 (3)
C10	0.052 (3)	0.061 (4)	0.051 (3)	−0.001 (3)	0.003 (2)	−0.003 (3)
C11	0.059 (3)	0.067 (4)	0.067 (3)	−0.010 (3)	0.011 (3)	−0.016 (4)
C12	0.068 (3)	0.054 (4)	0.060 (3)	0.005 (4)	0.023 (3)	0.008 (3)
C13	0.054 (3)	0.052 (4)	0.054 (3)	−0.006 (3)	0.004 (2)	−0.007 (3)
C14	0.048 (3)	0.068 (4)	0.043 (3)	−0.005 (3)	−0.004 (2)	−0.002 (3)
C15	0.038 (2)	0.054 (4)	0.053 (3)	−0.001 (3)	0.002 (2)	−0.001 (3)
C16	0.045 (3)	0.069 (4)	0.067 (3)	0.004 (3)	0.005 (3)	−0.003 (3)
C17	0.059 (3)	0.097 (5)	0.056 (3)	0.003 (4)	0.009 (3)	−0.013 (4)
C18	0.065 (3)	0.095 (5)	0.049 (3)	0.002 (4)	0.006 (3)	0.002 (4)
C19	0.056 (3)	0.075 (4)	0.053 (3)	−0.001 (4)	−0.003 (2)	0.007 (3)
C20	0.037 (2)	0.053 (4)	0.053 (3)	−0.009 (3)	0.001 (2)	−0.002 (3)

Geometric parameters (Å, °)

Cl1—C4	1.737 (6)	C7—H7	0.9300
Cl2—C6	1.744 (6)	C8—H8	0.9300
O1—N1	1.395 (5)	C9—C10	1.347 (6)
O1—C2	1.453 (6)	C9—C1	1.437 (7)
O2—C9	1.376 (5)	C10—H10	0.9300
O2—C12	1.348 (6)	C11—C10	1.401 (8)
N1—C1	1.287 (6)	C11—H11	0.9300
N2—C14	1.356 (6)	C12—C11	1.333 (7)
N2—C13	1.451 (6)	C12—H12	0.9300
N2—C20	1.389 (6)	C13—H13A	0.9700
N3—C14	1.300 (7)	C13—H13B	0.9700

N3—C15	1.393 (6)	C14—H14	0.9300
C1—C13	1.508 (6)	C15—C16	1.376 (6)
C2—H2A	0.9700	C15—C20	1.382 (7)
C2—H2B	0.9700	C16—C17	1.380 (7)
C3—C8	1.360 (7)	C16—H16	0.9300
C3—C4	1.373 (9)	C17—H17	0.9300
C3—C2	1.491 (7)	C18—C17	1.387 (9)
C5—C4	1.371 (7)	C18—H18	0.9300
C5—H5	0.9300	C19—C18	1.373 (7)
C6—C5	1.360 (8)	C19—C20	1.385 (6)
C7—C6	1.348 (9)	C19—H19	0.9300
C7—C8	1.388 (7)		
N1—O1—C2	106.6 (4)	C9—C10—C11	107.0 (5)
C12—O2—C9	106.4 (4)	C9—C10—H10	126.5
C1—N1—O1	111.3 (4)	C11—C10—H10	126.5
C14—N2—C20	105.6 (4)	C12—C11—C10	106.9 (5)
C14—N2—C13	126.8 (4)	C12—C11—H11	126.6
C20—N2—C13	127.5 (4)	C10—C11—H11	126.6
C14—N3—C15	104.1 (4)	C11—C12—O2	110.7 (5)
N1—C1—C9	128.1 (4)	C11—C12—H12	124.7
N1—C1—C13	112.0 (5)	O2—C12—H12	124.7
C9—C1—C13	119.9 (4)	N2—C13—C1	113.0 (4)
O1—C2—C3	110.4 (5)	N2—C13—H13A	109.0
O1—C2—H2A	109.6	C1—C13—H13A	109.0
C3—C2—H2A	109.6	N2—C13—H13B	109.0
O1—C2—H2B	109.6	C1—C13—H13B	109.0
C3—C2—H2B	109.6	H13A—C13—H13B	107.8
H2A—C2—H2B	108.1	N3—C14—N2	114.6 (4)
C8—C3—C4	116.5 (5)	N3—C14—H14	122.7
C8—C3—C2	120.3 (6)	N2—C14—H14	122.7
C4—C3—C2	123.2 (5)	C16—C15—C20	120.5 (5)
C5—C4—C3	122.7 (5)	C16—C15—N3	129.2 (5)
C5—C4—Cl1	117.6 (5)	C20—C15—N3	110.2 (4)
C3—C4—Cl1	119.7 (5)	C15—C16—C17	117.6 (5)
C6—C5—C4	118.4 (6)	C15—C16—H16	121.2
C6—C5—H5	120.8	C17—C16—H16	121.2
C4—C5—H5	120.8	C16—C17—C18	121.3 (5)
C7—C6—C5	121.6 (6)	C16—C17—H17	119.4
C7—C6—Cl2	120.2 (6)	C18—C17—H17	119.4
C5—C6—Cl2	118.2 (6)	C19—C18—C17	121.8 (5)
C6—C7—C8	118.3 (6)	C19—C18—H18	119.1
C6—C7—H7	120.8	C17—C18—H18	119.1
C8—C7—H7	120.8	C18—C19—C20	116.2 (6)
C3—C8—C7	122.5 (6)	C18—C19—H19	121.9
C3—C8—H8	118.7	C20—C19—H19	121.9
C7—C8—H8	118.7	C15—C20—C19	122.6 (5)
C10—C9—O2	109.0 (5)	C15—C20—N2	105.5 (4)
C10—C9—C1	137.0 (5)	C19—C20—N2	132.0 (5)
O2—C9—C1	113.9 (4)		

C2—O1—N1—C1	173.8 (4)	C2—C3—C8—C7	−175.9 (5)
N1—O1—C2—C3	−73.5 (5)	C6—C5—C4—C3	0.4 (8)
C12—O2—C9—C10	0.3 (5)	C6—C5—C4—Cl1	179.2 (5)
C12—O2—C9—C1	−179.6 (4)	C7—C6—C5—C4	1.0 (9)
C9—O2—C12—C11	0.0 (5)	Cl2—C6—C5—C4	−177.1 (4)
O1—N1—C1—C9	−1.8 (7)	C8—C7—C6—C5	−1.3 (9)
O1—N1—C1—C13	176.4 (4)	C8—C7—C6—Cl2	176.8 (5)
C14—N2—C13—C1	115.4 (5)	C6—C7—C8—C3	0.3 (9)
C20—N2—C13—C1	−62.9 (6)	C10—C9—C1—N1	0.7 (9)
C20—N2—C14—N3	−0.3 (6)	O2—C9—C1—N1	−179.5 (5)
C13—N2—C14—N3	−178.9 (4)	C10—C9—C1—C13	−177.5 (5)
C14—N2—C20—C15	−0.3 (5)	O2—C9—C1—C13	2.4 (6)
C13—N2—C20—C15	178.3 (4)	O2—C9—C10—C11	−0.5 (5)
C14—N2—C20—C19	−179.5 (5)	C1—C9—C10—C11	179.4 (5)
C13—N2—C20—C19	−0.9 (8)	C12—C11—C10—C9	0.5 (6)
C15—N3—C14—N2	0.8 (6)	O2—C12—C11—C10	−0.3 (6)
C14—N3—C15—C16	178.3 (5)	C20—C15—C16—C17	−1.4 (7)
C14—N3—C15—C20	−0.9 (5)	N3—C15—C16—C17	179.4 (5)
N1—C1—C13—N2	114.9 (5)	C16—C15—C20—C19	0.8 (7)
C9—C1—C13—N2	−66.6 (5)	N3—C15—C20—C19	−179.9 (5)
C8—C3—C2—O1	103.7 (6)	C16—C15—C20—N2	−178.6 (4)
C4—C3—C2—O1	−73.0 (6)	N3—C15—C20—N2	0.8 (5)
C8—C3—C4—C5	−1.3 (8)	C15—C16—C17—C18	1.0 (8)
C2—C3—C4—C5	175.5 (5)	C19—C18—C17—C16	0.2 (9)
C8—C3—C4—Cl1	179.9 (4)	C18—C19—C20—C15	0.4 (7)
C2—C3—C4—Cl1	−3.4 (7)	C18—C19—C20—N2	179.5 (5)
C4—C3—C8—C7	1.0 (8)	C20—C19—C18—C17	−0.8 (8)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···O1	0.93	2.43	2.823 (7)	105

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

Bond/Angle	(I)	(II)	(III)	(IV)	(V)	(VI)	(VII)
N1—O1	1.395 (5)	1.403 (2)	1.423 (3)	1.417 (1)	1.429 (4)	1.424 (2)	1.416 (3)
		1.396 (2)	1.396 (3)				1.397 (3)
N1—C1	1.287 (6)	1.281 (2)	1.290 (3)	1.290 (1)	1.241 (6)	1.289 (2)	1.282 (3)
		1.281 (2)	1.282 (3)				1.289 (3)
C1—C13	1.508 (6)	1.477 (3)	1.489 (3)	1.510 (1)	1.551 (7)	1.513 (2)	1.501 (4)
		1.473 (3)					1.502 (4)
C13—C1—N1	112.0 (5)	115.2 (2)	116.6 (2)	114.3 (1)	118.3 (5)	113.2 (1)	114.4 (2)
		115.0 (2)	115.0 (2)				113.4 (2)
C1—N1—O1	111.3 (4)	112.4 (1)	109.4 (2)	110.7 (1)	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-dimethylphenylamino)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); (VI): *N*-hydroxy-*N*'-(1-naphthyl)-2-phenylacetamidin-2-one (Hökelek *et al.*, 2004*a*); (VII): *N*-(3-chloro-4-methylphenyl)-*N*'-hydroxy-2-oxo-2-phenylacetamidine-2,3-dimethylquinoxaline–dimethylglyoxime (1/1) (Hökelek *et al.*, 2004*b*).

Fig. 1

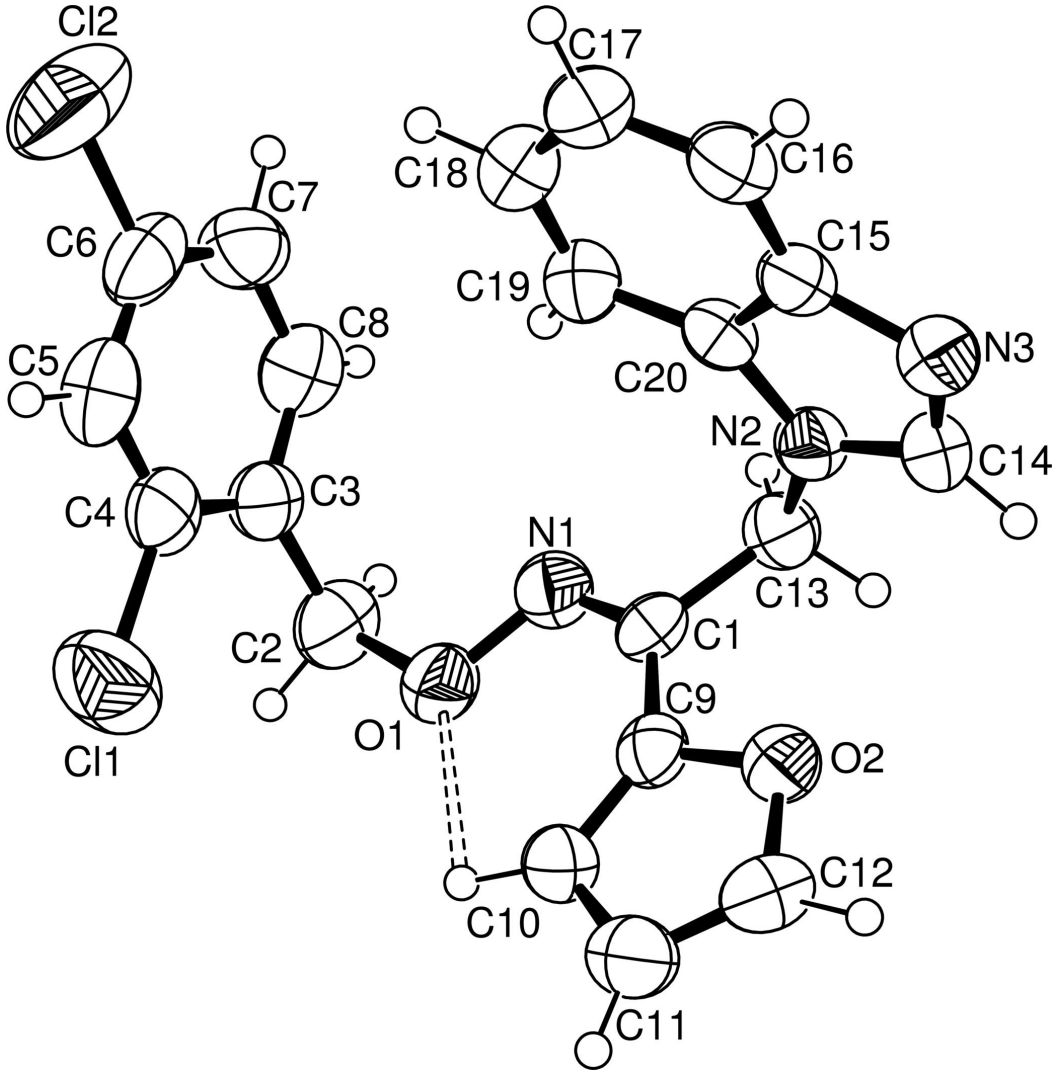

Fig. 2