



Crystal structure of 2-hydroxy-2-phenylacetophenone oxime

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Received 27 November 2020

Accepted 11 December 2020

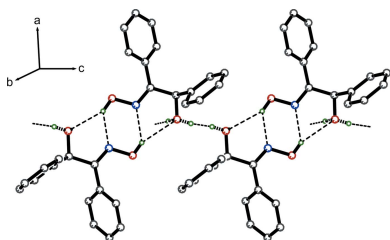
Edited by S. Parkin, University of Kentucky, USA

Keywords: crystal structure; hydrogen bond; phenylacetophenone; oxime.**CCDC reference:** 2049764**Supporting information:** this article has supporting information at journals.iucr.org/e

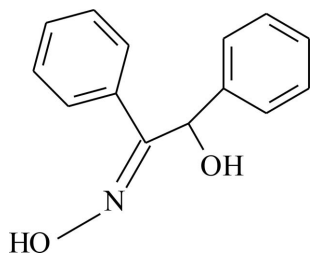
The title compound [systematic name: 2-(*N*-hydroxyimino)-1,2-diphenylethanol], $C_{14}H_{13}NO_2$, consists of hydroxy phenylacetophenone and oxime units, in which the phenyl rings are oriented at a dihedral angle of $80.54(7)^\circ$. In the crystal, intermolecular $O-H_{Oxm} \cdots N_{Oxm}$, $O-H_{Hydr} \cdots O_{Hydr}$, $O-H'_{Hydr} \cdots O_{Hydr}$ and $O-H_{Oxm} \cdots O_{Hydr}$ hydrogen bonds link the molecules into infinite chains along the *c*-axis direction. π - π contacts between inversion-related of the phenyl ring adjacent to the oxime group have a centroid-centroid separation of $3.904(3) \text{ \AA}$ and a weak $C-H \cdots \pi(\text{ring})$ interaction is also observed. A Hirshfeld surface analysis of the crystal structure indicates that the most important contributions for the crystal packing are from $H \cdots H$ (58.4%) and $H \cdots C/C \cdots H$ (26.4%) contacts. Hydrogen bonding and van der Waals contacts are the dominant interactions in the crystal packing.

1. Chemical context

Intermolecular hydrogen bonding has received considerable attention among the directional non-covalent intermolecular interactions (Etter *et al.*, 1990). Hydrogen bonds combine moderate strength and directionality (Karle *et al.*, 1996) in linking molecules to form supramolecular structures. The oxime ($-C=N-OH$) moiety, which is similar to carboxylic acid in that it contains one hydrogen-bond donor and two acceptor atoms, is a functional group that has not been extensively explored in crystal engineering. Structurally characterized oxime moieties are much less common than carboxylic acids and amides, but from a supramolecular perspective, this functionality does have some unique and desirable features (Aakeröy *et al.*, 2001). Oxime groups possess stronger hydrogen-bonding capabilities than alcohols, phenols and carboxylic acids (Marsman *et al.*, 1999). The hydrogen-bond systems in the crystals of oximes have been analysed and a correlation between patterns of hydrogen bonding and N—O bond lengths has been suggested (Bertolasi *et al.*, 1982). Oxime and dioxime derivatives are very important in the chemical industry, photography, agriculture, textiles, technological improvement, dye chemistry, semiconductor manufacturing and medicine (Sevagapandian *et al.*, 2000; Schrauzer *et al.*, 1965; Thomas & Underhill, 1972; Underhill *et al.*, 1973; Chakravorty, 1974; Kurita, 1998; Mathur & Narang, 1990; Ravi Kumar, 2000). They have a broad pharmacological activity spectrum, encompassing antibacterial, antidepressant and antifungal activities (Forman, 1964; Holan *et al.*, 1984). Some oxime complexes also have anticarcinogenic activities (Sevagapandian *et al.*, 2000; Srivastava *et al.*, 1997). The crystallization and the molecular



and crystal structures of the title compound, (I), are reported herein. Its magnetic properties have previously been studied by electron paramagnetic resonance (EPR) (Sayin *et al.*, 2012).



2. Structural commentary

As shown in Fig. 1, the title compound, (I), consists of hydroxy phenylacetophenone and oxime units, where the phenyl, *A* (C1–C6) and *B* (C9–C14), rings are oriented at a dihedral angle of 80.54 (7)°. The dihedral angle between the oxime plane *C* (O1/N1/C7) and phenyl rings *A* and *B* are 39.48 (9) and 80.11 (14)°, respectively. The base of the oxime moiety is approximately coplanar with the *A* phenyl ring plane, as indicated by the O1–N1–C7–C1 torsion angle of 1.0 (3)°. In the oxime moiety, the O1–N1 [1.4026 (18) Å] bond length and the O1–N1–C7 [115.36 (14)°] bond angle may be compared with the corresponding values of O1–N2 [1.423 (3) Å], O2–N3 [1.396 (3) Å], O2–N3–C10 [111.5 (2)°] and O1–N2–C9 [109.4 (2)°] in the glyoxime moiety reported in 1-(2,6-dimethylphenylamino)propane-1,2-dione dioxime [(II); (Hökelek *et al.*, 2001)], reflecting the types and electron-withdrawing or donating properties of the substituents bonded to the carbon atoms of the glyoxime moiety.

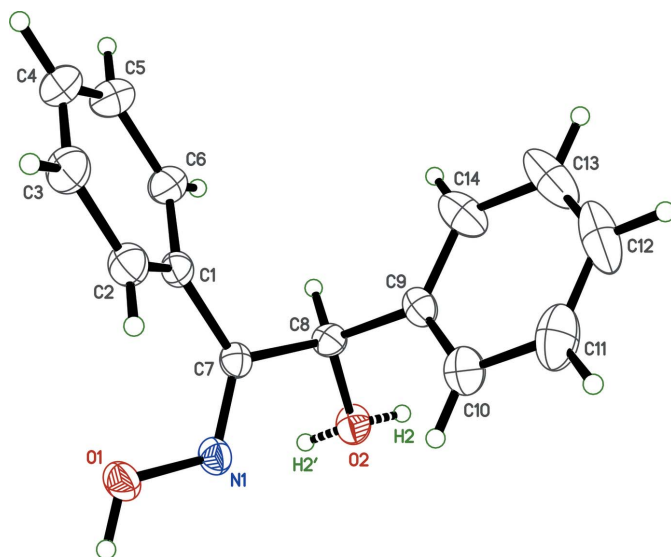


Figure 1

The asymmetric unit of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The hydrogen attached to hydroxyl oxygen O2 is disordered in a 50:50 ratio, as indicated by dashed bonds.

Table 1

Hydrogen-bond geometry (Å, °).

Cg2 is the centroid of the phenyl ring *B* (C9–C14).

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
O1–H1...O2 ⁱ	0.88 (2)	2.47 (2)	3.2638 (19)	151 (1.47)
O1–H1...N1 ⁱ	0.88 (2)	2.13 (2)	2.8236 (19)	135 (1.69)
O2–H2...O2 ⁱⁱⁱ	0.82 (4)	2.03 (2)	2.850 (3)	175 (1.99)
O2–H2...O2 ^{iv}	0.83 (4)	2.05 (3)	2.881 (3)	180 (2.38)
C4–H4...Cg2 ^{vi}	0.93	2.91	3.792 (3)	159

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

3. Supramolecular features

In the crystal, intermolecular O–H_{Oxm}...O_{Hydr}, O–H_{Oxm}...N_{Oxm}, O–H_{Hydr}...O_{Hydr} and O–H'_{Hydr}...O_{Hydr} hydrogen bonds (Table 1, Fig. 2) [Oxm = oxime and Hydr = hydroxy] form *R*₁²(5) and *R*₂²(6) ring motifs (Etter *et al.*, 1990) between inversion-related molecules, which link to form extended chains along the *c*-axis direction (Figs. 2 and 3). π – π contacts between inversion-related phenyl rings [Cg1...Cg1ⁱ = 3.904 (1) Å; symmetry code: (i) $\frac{1}{2} - x, \frac{3}{2} - y, 1 - z$], where Cg1 is the centroid of ring *A* (C1–C6)] and a weak C–H... π (ring) interaction (Table 1) are also observed. A Hirshfeld surface analysis of the crystal structure indicates that the most important contributions for the crystal packing are from H...H (58.4%) and H...C/C...H (26.4%) interactions, but a full Hirshfeld surface analysis is complicated by the disorder. Hydrogen bonding and van der Waals interactions comprise the dominant contacts in the crystal packing (Table 2).

4. Synthesis and crystallization

The alpha-benzoinoxime [ABO (C₁₄H₁₃NO₂) powder was purchased from Merck, and crystallized by slow evaporation from a concentrated solution in ethanol as colourless crystals at room temperature.

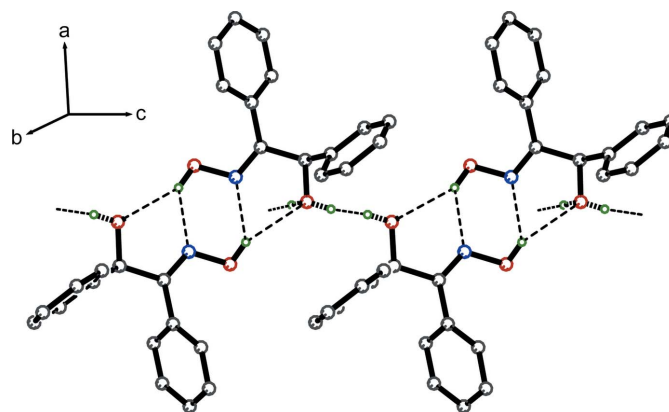


Figure 2

A partial packing diagram. The O–H_{Oxm}...N_{Oxm}, O–H_{Hydr}...O_{Hydr}, O–H'_{Hydr}...O_{Hydr} and O–H_{Oxm}...O_{Hydr} hydrogen bonds [Oxm = oxime and Hydr = hydroxy] are shown as thin dashed lines. Bonds involving the disordered hydroxyl hydrogen are shown as thick dashed lines. The remaining hydrogen atoms have been omitted for the sake of clarity.

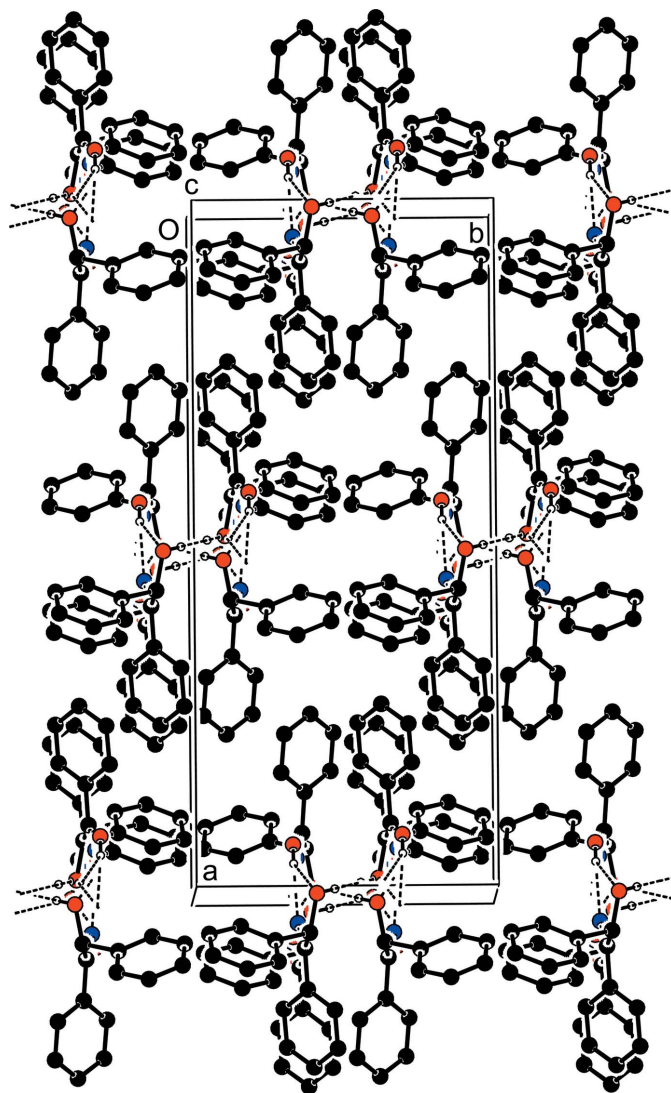


Figure 3
A packing diagram viewed down the *c* axis. The O—H_{Oxm}···N_{Oxm}, O—H_{Hydr}···O_{Hydr}, O—H_{Hydr}···O_{Hydr} and O—H_{Oxm}···O_{Hydr} hydrogen bonds [Oxm = oxime and Hydr = hydroxy] hydrogen bonds are shown as dashed lines. The remaining hydrogen atoms have been omitted for clarity.

5. Refinement

Experimental details including the crystal data, data collection and refinement are summarized in Table 3. The hydroxy H atoms were located in a difference-Fourier map and refined isotropically. The C-bound H atoms were positioned geometrically, with C—H = 0.93 Å (for aromatic H atoms), and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$. The hydrogen attached to O2 is disordered over two sites (H2 and H2') in a 0.5:0.5 ratio and was refined with restraints.

Acknowledgements

NA is grateful to Professor Tuncer Hökelek from Hacettepe University, Turkey for helpful discussions and technical fac-

Table 2
Selected interatomic distances (Å).

O1···C2	2.819 (3)	N1···H1 ⁱ	2.13 (2)
O1···N1 ⁱ	2.823 (2)	H2'···N1 ^{iv}	2.83 (2)
C8···O1 ⁱⁱⁱ	3.381 (2)	H14···C6 ⁱⁱ	2.79
O2···O2 ⁱⁱⁱ	2.850 (3)	C6···H8	2.66
O2···O2 ^{iv}	2.881 (3)	C7···H10	2.92
O2···N1	2.577 (2)	C8···H2 ⁱⁱⁱ	2.76 (2)
O1···H2A	2.41	C8···H6	2.75
H8···O1 ⁱⁱ	2.62	C8···H2 ^{iv}	2.87 (2)
O2···H10	2.87	C9···H2 ⁱⁱⁱ	2.92 (2)
O2···H1 ⁱ	2.465 (17)	H1···H2 ⁱ	2.31
H2···O2 ⁱⁱⁱ	2.03 (2)	H2'···H1 ⁱⁱ	2.59 (2)
H2'···O2 ^{iv}	2.05 (3)	H2A···H13 ^v	2.57
N1···N1 ⁱ	2.867 (2)	H6···H8	2.12
N1···H2A	2.90	H8···H14	2.30
N1···H2'	2.49 (2)		

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

Table 3
Experimental details.

Crystal data	
Chemical formula	C ₁₄ H ₁₃ NO ₂
<i>M_r</i>	227.25
Crystal system, space group	Monoclinic, C2/c
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	24.3559 (2), 10.7032 (2), 8.9667 (2)
β (°)	93.220 (2)
<i>V</i> (Å ³)	2333.80 (7)
<i>Z</i>	8
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.09
Crystal size (mm)	0.15 × 0.11 × 0.10
Data collection	
Diffractometer	Bruker APEXII QUAZAR three-circle
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	15784, 2673, 1781
<i>R</i> _{int}	0.048
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, <i>S</i>	0.048, 0.124, 1.03
No. of reflections	2673
No. of parameters	158
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³)	0.17, -0.24

Computer programs: APEX2 and SAINT (Bruker, 2012), SHELXT (Sheldrick, 2015a), SHELXL2018/3 (Sheldrick, 2015b), XP in SHELXTL (Sheldrick, 2008), ORTEP-3 for Windows and WinGX publication routines (Farrugia, 2012) and PLATON (Spek, 2020).

ities provided, and Professor Ülkü Sayın from Selçuk University, Turkey for her constant assistance during the crystallization process.

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supporting information

Acta Cryst. (2021). E77, 66-69 [https://doi.org/10.1107/S2056989020016163]

Crystal structure of 2-hydroxy-2-phenylacetophenone oxime

Nurcan Akduran

Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *ORTEP-3* for Windows (Farrugia, 2012) and *XP in SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 2012) and *PLATON* (Spek, 2020).

2-(*N*-Hydroxyimino)-1,2-diphenylethanol

Crystal data

$C_{14}H_{13}NO_2$

$M_r = 227.25$

Monoclinic, *C2/c*

$a = 24.3559(2) \text{ \AA}$

$b = 10.7032(2) \text{ \AA}$

$c = 8.9667(2) \text{ \AA}$

$\beta = 93.220(2)^\circ$

$V = 2333.80(7) \text{ \AA}^3$

$Z = 8$

$F(000) = 960$

$D_x = 1.294 \text{ Mg m}^{-3}$

Mo *K* α radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2607 reflections

$\theta = 3.1\text{--}21.7^\circ$

$\mu = 0.09 \text{ mm}^{-1}$

$T = 296 \text{ K}$

Block, colourless

$0.15 \times 0.11 \times 0.10 \text{ mm}$

Data collection

Bruker APEXII QUAZAR three-circle diffractometer

Detector resolution: $8.3333 \text{ pixels mm}^{-1}$

φ and ω scans

15784 measured reflections

2673 independent reflections

1781 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.048$

$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 1.7^\circ$

$h = -31 \rightarrow 31$

$k = -13 \rightarrow 13$

$l = -11 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.048$

$wR(F^2) = 0.124$

$S = 1.03$

2673 reflections

158 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 1.7468P]$

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

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

$\Delta\rho_{\text{max}} = 0.17 \text{ e \AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.24 \text{ e \AA}^{-3}$

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
O1	0.06576 (6)	0.67667 (13)	0.19541 (13)	0.0449 (3)	
H1	0.0363 (8)	0.676 (2)	0.1336 (17)	0.067*	
O2	0.01347 (5)	0.60393 (13)	0.59737 (16)	0.0451 (4)	
H2	0.0037 (6)	0.602 (4)	0.684 (4)	0.068*	0.5
H2'	0.0059 (5)	0.544 (4)	0.542 (5)	0.068*	0.5
N1	0.04995 (6)	0.66307 (14)	0.34255 (15)	0.0373 (4)	
C1	0.14866 (7)	0.63331 (17)	0.41569 (19)	0.0362 (4)	
C2	0.17398 (8)	0.71174 (19)	0.3165 (2)	0.0463 (5)	
H2A	0.153310	0.771694	0.263426	0.056*	
C3	0.22965 (8)	0.7011 (2)	0.2964 (2)	0.0582 (6)	
H3	0.246113	0.754405	0.230145	0.070*	
C4	0.26080 (9)	0.6132 (3)	0.3727 (3)	0.0644 (7)	
H4	0.298150	0.605990	0.357871	0.077*	
C5	0.23633 (9)	0.5359 (2)	0.4713 (3)	0.0627 (6)	
H5	0.257333	0.475965	0.523500	0.075*	
C6	0.18100 (8)	0.5459 (2)	0.4939 (2)	0.0483 (5)	
H6	0.165180	0.493550	0.562321	0.058*	
C7	0.08910 (7)	0.64245 (15)	0.44001 (19)	0.0330 (4)	
C8	0.07095 (7)	0.62830 (17)	0.59889 (19)	0.0359 (4)	
H8	0.090620	0.557401	0.645918	0.043*	
C9	0.08441 (7)	0.74454 (18)	0.68979 (19)	0.0390 (4)	
C10	0.06246 (10)	0.8580 (2)	0.6490 (3)	0.0572 (6)	
H10	0.038643	0.864319	0.564624	0.069*	
C11	0.07566 (12)	0.9636 (2)	0.7335 (3)	0.0782 (8)	
H11	0.060924	1.040773	0.705199	0.094*	
C12	0.11041 (13)	0.9541 (3)	0.8583 (3)	0.0877 (10)	
H12	0.119636	1.025026	0.914105	0.105*	
C13	0.13143 (13)	0.8414 (3)	0.9010 (3)	0.0878 (10)	
H13	0.154334	0.834930	0.987246	0.105*	
C14	0.11882 (10)	0.7366 (2)	0.8165 (2)	0.0632 (6)	
H14	0.133716	0.659731	0.845480	0.076*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0426 (7)	0.0630 (9)	0.0294 (6)	−0.0031 (7)	0.0029 (5)	0.0015 (6)
O2	0.0370 (7)	0.0526 (8)	0.0470 (8)	−0.0134 (6)	0.0130 (6)	−0.0077 (6)
N1	0.0383 (8)	0.0432 (9)	0.0308 (7)	−0.0034 (7)	0.0054 (6)	−0.0022 (6)
C1	0.0342 (9)	0.0406 (10)	0.0338 (9)	−0.0037 (8)	0.0034 (7)	−0.0074 (7)

C2	0.0434 (11)	0.0530 (12)	0.0429 (11)	-0.0069 (9)	0.0069 (8)	-0.0014 (9)
C3	0.0432 (12)	0.0805 (16)	0.0521 (12)	-0.0137 (11)	0.0145 (10)	-0.0048 (11)
C4	0.0346 (11)	0.0986 (19)	0.0609 (14)	0.0020 (12)	0.0093 (10)	-0.0156 (13)
C5	0.0434 (13)	0.0808 (17)	0.0636 (14)	0.0150 (11)	-0.0004 (11)	-0.0021 (12)
C6	0.0399 (11)	0.0557 (12)	0.0495 (11)	0.0024 (9)	0.0044 (9)	0.0001 (9)
C7	0.0340 (9)	0.0317 (9)	0.0335 (9)	-0.0053 (7)	0.0037 (7)	-0.0035 (7)
C8	0.0305 (9)	0.0408 (10)	0.0367 (9)	-0.0052 (7)	0.0049 (7)	0.0021 (8)
C9	0.0397 (10)	0.0472 (11)	0.0309 (9)	-0.0124 (8)	0.0087 (7)	-0.0013 (8)
C10	0.0651 (14)	0.0509 (13)	0.0559 (13)	-0.0012 (11)	0.0056 (11)	-0.0080 (10)
C11	0.093 (2)	0.0522 (15)	0.092 (2)	-0.0077 (13)	0.0314 (17)	-0.0185 (14)
C12	0.114 (2)	0.093 (2)	0.0601 (16)	-0.0545 (19)	0.0367 (16)	-0.0357 (16)
C13	0.108 (2)	0.112 (3)	0.0429 (14)	-0.059 (2)	-0.0020 (14)	-0.0092 (15)
C14	0.0712 (15)	0.0747 (16)	0.0428 (11)	-0.0246 (13)	-0.0062 (10)	0.0051 (11)

Geometric parameters (Å, °)

O1—N1	1.4026 (18)	C5—H5	0.9300
O1—H1	0.88 (2)	C6—H6	0.9300
O2—C8	1.424 (2)	C7—C8	1.523 (2)
O2—H2	0.82 (4)	C8—C9	1.513 (2)
O2—H2'	0.83 (4)	C8—H8	0.9800
N1—C7	1.276 (2)	C9—C10	1.368 (3)
C1—C6	1.388 (3)	C9—C14	1.376 (3)
C1—C2	1.392 (3)	C10—C11	1.388 (3)
C1—C7	1.482 (2)	C10—H10	0.9300
C2—C3	1.383 (3)	C11—C12	1.369 (4)
C2—H2A	0.9300	C11—H11	0.9300
C3—C4	1.368 (3)	C12—C13	1.356 (4)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.372 (3)	C13—C14	1.379 (4)
C4—H4	0.9300	C13—H13	0.9300
C5—C6	1.378 (3)	C14—H14	0.9300
O1...C2	2.819 (3)	N1...H1 ⁱ	2.13 (2)
O1...N1 ⁱ	2.823 (2)	H2'...N1 ^{iv}	2.83 (2)
C8...O1 ⁱⁱ	3.381 (2)	H14...C6 ⁱⁱ	2.79
O2...O2 ⁱⁱⁱ	2.850 (3)	C6...H8	2.66
O2...O2 ^{iv}	2.881 (3)	C7...H10	2.92
O2...N1	2.577 (2)	C8...H2 ⁱⁱⁱ	2.76 (2)
O1...H2A	2.41	C8...H6	2.75
H8...O1 ⁱⁱ	2.62	C8...H2 ^{iv}	2.87 (2)
O2...H10	2.87	C9...H2 ⁱⁱⁱ	2.92 (2)
O2...H1 ⁱ	2.465 (17)	H1...H2 ⁱ	2.31
H2...O2 ⁱⁱⁱ	2.03 (2)	H2'...H1 ⁱⁱ	2.59 (2)
H2'...O2 ^{iv}	2.05 (3)	H2A...H13 ^v	2.57
N1...N1 ⁱ	2.867 (2)	H6...H8	2.12
N1...H2A	2.90	H8...H14	2.30
N1...H2'	2.49 (2)		

N1—O1—H1	109.5	O2—C8—C9	109.82 (14)
C8—O2—H2	109.5	O2—C8—C7	110.26 (14)
C8—O2—H2'	109.5	C9—C8—C7	110.90 (14)
C7—N1—O1	115.36 (14)	O2—C8—H8	108.6
C6—C1—C2	118.06 (17)	C9—C8—H8	108.6
C6—C1—C7	120.16 (16)	C7—C8—H8	108.6
C2—C1—C7	121.77 (17)	C10—C9—C14	119.1 (2)
C3—C2—C1	120.5 (2)	C10—C9—C8	121.08 (17)
C3—C2—H2A	119.8	C14—C9—C8	119.82 (19)
C1—C2—H2A	119.8	C9—C10—C11	120.1 (2)
C4—C3—C2	120.8 (2)	C9—C10—H10	119.9
C4—C3—H3	119.6	C11—C10—H10	119.9
C2—C3—H3	119.6	C12—C11—C10	119.9 (3)
C3—C4—C5	119.3 (2)	C12—C11—H11	120.0
C3—C4—H4	120.4	C10—C11—H11	120.0
C5—C4—H4	120.4	C13—C12—C11	120.2 (2)
C4—C5—C6	120.8 (2)	C13—C12—H12	119.9
C4—C5—H5	119.6	C11—C12—H12	119.9
C6—C5—H5	119.6	C12—C13—C14	119.9 (3)
C5—C6—C1	120.7 (2)	C12—C13—H13	120.0
C5—C6—H6	119.7	C14—C13—H13	120.0
C1—C6—H6	119.7	C9—C14—C13	120.7 (3)
N1—C7—C1	127.62 (15)	C9—C14—H14	119.7
N1—C7—C8	114.40 (15)	C13—C14—H14	119.7
C1—C7—C8	117.97 (15)		
C6—C1—C2—C3	0.6 (3)	C1—C7—C8—O2	-163.47 (15)
C7—C1—C2—C3	179.89 (18)	N1—C7—C8—C9	-104.31 (17)
C1—C2—C3—C4	0.3 (3)	C1—C7—C8—C9	74.7 (2)
C2—C3—C4—C5	-0.7 (3)	O2—C8—C9—C10	-61.5 (2)
C3—C4—C5—C6	0.0 (4)	C7—C8—C9—C10	60.6 (2)
C4—C5—C6—C1	1.0 (3)	O2—C8—C9—C14	117.82 (19)
C2—C1—C6—C5	-1.3 (3)	C7—C8—C9—C14	-120.07 (19)
C7—C1—C6—C5	179.46 (18)	C14—C9—C10—C11	1.1 (3)
O1—N1—C7—C1	1.0 (3)	C8—C9—C10—C11	-179.54 (19)
O1—N1—C7—C8	179.88 (13)	C9—C10—C11—C12	-0.5 (4)
C6—C1—C7—N1	-141.68 (19)	C10—C11—C12—C13	-0.9 (4)
C2—C1—C7—N1	39.1 (3)	C11—C12—C13—C14	1.5 (4)
C6—C1—C7—C8	39.5 (2)	C10—C9—C14—C13	-0.5 (3)
C2—C1—C7—C8	-139.75 (17)	C8—C9—C14—C13	-179.8 (2)
N1—C7—C8—O2	17.5 (2)	C12—C13—C14—C9	-0.9 (4)

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

Hydrogen-bond geometry (\AA , $^\circ$)Cg2 is the centroid of the phenyl ring *B* (C9—C14).

<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 O2 ⁱ	0.88 (2)	2.47 (2)	3.2638 (19)	151 (1.47)
O1—H1 \cdots N1 ⁱ	0.88 (2)	2.13 (2)	2.8236 (19)	135 (1.69)
O2—H2 \cdots O2 ⁱⁱⁱ	0.82 (4)	2.03 (2)	2.850 (3)	175 (1.99)
O2—H2' \cdots O2 ^{iv}	0.83 (4)	2.05 (3)	2.881 (3)	180 (2.38)
C4—H4 \cdots Cg2 ^{vi}	0.93	2.91	3.792 (3)	159

Symmetry codes: (i) $-x, y, -z+1/2$; (iii) $-x, y, -z+3/2$; (iv) $-x, -y+1, -z+1$; (vi) $-x+1/2, -y+1/2, -z$.