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N-(2-{[(1*E*)-1-(2-Hydroxyphenyl)ethylidene]amino}phenyl)-2-methoxyacetamide

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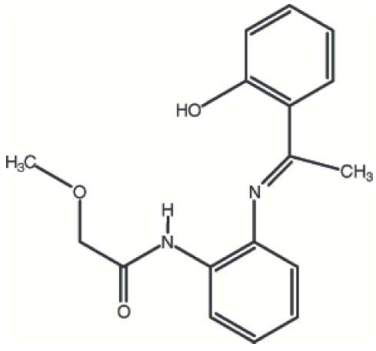
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.098; data-to-parameter ratio = 18.3.

Molecules of the title compound, $C_{17}H_{18}N_2O_3$, are linked by paired C—H···O hydrogen-bonding interactions into $R_2^2(8)$ dimers. The molecule is not planar. The dihedral angle between the two benzene rings is 64.17 (7)°. The molecular conformation is stabilized by intramolecular O—H···N, N—H···N and N—H···O hydrogen bonds.

Related literature

For related literature, see: Amirnasr, DehnoKhalaji & Falvello (2006); Amirnasr *et al.* (2001, 2002); Amirnasr, Schenk, Meghdadi & Morshedi (2006); Berkessel *et al.* (1997); Blower (1998); Habibi *et al.* (2006); Ho *et al.* (1996); Holla *et al.* (2005); Indreen *et al.* (2001); Irie *et al.* (1990); Jacobsen (1993); Jarrahpour, Motamedifar, Hadi & Zarei (2004); Jarrahpour, Motamedifar, Pakshir, Hadi & Zarei (2004); Kickelbick *et al.* (2003); Kovbasyuk *et al.* (1997); Larrow *et al.* (1994); Li & Chang (1991); Lozytska *et al.* (2004); Nawrocka *et al.* (2004); Srinivasan & Kochi (1985); Topich & Bachert (1992); Ünaleroğlu *et al.* (2001); Yıldız, Ünver, Dülger, Erdener, Ocak, Erdönmez & Durlu (2005).



Experimental

Crystal data

$C_{17}H_{18}N_2O_3$
M_r = 298.33
Monoclinic, $P2_1/n$
a = 8.4061 (8) Å
b = 11.2568 (5) Å
c = 16.4145 (16) Å
β = 98.988 (8)°
V = 1534.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 200 K
0.22 × 0.18 × 0.13 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.981, T_{max} = 0.988
35768 measured reflections
3829 independent reflections
2752 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.099
S = 1.01
3829 reflections
209 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—HO1···N1	0.894 (19)	1.725 (19)	2.5537 (14)	153.1 (17)
N2—HN1···O3	0.857 (15)	2.062 (15)	2.5578 (14)	116.2 (12)
N2—HN1···N1	0.857 (15)	2.363 (15)	2.7272 (15)	106.0 (11)
C13—H13···O2	0.93	2.34	2.9119 (16)	119
C16—H16*A*···O2^{i}	0.97	2.57	3.3941 (17)	143

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

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *EVALCCD* (Duisenberg *et al.*, 2003); data reduction: *EVALCCD* and *SADABS* (Sheldrick, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2432).

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supplementary materials

Acta Cryst. (2007). E**63**, o3478-o3479 [**doi:10.1107/S1600536807033673**]

N-(2-{[(1*E*)-1-(2-Hydroxyphenyl)ethylidene]amino}phenyl)-2-methoxyacetamide

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Comment

Schiff bases and their biologically active complexes have been often used as chelating ligands in the coordination chemistry of transition metals as radiopharmaceuticals for cancer targeting, agrochemicals, as model systems for biological macromolecules, as catalysts and as dioxygen carriers (Ünaleroğlu *et al.*, 2001; Li & Chang, 1991; Blower, 1998; Berkessel *et al.*, 1997). The phenyl derivatives of Schiff bases are used as corrosion inhibitors. Schiff bases derived from aldehyde and diamines constitute one of the most relevant synthetic ligand systems with importance in asymmetric catalysis and they appear to be of importance for a broad range of transition-metal catalyzed reactions including lactide polymerization, epoxidation of olefins, hydroxylation and asymmetric ring opening of epoxides (Kovbasyuk *et al.*, 1997; Ho *et al.*, 1996; Topich & Bachert, 1992; Larrow *et al.*, 1994; Jacobsen, 1993; Irie *et al.*, 1990; Srinivasan & Kochi, 1985; Kickelbick *et al.*, 2003). Although a series of Schiff base complexes have been studied crystallographically, there are only a very limited number of reports about the free Schiff bases in the literature (Amirnasr, Schenk, Meghdadi & Morshedi, 2006; Amirnasr, DehnoKhalaji & Falvello, 2006; Amirnasr *et al.*, 2002; Amirnasr *et al.*, 2001; Habibi *et al.*, 2006). Schiff bases have antibacterial, antimalarial, antiviral and antitumor activities (Yıldız *et al.*, 2005; Indreen *et al.*, 2001; Jarrahpour, Motamedifar, Pakshir, Hadi & Zarei,, 2004; Jarrahpour, Motamedifar, Hadi & Zarei, 2004; Holla *et al.*, 2005; Nawrocka *et al.*, 2004; Lozytska *et al.*, 2004).

In Fig. 1, the molecular conformation of the title compound was shown with the intramolecular N—H···O, N—H···N, O—H···N and C—H···O hydrogen-bond distances of 1.725 (19), 2.062 (15), 2.363 (15) and 2.34 Å, respectively. In the molecular structure all the bond distances and angles are normal. The molecular structure is not planar. The C1—C6 and C9—C14 benzene rings makes a dihedral angle of 64.17 (7) ° with each other.

The molecules of are linked by intermolecular C—H···O hydrogen bonding interactions, generating a centrosymmetric $R_2^2(8)$ dimer (Fig. 2).

Experimental

Schiff base {2-[(1E)-*N*-(2-aminophenyl)ethanimidoyl]phenol} (0.23 g, 1.0 mmol) was transformed to *N*-(2-{[(1E)-1-(2-hydroxyphenyl)- ethylidene]amino}phenyl)-2-methoxyacetamide, (I), by treatment with methoxyacetyl chloride (0.13 g, 1.2 mmol) and triethylamine (0.26 g, 2.6 mmol) in dry methylene chloride (10 ml) with cooling in ice-salt bath. The reaction progress was monitored by TLC and the presence of a new compound was confirmed. The IR spectrum showed the characteristic absorption of the amide carbonyl at 1752, the C=N moiety at 1689 and the amine group at 3386 cm^{-1}. The ^{1}H-NMR spectrum showed the methoxy protons at 3.27, methyl protons at 2.29, amine protons at 3.89, aromatic protons at 6.75–7.61, and hydroxyl proton at 13.97. The ^{13}C-NMR spectrum exhibited the following signals: CH_3 at 17.69, OCH_3 at 59.44, aromatic carbons at 118.31–133.68, Ph—C—N at 160.0, Ph—C—OH at 165.0, and the C=O at 174.0.The mass spectrum showed peaks at 298 (M^+), 299 (*M*+1), 300 (*M*+2) and the base peak at 253 ($C_{15}H_{13}N_2O_2$).

Refinement

The H atoms of the hydroxyl and amine groups were found from a difference Fourier map and refined freely. The other H atoms were located geometrically and treated as riding atoms with C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.2 U_{eq}(C) for aromatic and methelene H atoms and 1.5 U_{eq}(C) for methyl H atoms.

Figures

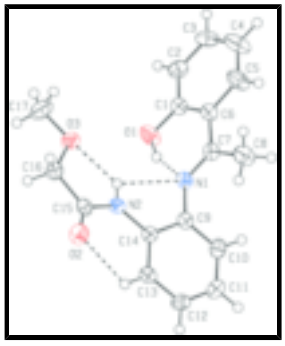


Figure 1.
View of the title compound (I) with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

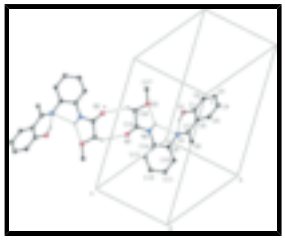


Figure 2.
View of the hydrogen bonding of the title compound. Dashed lines show hydrogen bonds. For clarity, H atoms not involved hydrogen bonding have been omitted.

N-(2-{[(1E)-1-(2-Hydroxyphenyl)ethylidene]amino}phenyl)-2-methoxyacetamide

Crystal data

$C_{17}H_{18}N_2O_3$	F_{000} = 632
M_r = 298.33	D_x = 1.292 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 117 reflections
a = 8.4061 (8) Å	θ = 6–20º
b = 11.2568 (5) Å	μ = 0.09 mm^{-1}
c = 16.4145 (16) Å	T = 200 K
β = 98.988 (8)º	Prism, colourless
V = 1534.2 (2) Å^3	0.22 × 0.18 × 0.13 mm
Z = 4	

Data collection

Bruker–Nonius KappaCCD diffractometer	3829 independent reflections
Radiation source: fine-focus sealed tube	2752 reflections with $I > 2\sigma(I)$

Monochromator: graphite	$R_{int} = 0.052$
Detector resolution: 9 pixels mm^{-1}	$\theta_{max} = 28.5°$
$T = 200$ K	$\theta_{min} = 3.6°$
ω scans	$h = -11 \rightarrow 11$
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	$k = -15 \rightarrow 15$
$T_{min} = 0.981$, $T_{max} = 0.988$	$l = -22 \rightarrow 21$
35768 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.099$	$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 0.3845P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
3829 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
209 parameters	$\Delta\rho_{min} = -0.21$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating –*R*-factor-obs *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}
O1	0.38697 (14)	0.26077 (9)	0.65758 (6)	0.0437 (3)
O2	0.86553 (11)	0.07956 (9)	0.42532 (6)	0.0392 (3)
O3	0.83793 (11)	0.24633 (9)	0.60472 (6)	0.0367 (3)
N1	0.36411 (12)	0.24204 (9)	0.50114 (6)	0.0265 (3)
N2	0.65482 (12)	0.14390 (9)	0.48630 (6)	0.0245 (3)
C1	0.33574 (15)	0.37372 (11)	0.64393 (8)	0.0279 (3)
C2	0.31560 (16)	0.44167 (12)	0.71259 (8)	0.0329 (4)
C3	0.26040 (18)	0.55646 (12)	0.70294 (9)	0.0385 (4)
C4	0.2252 (2)	0.60576 (14)	0.62526 (10)	0.0528 (6)

C5	0.2461 (2)	0.53965 (13)	0.55684 (9)	0.0447 (5)
C6	0.30137 (15)	0.42201 (11)	0.56370 (7)	0.0277 (3)
C7	0.31783 (15)	0.35103 (11)	0.48987 (7)	0.0271 (3)
C8	0.2818 (2)	0.40854 (13)	0.40636 (8)	0.0438 (5)
C9	0.37200 (14)	0.16073 (11)	0.43574 (7)	0.0250 (3)
C10	0.23477 (15)	0.12373 (12)	0.38351 (8)	0.0324 (4)
C11	0.24396 (16)	0.03598 (13)	0.32547 (8)	0.0346 (4)
C12	0.39076 (17)	−0.01639 (12)	0.31929 (8)	0.0317 (4)
C13	0.52882 (15)	0.01923 (11)	0.37099 (7)	0.0268 (3)
C14	0.52055 (14)	0.10719 (10)	0.42966 (7)	0.0230 (3)
C15	0.81256 (14)	0.12812 (11)	0.48183 (8)	0.0264 (3)
C16	0.92509 (15)	0.17935 (12)	0.55424 (8)	0.0323 (4)
C17	0.9274 (2)	0.27786 (17)	0.68146 (11)	0.0571 (6)
HO1	0.386 (2)	0.2308 (16)	0.6071 (12)	0.061 (5)*
H2	0.33960	0.40910	0.76520	0.0390*
HN1	0.6372 (17)	0.1835 (13)	0.5286 (9)	0.030 (4)*
H3	0.24670	0.60120	0.74900	0.0460*
H4	0.18740	0.68340	0.61900	0.0630*
H5	0.22290	0.57410	0.50480	0.0540*
H8A	0.31510	0.35680	0.36570	0.0660*
H8B	0.33900	0.48240	0.40700	0.0660*
H8C	0.16820	0.42320	0.39300	0.0660*
H10	0.13580	0.15830	0.38760	0.0390*
H11	0.15160	0.01210	0.29060	0.0410*
H12	0.39660	−0.07560	0.28030	0.0380*
H13	0.62730	−0.01580	0.36640	0.0320*
H16A	0.98160	0.11540	0.58620	0.0390*
H16B	1.00440	0.22960	0.53420	0.0390*
H17A	0.97260	0.20770	0.70920	0.0860*
H17B	0.85800	0.31640	0.71450	0.0860*
H17C	1.01260	0.33100	0.67300	0.0860*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0692 (7)	0.0355 (5)	0.0276 (5)	0.0188 (5)	0.0114 (5)	0.0043 (4)
O2	0.0296 (5)	0.0552 (6)	0.0349 (5)	0.0067 (4)	0.0116 (4)	−0.0097 (5)
O3	0.0303 (5)	0.0412 (5)	0.0378 (5)	0.0025 (4)	0.0030 (4)	−0.0139 (4)
N1	0.0239 (5)	0.0313 (6)	0.0255 (5)	0.0042 (4)	0.0076 (4)	−0.0011 (4)
N2	0.0235 (5)	0.0273 (5)	0.0239 (5)	0.0010 (4)	0.0071 (4)	−0.0042 (4)
C1	0.0280 (6)	0.0275 (6)	0.0292 (6)	0.0000 (5)	0.0077 (5)	0.0014 (5)
C2	0.0374 (7)	0.0363 (7)	0.0258 (6)	−0.0045 (6)	0.0076 (5)	−0.0015 (5)
C3	0.0500 (8)	0.0310 (7)	0.0386 (8)	−0.0077 (6)	0.0199 (6)	−0.0099 (6)
C4	0.0867 (13)	0.0264 (7)	0.0508 (9)	0.0102 (7)	0.0275 (9)	0.0020 (7)
C5	0.0708 (11)	0.0308 (7)	0.0354 (8)	0.0116 (7)	0.0176 (7)	0.0069 (6)
C6	0.0283 (6)	0.0279 (6)	0.0282 (6)	0.0009 (5)	0.0089 (5)	0.0017 (5)
C7	0.0252 (6)	0.0308 (6)	0.0265 (6)	0.0016 (5)	0.0076 (5)	0.0025 (5)
C8	0.0662 (10)	0.0382 (8)	0.0279 (7)	0.0095 (7)	0.0105 (7)	0.0051 (6)

C9	0.0274 (6)	0.0271 (6)	0.0219 (6)	0.0012 (5)	0.0079 (5)	0.0022 (5)
C10	0.0242 (6)	0.0405 (7)	0.0329 (7)	0.0016 (5)	0.0058 (5)	0.0022 (6)
C11	0.0319 (7)	0.0410 (7)	0.0295 (7)	−0.0069 (6)	0.0008 (5)	−0.0009 (6)
C12	0.0412 (7)	0.0298 (6)	0.0242 (6)	−0.0034 (6)	0.0055 (5)	−0.0030 (5)
C13	0.0317 (6)	0.0261 (6)	0.0241 (6)	0.0021 (5)	0.0092 (5)	0.0008 (5)
C14	0.0253 (6)	0.0238 (6)	0.0207 (5)	−0.0009 (5)	0.0065 (4)	0.0033 (4)
C15	0.0247 (6)	0.0267 (6)	0.0287 (6)	0.0029 (5)	0.0072 (5)	0.0028 (5)
C16	0.0247 (6)	0.0364 (7)	0.0363 (7)	0.0004 (5)	0.0061 (5)	−0.0041 (6)
C17	0.0466 (9)	0.0687 (12)	0.0525 (10)	0.0002 (8)	−0.0036 (8)	−0.0286 (9)

Geometric parameters (Å, °)

O1—C1	1.3499 (16)	C11—C12	1.386 (2)
O2—C15	1.2192 (16)	C12—C13	1.3857 (19)
O3—C16	1.4077 (16)	C13—C14	1.3905 (16)
O3—C17	1.408 (2)	C15—C16	1.5129 (18)
O1—HO1	0.894 (19)	C2—H2	0.9300
N1—C7	1.2916 (16)	C3—H3	0.9300
N1—C9	1.4202 (15)	C4—H4	0.9300
N2—C14	1.4076 (15)	C5—H5	0.9300
N2—C15	1.3511 (16)	C8—H8A	0.9600
N2—HN1	0.857 (15)	C8—H8B	0.9600
C1—C6	1.4122 (17)	C8—H8C	0.9600
C1—C2	1.3941 (18)	C10—H10	0.9300
C2—C3	1.3737 (19)	C11—H11	0.9300
C3—C4	1.380 (2)	C12—H12	0.9300
C4—C5	1.381 (2)	C13—H13	0.9300
C5—C6	1.4021 (19)	C16—H16A	0.9700
C6—C7	1.4760 (17)	C16—H16B	0.9700
C7—C8	1.5034 (18)	C17—H17A	0.9600
C9—C14	1.4041 (17)	C17—H17B	0.9600
C9—C10	1.3893 (18)	C17—H17C	0.9600
C10—C11	1.3829 (19)		
O1···N1	2.5537 (14)	C11···H17B^{viii}	2.7500
O1···C12^{i}	3.3138 (18)	C11···H16A^{i}	3.0800
O1···C13^{i}	3.2801 (16)	C12···H17B^{viii}	2.8200
O2···C13	2.9119 (16)	C13···HO1^{i}	2.913 (18)
O2···C16^{ii}	3.3941 (17)	C15···H13	2.7800
O2···C10^{iii}	3.3193 (16)	C15···H4^{vi}	2.6900
O3···N2	2.5578 (14)	HO1···N1	1.725 (19)
O1···H3^{iv}	2.7200	HO1···C7	2.349 (19)
O1···H13^{i}	2.7900	HO1···C9	2.906 (19)
O1···H12^{i}	2.8500	HO1···C13^{i}	2.913 (18)
O2···H13	2.3400	HO1···H13^{i}	2.4600
O2···H10^{iii}	2.6000	H2···O2^{xi}	2.6100
O2···H16A^{ii}	2.5700	HN1···O3	2.062 (15)

O2···H2^{v}	2.6100	HN1···N1	2.363 (15)
O2···H4^{vi}	2.7800	H3···O1^{xii}	2.7200
O3···HN1	2.062 (15)	H3···H13^{xi}	2.5000
O3···H5^{vi}	2.7000	H4···O2^{vi}	2.7800
N1···O1	2.5537 (14)	H4···C15^{vi}	2.6900
N1···N2	2.7272 (15)	H5···C8	2.5700
N2···N1	2.7272 (15)	H5···H8B	2.2500
N2···O3	2.5578 (14)	H5···H8C	2.4900
N1···HN1	2.363 (15)	H5···O3^{vi}	2.7000
N1···HO1	1.725 (19)	H8A···C9	2.5000
C4···C15^{vi}	3.463 (2)	H8A···C10	2.7400
C8···C10	3.245 (2)	H8B···C5	2.7700
C10···C8	3.245 (2)	H8B···H5	2.2500
C10···O2^{vii}	3.3193 (16)	H8C···C5	2.9700
C11···C16^{i}	3.5595 (19)	H8C···H5	2.4900
C12···O1^{i}	3.3138 (18)	H10···O2^{vii}	2.6000
C12···C17^{viii}	3.555 (2)	H10···C7	3.0100
C13···O2	2.9119 (16)	H10···C8	3.0700
C13···O1^{i}	3.2801 (16)	H11···C2^{viii}	2.9600
C14···C14^{i}	3.3948 (16)	H12···O1^{i}	2.8500
C15···C4^{vi}	3.463 (2)	H13···O2	2.3400
C16···O2^{ii}	3.3941 (17)	H13···C15	2.7800
C16···C11^{i}	3.5595 (19)	H13···O1^{i}	2.7900
C17···C12^{ix}	3.555 (2)	H13···HO1^{i}	2.4600
C1···H17C^{vii}	2.8700	H13···C3^{v}	3.1000
C2···H17C^{vii}	2.8200	H13···H3^{v}	2.5000
C2···H11^{ix}	2.9600	H16A···H17A	2.2800
C3···H17A^{x}	3.0000	H16A···O2^{ii}	2.5700
C3···H13^{xi}	3.1000	H16A···C11^{i}	3.0800
C5···H8C	2.9700	H16B···H17C	2.5400
C5···H8B	2.7700	H17A···H16A	2.2800
C7···HO1	2.349 (19)	H17A···C3^{xiii}	3.0000
C7···H10	3.0100	H17B···C11^{ix}	2.7500
C8···H10	3.0700	H17B···C12^{ix}	2.8200
C8···H5	2.5700	H17C···C1^{iii}	2.8700
C9···HO1	2.906 (19)	H17C···C2^{iii}	2.8200
C9···H8A	2.5000	H17C···H16B	2.5400
C10···H8A	2.7400		
C16—O3—C17	114.03 (11)	C1—C2—H2	120.00
C1—O1—HO1	104.2 (12)	C3—C2—H2	120.00
C7—N1—C9	123.54 (10)	C2—C3—H3	120.00
C14—N2—C15	128.17 (10)	C4—C3—H3	120.00
C15—N2—HN1	114.1 (10)	C3—C4—H4	120.00

C14—N2—HN1	117.7 (10)	C5—C4—H4	120.00
O1—C1—C6	122.06 (11)	C4—C5—H5	119.00
O1—C1—C2	117.29 (12)	C6—C5—H5	119.00
C2—C1—C6	120.64 (12)	C7—C8—H8A	109.00
C1—C2—C3	120.29 (12)	C7—C8—H8B	110.00
C2—C3—C4	120.31 (13)	C7—C8—H8C	109.00
C3—C4—C5	119.91 (14)	H8A—C8—H8B	109.00
C4—C5—C6	121.75 (13)	H8A—C8—H8C	109.00
C1—C6—C7	121.70 (11)	H8B—C8—H8C	109.00
C1—C6—C5	117.09 (11)	C9—C10—H10	120.00
C5—C6—C7	121.18 (11)	C11—C10—H10	120.00
N1—C7—C6	117.48 (10)	C10—C11—H11	120.00
N1—C7—C8	123.57 (11)	C12—C11—H11	120.00
C6—C7—C8	118.96 (11)	C11—C12—H12	120.00
C10—C9—C14	119.30 (11)	C13—C12—H12	120.00
N1—C9—C14	118.52 (10)	C12—C13—H13	120.00
N1—C9—C10	121.83 (11)	C14—C13—H13	120.00
C9—C10—C11	120.59 (12)	O3—C16—H16A	110.00
C10—C11—C12	120.04 (12)	O3—C16—H16B	110.00
C11—C12—C13	120.16 (12)	C15—C16—H16A	110.00
C12—C13—C14	120.17 (12)	C15—C16—H16B	110.00
C9—C14—C13	119.74 (11)	H16A—C16—H16B	108.00
N2—C14—C9	117.21 (10)	O3—C17—H17A	109.00
N2—C14—C13	123.01 (11)	O3—C17—H17B	109.00
O2—C15—N2	125.34 (12)	O3—C17—H17C	110.00
O2—C15—C16	120.72 (11)	H17A—C17—H17B	110.00
N2—C15—C16	113.94 (11)	H17A—C17—H17C	109.00
O3—C16—C15	110.34 (10)	H17B—C17—H17C	109.00
C17—O3—C16—C15	168.27 (12)	C4—C5—C6—C7	177.87 (14)
C9—N1—C7—C6	174.48 (11)	C5—C6—C7—N1	−177.62 (13)
C9—N1—C7—C8	−6.1 (2)	C1—C6—C7—C8	−179.04 (13)
C7—N1—C9—C14	121.72 (13)	C1—C6—C7—N1	0.45 (18)
C7—N1—C9—C10	−65.16 (17)	C5—C6—C7—C8	2.9 (2)
C14—N2—C15—C16	−179.91 (11)	C14—C9—C10—C11	−0.65 (19)
C14—N2—C15—O2	1.3 (2)	N1—C9—C14—C13	174.11 (11)
C15—N2—C14—C9	−163.09 (12)	N1—C9—C10—C11	−173.72 (12)
C15—N2—C14—C13	18.93 (19)	C10—C9—C14—N2	−177.24 (11)
C2—C1—C6—C7	−178.46 (12)	C10—C9—C14—C13	0.81 (18)
C2—C1—C6—C5	−0.31 (19)	N1—C9—C14—N2	−3.95 (16)
O1—C1—C6—C7	0.7 (2)	C9—C10—C11—C12	0.4 (2)
O1—C1—C6—C5	178.85 (13)	C10—C11—C12—C13	−0.2 (2)
O1—C1—C2—C3	−178.57 (13)	C11—C12—C13—C14	0.39 (19)
C6—C1—C2—C3	0.6 (2)	C12—C13—C14—N2	177.25 (11)
C1—C2—C3—C4	−0.3 (2)	C12—C13—C14—C9	−0.69 (18)
C2—C3—C4—C5	−0.3 (2)	O2—C15—C16—O3	170.90 (12)
C3—C4—C5—C6	0.6 (3)	N2—C15—C16—O3	−7.92 (15)
C4—C5—C6—C1	−0.3 (2)		

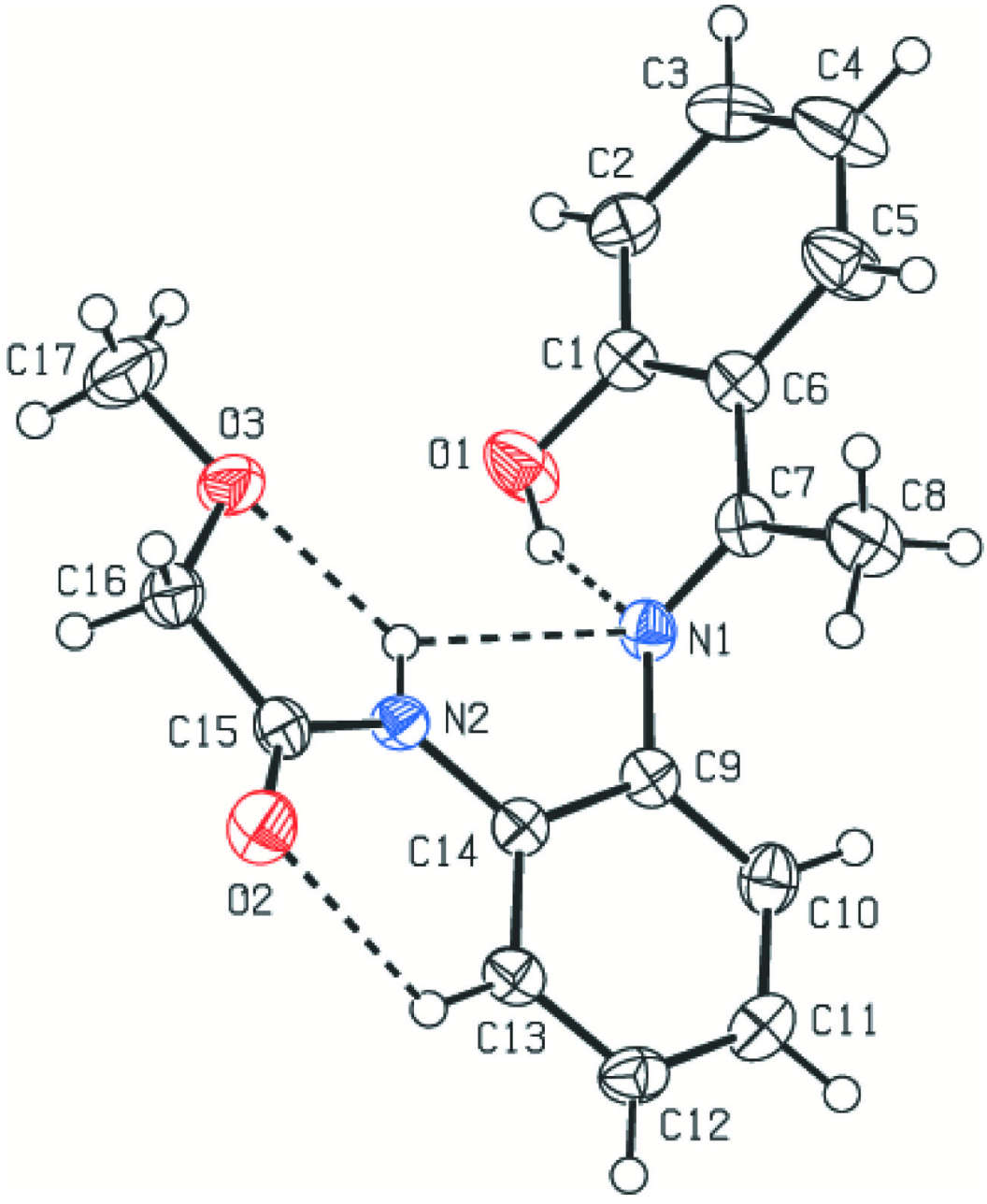
Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+2, −*y*, −*z*+1; (iii) *x*+1, *y*, *z*; (iv) −*x*+1/2, *y*−1/2, −*z*+3/2; (v) *x*+1/2, −*y*+1/2, *z*−1/2; (vi) −*x*+1, −*y*+1, −*z*+1; (vii) *x*−1, *y*, *z*; (viii) *x*−1/2, −*y*+1/2, *z*−1/2; (ix) *x*+1/2, −*y*+1/2, *z*+1/2; (x) −*x*+3/2, *y*+1/2, −*z*+3/2; (xi) *x*−1/2, −*y*+1/2, *z*+1/2; (xii) −*x*+1/2, *y*+1/2, −*z*+3/2; (xiii) −*x*+3/2, *y*−1/2, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—HO1···N1	0.894 (19)	1.725 (19)	2.5537 (14)	153.1 (17)
N2—HN1···O3	0.857 (15)	2.062 (15)	2.5578 (14)	116.2 (12)
N2—HN1···N1	0.857 (15)	2.363 (15)	2.7272 (15)	106.0 (11)
C13—H13···O2	0.93	2.34	2.9119 (16)	119
C16—H16A···O2^{ii}	0.97	2.57	3.3941 (17)	143

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

Fig. 1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O2
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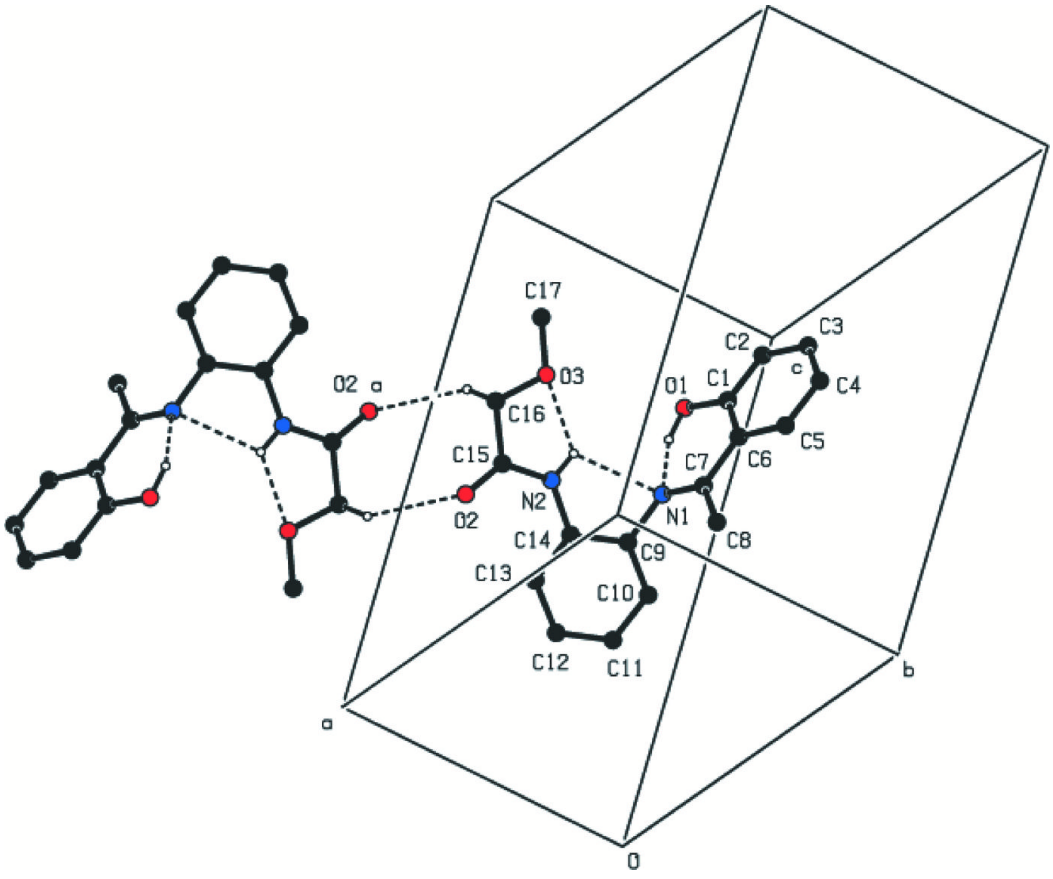
C11
C12

Fig. 2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C3
C4
C5
C6
C7
N1
C8
a
b
0