

Crystal structure and Hirshfeld surface analysis of (Z)-6-[(2-hydroxy-4-methylanilino)methylidene]-4-methylcyclohexa-2,4-dien-1-one

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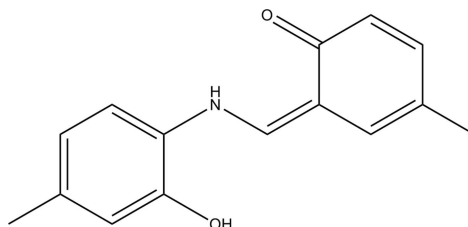
Keywords: crystal structure; Schiff base; hydrogen bonding; Hirshfeld surface analysis.**CCDC reference:** 1902148**Supporting information:** this article has supporting information at journals.iucr.org/e

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The title compound, C₁₅H₁₅NO₂, is a Schiff base that exists in the keto–enamine tautomeric form and adopts a *Z* configuration. The molecule is almost planar, with the two phenyl rings twisted relative to each other by 9.60 (18)°. There is an intramolecular N–H···O hydrogen bond present forming an *S*(6) ring motif. In the crystal, pairs of O–H···O hydrogen bonds link adjacent molecules into inversion dimers with an *R*₂²(18) ring motif. The dimers are linked by very weak π – π interactions, forming layers parallel to ($\bar{2}$ 01). Hirshfeld surface analysis, two-dimensional fingerprint plots and the molecular electrostatic potential surfaces were used to analyse the intermolecular interactions, indicating that the most important contributions for the crystal packing are from H···H (55.2%), C···H/H···C (22.3%) and O···H/H···O (13.6%) interactions.

1. Chemical context

Schiff bases contain the azomethine moiety (–RCH=N–R') and are prepared by condensation reactions between amines and active carbonyl compounds (Schiff, 1864). In the majority of cases, the synthesis involves an aromatic amine and an aldehyde (Schiff *et al.*, 1881). Schiff bases are very important for production of chemical specialties such as pharmaceuticals including antibiotics, and of antiallergic, antitumor, antifungal, antibacterial, antimalarial or antiviral drugs. Schiff bases are also employed as catalyst carriers (Grigoras *et al.*, 2001), thermo-stable materials (Vančo *et al.*, 2004), metal–cation complexing agents or in biological systems (Taggi *et al.*, 2002). Schiff bases containing phenol indicate two possible tautomeric forms, *viz.* phenol–imine and keto–enamine.



In the current study, a new Schiff base, (Z)-6-[[2-(2-hydroxy-4-methylphenyl)amino]methylidene]-4-methylcyclohexa-2,4-dien-1-one, was obtained in crystalline form from the reaction of 2-amino-5-methylphenol with 2-hydroxy-5-methylbenzaldehyde. We report here its synthesis conditions and the molecular and crystal structures, supplemented by Hirshfeld surface analysis.

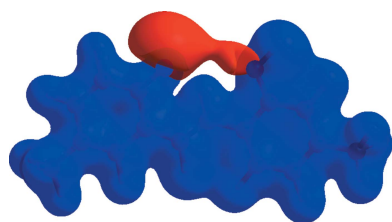


Table 1
Hydrogen-bond geometry (Å, °).

<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	0.82	1.82	2.627 (3)	168
N1–H1A···O2	0.87 (4)	1.83 (4)	2.585 (4)	144 (3)

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

2. Structural commentary

The molecular structure of the title compound is illustrated in Fig. 1. The asymmetric unit comprises one molecule that adopts the keto–enamine tautomeric form, *i.e.* the H atom is located at the amine functionality (N1). The molecule is almost planar, with an r.m.s. deviation of 0.1061 Å for the complete molecule except the H atoms [largest deviation 0.176 (3) Å for C8]. The two phenyl rings (C1–C6 and C9–C14) are inclined by 9.60 (18)°. The C1–O1 bond length [1.356 (3) Å] to the hydroxy group is in the normal range, while the C14=O2 bond length is comparatively elongated [1.302 (4) Å] due to the involvement of the carbonyl O atom in an intramolecular N–H···O hydrogen bond, forming an *S*(6) ring motif. The C6–N1 and C8=N1 bond lengths are 1.404 (4) and 1.310 (4) Å, respectively. Overall, the bond lengths in the title structure compare well with those of other keto–enamine tautomers known from the literature (see: *Database Survey*).

3. Supramolecular features

The molecules are linked by mutual O–H···O hydrogen bonds forming pairs of inversion dimers with an $R_2^2(18)$ ring motif (Table 1, Figs. 2 and 3). The dimers are linked by very weak π -stacking interactions [$Cg1 \cdots Cg2 = 4.721$ (2) Å; *Cg*1 and *Cg*2 are the centroids of the C1–C6 and C9–C14 rings, respectively], forming layers parallel to ($\bar{2}$ 01).

4. Database survey

A search of the Cambridge Structural Database (CSD, version 5.40, update November 2018; Groom *et al.*, 2016) for the (*E*)-2-[(2-hydroxyphenyliminio)methyl]phenolate fragment revealed 25 hits where this fragment adopts the keto–enamine

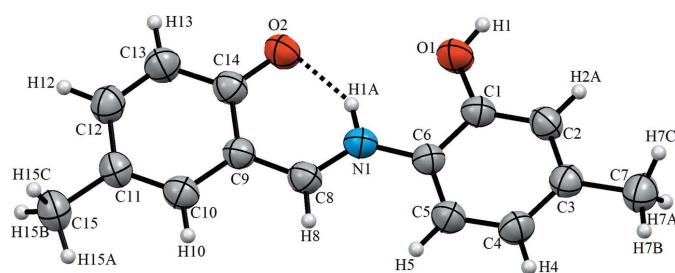


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 40% probability level. Dashed lines denote the intramolecular N–H···O hydrogen bond (Table 1) forming an *S*(6) ring motif.

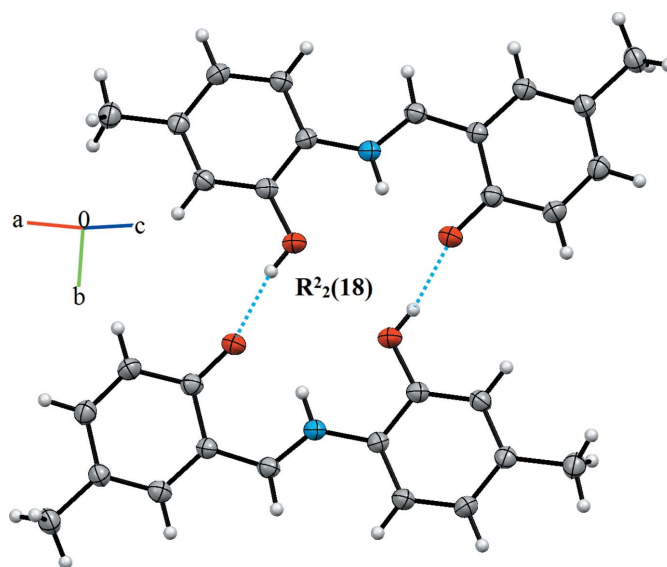


Figure 2
A view of the crystal packing of the title compound. Dashed lines denote the intermolecular O–H···O hydrogen bonds (Table 1) forming an inversion dimer with an $R_2^2(18)$ ring motif.

tautomeric form. Nearly all bond lengths in the title structure are the same within standard uncertainties as the corresponding bond lengths in the structures of 2,4-dichloro-6-[[2-methoxyphenyl]iminio]methyl]phenolate hydrate (VUYFEC; Tsuchimoto *et al.*, 2016), 2-[(*E*)-[(2-hydroxyphenyl)iminio]methyl]-4-methylphenolate (XULSOO; Shalini *et al.*, 2015), (*E*)-4-hydroxy-2-[(2-hydroxyphenyl)iminio]methyl]phenolate (QUYGOH; Eltayeb *et al.*, 2010) or 2-[(*E*)-[(2-hydroxy-5-methylphenyl)iminio]methyl]-4-(trifluoromethoxy)phenolate (QAJYUX; Karadağ *et al.*, 2011). For example, in the structures of these typical keto–enamine tautomers, the corresponding C14=O2 and C8–C9 bond lengths are in the ranges 1.279–1.316 Å and 1.410–1.427 Å, respectively. It is likely that the intermolecular O–H···O hydrogen bond, where the keto O atom acts as an hydrogen-bond acceptor, is an important prerequisite for the tautomeric shift toward the keto–enamine form. In fact, in all 25 structures of the keto–enamine tautomers, hydrogen bonds of this type are observed.

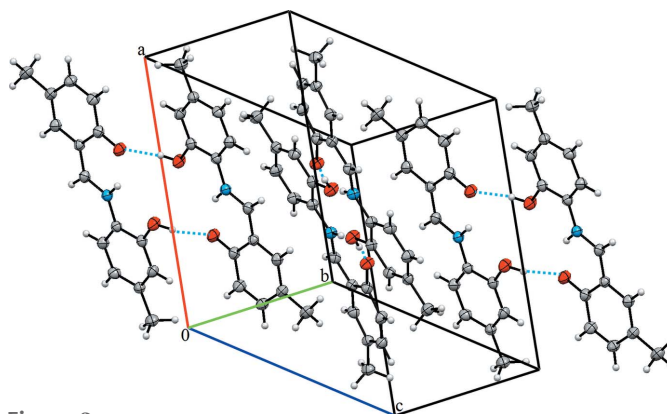


Figure 3
The crystal packing of the title compound.

5. Hirshfeld surface analysis

A Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) and the associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007) were performed with *Crystal-Explorer17* (Turner *et al.*, 2017) for specifying the intermolecular interactions in the title compound. Fig. 4*a* illustrates the Hirshfeld surface mapped over d_{norm} . The red spots highlight the interatomic contacts included in O–H...O hydrogen bonding. The three-dimensional d_{norm} surfaces were plotted with a colour scale of -0.7370 to 1.3366 Å with a standard (high) surface resolution. Fig. 4*b* shows the molecular electrostatic potential plotted over the three-dimensional Hirshfeld surface using the STO-3G basis set in the range -0.0975 to 0.2197 a.u. within the Hartree–Fock level of theory. The O–H...O hydrogen-bond donors and acceptors are shown as blue and red areas around the atoms related with positive (hydrogen-bond donors) and negative (hydrogen-bond acceptors) electrostatic potentials, respectively.

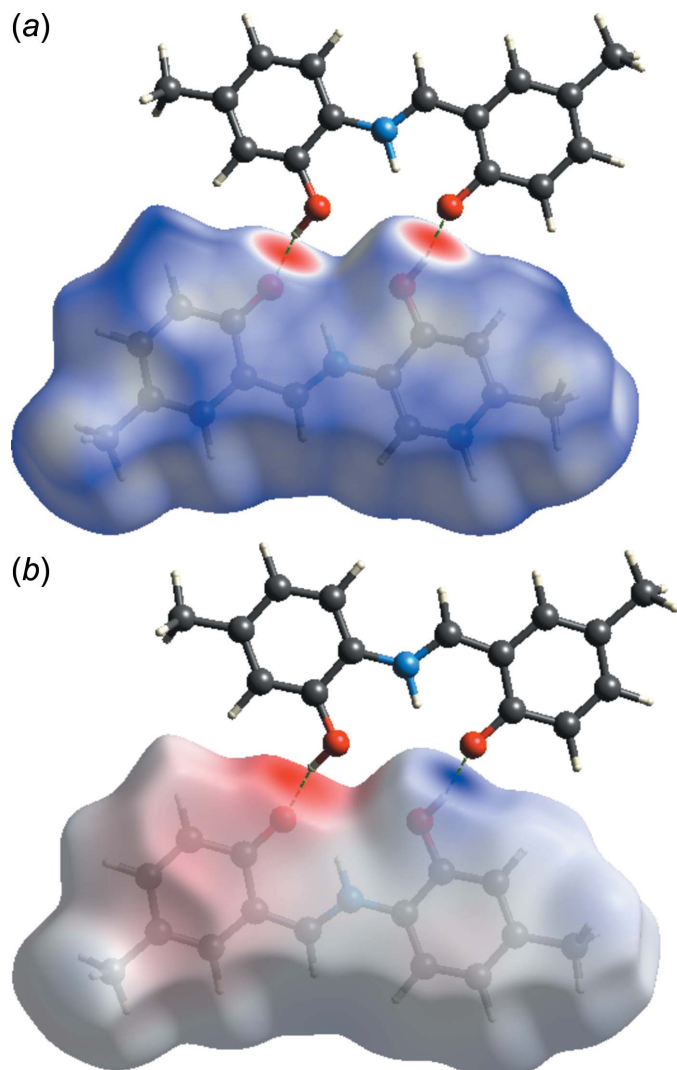


Figure 4
(*a*) The Hirshfeld surface mapped over d_{norm} , and (*b*) the molecular electrostatic potential surface showing the O–H...O interactions.

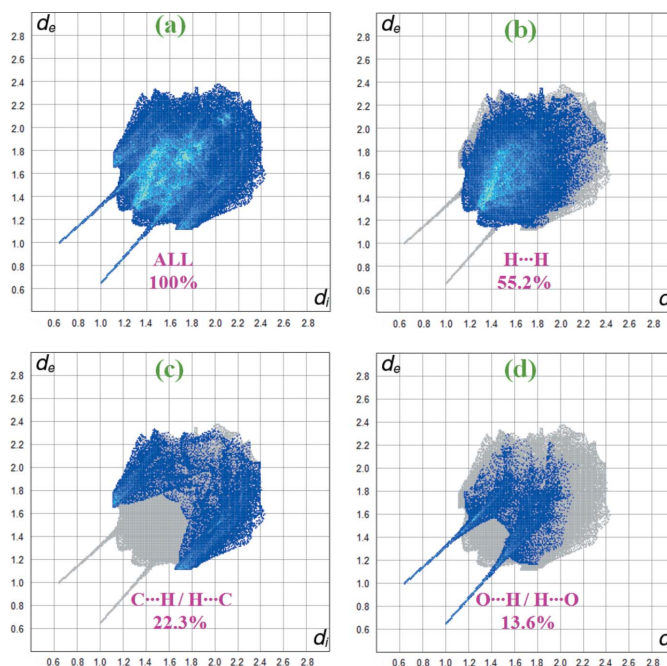


Figure 5
Two-dimensional fingerprint plots for the title compound giving the relative contribution of atom pairs to the Hirshfeld surface.

Fig. 5*a* shows the two-dimensional fingerprint of the sum of all contacts contributing to the Hirshfeld surface indicated in normal mode. Fig. 5*b* illustrates the two-dimensional fingerprint of (d_i , d_e) points related to H...H contacts that represent a 55.2% contribution in the title structure. In Fig. 5*c*, two symmetrical wings on the left and right sides indicate C...H/H...C interactions with a contribution of 22.3%. Furthermore, there are O...H/H...O (13.6%; Fig. 5*d*), C...C (4.9%) and C...N/N...C (2.6%) contacts.

Fig. 6 shows the molecular electrostatic potential surface generated using the STO-3G basis set in the range -0.050 to 0.050 a.u. within the Hartree–Fock level of theory. The blue and red regions are associated with positive and negative molecular electrostatic potentials and represent the donor and acceptor groups, respectively, in hydrogen bonding.

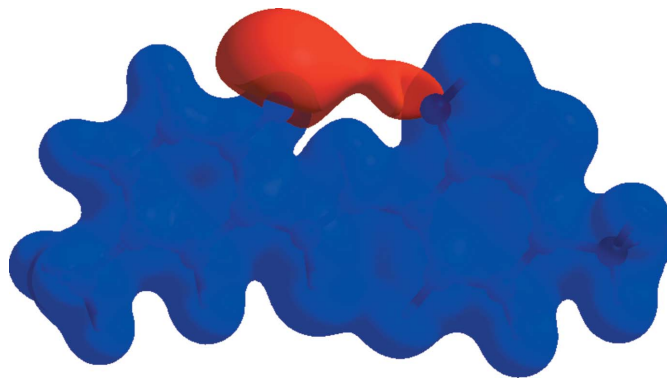


Figure 6
A view of the molecular electrostatic potential, in the range -0.0500 to 0.0500 a.u. calculated using the STO-3 G basis set in the range -0.050 to 0.050 a.u. within the Hartree–Fock level of theory.

6. Synthesis and crystallization

The title compound was prepared by refluxing a mixture of 2-hydroxy-5-methylbenzaldehyde (34.0 mg, 0.25 mmol) in ethanol (15 ml) and 2-amino-5-methylphenol (30.8 mg, 0.25 mmol) in ethanol (15 ml) for 5 h. Single crystals of the title compound for X-ray analysis were obtained by slow evaporation of an ethanol solution (yield 65%, m.p. 446–448 K).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The O- and N-bound H atoms were located in a difference-Fourier map and refined with O–H = 0.82 Å and N–H = 0.85 Å, and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{N}, \text{O})$. The C-bound H atoms were positioned geometrically and refined using a riding model with C–H = 0.93 and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic H atoms, and with C–H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms.

Funding information

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Table 2

Experimental details.

Crystal data	
Chemical formula	C ₁₅ H ₁₅ NO ₂
<i>M_r</i>	241.28
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.3954 (19), 11.746 (2), 10.3067 (17)
β (°)	115.940 (12)
<i>V</i> (Å ³)	1240.6 (4)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.09
Crystal size (mm)	0.57 × 0.50 × 0.44
Data collection	
Diffractometer	Stoe <i>IPDS 2</i>
Absorption correction	Integration (<i>X-RED32</i> ; Stoe & Cie, 2002)
<i>T_{min}</i> , <i>T_{max}</i>	0.962, 0.975
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	6997, 2417, 1261
<i>R_{int}</i>	0.061
(sin θ/λ) _{max} (Å ⁻¹)	0.617
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.064, 0.156, 0.99
No. of reflections	2417
No. of parameters	171
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.16, -0.14

Computer programs: *X-AREA* and *X-RED* (Stoe & Cie, 2002), *SHELXT2017* (Sheldrick, 2015a), *SHELXL2018* (Sheldrick, 2015b), *WinGX* (Farrugia, 2012), *PLATON* (Spek, 2009) and *pubCIF* (Westrip, 2010).

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supporting information

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Computing details

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXT2017* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012), *SHELXL2018* (Sheldrick, 2015b), *PLATON* (Spek, 2009) and *pubCIF* (Westrip, 2010).

(Z)-6-[(2-Hydroxy-4-methylanilino)methylidene]-4-methylcyclohexa-2,4-dien-1-one

Crystal data

C₁₅H₁₅NO₂

M_r = 241.28

Monoclinic, *P2₁/c*

a = 11.3954 (19) Å

b = 11.746 (2) Å

c = 10.3067 (17) Å

β = 115.940 (12)°

V = 1240.6 (4) Å³

Z = 4

F(000) = 512

D_x = 1.292 Mg m⁻³

Mo *Kα* radiation, λ = 0.71073 Å

Cell parameters from 15101 reflections

θ = 2.8–30.9°

μ = 0.09 mm⁻¹

T = 296 K

Prism, red

0.57 × 0.50 × 0.44 mm

Data collection

Stoe IPDS 2

diffractometer

Radiation source: sealed X-ray tube, 12 x 0.4

mm long-fine focus

Detector resolution: 6.67 pixels mm⁻¹

rotation method scans

Absorption correction: integration

(*X-RED32*; Stoe & Cie, 2002)

T_{min} = 0.962, *T_{max}* = 0.975

6997 measured reflections

2417 independent reflections

1261 reflections with *I* > 2σ(*I*)

R_{int} = 0.061

θ_{max} = 26.0°, θ_{min} = 2.8°

h = -14→13

k = -14→11

l = -12→12

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.064

wR(*F*²) = 0.156

S = 0.99

2417 reflections

171 parameters

0 restraints

Hydrogen site location: mixed

H atoms treated by a mixture of independent

and constrained refinement

w = 1/[σ²(*F_o*²) + (0.0717*P*)²]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} < 0.001

$$\Delta\rho_{\max} = 0.16 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.14 \text{ e } \text{\AA}^{-3}$$

Extinction correction: SHELXL2017
(Sheldrick, 2015b),
 $F_c^* = kF_c [1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.007 (2)

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>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.3892 (2)	0.58075 (18)	0.4721 (3)	0.0775 (7)
H1	0.379271	0.539357	0.530605	0.116*
O2	0.6238 (2)	0.57505 (18)	0.3518 (2)	0.0735 (7)
N1	0.4922 (3)	0.7437 (3)	0.3822 (3)	0.0581 (7)
C9	0.6549 (3)	0.7665 (2)	0.2975 (3)	0.0544 (7)
C1	0.3454 (3)	0.6868 (3)	0.4791 (3)	0.0563 (7)
C8	0.5565 (3)	0.8082 (3)	0.3317 (3)	0.0599 (8)
H8	0.536018	0.885293	0.317983	0.072*
C6	0.3978 (3)	0.7746 (2)	0.4288 (3)	0.0546 (7)
C2	0.2544 (3)	0.7113 (3)	0.5301 (3)	0.0613 (8)
H2A	0.219587	0.652120	0.562261	0.074*
C3	0.2140 (3)	0.8211 (3)	0.5343 (3)	0.0592 (8)
C11	0.8287 (3)	0.8104 (3)	0.2270 (3)	0.0603 (8)
C14	0.6898 (3)	0.6484 (3)	0.3155 (3)	0.0599 (8)
C10	0.7254 (3)	0.8436 (3)	0.2515 (3)	0.0628 (8)
H10	0.700067	0.919577	0.237683	0.075*
C5	0.3571 (3)	0.8851 (3)	0.4324 (3)	0.0642 (8)
H5	0.390952	0.944514	0.399559	0.077*
C4	0.2668 (3)	0.9080 (3)	0.4843 (3)	0.0670 (8)
H4	0.240644	0.982737	0.485967	0.080*
C12	0.8638 (3)	0.6949 (3)	0.2488 (3)	0.0681 (9)
H12	0.934719	0.670249	0.234291	0.082*
C13	0.7972 (3)	0.6170 (3)	0.2906 (3)	0.0688 (9)
H13	0.823971	0.541368	0.302935	0.083*
C7	0.1151 (3)	0.8461 (3)	0.5909 (3)	0.0762 (10)
H7A	0.031563	0.816866	0.524800	0.114*
H7B	0.109049	0.926922	0.600598	0.114*
H7C	0.141812	0.810509	0.683322	0.114*
C15	0.9064 (3)	0.8936 (3)	0.1829 (4)	0.0769 (10)
H15A	0.861304	0.965184	0.157474	0.115*
H15B	0.916047	0.863810	0.101333	0.115*
H15C	0.990962	0.904493	0.261813	0.115*
H1A	0.516 (4)	0.673 (4)	0.387 (4)	0.088 (12)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1026 (18)	0.0475 (13)	0.1056 (17)	0.0073 (13)	0.0671 (15)	0.0093 (11)
O2	0.0894 (16)	0.0526 (13)	0.0949 (14)	-0.0002 (12)	0.0555 (13)	0.0079 (11)
N1	0.0611 (17)	0.0488 (17)	0.0674 (15)	0.0035 (14)	0.0308 (13)	0.0064 (12)
C9	0.0583 (18)	0.0501 (18)	0.0558 (16)	0.0016 (15)	0.0259 (15)	0.0034 (13)
C1	0.0612 (19)	0.0484 (18)	0.0586 (16)	0.0013 (16)	0.0254 (15)	0.0019 (13)
C8	0.0620 (19)	0.0505 (18)	0.0669 (17)	-0.0019 (16)	0.0281 (15)	0.0050 (14)
C6	0.0550 (18)	0.0498 (18)	0.0602 (16)	0.0033 (15)	0.0262 (14)	0.0031 (13)
C2	0.068 (2)	0.056 (2)	0.0655 (17)	-0.0049 (16)	0.0342 (16)	0.0039 (14)
C3	0.0591 (19)	0.063 (2)	0.0557 (16)	0.0044 (17)	0.0251 (14)	0.0027 (14)
C11	0.063 (2)	0.063 (2)	0.0601 (16)	-0.0045 (17)	0.0318 (15)	-0.0012 (14)
C14	0.065 (2)	0.0535 (19)	0.0620 (16)	-0.0024 (16)	0.0288 (15)	-0.0002 (14)
C10	0.067 (2)	0.0563 (19)	0.0648 (17)	-0.0033 (17)	0.0283 (16)	0.0005 (14)
C5	0.0658 (19)	0.0512 (19)	0.0800 (19)	-0.0004 (17)	0.0359 (17)	0.0060 (15)
C4	0.072 (2)	0.0526 (19)	0.084 (2)	0.0078 (17)	0.0406 (18)	0.0011 (16)
C12	0.071 (2)	0.069 (2)	0.0735 (19)	0.0016 (18)	0.0400 (17)	-0.0055 (16)
C13	0.082 (2)	0.0532 (19)	0.081 (2)	0.0030 (18)	0.0450 (19)	-0.0030 (16)
C7	0.073 (2)	0.085 (3)	0.078 (2)	0.0082 (19)	0.0403 (18)	0.0022 (17)
C15	0.078 (2)	0.081 (3)	0.084 (2)	-0.011 (2)	0.0477 (19)	-0.0013 (18)

Geometric parameters (\AA , $^\circ$)

O1—C1	1.356 (3)	C11—C10	1.365 (4)
O1—H1	0.8200	C11—C12	1.405 (4)
O2—C14	1.302 (4)	C11—C15	1.516 (4)
N1—C8	1.310 (4)	C14—C13	1.404 (4)
N1—C6	1.404 (4)	C10—H10	0.9300
N1—H1A	0.87 (4)	C5—C4	1.377 (4)
C9—C8	1.403 (4)	C5—H5	0.9300
C9—C10	1.422 (4)	C4—H4	0.9300
C9—C14	1.433 (4)	C12—C13	1.373 (4)
C1—C2	1.383 (4)	C12—H12	0.9300
C1—C6	1.400 (4)	C13—H13	0.9300
C8—H8	0.9300	C7—H7A	0.9600
C6—C5	1.385 (4)	C7—H7B	0.9600
C2—C3	1.377 (4)	C7—H7C	0.9600
C2—H2A	0.9300	C15—H15A	0.9600
C3—C4	1.393 (4)	C15—H15B	0.9600
C3—C7	1.506 (4)	C15—H15C	0.9600
C1—O1—H1	109.5	C11—C10—C9	122.6 (3)
C8—N1—C6	129.1 (3)	C11—C10—H10	118.7
C8—N1—H1A	111 (2)	C9—C10—H10	118.7
C6—N1—H1A	120 (2)	C4—C5—C6	120.6 (3)
C8—C9—C10	119.4 (3)	C4—C5—H5	119.7
C8—C9—C14	120.9 (2)	C6—C5—H5	119.7

C10—C9—C14	119.6 (3)	C5—C4—C3	121.2 (3)
O1—C1—C2	124.5 (3)	C5—C4—H4	119.4
O1—C1—C6	115.5 (2)	C3—C4—H4	119.4
C2—C1—C6	120.0 (3)	C13—C12—C11	122.4 (3)
N1—C8—C9	123.0 (3)	C13—C12—H12	118.8
N1—C8—H8	118.5	C11—C12—H12	118.8
C9—C8—H8	118.5	C12—C13—C14	121.9 (3)
C5—C6—C1	118.5 (3)	C12—C13—H13	119.1
C5—C6—N1	124.6 (3)	C14—C13—H13	119.1
C1—C6—N1	116.8 (3)	C3—C7—H7A	109.5
C3—C2—C1	121.6 (3)	C3—C7—H7B	109.5
C3—C2—H2A	119.2	H7A—C7—H7B	109.5
C1—C2—H2A	119.2	C3—C7—H7C	109.5
C2—C3—C4	118.0 (3)	H7A—C7—H7C	109.5
C2—C3—C7	120.8 (3)	H7B—C7—H7C	109.5
C4—C3—C7	121.2 (3)	C11—C15—H15A	109.5
C10—C11—C12	117.0 (3)	C11—C15—H15B	109.5
C10—C11—C15	122.4 (3)	H15A—C15—H15B	109.5
C12—C11—C15	120.5 (3)	C11—C15—H15C	109.5
O2—C14—C13	122.6 (3)	H15A—C15—H15C	109.5
O2—C14—C9	121.0 (3)	H15B—C15—H15C	109.5
C13—C14—C9	116.4 (3)		
C6—N1—C8—C9	175.8 (3)	C10—C9—C14—C13	2.3 (4)
C10—C9—C8—N1	-176.2 (3)	C12—C11—C10—C9	0.1 (4)
C14—C9—C8—N1	0.5 (4)	C15—C11—C10—C9	-177.9 (3)
O1—C1—C6—C5	179.8 (3)	C8—C9—C10—C11	174.9 (3)
C2—C1—C6—C5	0.4 (4)	C14—C9—C10—C11	-1.8 (4)
O1—C1—C6—N1	-2.2 (4)	C1—C6—C5—C4	-0.1 (4)
C2—C1—C6—N1	178.4 (3)	N1—C6—C5—C4	-177.9 (3)
C8—N1—C6—C5	-1.7 (5)	C6—C5—C4—C3	0.0 (5)
C8—N1—C6—C1	-179.5 (3)	C2—C3—C4—C5	-0.2 (4)
O1—C1—C2—C3	180.0 (3)	C7—C3—C4—C5	-179.9 (3)
C6—C1—C2—C3	-0.7 (4)	C10—C11—C12—C13	1.0 (5)
C1—C2—C3—C4	0.6 (4)	C15—C11—C12—C13	179.1 (3)
C1—C2—C3—C7	-179.7 (3)	C11—C12—C13—C14	-0.5 (5)
C8—C9—C14—O2	6.1 (4)	O2—C14—C13—C12	178.3 (3)
C10—C9—C14—O2	-177.2 (3)	C9—C14—C13—C12	-1.2 (4)
C8—C9—C14—C13	-174.4 (3)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots O2 ⁱ	0.82	1.82	2.627 (3)	168
N1—H1A \cdots O2	0.87 (4)	1.83 (4)	2.585 (4)	144 (3)

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