



Crystal structure and Hirshfeld surface analysis of 3-[(1*E*)-(4-{4-[(*E*)-(3-hydroxybenzylidene)amino]-phenoxy}phenylimino)methyl]phenol

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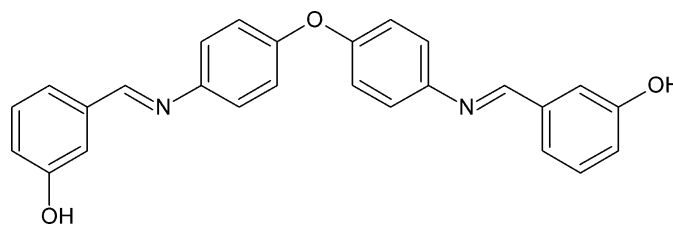
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In the crystal, the molecule of the title compound, C₂₆H₂₀N₂O₃, has crystallographically imposed twofold rotation symmetry. The crystal packing consists of layers parallel to the *ab* plane formed by O—H···N and C—H···O hydrogen bonds. Between the layers, C—H···π interactions are observed.

1. Chemical context

Several Schiff bases have been reported for their significant biological activities such as antitumor (Mansouri *et al.*, 2013), anti-inflammatory (Shukla & Mishra, 2019), antibacterial (Van Zee & Coates, 2015) or antimicrobial (Pagadala *et al.*, 2015). Schiff bases are also used as versatile components in nucleophilic addition with organometallic reagents and in cycloaddition reactions (Mohan *et al.*, 2012). These findings prompted us to investigate the crystal structure of the title compound.



2. Structural commentary

The molecule of the title compound has crystallographically imposed twofold rotation symmetry (Fig. 1). The dihedral angle between the two unique benzene rings is 40.68 (6)° while the dihedral angle between the two central benzene rings is 77.71 (6)°. Bond lengths are typical for this kind of compounds.

3. Supramolecular features

In the crystal, O2—H2A···N1 and C5—H5···O2 hydrogen bonds link the molecules into layers parallel to the *ab* plane

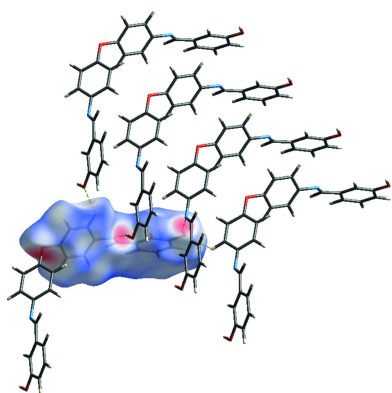


Table 1
Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C1–C6 benzene ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O2-H2A\cdots N1^i$	0.972 (19)	1.828 (19)	2.7615 (12)	160.1 (16)
$C5-H5\cdots O2^{ii}$	0.973 (13)	2.431 (14)	3.1121 (14)	126.7 (10)
$C12-H11\cdots Cg1^{ii}$	1.004 (14)	2.986 (15)	3.9882 (12)	178.7 (19)

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

(Table 1, Fig. 2). The layers are held together by $C-H\cdots\pi$ contacts (Table 1, Fig. 3) and by other van der Waals interactions (Table 2).

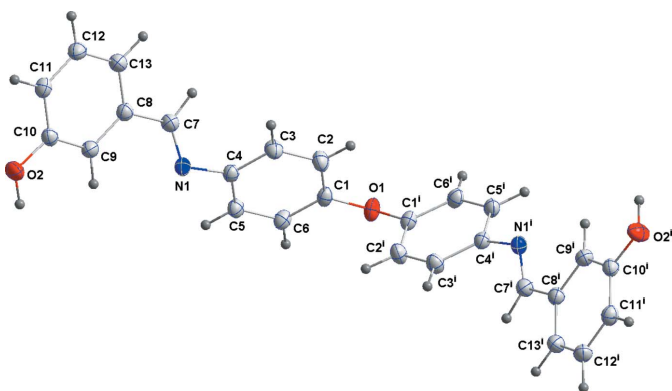


Figure 1
The title molecule with labeling scheme and 50% probability ellipsoids [symmetry code: (i) $-x + 1, y, -z + \frac{1}{2}$].

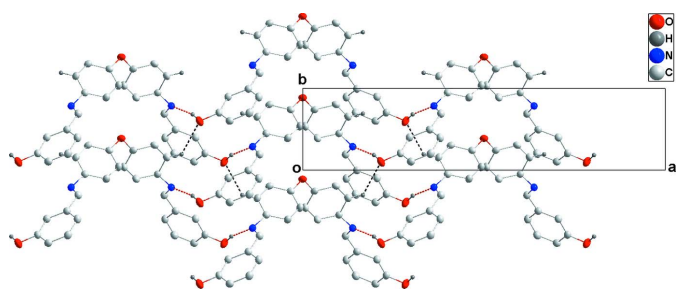


Figure 2
The layer structure viewed along the c -axis direction. The intermolecular $O-H\cdots N$ and $C-H\cdots O$ hydrogen bonds are shown as red and black dashed lines, respectively.

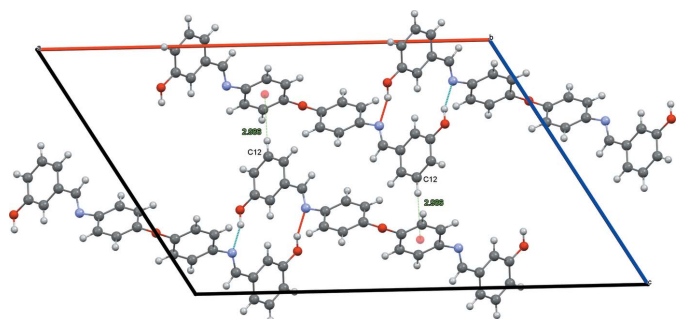


Figure 3
Side view of two layers seen along the b -axis direction. Hydrogen bonds and $C-H\cdots\pi$ interactions are depicted by dashed lines.

Table 2
Short intermolecular contacts (Å) in the title structure.

Contact	Distance	Symmetry operation
$H12\cdots O1$	2.763 (14)	$1 - x, 2 - y, 1 - z$
$H6\cdots H11$	2.53 (2)	$x, 2 - y, -\frac{1}{2} + z$
$C3\cdots C6$	3.5155 (15)	$x, -1 + y, z$
$C6\cdots H11$	2.892 (15)	$x, 1 - y, -\frac{1}{2} + z$
$C11\cdots C11$	3.319 (2)	$\frac{1}{2} - x, \frac{1}{2} - y, 1 - z$
$H11\cdots H2$	2.40 (3)	$1 - x, 1 - y, 1 - z$

4. Hirshfeld surface analysis

Hirshfeld surface analysis, together with two-dimensional fingerprint plots, is an important tool for visualizing and analyzing intermolecular contacts in molecular crystals. The corresponding surfaces and fingerprint plots were prepared by *CrystalExplorer* (Turner *et al.*, 2017). Fig. 4 shows the d_{norm} map for the title molecule, with red spots indicating the positions of $H\cdots N$ contacts arising from the $O-H\cdots N$ hydrogen bonds.

Fig. 5 shows the two-dimensional fingerprint plots, which give the contributions of intermolecular contacts to the Hirshfeld surface. The most important contribution to the Hirshfeld surface (41.6%) is from $H\cdots H$ contacts. $C\cdots H/H\cdots C$ and $O\cdots H/H\cdots O$ interactions follow with 28.1% and 13.8% contributions, respectively. Other minor contributors are $C\cdots C$ (5.3%), $N\cdots H/H\cdots N$ (4.8%), $O\cdots C/C\cdots O$ (3.8%) and $N\cdots C/C\cdots N$ (2.6%) contacts.

5. Database survey

Five related compounds with a 4-[(*E*)-benzylideneamino]-phenol skeleton are: (*E*)-2-[(2-aminophenyl)imino]methyl]-

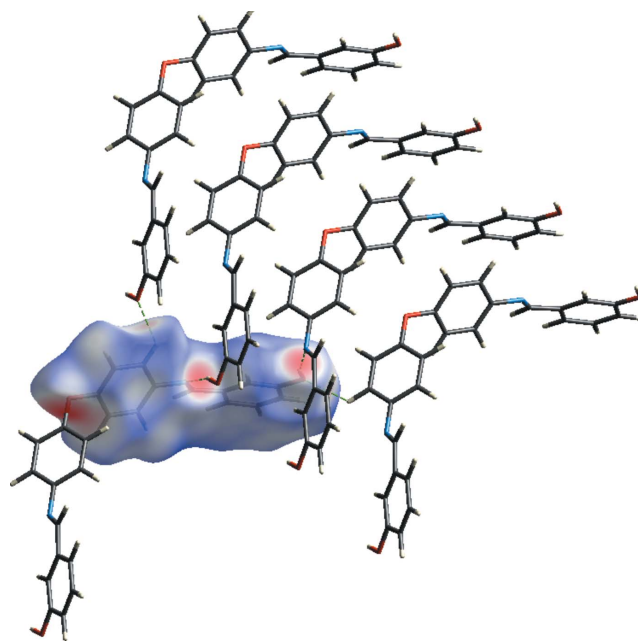


Figure 4
A view of the three-dimensional Hirshfeld surface for the title compound, plotted over d_{norm} in the range -1.1242 to 1.4437 a.u.

5-(benzyloxy)phenol (NIBRIC; Ghichi *et al.*, 2018), (*Z*)-3-(benzyloxy)-6-[[5-(chloro-2-hydroxyphenyl)amino]methylidene]cyclohexa-2,4-dien-1-one (NIBROI; Ghichi *et al.*, 2018), 2-[(*E*)-[(2-methyl-3-nitrophenyl)imino]methyl]-4-nitrophenol (AFOPUI; Tanak *et al.*, 2013), 2-[(*E*)-(2-chlorophenyl)imino]methyl]-6-methylphenol (SABKOX; Zhu *et al.*, 2010) and 2-[[2,4-dimethylphenyl]imino]methyl]-6-methylphenol (MUCDIY; Tanak *et al.*, 2009).

In the crystal of NIBRIC, strong N—H···O hydrogen bonds form zigzag chains of molecules along the *b*-axis direction. Weaker C—H··· π and offset π – π stacking interactions also contribute to the packing. For NIBROI, pairs of strong O—H···O hydrogen bonds form centrosymmetric dimers that enclose $R_2^2(18)$ rings. These combine with weaker C—H···Cl hydrogen bonds, which also generate centrosymmetric dimers, but with $R_2^2(14)$ motifs. Inversion-related C—H··· π contacts lead to the formation of sheets of molecules parallel to (120), which are stacked approximately along the *b*-axis direction. In the crystal of AFOPUI, molecules are linked by C—H···O interactions, forming two-dimensional sheets parallel to the *bc* plane. In the structure of SABKOX, the hydroxy H atom is involved in a strong intramolecular O—H···N hydrogen bond, generating a *S*(6) ring. The molecular structure of MUCDIY is stabilized by an intramolecular O—H···N hydrogen bond, which generates a six membered ring.

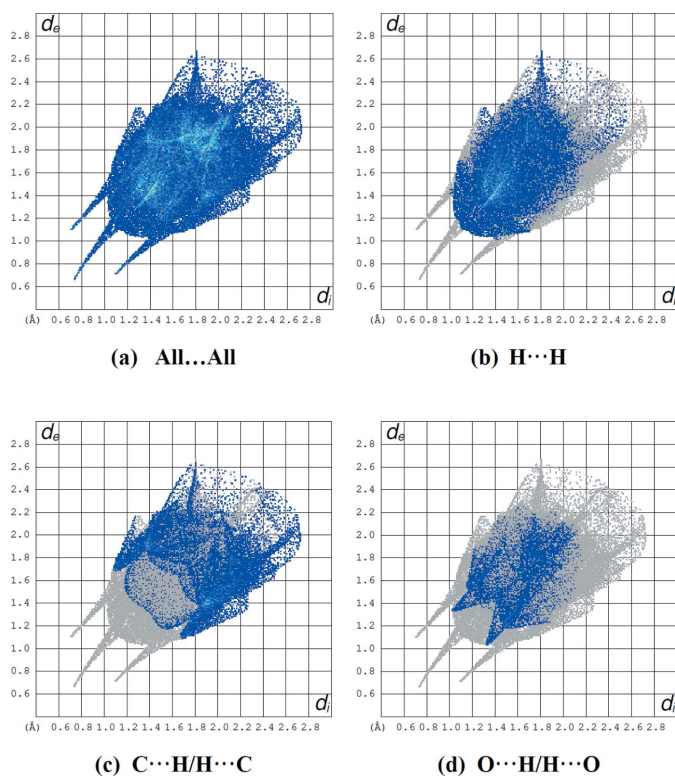


Figure 5
A view of the two-dimensional fingerprint plots for the title compound, showing (a) all interactions, and delineated into (b) H···H, (c) C···H/H···C and (d) O···H/H···O interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{20}N_2O_3$
M_r	408.44
Crystal system, space group	Monoclinic, <i>C2/c</i>
Temperature (K)	150
a, b, c (Å)	26.8396 (6), 5.1174 (1), 17.2574 (4)
β (°)	121.764 (1)
V (Å ³)	2015.27 (8)
Z	4
Radiation type	Cu $K\alpha$
μ (mm ⁻¹)	0.72
Crystal size (mm)	0.25 × 0.06 × 0.06
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
T_{min}, T_{max}	0.90, 0.96
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15449, 1880, 1767
R_{int}	0.031
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.609
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.033, 0.086, 1.05
No. of reflections	1880
No. of parameters	182
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.19, -0.16

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL2016/6* (Sheldrick, 2015b), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

6. Synthesis and crystallization

Condensation of 1 mmol of 4,4'-oxydibenzaldehyde (226 mg) with 2 mmol of 3-aminophenol (218 mg) in ethanol under reflux for 4 h afforded the crude product of the title compound. The product was crystallized from ethanol by slow evaporation to obtain good quality crystals for X-ray diffraction. Yield 82%.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were located in a difference-Fourier map and refined freely.

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Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINTE* (Bruker, 2016); data reduction: *SAINTE* (Bruker, 2016); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2016/6* (Sheldrick, 2015*b*); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2012); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

3-[(1*E*)-(4-{4-[(*E*)-(3-Hydroxybenzylidene)amino]phenoxy}phenylimino)methyl]phenol

Crystal data

$C_{26}H_{20}N_2O_3$

$M_r = 408.44$

Monoclinic, *C2/c*

$a = 26.8396$ (6) Å

$b = 5.1174$ (1) Å

$c = 17.2574$ (4) Å

$\beta = 121.764$ (1)°

$V = 2015.27$ (8) Å³

$Z = 4$

$F(000) = 856$

$D_x = 1.346$ Mg m⁻³

Cu *K* α radiation, $\lambda = 1.54178$ Å

Cell parameters from 9934 reflections

$\theta = 3.9$ – 69.8 °

$\mu = 0.72$ mm⁻¹

$T = 150$ K

Column, colourless

$0.25 \times 0.06 \times 0.06$ mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer

Radiation source: INCOATEC I μ S micro-focus source

Mirror monochromator

Detector resolution: 10.4167 pixels mm⁻¹

ω scans

Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)

$T_{\min} = 0.90$, $T_{\max} = 0.96$

15449 measured reflections

1880 independent reflections

1767 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\max} = 69.8$ °, $\theta_{\min} = 3.9$ °

$h = -32$ → 32

$k = -6$ → 6

$l = -20$ → 20

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.033$

$wR(F^2) = 0.086$

$S = 1.05$

1880 reflections

182 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: difference Fourier map

All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 1.3008P]$

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

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

$$\Delta\rho_{\max} = 0.19 \text{ e } \text{\AA}^{-3}$$

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

Extinction correction: *SHELXL* 2016/6
(Sheldrick, 2015b),
 $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0031 (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.

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.500000	1.3874 (2)	0.250000	0.0267 (3)
O2	0.21618 (3)	0.09976 (18)	0.33558 (6)	0.0336 (2)
H2A	0.1966 (8)	0.182 (4)	0.2759 (13)	0.066 (5)*
N1	0.36195 (4)	0.78690 (18)	0.33726 (6)	0.0233 (2)
C1	0.46708 (5)	1.2402 (2)	0.27573 (7)	0.0228 (3)
C2	0.49250 (5)	1.0380 (2)	0.33777 (8)	0.0288 (3)
H2	0.5331 (6)	0.994 (3)	0.3625 (9)	0.035 (3)*
C3	0.45903 (5)	0.8917 (2)	0.36148 (8)	0.0276 (3)
H3	0.4769 (6)	0.743 (3)	0.4038 (9)	0.033 (3)*
C4	0.39966 (4)	0.9482 (2)	0.32294 (7)	0.0220 (3)
C5	0.37512 (5)	1.1545 (2)	0.26182 (7)	0.0244 (3)
H5	0.3337 (6)	1.192 (3)	0.2353 (9)	0.031 (3)*
C6	0.40866 (5)	1.3034 (2)	0.23883 (7)	0.0242 (3)
H6	0.3914 (5)	1.445 (3)	0.1965 (9)	0.030 (3)*
C7	0.38127 (5)	0.6916 (2)	0.41641 (7)	0.0254 (3)
H7	0.4211 (6)	0.744 (3)	0.4696 (10)	0.035 (4)*
C8	0.35036 (5)	0.4960 (2)	0.43754 (7)	0.0238 (3)
C9	0.29481 (5)	0.4001 (2)	0.37197 (7)	0.0242 (3)
H9	0.2735 (5)	0.460 (3)	0.3094 (9)	0.026 (3)*
C10	0.26950 (5)	0.2038 (2)	0.39519 (7)	0.0242 (3)
H10	0.2803 (6)	-0.038 (3)	0.4990 (9)	0.030 (3)*
C11	0.29889 (5)	0.1028 (2)	0.48379 (8)	0.0262 (3)
H11	0.3729 (6)	0.127 (3)	0.6118 (10)	0.034 (3)*
C12	0.35320 (5)	0.2004 (2)	0.54851 (8)	0.0278 (3)
H12	0.4190 (6)	0.465 (3)	0.5730 (9)	0.030 (3)*
C13	0.37916 (5)	0.3963 (2)	0.52590 (8)	0.0268 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0298 (6)	0.0206 (5)	0.0400 (6)	0.000	0.0254 (5)	0.000

O2	0.0266 (4)	0.0395 (5)	0.0285 (5)	-0.0111 (4)	0.0103 (4)	-0.0010 (4)
N1	0.0218 (5)	0.0235 (5)	0.0265 (5)	0.0009 (4)	0.0141 (4)	0.0018 (4)
C1	0.0256 (5)	0.0208 (5)	0.0278 (6)	-0.0023 (4)	0.0181 (5)	-0.0032 (4)
C2	0.0204 (5)	0.0313 (6)	0.0344 (6)	0.0025 (5)	0.0142 (5)	0.0046 (5)
C3	0.0240 (6)	0.0273 (6)	0.0304 (6)	0.0030 (5)	0.0136 (5)	0.0066 (5)
C4	0.0224 (5)	0.0226 (5)	0.0235 (5)	-0.0011 (4)	0.0138 (4)	-0.0019 (4)
C5	0.0221 (5)	0.0262 (6)	0.0275 (6)	0.0037 (4)	0.0148 (5)	0.0013 (4)
C6	0.0276 (6)	0.0215 (5)	0.0277 (6)	0.0042 (4)	0.0175 (5)	0.0020 (4)
C7	0.0237 (5)	0.0276 (6)	0.0247 (6)	-0.0018 (4)	0.0125 (5)	-0.0010 (4)
C8	0.0235 (5)	0.0251 (6)	0.0249 (6)	-0.0002 (4)	0.0142 (5)	-0.0010 (4)
C9	0.0238 (5)	0.0275 (6)	0.0219 (6)	0.0008 (4)	0.0124 (5)	0.0012 (4)
C10	0.0209 (5)	0.0267 (6)	0.0257 (6)	-0.0014 (4)	0.0128 (5)	-0.0035 (4)
C11	0.0274 (6)	0.0254 (6)	0.0299 (6)	-0.0001 (4)	0.0179 (5)	0.0021 (4)
C12	0.0271 (6)	0.0317 (6)	0.0249 (6)	0.0033 (5)	0.0140 (5)	0.0046 (5)
C13	0.0224 (5)	0.0325 (6)	0.0237 (6)	-0.0011 (5)	0.0109 (5)	-0.0003 (5)

Geometric parameters (Å, °)

O1—C1 ⁱ	1.3992 (12)	C5—H5	0.973 (13)
O1—C1	1.3993 (12)	C6—H6	0.959 (14)
O2—C10	1.3563 (13)	C7—C8	1.4634 (15)
O2—H2A	0.972 (19)	C7—H7	1.012 (14)
N1—C7	1.2755 (14)	C8—C13	1.3935 (15)
N1—C4	1.4250 (13)	C8—C9	1.4028 (15)
C1—C2	1.3831 (16)	C9—C10	1.3848 (16)
C1—C6	1.3849 (15)	C9—H9	0.967 (13)
C2—C3	1.3865 (16)	C10—C11	1.3991 (16)
C2—H2	0.965 (14)	C11—C12	1.3812 (16)
C3—C4	1.3961 (15)	C11—H10	0.988 (14)
C3—H3	0.988 (15)	C12—C13	1.3888 (16)
C4—C5	1.3891 (16)	C12—H11	1.004 (14)
C5—C6	1.3871 (15)	C13—H12	1.007 (13)
C1 ⁱ —O1—C1	114.87 (11)	N1—C7—C8	124.35 (10)
C10—O2—H2A	113.5 (11)	N1—C7—H7	120.7 (8)
C7—N1—C4	118.81 (9)	C8—C7—H7	114.9 (8)
C2—C1—C6	120.56 (10)	C13—C8—C9	119.77 (10)
C2—C1—O1	120.77 (9)	C13—C8—C7	117.53 (10)
C6—C1—O1	118.66 (9)	C9—C8—C7	122.65 (10)
C1—C2—C3	120.01 (10)	C10—C9—C8	119.69 (10)
C1—C2—H2	119.8 (9)	C10—C9—H9	117.3 (8)
C3—C2—H2	120.1 (9)	C8—C9—H9	122.9 (8)
C2—C3—C4	120.12 (10)	O2—C10—C9	123.21 (10)
C2—C3—H3	119.8 (8)	O2—C10—C11	116.53 (10)
C4—C3—H3	120.0 (8)	C9—C10—C11	120.26 (10)
C5—C4—C3	119.03 (10)	C12—C11—C10	119.88 (10)
C5—C4—N1	118.41 (9)	C12—C11—H10	121.0 (8)
C3—C4—N1	122.28 (10)	C10—C11—H10	119.1 (8)

C6—C5—C4	120.99 (10)	C11—C12—C13	120.38 (10)
C6—C5—H5	120.6 (8)	C11—C12—H11	118.1 (8)
C4—C5—H5	118.4 (8)	C13—C12—H11	121.5 (8)
C1—C6—C5	119.23 (10)	C12—C13—C8	120.02 (10)
C1—C6—H6	120.2 (8)	C12—C13—H12	120.2 (8)
C5—C6—H6	120.5 (8)	C8—C13—H12	119.8 (8)
C1 ⁱ —O1—C1—C2	49.26 (9)	C4—N1—C7—C8	-171.34 (10)
C1 ⁱ —O1—C1—C6	-131.68 (11)	N1—C7—C8—C13	175.25 (11)
C6—C1—C2—C3	1.91 (17)	N1—C7—C8—C9	-2.15 (18)
O1—C1—C2—C3	-179.04 (10)	C13—C8—C9—C10	-1.16 (16)
C1—C2—C3—C4	-0.10 (18)	C7—C8—C9—C10	176.18 (10)
C2—C3—C4—C5	-0.88 (17)	C8—C9—C10—O2	-179.55 (10)
C2—C3—C4—N1	173.02 (10)	C8—C9—C10—C11	0.54 (16)
C7—N1—C4—C5	-145.80 (11)	O2—C10—C11—C12	-179.50 (10)
C7—N1—C4—C3	40.26 (15)	C9—C10—C11—C12	0.42 (17)
C3—C4—C5—C6	0.06 (16)	C10—C11—C12—C13	-0.76 (17)
N1—C4—C5—C6	-174.08 (10)	C11—C12—C13—C8	0.15 (17)
C2—C1—C6—C5	-2.71 (16)	C9—C8—C13—C12	0.82 (17)
O1—C1—C6—C5	178.23 (9)	C7—C8—C13—C12	-176.66 (10)
C4—C5—C6—C1	1.72 (16)		

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

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

Cg1 is the centroid of the C1–C6 benzene ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H2A \cdots N1 ⁱⁱ	0.972 (19)	1.828 (19)	2.7615 (12)	160.1 (16)
C5—H5 \cdots O2 ⁱⁱⁱ	0.973 (13)	2.431 (14)	3.1121 (14)	126.7 (10)
C12—H11 \cdots Cg1 ⁱⁱⁱ	1.004 (14)	2.986 (15)	3.9882 (12)	178.7 (19)

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