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4-[(*E*)-(4-Ethoxybenzylidene)amino]-phenol

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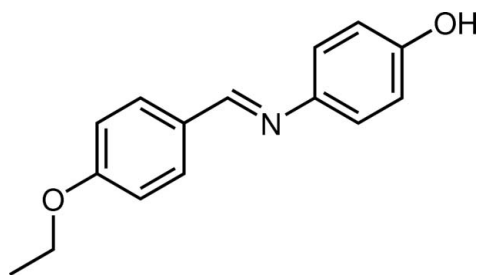
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 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.030; wR factor = 0.086; data-to-parameter ratio = 14.2.

The molecule of the title compound, $\text{C}_{15}\text{H}_{15}\text{NO}_2$, adopts a *trans* conformation with respect to the methyldene $\text{C}=\text{N}$ bond and is twisted with a dihedral angle of $26.31(5)^\circ$ between the two substituted benzene rings. The ethoxy group is almost coplanar with the bound benzene ring with a $\text{C}-\text{O}-\text{C}$ torsion angle of $-179.08(9)^\circ$. In the crystal, molecules are linked by $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds and weak $\text{C}-\text{H}\cdots\text{O}$ interactions into chains propagating in the $[011]$ and $[01\bar{1}]$ directions. $\text{C}-\text{H}\cdots\pi$ interactions are also present.

Related literature

For standard bond lengths, see: Allen *et al.* (1987). For background to and applications of aza-stilbene, see: Cheng *et al.* (2010); da Silva *et al.* (2011); Kabir *et al.* (2008); Lu *et al.* (2012); Pavan *et al.* (2011). For related structures, see: Sun *et al.* (2011); Wang (2009).



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Experimental

Crystal data

$\text{C}_{15}\text{H}_{15}\text{NO}_2$	$V = 1268.45(13) \text{ \AA}^3$
$M_r = 241.28$	$Z = 4$
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation
$a = 18.6882(11) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$b = 10.7420(6) \text{ \AA}$	$T = 100 \text{ K}$
$c = 6.3186(4) \text{ \AA}$	$0.59 \times 0.27 \times 0.25 \text{ mm}$

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	16922 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2009)	2382 independent reflections
$T_{\min} = 0.952, T_{\max} = 0.979$	2319 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.086$	
$S = 1.10$	
2382 reflections	
168 parameters	$\Delta\rho_{\text{max}} = 0.35 \text{ e \AA}^{-3}$
1 restraint	$\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C8–C13 ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O2}-\text{H1O2}\cdots\text{N1}^{\text{i}}$	0.83 (2)	1.87 (2)	2.6971 (12)	172 (2)
$\text{C6}-\text{H6A}\cdots\text{O2}^{\text{ii}}$	0.95	2.51	3.3956 (14)	156
$\text{C9}-\text{H9A}\cdots\text{O2}^{\text{iii}}$	0.95	2.38	3.3229 (13)	171
$\text{C14}-\text{H14B}\cdots\text{Cg1}^{\text{iv}}$	0.99	2.90	3.7668 (12)	147

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

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ5061).

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Acta Cryst. (2013). E69, o903–o904 [doi:10.1107/S1600536813012580]

4-[(*E*)-(4-Ethoxybenzylidene)amino]phenol

Narissara Kaewmanee, Suchada Chantrapromma, Nawong Boonnak and Hoong-Kun Fun

S1. Comment

Aza-stilbene derivatives derived from the reaction of an aldehyde with hydrazine have been shown to possess potent biological activities such as antibacterial (Kabir *et al.*, 2008), antifungal (da Silva *et al.*, 2011), antimycobacterium tuberculosis (Pavan *et al.*, 2011) and antioxidation (Cheng *et al.*, 2010; Lu *et al.*, 2012) properties. These interesting biological activities of aza-stilbene led us to synthesize the title compound, (I), and study its antibacterial activity. Our antibacterial assay showed that (I) exhibits moderate activity against *Salmonella typhi* with the minimum inhibition concentration (MIC) value of 18.75 $\mu\text{g/ml}$. We report here the crystal structure of the title compound.

The molecule of (I) (Fig. 1), $\text{C}_{15}\text{H}_{15}\text{NO}_2$, is twisted and exists in a *trans* configuration with respect to the methylenide $\text{C7}=\text{N1}$ double bond [1.2867 (13) Å] with the torsion angle $\text{C8-N1-C7-C1} = 179.23 (8)^\circ$. The dihedral angle between the two substituted benzene rings is $26.31 (5)^\circ$. The ethoxy group is co-planar with the bound benzene ring with the *r.m.s.* deviation of 0.0155 (1) Å for the nine non H-atoms and the C4-O1-C14-C15 angle is $-179.08 (9)^\circ$. The bond distances are within the normal range (Allen *et al.*, 1987) and are in agreement with those reported for related structures (Sun *et al.*, 2011; Wang, 2009).

In the crystal structure (Fig. 2), the molecules are linked by $\text{O-H}\cdots\text{N}$ hydrogen bond and weak $\text{C-H}\cdots\text{O}$ interactions (Table 1) into chains propagating in the [011] and $[0\bar{1}\bar{1}]$ directions. $\text{C-H}\cdots\pi$ interactions between the ethoxy group and the hydroxy substituted rings are also present (Table 1).

S2. Experimental

The title compound (I) was prepared by dissolving 4-benzylideneaniline (5 mmol, 0.50 g) in ethanol (30 ml) and 4-ethoxybenzaldehyde (5 mmol, 0.70 ml) was slowly added with stirring. The solution was stirred at room temperature for around 3 hr yielding a white solid, which was filtered off and washed with cold ethanol and dried in air. Colourless block-shaped single crystals of (I) suitable for X-ray structure determination were recrystallized from methanol by slow evaporation at room temperature after several days, M. p. 470–472 K.

S3. Refinement

The hydroxyl H atom was located in a difference map and refined isotropically. The remaining H atoms were fixed geometrically and allowed to ride on their parent atoms, with $d(\text{C-H}) = 0.95$ Å for aromatic and CH, 0.99 Å for CH_2 and 0.98 Å for CH_3 atoms. The U_{iso} values were constrained to be $1.5U_{\text{eq}}$ of the carrier atom for methyl H atoms and $1.2U_{\text{eq}}$ for the remaining H atoms. A rotating group model was used for the methyl group. 1762 Friedel pairs were merged as there is insufficient anomalous dispersion to determine the absolute structure since Mo radiation was used for data collection.

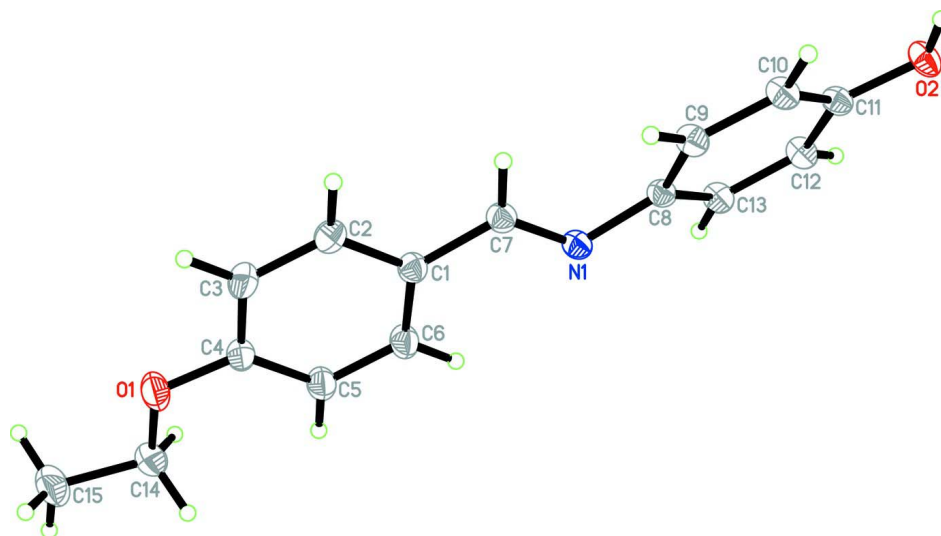


Figure 1

The asymmetric unit of the title compound showing 65% probability displacement ellipsoids.

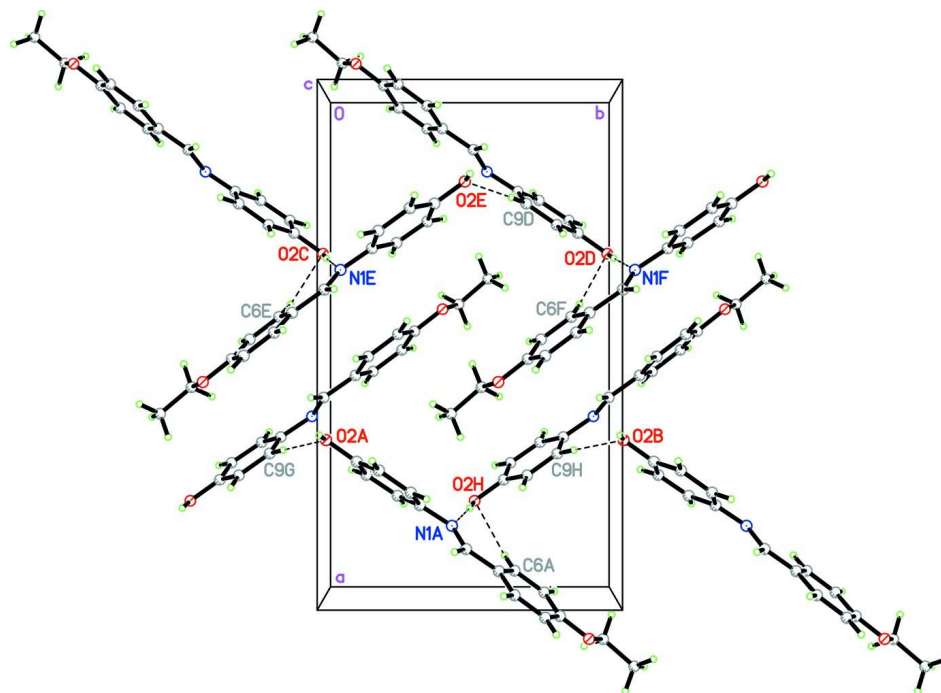


Figure 2

Crystal packing of the title compound viewed along the *c* axis. Hydrogen bonds are drawn as dashed lines.

4-[(*E*)-(4-Ethoxybenzylidene)amino]phenol

Crystal data

$C_{15}H_{15}NO_2$

$M_r = 241.28$

Orthorhombic, $Pna2_1$

Hall symbol: $P\ 2c\ -2n$

$a = 18.6882\ (11)\ \text{\AA}$

$b = 10.7420\ (6)\ \text{\AA}$

$c = 6.3186\ (4)\ \text{\AA}$

$V = 1268.45\ (13)\ \text{\AA}^3$

$Z = 4$

$F(000) = 512$

$D_x = 1.263 \text{ Mg m}^{-3}$
 Melting point = 470–472 K
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 2382 reflections
 $\theta = 2.2\text{--}32.0^\circ$

$\mu = 0.08 \text{ mm}^{-1}$
 $T = 100 \text{ K}$
 Block, colourless
 $0.59 \times 0.27 \times 0.25 \text{ mm}$

Data collection

Bruker SMART APEXII CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 Detector resolution: 8.33 pixels mm^{-1}
 ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2009)
 $T_{\min} = 0.952$, $T_{\max} = 0.979$

16922 measured reflections
 2382 independent reflections
 2319 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$
 $\theta_{\max} = 32.0^\circ$, $\theta_{\min} = 2.2^\circ$
 $h = -27 \rightarrow 27$
 $k = -16 \rightarrow 15$
 $l = -9 \rightarrow 9$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.086$
 $S = 1.10$
 2382 reflections
 168 parameters
 1 restraint
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.1397P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.35 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.19 \text{ e \AA}^{-3}$

Special details

Experimental. The data was collected with the Oxford Cryosystem Cobra low-temperature attachment.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	1.07262 (4)	0.90374 (7)	0.65280 (16)	0.02092 (17)
O2	0.68429 (4)	0.01683 (7)	0.72655 (13)	0.01662 (15)
H1O2	0.6732 (11)	0.000 (2)	0.851 (4)	0.038 (5)*
N1	0.85372 (4)	0.43914 (7)	0.61658 (15)	0.01367 (16)
C1	0.93803 (5)	0.59761 (9)	0.72367 (18)	0.01420 (18)
C2	0.97668 (5)	0.64779 (9)	0.89339 (19)	0.01686 (19)
H2A	0.9725	0.6113	1.0298	0.020*
C3	1.02104 (6)	0.75025 (10)	0.86479 (19)	0.0181 (2)
H3A	1.0468	0.7835	0.9813	0.022*

C4	1.02770 (5)	0.80430 (9)	0.66463 (19)	0.01595 (19)
C5	0.98933 (6)	0.75587 (10)	0.49369 (19)	0.01789 (19)
H5A	0.9934	0.7928	0.3576	0.021*
C6	0.94517 (6)	0.65320 (10)	0.52393 (19)	0.01713 (19)
H6A	0.9194	0.6201	0.4072	0.021*
C7	0.89365 (5)	0.48741 (8)	0.76077 (17)	0.01413 (18)
H7A	0.8944	0.4500	0.8970	0.017*
C8	0.81221 (5)	0.33104 (9)	0.65972 (16)	0.01283 (17)
C9	0.78245 (5)	0.30394 (9)	0.85792 (16)	0.01439 (18)
H9A	0.7915	0.3572	0.9750	0.017*
C10	0.73949 (5)	0.19880 (9)	0.88339 (16)	0.01468 (17)
H10A	0.7190	0.1811	1.0176	0.018*
C11	0.72652 (5)	0.11939 (8)	0.71249 (17)	0.01325 (17)
C12	0.75683 (6)	0.14583 (9)	0.51485 (17)	0.01527 (18)
H12A	0.7489	0.0913	0.3988	0.018*
C13	0.79848 (5)	0.25179 (9)	0.48866 (16)	0.01442 (17)
H13A	0.8178	0.2707	0.3534	0.017*
C14	1.08402 (6)	0.95958 (10)	0.4482 (2)	0.0215 (2)
H14A	1.0383	0.9914	0.3904	0.026*
H14B	1.1037	0.8975	0.3482	0.026*
C15	1.13632 (6)	1.06515 (11)	0.4787 (3)	0.0285 (3)
H15A	1.1448	1.1065	0.3427	0.043*
H15B	1.1816	1.0323	0.5335	0.043*
H15C	1.1165	1.1253	0.5795	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0213 (3)	0.0180 (3)	0.0234 (4)	-0.0072 (3)	-0.0018 (3)	-0.0007 (3)
O2	0.0230 (3)	0.0138 (3)	0.0131 (3)	-0.0056 (2)	0.0018 (3)	-0.0011 (3)
N1	0.0156 (3)	0.0116 (3)	0.0138 (4)	-0.0003 (3)	0.0002 (3)	0.0000 (3)
C1	0.0144 (4)	0.0133 (3)	0.0148 (4)	-0.0003 (3)	-0.0007 (3)	-0.0011 (3)
C2	0.0177 (4)	0.0183 (4)	0.0146 (4)	-0.0008 (3)	-0.0029 (4)	-0.0003 (4)
C3	0.0174 (4)	0.0193 (4)	0.0176 (5)	-0.0023 (3)	-0.0036 (4)	-0.0023 (4)
C4	0.0146 (4)	0.0140 (4)	0.0193 (5)	-0.0013 (3)	-0.0018 (4)	-0.0007 (4)
C5	0.0199 (4)	0.0175 (4)	0.0162 (5)	-0.0045 (3)	-0.0025 (4)	0.0009 (4)
C6	0.0188 (4)	0.0176 (4)	0.0150 (4)	-0.0044 (3)	-0.0017 (4)	-0.0002 (4)
C7	0.0153 (4)	0.0132 (4)	0.0139 (4)	-0.0001 (3)	0.0000 (3)	-0.0002 (3)
C8	0.0144 (3)	0.0114 (3)	0.0126 (4)	0.0002 (3)	-0.0005 (3)	0.0001 (3)
C9	0.0184 (4)	0.0128 (4)	0.0119 (4)	-0.0005 (3)	0.0006 (3)	-0.0015 (3)
C10	0.0192 (4)	0.0137 (4)	0.0111 (4)	-0.0010 (3)	0.0012 (4)	-0.0007 (3)
C11	0.0161 (4)	0.0113 (3)	0.0123 (4)	-0.0001 (3)	0.0005 (3)	-0.0001 (3)
C12	0.0196 (4)	0.0143 (4)	0.0119 (4)	-0.0018 (3)	0.0011 (4)	-0.0015 (3)
C13	0.0181 (4)	0.0146 (4)	0.0106 (4)	-0.0011 (3)	0.0009 (4)	-0.0010 (3)
C14	0.0199 (4)	0.0176 (4)	0.0269 (6)	-0.0038 (3)	-0.0014 (4)	0.0044 (4)
C15	0.0236 (5)	0.0201 (5)	0.0420 (8)	-0.0071 (4)	0.0000 (5)	0.0019 (5)

Geometric parameters (Å, °)

O1—C4	1.3605 (11)	C7—H7A	0.9500
O1—C14	1.4412 (16)	C8—C13	1.3996 (14)
O2—C11	1.3581 (11)	C8—C9	1.4009 (14)
O2—H1O2	0.83 (3)	C9—C10	1.3951 (13)
N1—C7	1.2867 (13)	C9—H9A	0.9500
N1—C8	1.4228 (12)	C10—C11	1.3973 (14)
C1—C2	1.4008 (15)	C10—H10A	0.9500
C1—C6	1.4026 (16)	C11—C12	1.4004 (15)
C1—C7	1.4643 (13)	C12—C13	1.3887 (13)
C2—C3	1.3898 (14)	C12—H12A	0.9500
C2—H2A	0.9500	C13—H13A	0.9500
C3—C4	1.3972 (16)	C14—C15	1.5094 (15)
C3—H3A	0.9500	C14—H14A	0.9900
C4—C5	1.3970 (15)	C14—H14B	0.9900
C5—C6	1.3906 (14)	C15—H15A	0.9800
C5—H5A	0.9500	C15—H15B	0.9800
C6—H6A	0.9500	C15—H15C	0.9800
C4—O1—C14	117.86 (9)	C10—C9—C8	119.99 (9)
C11—O2—H1O2	112.7 (15)	C10—C9—H9A	120.0
C7—N1—C8	120.62 (9)	C8—C9—H9A	120.0
C2—C1—C6	118.43 (9)	C9—C10—C11	120.33 (9)
C2—C1—C7	118.72 (10)	C9—C10—H10A	119.8
C6—C1—C7	122.83 (9)	C11—C10—H10A	119.8
C3—C2—C1	120.85 (11)	O2—C11—C10	123.06 (9)
C3—C2—H2A	119.6	O2—C11—C12	117.25 (9)
C1—C2—H2A	119.6	C10—C11—C12	119.68 (9)
C2—C3—C4	120.00 (10)	C13—C12—C11	119.95 (9)
C2—C3—H3A	120.0	C13—C12—H12A	120.0
C4—C3—H3A	120.0	C11—C12—H12A	120.0
O1—C4—C5	124.52 (10)	C12—C13—C8	120.62 (9)
O1—C4—C3	115.52 (9)	C12—C13—H13A	119.7
C5—C4—C3	119.96 (9)	C8—C13—H13A	119.7
C6—C5—C4	119.59 (10)	O1—C14—C15	107.10 (11)
C6—C5—H5A	120.2	O1—C14—H14A	110.3
C4—C5—H5A	120.2	C15—C14—H14A	110.3
C5—C6—C1	121.18 (10)	O1—C14—H14B	110.3
C5—C6—H6A	119.4	C15—C14—H14B	110.3
C1—C6—H6A	119.4	H14A—C14—H14B	108.5
N1—C7—C1	122.74 (9)	C14—C15—H15A	109.5
N1—C7—H7A	118.6	C14—C15—H15B	109.5
C1—C7—H7A	118.6	H15A—C15—H15B	109.5
C13—C8—C9	119.41 (9)	C14—C15—H15C	109.5
C13—C8—N1	116.65 (9)	H15A—C15—H15C	109.5
C9—C8—N1	123.87 (9)	H15B—C15—H15C	109.5

C6—C1—C2—C3	0.01 (15)	C6—C1—C7—N1	-5.42 (15)
C7—C1—C2—C3	178.24 (9)	C7—N1—C8—C13	-150.56 (9)
C1—C2—C3—C4	-0.20 (15)	C7—N1—C8—C9	32.46 (13)
C14—O1—C4—C5	-2.99 (14)	C13—C8—C9—C10	-0.07 (14)
C14—O1—C4—C3	177.23 (9)	N1—C8—C9—C10	176.84 (9)
C2—C3—C4—O1	-179.72 (9)	C8—C9—C10—C11	0.67 (14)
C2—C3—C4—C5	0.48 (15)	C9—C10—C11—O2	-178.92 (9)
O1—C4—C5—C6	179.64 (9)	C9—C10—C11—C12	-0.06 (15)
C3—C4—C5—C6	-0.58 (16)	O2—C11—C12—C13	177.76 (9)
C4—C5—C6—C1	0.40 (16)	C10—C11—C12—C13	-1.16 (15)
C2—C1—C6—C5	-0.12 (15)	C11—C12—C13—C8	1.78 (15)
C7—C1—C6—C5	-178.27 (9)	C9—C8—C13—C12	-1.16 (14)
C8—N1—C7—C1	179.23 (8)	N1—C8—C13—C12	-178.29 (9)
C2—C1—C7—N1	176.43 (9)	C4—O1—C14—C15	-179.08 (9)

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

Cg1 is the centroid of the C8—C13 ring.

<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>
O2—H1O2 \cdots N1 ⁱ	0.83 (2)	1.87 (2)	2.6971 (12)	172 (2)
C6—H6A \cdots O2 ⁱⁱ	0.95	2.51	3.3956 (14)	156
C9—H9A \cdots O2 ⁱⁱⁱ	0.95	2.38	3.3229 (13)	171
C14—H14B \cdots Cg1 ^{iv}	0.99	2.90	3.7668 (12)	147

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