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N-(3,4-Dimethoxybenzylidene)-4-methylaniline

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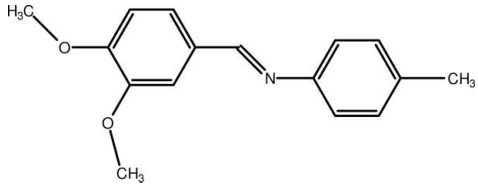
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.063; wR factor = 0.229; data-to-parameter ratio = 17.7.

The title compound, $C_{16}H_{17}NO_2$, crystallizes with two independent molecules in the asymmetric unit. In these molecules, the two benzene rings form dihedral angles of 26.44 (15) and 35.97 (16)°. There are weak intermolecular C—H···O hydrogen-bonding interactions in the crystal structure.

Related literature

For related literature, see: Allen *et al.* (1987); Li *et al.* (2006); Tian *et al.* (2006).



Experimental

Crystal data

$C_{16}H_{17}NO_2$
M_r = 255.31
Triclinic, $P\overline{1}$
a = 9.777 (2) Å
b = 12.304 (3) Å
c = 13.716 (3) Å
α = 67.84 (3)°
β = 81.97 (3)°
γ = 68.41 (3)°
V = 1420.9 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.54 × 0.34 × 0.18 mm

Data collection

Bruker *P*4 diffractometer
Absorption correction: none
6427 measured reflections
6059 independent reflections
2536 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.229
S = 1.01
6059 reflections
343 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···O1^{i}	0.96	2.52	3.439 (4)	161
C17—H17A···O4^{ii}	0.96	2.51	3.459 (4)	169

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2373).

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supplementary materials

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N-(3,4-Dimethoxybenzylidene)-4-methylaniline

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Comment

Schiff base compounds and its derivatives have broad application in biological activity of antibacterial drugs, anti-virus, and anti-cancer (Tian, *et al.*, 2006). Due to their important biological activities, these compounds have received a great deal of attention in connection with their syntheses and in the elucidation of their crystal structures. In search for new Schiff base compounds with higher biological activities, the title compound (I) was synthesized. We report herein its crystal structure.

The asymmetric unit of (I) contains two independent molecules (Fig. 1). In these molecules, the benzene rings A(C3—C8), B(C10—C15) and C(C19—C24), D(C26—C31) deviate only slightly from coplanarity with the dihedral angles of 26.44 (15) and 35.97 (16)°, respectively. The dihedral angles A/C and B/D are 11.42 (16) and 72.31 (15)°, respectively. In (I), all the bond lengths and angles are generally normal (Allen *et al.*, 1987). In the title molecule, the average C═N, C—C and C—O bond distances [1.274 (4), 1.507 (4) and 1.374 (3) Å, respectively] are also in good agreement with an earlier report (Li *et al.*, 2006). The torsion angles C10—N1═ C9—C6 and C26—N2═C25—C21 are −177.7 (2)° and 178.0 (2) °, respectively.

There are some weak intermolecular C—H···O hydrogen bonding interactions in the crystal structure, providing stabilization (Table 1, Fig. 2).

Experimental

The title compound (I) was prepared by reaction of [(3,4-dimethoxy-benzylidene)-amino]-ethanol and (right) toluidine in ethanol at room temperature. Single crystals of the title compound suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Refinement

All H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C).

Figures

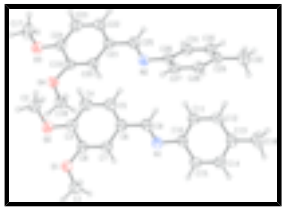
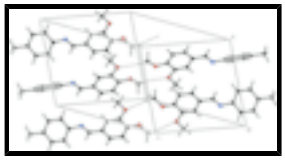


Fig. 1. View of the title compound (I), with displacement ellipsoids drawn at the 30% probability level.



_N_-(3,4-Dimethoxybenzylidene)-4-methylaniline

Crystal data

$C_{16}H_{17}NO_2$	$Z = 4$
$M_r = 255.31$	$F_{000} = 544$
Triclinic, $P\overline{1}$	$D_x = 1.194$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.777$ (2) Å	Cell parameters from 2566 reflections
$b = 12.304$ (3) Å	$\theta = 1.6$–27.0º
$c = 13.716$ (3) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 67.84$ (3)º	$T = 293$ (2) K
$\beta = 81.97$ (3)º	Slice, colourless
$\gamma = 68.41$ (3)º	0.54 × 0.34 × 0.18 mm
$V = 1420.9$ (5) Å^3	

Data collection

Bruker P4 diffractometer	$R_{int} = 0.018$
Radiation source: fine-focus sealed tube	$\theta_{max} = 27.0$º
Monochromator: graphite	$\theta_{min} = 1.6$º
$T = 293$(2) K	$h = 0 \rightarrow 11$
ω scans	$k = -14 \rightarrow 14$
Absorption correction: none	$l = -16 \rightarrow 16$
6427 measured reflections	3 standard reflections
6059 independent reflections	every 200 reflections
2536 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.063$	H-atom parameters constrained
$wR(F^2) = 0.229$	$w = 1/[\sigma^2(F_o^2) + (0.1145P)^2 + 0.0112P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
6059 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
343 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

Special details

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.0106 (2)	0.25461 (19)	0.48495 (17)	0.0722 (6)
O2	0.1218 (2)	0.42907 (18)	0.42852 (17)	0.0717 (6)
N1	0.2567 (3)	−0.0024 (2)	0.24077 (19)	0.0627 (7)
C1	−0.0405 (4)	0.1520 (3)	0.5273 (3)	0.0725 (9)
H1B	−0.1079	0.1623	0.5838	0.109*
H1C	0.0414	0.0759	0.5534	0.109*
H1D	−0.0897	0.1484	0.4733	0.109*
C2	0.1898 (4)	0.5212 (3)	0.4088 (3)	0.0797 (10)
H2A	0.1461	0.5691	0.4536	0.120*
H2B	0.1753	0.5758	0.3365	0.120*
H2C	0.2932	0.4801	0.4233	0.120*
C3	0.1688 (3)	0.3528 (3)	0.3719 (2)	0.0593 (8)
C4	0.2673 (4)	0.3626 (3)	0.2896 (3)	0.0697 (9)
H4A	0.3061	0.4267	0.2682	0.084*
C5	0.3089 (4)	0.2773 (3)	0.2383 (2)	0.0706 (9)
H5A	0.3758	0.2848	0.1830	0.085*
C6	0.2528 (3)	0.1816 (3)	0.2678 (2)	0.0611 (8)
C7	0.1506 (3)	0.1716 (3)	0.3515 (2)	0.0584 (8)
H7A	0.1118	0.1077	0.3721	0.070*
C8	0.1082 (3)	0.2557 (3)	0.4025 (2)	0.0562 (7)
C9	0.3004 (3)	0.0904 (3)	0.2150 (2)	0.0650 (8)
H9A	0.3664	0.1007	0.1593	0.078*
C10	0.3127 (3)	−0.0892 (3)	0.1876 (2)	0.0555 (7)
C11	0.4502 (3)	−0.1165 (3)	0.1398 (2)	0.0644 (8)
H11A	0.5126	−0.0751	0.1405	0.077*
C12	0.4950 (3)	−0.2034 (3)	0.0918 (2)	0.0677 (9)
H12A	0.5875	−0.2200	0.0606	0.081*
C13	0.4047 (4)	−0.2682 (3)	0.0885 (2)	0.0650 (8)
C14	0.2682 (3)	−0.2403 (3)	0.1360 (2)	0.0670 (9)
H14A	0.2053	−0.2808	0.1344	0.080*
C15	0.2223 (3)	−0.1537 (3)	0.1862 (2)	0.0637 (8)

H15A	0.1309	−0.1386	0.2190	0.076*
C16	0.4536 (5)	−0.3650 (3)	0.0369 (3)	0.0969 (12)
H16A	0.3779	−0.3998	0.0442	0.145*
H16B	0.5420	−0.4302	0.0700	0.145*
H16C	0.4722	−0.3267	−0.0365	0.145*
O3	0.5841 (2)	0.44440 (17)	0.40783 (16)	0.0687 (6)
O4	0.5223 (2)	0.24385 (17)	0.49333 (16)	0.0646 (6)
N2	0.7675 (3)	−0.0204 (2)	0.25563 (19)	0.0574 (6)
C17	0.5994 (5)	0.5632 (3)	0.3599 (3)	0.0958 (13)
H17A	0.5550	0.6120	0.4039	0.144*
H17B	0.5516	0.6050	0.2926	0.144*
H17C	0.7019	0.5533	0.3508	0.144*
C18	0.4808 (4)	0.1364 (2)	0.5426 (2)	0.0670 (9)
H18A	0.4218	0.1435	0.6036	0.100*
H18B	0.5673	0.0632	0.5635	0.100*
H18C	0.4250	0.1298	0.4941	0.100*
C19	0.6072 (3)	0.2496 (2)	0.4041 (2)	0.0522 (7)
C20	0.6583 (3)	0.1595 (2)	0.3597 (2)	0.0536 (7)
H20A	0.6346	0.0871	0.3901	0.064*
C21	0.7467 (3)	0.1750 (3)	0.2685 (2)	0.0562 (7)
C22	0.7822 (4)	0.2827 (3)	0.2256 (3)	0.0709 (9)
H22A	0.8426	0.2930	0.1666	0.085*
C23	0.7294 (4)	0.3750 (3)	0.2692 (2)	0.0695 (9)
H23A	0.7531	0.4473	0.2386	0.083*
C24	0.6415 (3)	0.3607 (3)	0.3581 (2)	0.0553 (7)
C25	0.7994 (3)	0.0788 (3)	0.2206 (2)	0.0628 (8)
H25A	0.8595	0.0908	0.1615	0.075*
C26	0.8191 (3)	−0.1072 (3)	0.2028 (2)	0.0521 (7)
C27	0.8563 (3)	−0.2335 (3)	0.2632 (2)	0.0600 (8)
H27A	0.8492	−0.2584	0.3361	0.072*
C28	0.9039 (3)	−0.3226 (3)	0.2161 (3)	0.0638 (8)
H28A	0.9299	−0.4068	0.2579	0.077*
C29	0.9134 (3)	−0.2882 (3)	0.1071 (3)	0.0637 (8)
C30	0.8748 (3)	−0.1628 (3)	0.0483 (3)	0.0700 (9)
H30A	0.8808	−0.1382	−0.0247	0.084*
C31	0.8277 (3)	−0.0725 (3)	0.0934 (2)	0.0616 (8)
H31A	0.8016	0.0115	0.0511	0.074*
C32	0.9638 (4)	−0.3868 (4)	0.0562 (3)	0.0951 (12)
H32A	0.9644	−0.3470	−0.0189	0.143*
H32B	0.8977	−0.4331	0.0753	0.143*
H32C	1.0612	−0.4426	0.0800	0.143*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0888 (16)	0.0727 (14)	0.0692 (15)	−0.0405 (12)	0.0212 (13)	−0.0353 (12)
O2	0.0855 (16)	0.0604 (12)	0.0766 (15)	−0.0309 (11)	0.0077 (13)	−0.0291 (12)
N1	0.0647 (16)	0.0733 (17)	0.0546 (16)	−0.0276 (14)	0.0007 (13)	−0.0239 (14)

C1	0.083 (2)	0.079 (2)	0.064 (2)	−0.0421 (19)	0.0124 (18)	−0.0262 (18)
C2	0.078 (2)	0.071 (2)	0.103 (3)	−0.0294 (18)	−0.006 (2)	−0.039 (2)
C3	0.065 (2)	0.0547 (18)	0.0549 (19)	−0.0182 (15)	−0.0088 (16)	−0.0155 (15)
C4	0.079 (2)	0.065 (2)	0.065 (2)	−0.0329 (17)	0.0000 (19)	−0.0145 (17)
C5	0.082 (2)	0.080 (2)	0.0513 (19)	−0.0373 (19)	0.0063 (17)	−0.0174 (17)
C6	0.069 (2)	0.0673 (19)	0.0460 (17)	−0.0223 (16)	−0.0066 (16)	−0.0175 (15)
C7	0.0627 (19)	0.0593 (18)	0.0534 (19)	−0.0239 (15)	−0.0067 (16)	−0.0149 (15)
C8	0.0638 (19)	0.0568 (17)	0.0465 (17)	−0.0194 (15)	−0.0010 (15)	−0.0177 (15)
C9	0.072 (2)	0.082 (2)	0.0430 (18)	−0.0313 (18)	0.0042 (16)	−0.0216 (17)
C10	0.0565 (19)	0.0662 (18)	0.0445 (17)	−0.0235 (15)	0.0003 (14)	−0.0180 (15)
C11	0.0546 (19)	0.080 (2)	0.061 (2)	−0.0280 (16)	0.0021 (16)	−0.0241 (17)
C12	0.0541 (19)	0.080 (2)	0.063 (2)	−0.0200 (16)	0.0120 (16)	−0.0258 (18)
C13	0.078 (2)	0.071 (2)	0.0435 (17)	−0.0237 (18)	−0.0001 (17)	−0.0194 (16)
C14	0.067 (2)	0.084 (2)	0.061 (2)	−0.0358 (18)	0.0003 (17)	−0.0282 (18)
C15	0.0558 (18)	0.084 (2)	0.0563 (19)	−0.0318 (16)	0.0070 (15)	−0.0254 (17)
C16	0.119 (3)	0.102 (3)	0.077 (3)	−0.036 (2)	0.015 (2)	−0.046 (2)
O3	0.0907 (16)	0.0543 (12)	0.0674 (14)	−0.0357 (11)	0.0120 (12)	−0.0221 (11)
O4	0.0832 (15)	0.0566 (12)	0.0595 (14)	−0.0342 (11)	0.0207 (12)	−0.0237 (10)
N2	0.0576 (15)	0.0620 (15)	0.0515 (15)	−0.0195 (12)	0.0045 (12)	−0.0216 (13)
C17	0.172 (4)	0.069 (2)	0.064 (2)	−0.065 (2)	0.012 (2)	−0.0236 (18)
C18	0.085 (2)	0.0540 (18)	0.058 (2)	−0.0311 (16)	0.0137 (18)	−0.0136 (15)
C19	0.0545 (17)	0.0520 (16)	0.0482 (17)	−0.0224 (13)	0.0028 (14)	−0.0126 (14)
C20	0.0580 (18)	0.0483 (15)	0.0530 (18)	−0.0200 (13)	−0.0011 (15)	−0.0145 (14)
C21	0.0561 (18)	0.0637 (18)	0.0494 (17)	−0.0231 (15)	0.0018 (15)	−0.0187 (15)
C22	0.087 (2)	0.079 (2)	0.056 (2)	−0.0466 (19)	0.0202 (18)	−0.0237 (18)
C23	0.092 (2)	0.068 (2)	0.058 (2)	−0.0460 (19)	0.0091 (19)	−0.0188 (17)
C24	0.0635 (19)	0.0545 (17)	0.0502 (18)	−0.0257 (15)	−0.0024 (15)	−0.0151 (15)
C25	0.064 (2)	0.072 (2)	0.0532 (19)	−0.0241 (16)	0.0066 (16)	−0.0245 (17)
C26	0.0444 (16)	0.0606 (18)	0.0504 (17)	−0.0164 (13)	0.0037 (14)	−0.0214 (15)
C27	0.0542 (18)	0.074 (2)	0.0518 (18)	−0.0234 (15)	0.0014 (15)	−0.0211 (16)
C28	0.0553 (18)	0.0662 (19)	0.070 (2)	−0.0195 (15)	0.0021 (16)	−0.0259 (17)
C29	0.0544 (19)	0.082 (2)	0.067 (2)	−0.0250 (17)	0.0045 (17)	−0.0398 (19)
C30	0.070 (2)	0.091 (2)	0.053 (2)	−0.0255 (19)	−0.0013 (17)	−0.0310 (19)
C31	0.0617 (19)	0.0698 (19)	0.0503 (18)	−0.0208 (15)	−0.0022 (15)	−0.0192 (16)
C32	0.108 (3)	0.098 (3)	0.095 (3)	−0.033 (2)	0.015 (2)	−0.059 (2)

Geometric parameters (Å, °)

O1—C8	1.374 (3)	O3—C24	1.356 (3)
O1—C1	1.418 (3)	O3—C17	1.414 (3)
O2—C3	1.352 (3)	O4—C19	1.373 (3)
O2—C2	1.440 (3)	O4—C18	1.420 (3)
N1—C9	1.274 (4)	N2—C25	1.270 (3)
N1—C10	1.420 (3)	N2—C26	1.416 (3)
C1—H1B	0.9600	C17—H17A	0.9600
C1—H1C	0.9600	C17—H17B	0.9600
C1—H1D	0.9600	C17—H17C	0.9600
C2—H2A	0.9600	C18—H18A	0.9600
C2—H2B	0.9600	C18—H18B	0.9600

C2—H2C	0.9600	C18—H18C	0.9600
C3—C4	1.377 (4)	C19—C20	1.366 (3)
C3—C8	1.424 (4)	C19—C24	1.416 (4)
C4—C5	1.387 (4)	C20—C21	1.410 (4)
C4—H4A	0.9300	C20—H20A	0.9300
C5—C6	1.381 (4)	C21—C22	1.384 (4)
C5—H5A	0.9300	C21—C25	1.464 (4)
C6—C7	1.412 (4)	C22—C23	1.382 (4)
C6—C9	1.461 (4)	C22—H22A	0.9300
C7—C8	1.372 (4)	C23—C24	1.382 (4)
C7—H7A	0.9300	C23—H23A	0.9300
C9—H9A	0.9300	C25—H25A	0.9300
C10—C11	1.391 (4)	C26—C27	1.389 (4)
C10—C15	1.394 (4)	C26—C31	1.396 (4)
C11—C12	1.370 (4)	C27—C28	1.382 (4)
C11—H11A	0.9300	C27—H27A	0.9300
C12—C13	1.405 (4)	C28—C29	1.392 (4)
C12—H12A	0.9300	C28—H28A	0.9300
C13—C14	1.383 (4)	C29—C30	1.375 (4)
C13—C16	1.507 (4)	C29—C32	1.518 (4)
C14—C15	1.388 (4)	C30—C31	1.376 (4)
C14—H14A	0.9300	C30—H30A	0.9300
C15—H15A	0.9300	C31—H31A	0.9300
C16—H16A	0.9600	C32—H32A	0.9600
C16—H16B	0.9600	C32—H32B	0.9600
C16—H16C	0.9600	C32—H32C	0.9600
C8—O1—C1	117.5 (2)	C24—O3—C17	118.5 (2)
C3—O2—C2	117.9 (3)	C19—O4—C18	117.4 (2)
C9—N1—C10	120.0 (3)	C25—N2—C26	120.0 (3)
O1—C1—H1B	109.5	O3—C17—H17A	109.5
O1—C1—H1C	109.5	O3—C17—H17B	109.5
H1B—C1—H1C	109.5	H17A—C17—H17B	109.5
O1—C1—H1D	109.5	O3—C17—H17C	109.5
H1B—C1—H1D	109.5	H17A—C17—H17C	109.5
H1C—C1—H1D	109.5	H17B—C17—H17C	109.5
O2—C2—H2A	109.5	O4—C18—H18A	109.5
O2—C2—H2B	109.5	O4—C18—H18B	109.5
H2A—C2—H2B	109.5	H18A—C18—H18B	109.5
O2—C2—H2C	109.5	O4—C18—H18C	109.5
H2A—C2—H2C	109.5	H18A—C18—H18C	109.5
H2B—C2—H2C	109.5	H18B—C18—H18C	109.5
O2—C3—C4	125.5 (3)	C20—C19—O4	125.7 (3)
O2—C3—C8	115.1 (3)	C20—C19—C24	120.1 (3)
C4—C3—C8	119.3 (3)	O4—C19—C24	114.2 (2)
C3—C4—C5	120.2 (3)	C19—C20—C21	120.7 (3)
C3—C4—H4A	119.9	C19—C20—H20A	119.7
C5—C4—H4A	119.9	C21—C20—H20A	119.7
C6—C5—C4	121.3 (3)	C22—C21—C20	118.6 (3)
C6—C5—H5A	119.4	C22—C21—C25	121.0 (3)

C4—C5—H5A	119.4	C20—C21—C25	120.4 (3)
C5—C6—C7	118.9 (3)	C23—C22—C21	121.0 (3)
C5—C6—C9	120.7 (3)	C23—C22—H22A	119.5
C7—C6—C9	120.4 (3)	C21—C22—H22A	119.5
C8—C7—C6	120.4 (3)	C22—C23—C24	120.5 (3)
C8—C7—H7A	119.8	C22—C23—H23A	119.8
C6—C7—H7A	119.8	C24—C23—H23A	119.8
C7—C8—O1	125.4 (3)	O3—C24—C23	125.7 (3)
C7—C8—C3	119.9 (3)	O3—C24—C19	115.3 (3)
O1—C8—C3	114.7 (3)	C23—C24—C19	119.0 (3)
N1—C9—C6	123.8 (3)	N2—C25—C21	123.4 (3)
N1—C9—H9A	118.1	N2—C25—H25A	118.3
C6—C9—H9A	118.1	C21—C25—H25A	118.3
C11—C10—C15	118.2 (3)	C27—C26—C31	118.3 (3)
C11—C10—N1	125.5 (3)	C27—C26—N2	118.1 (3)
C15—C10—N1	116.3 (3)	C31—C26—N2	123.6 (3)
C12—C11—C10	121.0 (3)	C28—C27—C26	120.8 (3)
C12—C11—H11A	119.5	C28—C27—H27A	119.6
C10—C11—H11A	119.5	C26—C27—H27A	119.6
C11—C12—C13	121.6 (3)	C27—C28—C29	121.0 (3)
C11—C12—H12A	119.2	C27—C28—H28A	119.5
C13—C12—H12A	119.2	C29—C28—H28A	119.5
C14—C13—C12	117.0 (3)	C30—C29—C28	117.6 (3)
C14—C13—C16	121.0 (3)	C30—C29—C32	121.9 (3)
C12—C13—C16	122.0 (3)	C28—C29—C32	120.5 (3)
C13—C14—C15	121.9 (3)	C29—C30—C31	122.5 (3)
C13—C14—H14A	119.0	C29—C30—H30A	118.8
C15—C14—H14A	119.0	C31—C30—H30A	118.8
C14—C15—C10	120.3 (3)	C30—C31—C26	119.9 (3)
C14—C15—H15A	119.9	C30—C31—H31A	120.1
C10—C15—H15A	119.9	C26—C31—H31A	120.1
C13—C16—H16A	109.5	C29—C32—H32A	109.5
C13—C16—H16B	109.5	C29—C32—H32B	109.5
H16A—C16—H16B	109.5	H32A—C32—H32B	109.5
C13—C16—H16C	109.5	C29—C32—H32C	109.5
H16A—C16—H16C	109.5	H32A—C32—H32C	109.5
H16B—C16—H16C	109.5	H32B—C32—H32C	109.5
C2—O2—C3—C4	−6.4 (4)	C18—O4—C19—C20	−1.6 (4)
C2—O2—C3—C8	173.8 (3)	C18—O4—C19—C24	178.6 (2)
O2—C3—C4—C5	179.1 (3)	O4—C19—C20—C21	−179.1 (3)
C8—C3—C4—C5	−1.1 (5)	C24—C19—C20—C21	0.6 (4)
C3—C4—C5—C6	0.3 (5)	C19—C20—C21—C22	0.9 (4)
C4—C5—C6—C7	0.4 (5)	C19—C20—C21—C25	−179.2 (3)
C4—C5—C6—C9	−178.4 (3)	C20—C21—C22—C23	−1.8 (5)
C5—C6—C7—C8	−0.1 (4)	C25—C21—C22—C23	178.3 (3)
C9—C6—C7—C8	178.6 (3)	C21—C22—C23—C24	1.1 (5)
C6—C7—C8—O1	−179.6 (3)	C17—O3—C24—C23	7.8 (4)
C6—C7—C8—C3	−0.8 (4)	C17—O3—C24—C19	−172.9 (3)
C1—O1—C8—C7	6.1 (4)	C22—C23—C24—O3	179.7 (3)

C1—O1—C8—C3	−172.8 (3)	C22—C23—C24—C19	0.4 (5)
O2—C3—C8—C7	−178.8 (2)	C20—C19—C24—O3	179.4 (2)
C4—C3—C8—C7	1.4 (4)	O4—C19—C24—O3	−0.8 (4)
O2—C3—C8—O1	0.2 (4)	C20—C19—C24—C23	−1.2 (4)
C4—C3—C8—O1	−179.6 (3)	O4—C19—C24—C23	178.5 (3)
C10—N1—C9—C6	−177.7 (2)	C26—N2—C25—C21	178.0 (2)
C5—C6—C9—N1	177.5 (3)	C22—C21—C25—N2	−178.5 (3)
C7—C6—C9—N1	−1.2 (5)	C20—C21—C25—N2	1.6 (4)
C9—N1—C10—C11	27.7 (4)	C25—N2—C26—C27	145.1 (3)
C9—N1—C10—C15	−154.0 (3)	C25—N2—C26—C31	−38.2 (4)
C15—C10—C11—C12	0.6 (4)	C31—C26—C27—C28	1.5 (4)
N1—C10—C11—C12	179.0 (3)	N2—C26—C27—C28	178.4 (3)
C10—C11—C12—C13	0.1 (5)	C26—C27—C28—C29	−1.1 (4)
C11—C12—C13—C14	0.0 (5)	C27—C28—C29—C30	0.5 (4)
C11—C12—C13—C16	−179.3 (3)	C27—C28—C29—C32	−179.2 (3)
C12—C13—C14—C15	−0.9 (5)	C28—C29—C30—C31	−0.2 (5)
C16—C13—C14—C15	178.4 (3)	C32—C29—C30—C31	179.4 (3)
C13—C14—C15—C10	1.7 (5)	C29—C30—C31—C26	0.6 (5)
C11—C10—C15—C14	−1.5 (4)	C27—C26—C31—C30	−1.2 (4)
N1—C10—C15—C14	−180.0 (3)	N2—C26—C31—C30	−177.9 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2A···O1^{i}	0.96	2.52	3.439 (4)	161
C17—H17A···O4^{ii}	0.96	2.51	3.459 (4)	169

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

Fig. 1

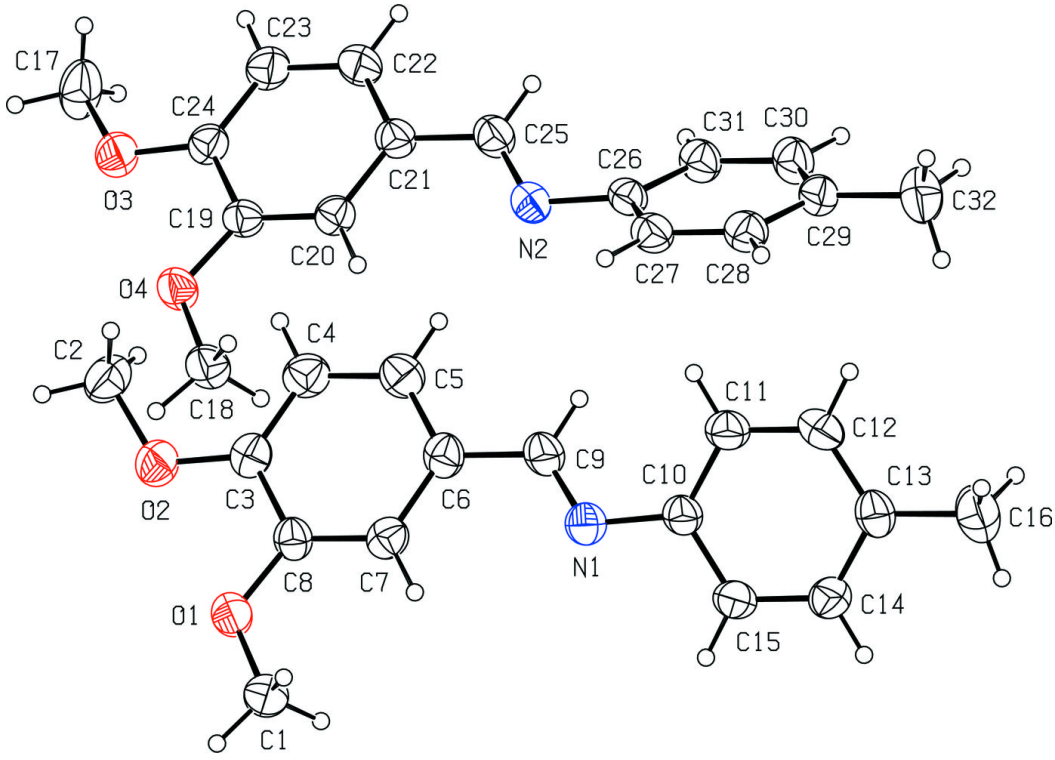

C17
C23
C22
C24
C25
C31
C30
C26
C21
O3
C19
N2
C32
C20
C29
C27
C28
O4
C4
C2
C5
C11
C18
C12
C9
C10
C13
O2
C3
C6
C16
N1
C8
C7
C14
O1
C15
C1

Fig. 2