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6,6′-Dimethoxy-2,2′-(2,2,4-trimethylimidazolidine-1,3-diyldimethylene)diphenol

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.055
wR factor = 0.138
Data-to-parameter ratio = 14.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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In the title compound, $C_{22}H_{30}N_2O_4$, the molecules are linked into a dimer by a pair of C—H$\cdots\pi$ hydrogen bonds. Neighbouring dimers are linked by C—H$\cdots$O and C—H$\cdots\pi$ hydrogen bonds into chains running parallel to the [011] and [$1\bar{1}0$] directions.

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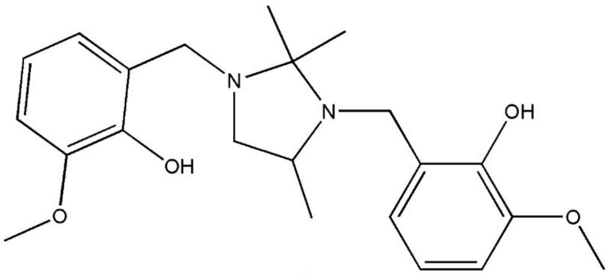
Comment

As part of our investigations of the crystal structures of *o*-vanillin diamine derivatives, we report here the crystal structure of the title compound, (I) (Fig. 1). The dihedral angle between the two benzene rings in the molecule is 65.27 (12)°.



(I)

The molecules of (I) are linked by a pair of C—H$\cdots\pi$ hydrogen bonds (Fig. 2). Atom C19 in the molecule at (x, y, z) acts as a hydrogen-bond donor, *via* H19, to the C8–C13 aryl ring of the molecule at ($1 - x$, $1 - y$, $1 - z$), generating a dimer. Neighbouring dimers are linked by pair of C—H$\cdots$O hydrogen bonds into a chain (Fig. 3 and Table 1). Atom C22 in the molecule at (x, y, z) acts as a hydrogen-bond donor, *via* H22*B*, to atom O4 in the molecule at ($1 - x$, $-y$, $2 - z$), generating a chain of $R_2^2(6)$ rings (Bernstein *et al.*, 1995)

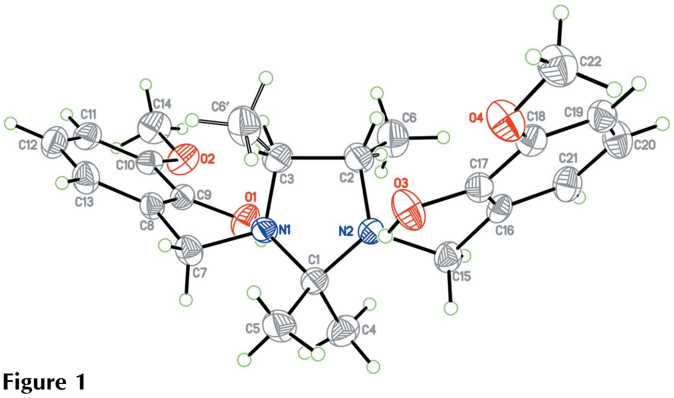


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Only one disorder component is shown.

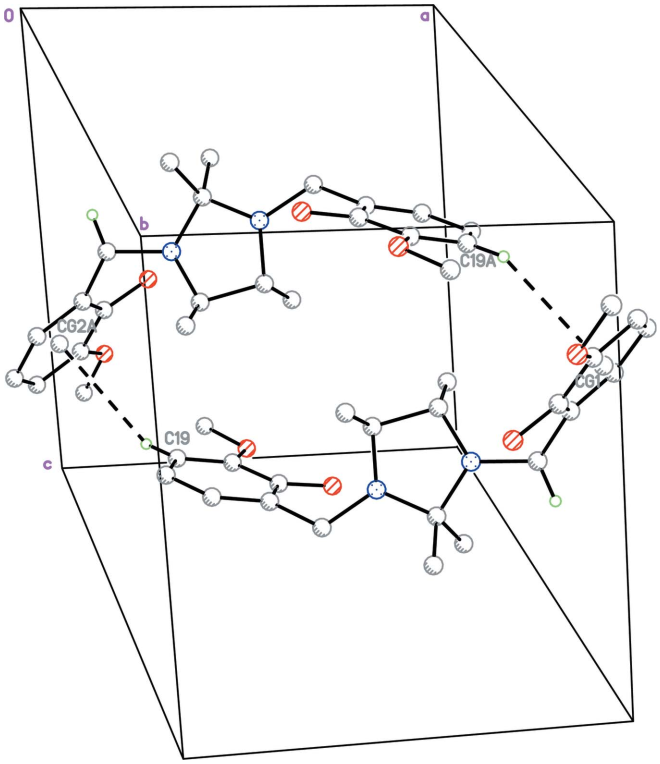


Figure 2
A portion of the crystal structure of (I), showing the formation of a hydrogen-bonded dimer built from C—H$\cdots\pi$ interactions (dashed lines). For clarity, H atoms not involved in hydrogen bonds have been omitted, and only one disorder component is shown. [Symmetry code: (A) $1-x$, $1-y$, $1-z$.]

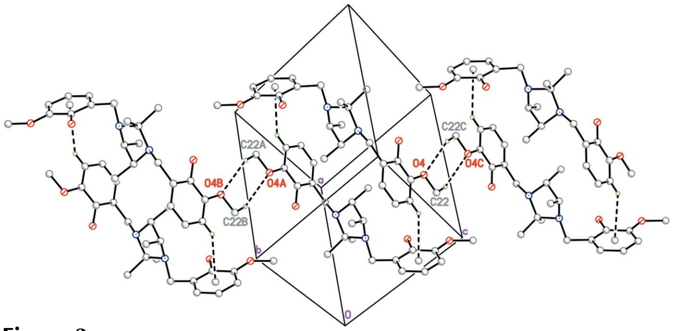


Figure 3
A portion of the crystal structure of (I), showing the formation of a hydrogen-bonded chain built from C—H$\cdots$O interactions (dashed lines). For clarity, H atoms not involved in hydrogen bonds have been omitted, and only one disorder component is shown. [Symmetry code: (A) $1-x$, $1-y$, $1-z$; (B) x, $1+y$, $-1+z$; (C) $1-x$, $-y$, $2-z$.]

running parallel to the [011] direction. In addition, atom C7 in the molecule at (x, y, z) acts as a hydrogen-bond donor, *via* H7*B*, to the C8–C13 aryl ring of the molecule at ($2-x$, $2-y$, $1-z$), forming a chain running parallel to the [$1\overline{1}0$] direction (Fig. 4). There are no significant intermolecular interactions between sheets formed from the [011] and [$1\overline{1}0$] chains.

Experimental

A solution of *N*,*N*′-bis(2-hydroxy-3-methoxybenzylene)propane-1,2-diamine (10 mmol) in methanol–acetone (1:1 *v*/*v*, 20 ml) and solid NaBH$_4$ (40 mmol) were mixed. The mixture was stirred overnight and then filtered. The filtrate was allowed to evaporate slowly, giving single crystals of (I).

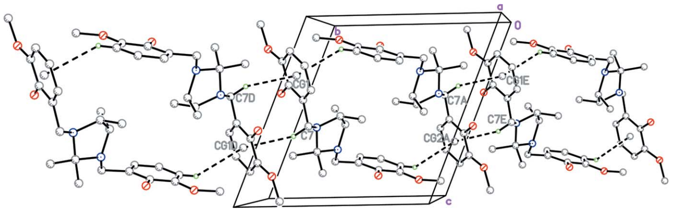


Figure 4
A portion of the crystal structure of (I), showing the formation of a hydrogen-bonded chain built from C—H$\cdots\pi$ interactions (dashed lines). For clarity, H atoms not involved in hydrogen bonds have been omitted, and only one disorder component is shown. [Symmetry code: (A) $1-x$, $1-y$, $1-z$; (D) $2-x$, $1-y$, 1 - z; (E) $-1+x$, $-1+y$, z.]

Crystal data

$C_{22}H_{30}N_2O_4$
$M_r = 386.48$
Triclinic, $P\overline{1}$
$a = 9.879$ (2) Å
$b = 10.443$ (2) Å
$c = 10.941$ (3) Å
$\alpha = 68.260$ (3)°
$\beta = 85.659$ (3)°
$\gamma = 84.541$ (4)°
$V = 1042.7$ (4) Å^3
$Z = 2$
$D_x = 1.231$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 298$ (2) K
Block, colourless
0.40 × 0.21 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.967$, $T_{\max} = 0.990$
5397 measured reflections
3598 independent reflections
1679 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.035$
$\theta_{\max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.138$
$S = 0.95$
3598 reflections
257 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.003$
$\Delta\rho_{\max} = 0.17$ e Å^{-3}
$\Delta\rho_{\min} = -0.18$ e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C22—H22$B\cdots$O4$^{\rm i}$	0.96	2.50	3.289 (4)	140

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

All H atoms were located in a difference Fourier map and then treated as riding atoms, with C—H = 0.93–0.97 and O—H = 0.82 Å, and with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(aryl and methylene C) and 1.5$U_{\rm eq}$(methyl C, and O). A methyl group is disordered over two positions, bonded to either C2 or C3. The coordinates of these two positions were refined with the occupancies tied to sum to unity. The site occupancies for C6 and attached H atoms and C6′ with attached H atoms refined to 0.701 (4) and 0.299 (4), respectively.

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Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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