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6,6′-Dimethoxy-2,2′-(propane-1,3-diyldiimino-dimethylene)diphenol

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In the title compound, $C_{19}H_{26}N_2O_4$, the molecules are linked into sheets *via* C—H···O, N—H···O and O—H···N hydrogen bonds. There are no significant intermolecular interactions between adjacent sheets.

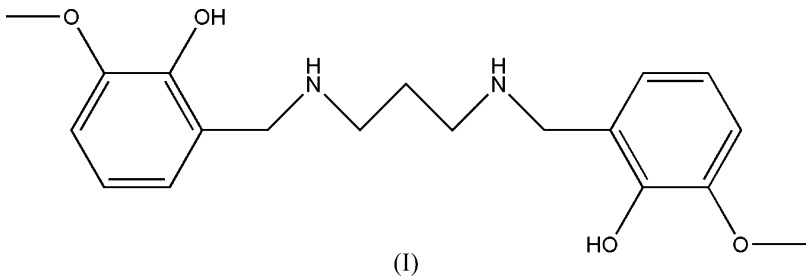
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.054
wR factor = 0.152
Data-to-parameter ratio = 14.2

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

Comment

As part of our ongoing research into the crystal structures of *o*-vanillin diamine derivatives, we have recently reported the crystal structure of 6,6′-dimethoxy-2,2′-(ethane-1,3-diyldiiminodimethylene)diphenol (Xia *et al.*, 2006). We report here a similar structure of 6,6′-dimethoxy-2,2′-(propane-1,3-diyldiiminodimethylene)diphenol, (I) (Fig. 1). In (I), the dihedral angle between the two benzene rings is 30.51 (10)°. The molecules are linked into chains through intermolecular N—H···O and O—H···N hydrogen bonds (Fig. 2 and Table 1), generating an $R_2^2(7)$ ring (Bernstein *et al.*, 1995). In addition, there is an $R_2^2(9)[R_1^2(5)R_2^2(12)R_6^6(40)]$ motif (García-Báez *et al.*, 2002) in the molecular chains, formed from intermolecular N—H···O, C—H···O and O—H···N hydrogen bonds. There are no direction-specific interactions between adjacent chains in the three-dimensional network structure.



(I)

Experimental

A solution of *N*,*N*′-bis(2-hydroxy-3-methoxybenzyl)propanediamine (10 mmol) in methanol–chloroform (1:2 *v*/*v*, 30 ml) and solid $NaBH_4$ (40 mmol) were mixed. The mixture was stirred at room temperature for 24 h and then filtered. The filtrate was allowed to evaporate slowly, giving single crystals of (I).

Crystal data

$C_{19}H_{26}N_2O_4$
M_r = 346.42
Triclinic, $P\overline{1}$
a = 9.278 (3) Å
b = 10.013 (4) Å
c = 10.816 (4) Å
α = 92.144 (4)°
β = 98.550 (4)°
γ = 109.215 (4)°
V = 934.2 (6) Å^3
Z = 2
D_x = 1.231 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
Block, colourless
0.23 × 0.21 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.980, T_{max} = 0.985

4873 measured reflections
3234 independent reflections
2033 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.152
S = 1.02
3234 reflections
228 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0655P)^2 + 0.3501P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O4^{i}	0.90	2.45	2.895 (3)	111
O3—H3···N1^{i}	0.82	1.90	2.674 (3)	157
N2—H2···O1^{ii}	0.90	1.83	2.721 (3)	170
N2—H2···O2^{ii}	0.90	2.65	2.951 (3)	101
C7—H7*B*···O3^{ii}	0.96	2.69	3.536 (4)	148
C19—H19*B*···O1^{i}	0.96	2.69	3.491 (4)	141

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

All H atoms were located in difference Fourier maps but were treated as riding atoms, with C—H distances of 0.93 Å (aryl), 0.96 Å (methyl), 0.97 Å (methylene), O—H distances of 0.82 Å and N—H distances of 0.90 Å (amino), and with U_{iso}(H) = 1.2(C,N) (aryl, methylene, amino) or 1.5U_{eq}(C,O) (methyl or hydroxy).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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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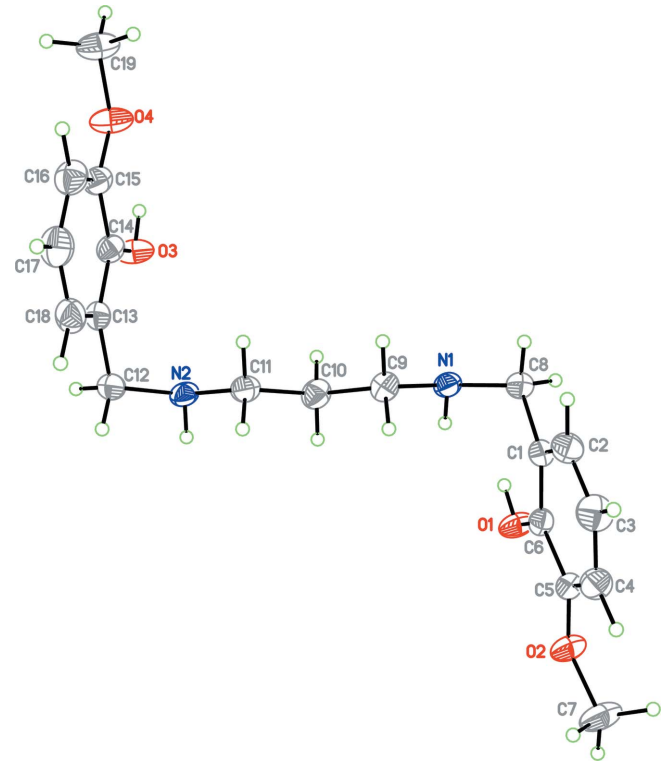

Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

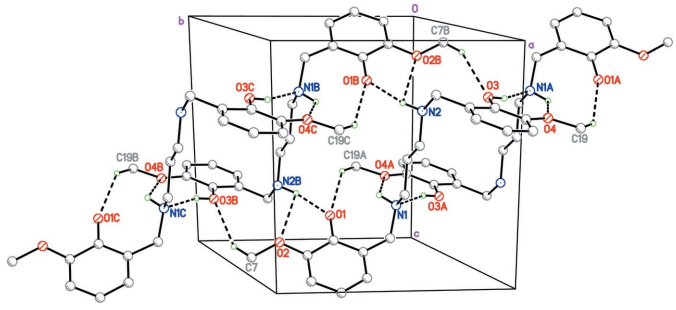

Figure 2
A portion of the crystal structure of (I), showing the formation of a hydrogen-bonded chain built from C—H···O, N—H···O and O—H···N interactions. For clarity, H atoms not involved in hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [Symmetry codes: (A) $1-x, -y, 1-z$; (B) $1-x, 1-y, 1-z$; (C) $x, 1+y, z$.]