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N′-(2,3-Dimethoxybenzylidene)-2-hydroxy-3-methylbenzohydrazide

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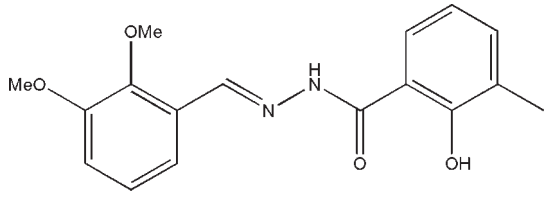
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.067; wR factor = 0.175; data-to-parameter ratio = 16.4.

In the title compound, $C_{17}H_{18}N_2O_4$, the dihedral angle between the two benzene rings is 6.0 (2)° and the molecule adopts an *E* configuration with respect to the C=N bond. There is an intramolecular O—H···O hydrogen bond in the molecule, which generates an *S*(6) ring. In the crystal, molecules are linked through intermolecular N—H···O hydrogen bonds, forming *C*(4) chains running along the *c* axis.

Related literature

For a related structure and background information, see: Han & Zhao (2010). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{17}H_{18}N_2O_4$ M_r = 314.33
Orthorhombic, *Pccn*
a = 14.923 (3) Å
b = 24.329 (5) Å
c = 8.7422 (17) Å
V = 3174.0 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 K
0.17 × 0.15 × 0.15 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.984, T_{max} = 0.986
17128 measured reflections
3461 independent reflections
1998 reflections with $I > 2\sigma(I)$
R_{int} = 0.223

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.175
S = 0.92
3461 reflections
211 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O3	0.82	1.91	2.630 (2)	146
N2—H2A···O3^{i}	0.90	2.17	3.030 (2)	158

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5386).

References

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Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Han, Y.-Y. & Zhao, Q.-R. (2010). Acta Cryst. E66, o1025.
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supporting information

Acta Cryst. (2010). E**66**, o1026 [https://doi.org/10.1107/S1600536810012122]

N′-(2,3-Dimethoxybenzylidene)-2-hydroxy-3-methylbenzohydrazide

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S1. Comment

As part of our ongoing studies of hydrazones (Han & Zhao, 2010), we now report the structure of the title compound, (I).

In the molecule of the title compound, Fig. 1, the dihedral angle between the two benzene rings is 6.0 (2)°. The molecule adopts an *E* configuration with respect to the C═N bond. There is an intramolecular O–H···O hydrogen bond (Table 1) in the molecule. All the bond lengths are within normal ranges (Allen *et al.*, 1987).

In the crystal structure, molecules are linked through intermolecular N–H···O hydrogen bonds (Table 1) to form chains running along the *c* axis (Fig. 2).

S2. Experimental

A mixture of 2,3-dimethoxybenzaldehyde (0.166 g, 1 mmol) and 2-hydroxy-3-methylbenzohydrazide (0.166 g, 1 mmol) in 50 ml me thanol was stirred at room temperature for 1 h. The mixture was filtered to remove impurities, and then left at room temperature. After a few days, colourless blocks of (I) were formed.

S3. Refinement

H atoms were positioned geometrically and refined using the riding-model approximation, with C–H = 0.93 or 0.96 Å, O–H = 0.82 Å, N–H = 0.90 Å, and U_{iso}(H) = 1.2U_{eq}(C,*N*) or U_{iso}(H) = 1.5U_{eq}(methyl C and O).

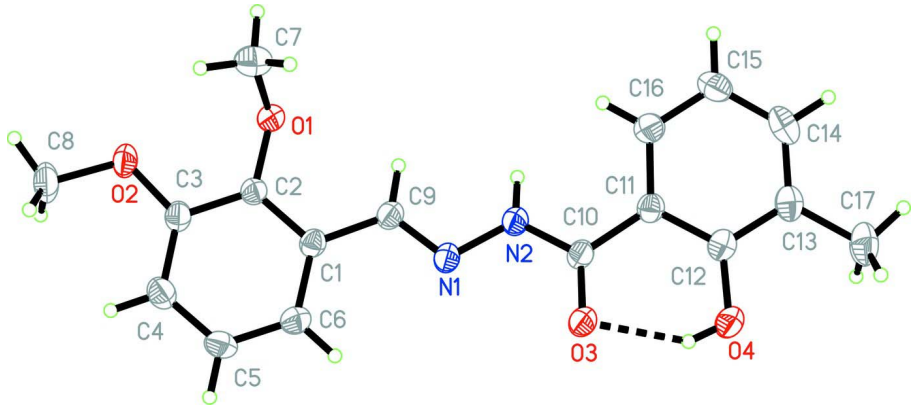

Figure 1

The molecular structure of (I) with 30% probability displacement ellipsoids for non-H atoms. Intramolecular O–H···O hydrogen bond is shown as a dashed line.

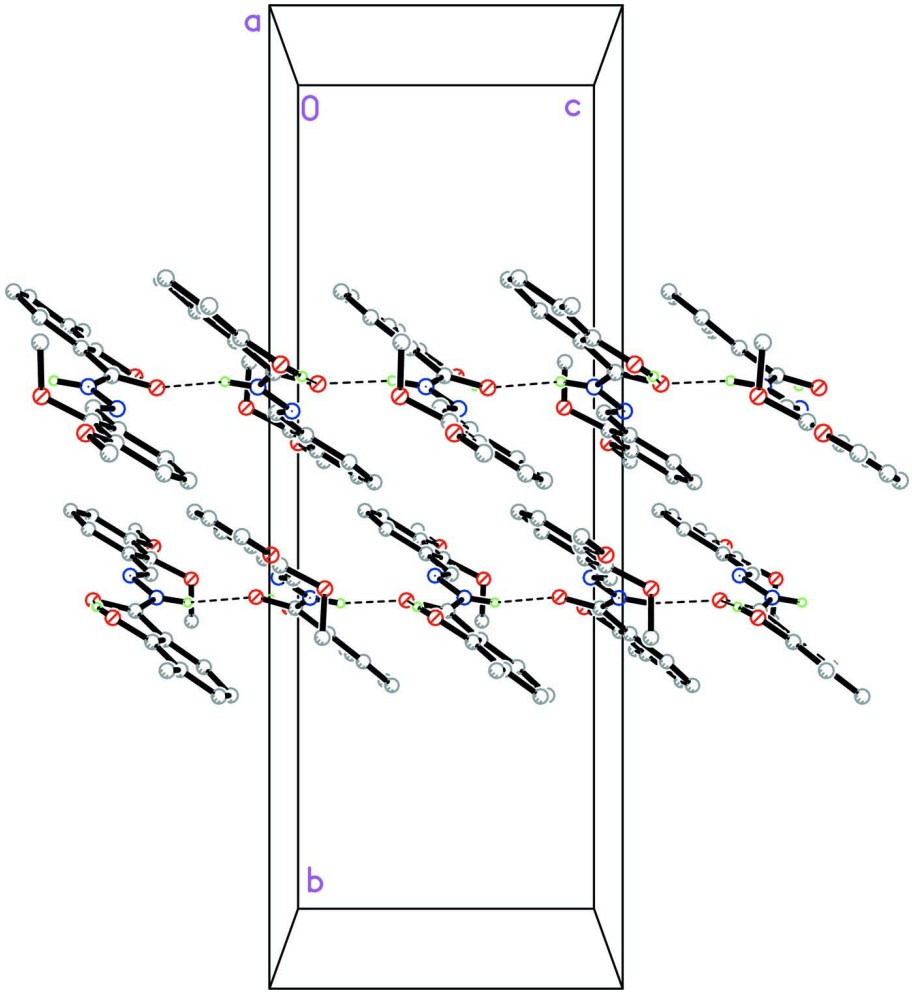

Figure 2

The molecular packing of the title compound, viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

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Crystal data

$C_{17}H_{18}N_2O_4$
$M_r = 314.33$
Orthorhombic, *Pccn*
Hall symbol: -P 2ab 2ac
$a = 14.923\ (3)$ Å
$b = 24.329\ (5)$ Å
$c = 8.7422\ (17)$ Å
$V = 3174.0\ (11)$ Å^3
$Z = 8$
$F(000) = 1328$
$D_x = 1.316$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2994 reflections
$\theta = 2.7–24.9°$
$\mu = 0.10$ mm^{-1}
$T = 298$ K
Block, colorless
0.17 × 0.15 × 0.15 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.984$, $T_{max} = 0.986$
17128 measured reflections
3461 independent reflections

1998 reflections with $I > 2\sigma(I)$
$R_{int} = 0.223$
$\theta_{max} = 27.0°$, $\theta_{min} = 1.6°$

$h = -18 \rightarrow 18$
$k = -30 \rightarrow 31$
$l = -8 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.067$
$wR(F^2) = 0.175$
$S = 0.92$
3461 reflections
211 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0754P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.42606 (9)	0.10101 (6)	0.37153 (16)	0.0482 (4)
O2	0.28300 (9)	0.06224 (8)	0.52262 (16)	0.0602 (5)
O3	0.84543 (10)	0.11847 (7)	0.62612 (16)	0.0586 (5)
O4	1.01095 (9)	0.13449 (7)	0.53290 (16)	0.0601 (5)
H4	0.9716	0.1232	0.5903	0.072*
N1	0.67827 (11)	0.09279 (7)	0.53655 (18)	0.0464 (5)
N2	0.74005 (11)	0.11742 (7)	0.44045 (19)	0.0474 (5)
H2A	0.7274	0.1235	0.3411	0.057*
C1	0.52468 (13)	0.06866 (8)	0.5673 (2)	0.0402 (5)
C2	0.43791 (13)	0.07538 (9)	0.5098 (2)	0.0396 (5)
C3	0.36482 (13)	0.05310 (9)	0.5889 (2)	0.0443 (5)
C4	0.37887 (16)	0.02333 (10)	0.7208 (2)	0.0521 (6)
H4A	0.3306	0.0079	0.7727	0.063*
C5	0.46507 (16)	0.01651 (10)	0.7758 (2)	0.0536 (6)
H5	0.4743	−0.0036	0.8649	0.064*
C6	0.53705 (15)	0.03885 (9)	0.7014 (2)	0.0473 (5)
H6	0.5945	0.0341	0.7406	0.057*
C7	0.38589 (19)	0.15360 (11)	0.3766 (3)	0.0724 (8)
H7A	0.3336	0.1523	0.4405	0.109*
H7B	0.3690	0.1646	0.2751	0.109*
H7C	0.4278	0.1797	0.4178	0.109*
C8	0.20603 (16)	0.04196 (12)	0.6008 (3)	0.0701 (8)

H8A	0.2071	0.0025	0.6009	0.105*
H8B	0.1529	0.0546	0.5500	0.105*
H8C	0.2063	0.0551	0.7043	0.105*
C9	0.59903 (13)	0.09237 (9)	0.4826 (2)	0.0445 (5)
H9	0.5885	0.1076	0.3867	0.053*
C10	0.82117 (13)	0.13106 (9)	0.4951 (2)	0.0428 (5)
C11	0.88015 (14)	0.16270 (8)	0.3910 (2)	0.0421 (5)
C12	0.97309 (14)	0.16251 (8)	0.4165 (2)	0.0456 (5)
C13	1.03102 (15)	0.19180 (10)	0.3209 (3)	0.0532 (6)
C14	0.99399 (18)	0.22279 (10)	0.2061 (3)	0.0650 (7)
H14	1.0318	0.2430	0.1429	0.078*
C15	0.90212 (19)	0.22521 (11)	0.1802 (3)	0.0671 (7)
H15	0.8789	0.2469	0.1021	0.081*
C16	0.84659 (15)	0.19497 (9)	0.2724 (2)	0.0538 (6)
H16	0.7851	0.1960	0.2554	0.065*
C17	1.13038 (15)	0.18931 (13)	0.3465 (3)	0.0768 (8)
H17A	1.1502	0.1519	0.3392	0.115*
H17B	1.1442	0.2034	0.4464	0.115*
H17C	1.1603	0.2111	0.2705	0.115*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0396 (8)	0.0589 (10)	0.0462 (9)	0.0034 (7)	−0.0010 (6)	0.0099 (7)
O2	0.0318 (8)	0.0918 (13)	0.0569 (10)	−0.0080 (8)	0.0014 (7)	0.0109 (8)
O3	0.0378 (8)	0.0921 (13)	0.0459 (9)	−0.0056 (8)	−0.0042 (7)	0.0152 (8)
O4	0.0370 (9)	0.0835 (12)	0.0597 (10)	0.0003 (8)	−0.0035 (7)	0.0124 (8)
N1	0.0348 (10)	0.0580 (12)	0.0463 (10)	−0.0030 (8)	−0.0004 (8)	0.0027 (8)
N2	0.0375 (10)	0.0623 (12)	0.0422 (10)	−0.0061 (9)	−0.0030 (8)	0.0055 (8)
C1	0.0371 (11)	0.0444 (12)	0.0390 (11)	−0.0017 (9)	−0.0027 (9)	−0.0038 (9)
C2	0.0373 (11)	0.0444 (11)	0.0372 (11)	−0.0011 (9)	−0.0012 (9)	0.0006 (9)
C3	0.0377 (12)	0.0543 (13)	0.0409 (11)	−0.0030 (10)	0.0018 (9)	−0.0034 (10)
C4	0.0520 (14)	0.0595 (15)	0.0448 (12)	−0.0075 (11)	0.0059 (11)	0.0020 (10)
C5	0.0616 (15)	0.0590 (14)	0.0403 (12)	0.0016 (12)	−0.0011 (11)	0.0102 (10)
C6	0.0470 (13)	0.0505 (13)	0.0445 (12)	0.0015 (10)	−0.0070 (10)	0.0015 (10)
C7	0.0754 (19)	0.0632 (18)	0.0787 (17)	0.0105 (14)	−0.0018 (15)	0.0187 (14)
C8	0.0411 (14)	0.102 (2)	0.0677 (16)	−0.0099 (13)	0.0149 (11)	−0.0004 (14)
C9	0.0368 (12)	0.0531 (13)	0.0436 (12)	0.0003 (9)	−0.0030 (9)	0.0007 (10)
C10	0.0348 (11)	0.0501 (12)	0.0437 (12)	0.0008 (10)	−0.0017 (9)	−0.0012 (9)
C11	0.0410 (12)	0.0432 (12)	0.0422 (11)	−0.0039 (9)	−0.0031 (9)	−0.0042 (9)
C12	0.0440 (13)	0.0456 (12)	0.0472 (12)	−0.0001 (10)	−0.0006 (10)	−0.0079 (10)
C13	0.0461 (13)	0.0532 (14)	0.0602 (14)	−0.0050 (11)	0.0092 (11)	−0.0077 (11)
C14	0.0723 (18)	0.0547 (15)	0.0680 (16)	−0.0191 (13)	0.0149 (14)	0.0024 (12)
C15	0.0768 (19)	0.0569 (16)	0.0678 (16)	−0.0098 (13)	−0.0064 (14)	0.0206 (12)
C16	0.0519 (13)	0.0512 (14)	0.0584 (14)	−0.0029 (11)	−0.0090 (11)	0.0061 (11)
C17	0.0450 (15)	0.087 (2)	0.098 (2)	−0.0091 (14)	0.0176 (14)	−0.0022 (16)

Geometric parameters (Å, º)

O1—C2	1.372 (2)	C7—H7A	0.9600
O1—C7	1.414 (3)	C7—H7B	0.9600
O2—C3	1.370 (2)	C7—H7C	0.9600
O2—C8	1.425 (3)	C8—H8A	0.9600
O3—C10	1.240 (2)	C8—H8B	0.9600
O4—C12	1.349 (2)	C8—H8C	0.9600
O4—H4	0.8195	C9—H9	0.9300
N1—C9	1.273 (3)	C10—C11	1.482 (3)
N1—N2	1.384 (2)	C11—C16	1.394 (3)
N2—C10	1.343 (2)	C11—C12	1.405 (3)
N2—H2A	0.9005	C12—C13	1.398 (3)
C1—C6	1.391 (3)	C13—C14	1.372 (3)
C1—C2	1.398 (3)	C13—C17	1.501 (3)
C1—C9	1.453 (3)	C14—C15	1.391 (4)
C2—C3	1.401 (3)	C14—H14	0.9300
C3—C4	1.378 (3)	C15—C16	1.370 (3)
C4—C5	1.383 (3)	C15—H15	0.9300
C4—H4A	0.9300	C16—H16	0.9300
C5—C6	1.368 (3)	C17—H17A	0.9600
C5—H5	0.9300	C17—H17B	0.9600
C6—H6	0.9300	C17—H17C	0.9600
C2—O1—C7	115.99 (16)	O2—C8—H8C	109.5
C3—O2—C8	117.34 (18)	H8A—C8—H8C	109.5
C12—O4—H4	109.3	H8B—C8—H8C	109.5
C9—N1—N2	113.41 (17)	N1—C9—C1	121.57 (19)
C10—N2—N1	119.45 (17)	N1—C9—H9	119.2
C10—N2—H2A	119.4	C1—C9—H9	119.2
N1—N2—H2A	121.1	O3—C10—N2	122.05 (19)
C6—C1—C2	119.12 (18)	O3—C10—C11	121.49 (18)
C6—C1—C9	122.34 (18)	N2—C10—C11	116.46 (17)
C2—C1—C9	118.53 (18)	C16—C11—C12	118.3 (2)
O1—C2—C1	119.28 (17)	C16—C11—C10	122.42 (19)
O1—C2—C3	120.71 (17)	C12—C11—C10	119.17 (18)
C1—C2—C3	119.90 (18)	O4—C12—C13	116.7 (2)
O2—C3—C4	125.12 (18)	O4—C12—C11	122.34 (19)
O2—C3—C2	114.99 (18)	C13—C12—C11	120.9 (2)
C4—C3—C2	119.87 (19)	C14—C13—C12	117.9 (2)
C3—C4—C5	119.7 (2)	C14—C13—C17	122.0 (2)
C3—C4—H4A	120.2	C12—C13—C17	120.1 (2)
C5—C4—H4A	120.2	C13—C14—C15	122.6 (2)
C6—C5—C4	121.1 (2)	C13—C14—H14	118.7
C6—C5—H5	119.4	C15—C14—H14	118.7
C4—C5—H5	119.4	C16—C15—C14	118.6 (2)
C5—C6—C1	120.25 (19)	C16—C15—H15	120.7
C5—C6—H6	119.9	C14—C15—H15	120.7

C1—C6—H6	119.9	C15—C16—C11	121.5 (2)
O1—C7—H7A	109.5	C15—C16—H16	119.2
O1—C7—H7B	109.5	C11—C16—H16	119.2
H7A—C7—H7B	109.5	C13—C17—H17A	109.5
O1—C7—H7C	109.5	C13—C17—H17B	109.5
H7A—C7—H7C	109.5	H17A—C17—H17B	109.5
H7B—C7—H7C	109.5	C13—C17—H17C	109.5
O2—C8—H8A	109.5	H17A—C17—H17C	109.5
O2—C8—H8B	109.5	H17B—C17—H17C	109.5
H8A—C8—H8B	109.5		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O3	0.82	1.91	2.630 (2)	146
N2—H2*A*···O3^{i}	0.90	2.17	3.030 (2)	158

Symmetry code: (i) −*x*+3/2, *y*, *z*−1/2.