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(*E*)-2-Hydroxy-*N*′-(2-naphthylmethylene)-benzohydrazide

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The title compound, $C_{18}H_{14}N_2O_2$, is approximately planar and displays a *trans* configuration with respect to the C=N double bond. In the crystal structure, the molecules are linked through weak intermolecular O—H···O hydrogen bonds, forming a network structure.

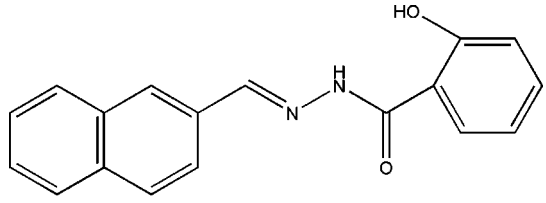
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.126
Data-to-parameter ratio = 12.0

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

Comment

Recently, we have reported a number of Schiff base complexes (Qiu, Yang *et al.*, 2006; Qiu, Ma *et al.*, 2006). As an extension of our work on the structural characterization of these compounds, the title compound, (I), is reported here (Fig. 1).



(I)

In the title compound, all bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The C8=N1 bond length of 1.277 (3) Å conforms to the value for a double bond. The dihedral angle between the benzene ring and naphthalene ring system is 8.8 (2)°.

In the crystal structure, the molecules are linked through weak intermolecular O—H···O hydrogen bonds, forming a network structure, and there is also an intramolecular N—H···O hydrogen bond (Table 1 and Fig. 2).

Experimental

The reagents were commercial products and were used without further purification. 2-Naphthaldehyde (0.1 mmol, 15.6 mg) and 2-hydroxybenzohydrazide (0.1 mmol, 15.2 mg) were dissolved in ethanol (10 ml). The reaction mixture was stirred for 10 min to give a clear yellow solution. After allowing this solution to stand at room temperature in air for 12 d, large yellow crystals were formed at the bottom of the vessel on slow evaporation of the solvent. The crystals were isolated, washed three times with ethanol and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 63%).

Crystal data

$C_{18}H_{14}N_2O_2$
M_r = 290.31
Monoclinic, $P2_1/n$
a = 4.7771 (10) Å
b = 26.881 (5) Å
c = 11.242 (2) Å
β = 100.72 (3)°
V = 1418.5 (5) Å^3
Z = 4
D_x = 1.359 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
Block, yellow
0.34 × 0.18 × 0.06 mm

Data collection

Bruker SMART APEX area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.978, T_{max} = 0.993
8509 measured reflections
2437 independent reflections
1146 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.127
S = 0.85
2437 reflections
203 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0713P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1	0.86	1.94	2.631 (2)	137
O1—H1···O2^{i}	0.94 (3)	1.75 (3)	2.656 (2)	160 (2)

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

Atom H1, attached to O1, was located in a difference Fourier map and refined isotropically, with the U_{iso}(H) value fixed at 0.08 Å^2. All remaining H atoms were placed in geometrically idealized positions (C—H = 0.93 Å and N—H = 0.86 Å) and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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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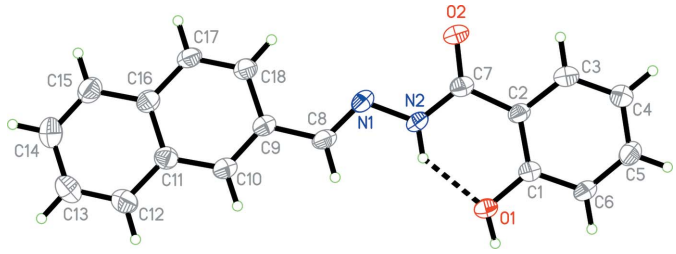

Figure 1
The structure of (I) showing 30% probability displacement ellipsoids and the atom-numbering scheme. The dashed line indicates the intramolecular hydrogen bond.

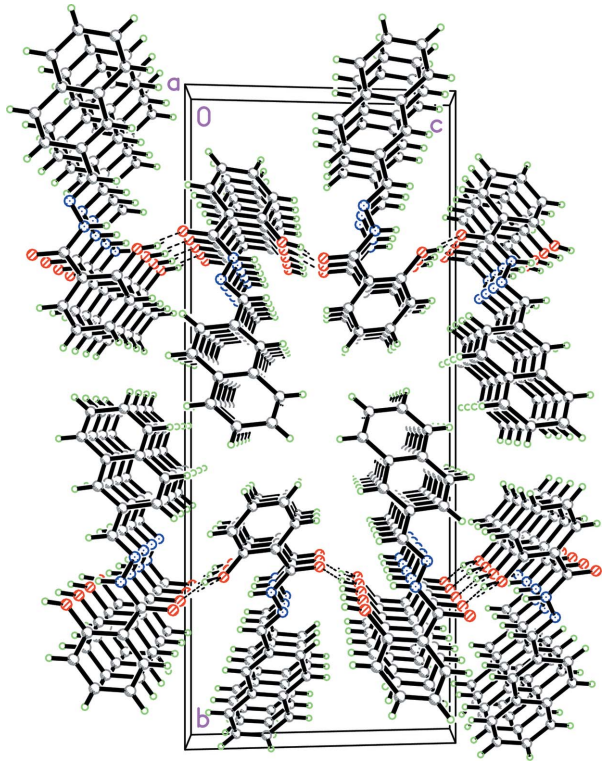

Figure 2
The crystal packing of (I), viewed along the *a* axis. Dashed lines show intermolecular hydrogen bonds.