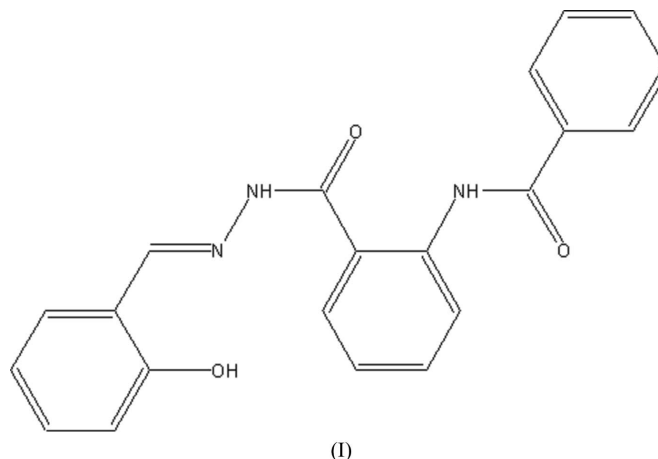


***N*-[2-[[*(2E)*-2-(2-Hydroxybenzylidene)-hydrazino]carbonyl]phenyl]benzamide**Shashidhar,^a Deepak Chopra,^b
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ssctng@sscu.iisc.ernet.in**Key indicators**Single-crystal X-ray study
T = 290 K
Mean $\sigma(\text{C}-\text{C}) = 0.008 \text{ \AA}$
R factor = 0.098
wR factor = 0.157
Data-to-parameter ratio = 10.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $\text{C}_{21}\text{H}_{17}\text{N}_3\text{O}_3$ exhibits antifungal and antibacterial properties. The crystal structure is stabilized by a co-operative interplay of both intra- and intermolecular strong and weak hydrogen bonds of types $\text{O}-\text{H}\cdots\text{N}$, $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}/\text{N}$.

Received 1 September 2006
Accepted 7 September 2006**Comment**

Crystal engineering *via* manipulation of hydrogen bonding has attracted much interest in recent years (Aakeröy, 1997; Desiraju, 2000). Fig. 1 shows the molecular structure of the title compound, (I). Relevant bond lengths and torsion angles are given in Table 1. A related compound exhibits antifungal and antibacterial properties (Gudasi *et al.*, 2005).



The bond lengths involving atoms N1, N2 and N3 are different, indicating that the environments around the N atoms are different because of electronic effects. The molecular conformation is stabilized by intramolecular hydrogen bonds (Table 2) of the types $\text{O}-\text{H}\cdots\text{N}$ [Etter symbol *S*(6)], $\text{N}-\text{H}\cdots\text{O}$ [Etter symbol *S*(6)], two $\text{C}-\text{H}\cdots\text{O}$ interactions involving H17 and H11 [Etter symbols *S*(5) and *S*(6)], and a $\text{C}-\text{H}\cdots\text{N}$ interaction [Etter symbol *S*(5)], which eliminates conformational flexibility and results in near-planarity. In addition, an intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bond involving H3N [Etter symbol *R*22 (16)] forms molecular dimers; these dimers are held together by $\text{C}-\text{H}\cdots\text{O}$ interactions, forming molecular chains along the *b* axis [Etter symbol *C*(8)].

Experimental

Compound (I) was prepared by condensation of *N*-[2-(hydrazinocarbonyl)phenyl]benzamide (0.1 mol, 12.1 g) and salicylaldehyde (0.1 mol, 12.2 g) in ethanol (50 ml). The resulting mixture

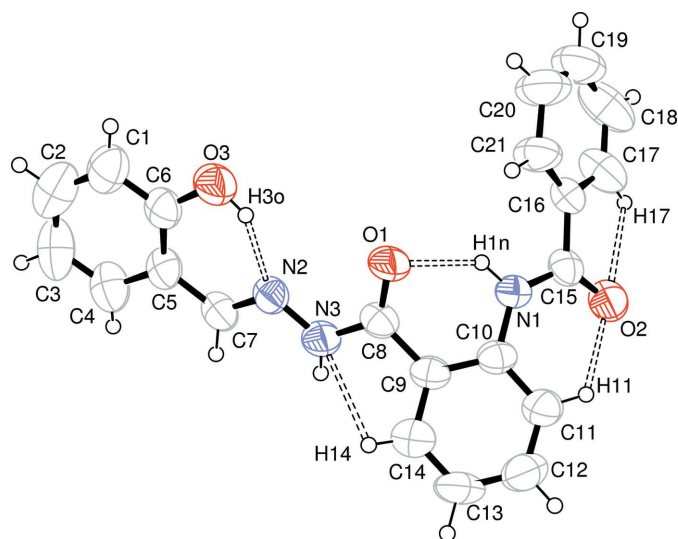


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.

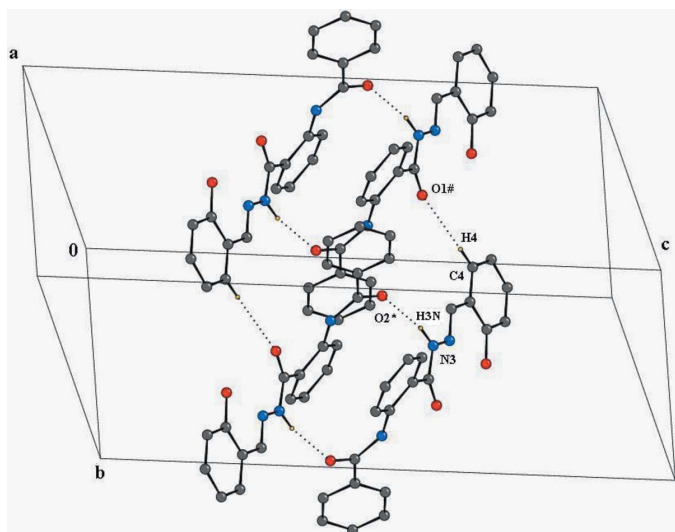


Figure 2
N—H...O-generated molecular dimers and C—H...O-generated molecular chains. Dashed lines indicate hydrogen bonds. The symbols * and # represent the symmetry codes $(1 - x, -y, 1 - z)$ and $(x, y - 1, z)$, respectively.

was refluxed in a water bath for 5–6 h in the presence of a few drops of acetic acid. On partial removal of the solvent and upon cooling, compound (I) was separated and filtered off, washed and recrystallized from ethanol to obtain good quality crystals (yield 96%). Their purity was confirmed by thin-layer chromatography.

Crystal data

$C_{21}H_{17}N_3O_3$ $Z = 8$
 $M_r = 359.38$ $D_x = 1.300 \text{ Mg m}^{-3}$
 Monoclinic, $C2/c$ $Mo \text{ K}\alpha$ radiation
 $a = 21.226(4) \text{ \AA}$ $\mu = 0.09 \text{ mm}^{-1}$
 $b = 8.362(2) \text{ \AA}$ $T = 290(2) \text{ K}$
 $c = 22.497(4) \text{ \AA}$ Block, colourless
 $\beta = 113.085(4)^\circ$ $0.30 \times 0.25 \times 0.20 \text{ mm}$
 $V = 3673.1(12) \text{ \AA}^3$

Data collection

Bruker SMART APEX CCD 12677 measured reflections
 diffractometer 3185 independent reflections
 φ and ω scans 1832 reflections with $I > 2\sigma(I)$
 Absorption correction: multi-scan $R_{int} = 0.068$
 (SADABS; Sheldrick, 1996) $\theta_{max} = 25.0^\circ$
 $T_{min} = 0.933, T_{max} = 0.982$

Refinement

Refinement on F^2 $w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 0.2154P]$
 $R[F^2 > 2\sigma(F^2)] = 0.098$ where $P = (F_o^2 + 2F_c^2)/3$
 $wR(F^2) = 0.157$ $(\Delta/\sigma)_{max} < 0.001$
 $S = 1.21$ $\Delta\rho_{max} = 0.14 \text{ e \AA}^{-3}$
 3185 reflections $\Delta\rho_{min} = -0.15 \text{ e \AA}^{-3}$
 312 parameters
 All H-atom parameters refined

Table 1

Selected geometric parameters ($\text{\AA}, ^\circ$).

O3—C6	1.354 (5)	C10—N1	1.400 (4)
N2—C7	1.281 (4)	C15—N1	1.344 (4)
N2—N3	1.371 (4)	C8—N3	1.353 (4)
O1—C8	1.229 (4)		
C10—C9—C8—N3	145.5 (3)	C16—C15—N1—C10	−179.5 (3)
C7—N2—N3—C8	174.6 (3)	N3—N2—C7—C5	177.1 (3)
N1—C15—C16—C21	26.1 (5)	N2—C7—C5—C6	−1.1 (6)

Table 2

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3O...N2	0.88 (7)	1.81 (7)	2.601 (6)	150 (5)
N1—H1N...O1	0.92 (4)	1.97 (4)	2.728 (5)	139 (3)
N3—H3N...O2 ⁱ	0.89 (5)	1.99 (5)	2.857 (5)	165 (4)
C4—H4...O1 ⁱⁱ	0.95 (5)	2.49 (4)	3.317 (6)	146 (3)
C11—H11...O2	0.96 (4)	2.27 (3)	2.913 (5)	124 (3)
C14—H14...N3	0.93 (3)	2.55 (4)	2.858 (7)	100 (3)
C17—H17...O2	0.98 (5)	2.41 (4)	2.812 (7)	104 (3)

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

All H atoms were located in difference Fourier maps and refined isotropically. The O—H, N—H and C—H bond lengths are 0.88 (7), 0.89 (5)–0.92 (4) and 0.91 (3)–1.01 (3) \AA , respectively.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SIR92 (Altomare *et al.*, 1993); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and CAMERON (Watkin *et al.*, 1993); software used to prepare material for publication: PLATON (Spek, 2003).

The authors thank the Department of Science and Technology, Government of India, for data collection on the CCD facility set up under the IRHPA–DST programme. DC thanks the CSIR, Government of India, for a senior research fellowship.

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