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# 3-Hydroxysalicylaldehyde benzoylhydrazone

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**Key indicators**

Single-crystal X-ray study
$T$ = 295 K
Mean $\sigma$(C–C) = 0.003 Å
$R$ factor = 0.040
$wR$ factor = 0.124
Data-to-parameter ratio = 15.5

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

The molecules of the title compound, $C_{14}H_{12}N_2O_3$, are linked *via* hydrogen bonds into a chain running along the shortest axis of the orthorhombic cell.

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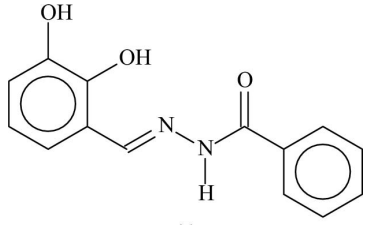
## Comment

The planar conformation of the salicylaldehyde–benzoylhydrazone class of Schiff bases originates from water molecules that stabilize the structures (Huo *et al.*, 2004).




(I)

3-Hydroxysalicylaldehyde benzoylhydrazone, (I) (Fig. 1), possesses a 3-hydroxy substituent that is capable of stabilization, but the compound does not contain water. This substituent engages in intramolecular and also intermolecular hydrogen-bonding interactions. Meanwhile, the amido H atom forms a short hydrogen bond with the amido O atom of an adjacent molecule to give rise to a linear chain running along the shortest axis of the orthorhombic unit cell. Adjacent chains are linked through the 3-hydroxy unit (Table 1). The hydroxy-substituted aromatic system is twisted by 8.3 (1) Å with respect to the planar —N═N—C(═O)— fragment, whereas the other aromatic ring is twisted by 23.5 (1)°.

## t>Experimental

3-Hydroxysalicyldehyde (0.22 g, 1.59 mmol) and benzoylhydrazide (0.21 g, 1.54 mmol) were heated in ethanol. The solvent was removed and the solid compound recrystallized from ethanol to furnish yellow prisms.

*Crystal data*

$C_{14}H_{12}N_2O_3$
$M_r$ = 256.26
Orthorhombic, *Pbca*
$a$ = 10.6030 (6) Å
$b$ = 9.7780 (6) Å
$c$ = 25.203 (2) Å
$V$ = 2612.9 (3) Å$^3$
$Z$ = 8
$D_x$ = 1.303 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 3480 reflections
$\theta$ = 2.5–23.8°
$\mu$ = 0.09 mm$^{-1}$
$T$ = 295 (2) K
Prism, yellow
0.39 × 0.31 × 0.20 mm

*Data collection*

Bruker SMART area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: none
14751 measured reflections
2855 independent reflections
1651 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 27.0^{\circ}$
$h = -13 \rightarrow 13$
$k = -12 \rightarrow 12$
$l = -32 \rightarrow 19$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.124$
$S = 0.99$
2855 reflections
184 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0597P)^2 + 0.3349P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.14$ e Å$^{-3}$
$\Delta\rho_{min} = -0.15$ e Å$^{-3}$

**Table 1**
Hydrogen-bonding geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1*o*···O2 | 0.86 (1) | 2.25 (3) | 2.706 (2) | 113 (2) |
| O1—H1*o*···O2$^{i}$ | 0.86 (1) | 2.14 (2) | 2.874 (2) | 144 (3) |
| O2—H2*o*···N1 | 0.86 (1) | 1.77 (1) | 2.564 (2) | 153 (2) |
| N2—H2*n*···O3$^{ii}$ | 0.86 (1) | 1.94 (1) | 2.783 (2) | 165 (2) |

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

The carbon-bound H atoms were positioned geometrically (C—H = 0.93 Å) and were included in the refinement in the riding-model approximation, with $U_{iso}$(H) values set at $1.2U_{eq}$ of the parent atoms. The hydroxy and amino H atoms were refined with a distance restraint of 0.85 (1) Å; their displacement parameters were also refined.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

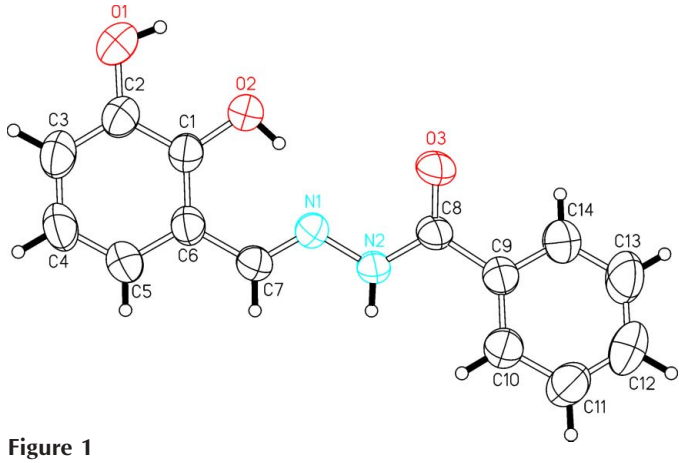



**Figure 1**
*ORTEPII* plot (Johnson, 1976) of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii.

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