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N′-[(1*E*)-(5-Chloro-2-hydroxyphenyl)(phenyl)-methylene]-2-hydroxybenzohydrazide

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.003 Å
R factor = 0.040
wR factor = 0.115
Data-to-parameter ratio = 13.7

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

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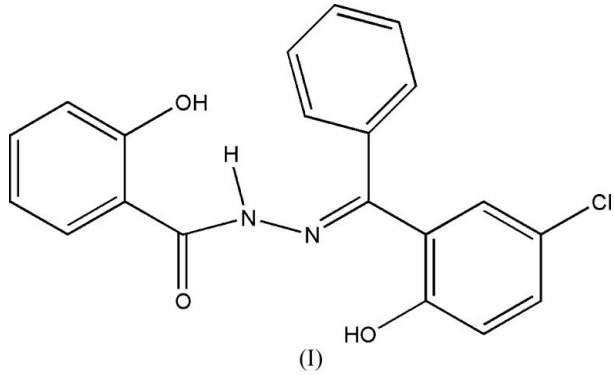
The title compound, $C_{20}H_{15}ClN_2O_3$, displays a *trans* configuration with respect to the C=N double bond. The crystal structure is stabilized by intramolecular O—H···N and N—H···O and intermolecular O—H···O hydrogen bonds.

Comment

The chemistry of aroylhydrazones continues to attract much attention due to their ability to coordinate to metal ions (Singh *et al.*, 1982; Salem, 1998) and their biological activity (Singh *et al.*, 1982; Carcelli *et al.*, 1995). As an extension of our work on the structural characterization of aroylhydrazone derivatives, the title compound, (I), was synthesized and characterized.



(I)

The molecule of (I) displays a *trans* configuration with respect to the C7=N1 double bond (Fig. 1). The three benzene rings, C1–C6 (*A*), C8–C13 (*B*) and C15–C20 (*C*), make dihedral angles of 80.05 (7) (*A*/*B*), 6.16 (13) (*A*/*C*) and 81.95 (7)° (*B*/*C*).

Intramolecular N—H···O and O—H···N hydrogen bonds stabilize the conformation of the molecule, while O—H···O intermolecular hydrogen bonds lead to the formation of infinite chains parallel to the *b* axis (Table 1, Fig. 2).

Experimental

2-Hydroxybenzoylhydrazine (0.01 mol, 1.52 g) was dissolved in anhydrous ethanol (50 ml) and (5-chloro-2-hydroxyphenyl)-(phenyl)methanone (0.01 mol, 2.32 g) was added. The reaction mixture was refluxed for 8 h with stirring, and then the resulting precipitate was collected by filtration, washed several times with ethanol and dried *in vacuo* (yield 78%). The compound (1.0 mmol, 0.37 g) was dissolved in dimethylformamide (15 ml) and kept at room temperature for 25 d to obtain colourless single crystals suitable for X-ray diffraction.

Crystal data

$C_{20}H_{15}ClN_2O_3$
M_r = 366.79
Orthorhombic, *Pbca*
a = 15.3237 (6) Å
b = 12.0171 (5) Å
c = 20.0773 (8) Å
V = 3697.2 (3) Å^3
Z = 8
D_x = 1.318 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 273 (2) K
Block, colourless
0.45 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.924, T_{max} = 0.978
39233 measured reflections
3248 independent reflections
2261 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.115
S = 1.00
3248 reflections
237 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2 + 1.2845P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.84	2.551 (1)	145
N2—H2···O3	0.86	1.90	2.567 (1)	133
O3—H3···O2^{i}	0.82	1.77	2.578 (1)	169

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

All H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H(aromatic) = 0.93, O—H = 0.82 and N—H = 0.86 Å, and with U_{iso}(H) = 1.5U_{eq}(O) or 1.2U_{eq}($C_{aromatic}$,N).

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*) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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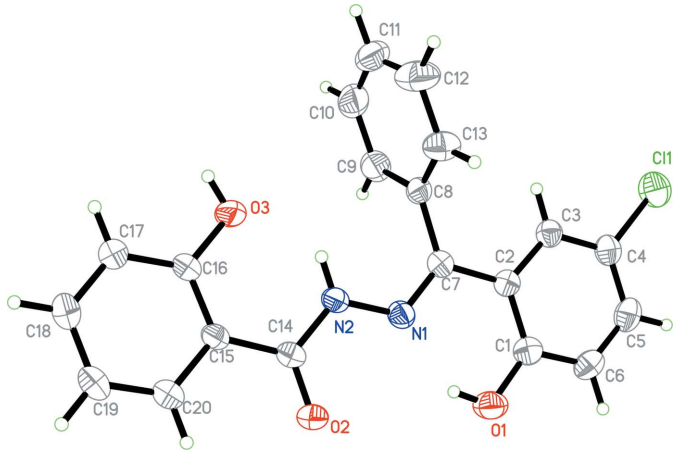

Figure 1
The molecular structure of compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as spheres of arbitrary radii.

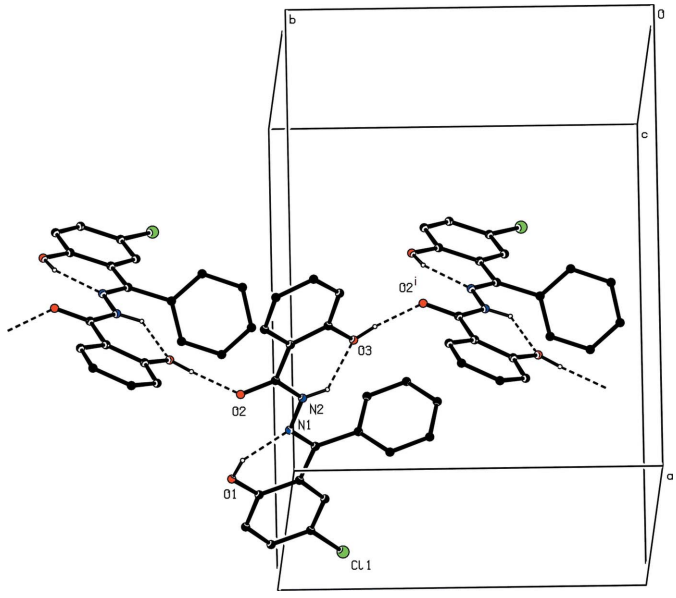

Figure 2
A partial packing view of (I), showing the formation of chains. Dashed lines show intra- and intermolecular hydrogen bonds. H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry code: (i) $\frac{3}{2}-x, y-\frac{1}{2}, z$].

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