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# 4-Chloro-2-(1-naphthyliminomethyl)phenol

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**Key indicators**

Single-crystal X-ray study
*T* = 298 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.055
*wR* factor = 0.125
Data-to-parameter ratio = 13.1

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

The title compound, $C_{17}H_{12}ClNO$, is a Schiff base compound derived from the condensation of equimolar quantities of 5-chlorosalicylaldehyde and 1-naphthylamine. The structure displays a *trans* configuration with respect to the imine C=N double bond. The N atom is also involved in an intramolecular O—H···N hydrogen bond. In the crystal structure, the molecules stack along the *b* axis.

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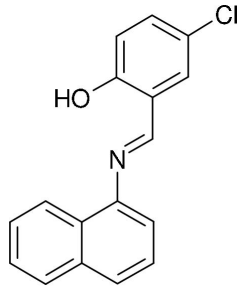
## Comment

Schiff base compounds have been of great interest for many years. These compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures. As an extension of the work on the structural characterization of Schiff base compounds, the crystal structure of the title compound, (I), is reported here.




(I)

The molecular structure of (I) is illustrated in Fig. 1. All the bond lengths and angles in (I) are within normal ranges (Allen

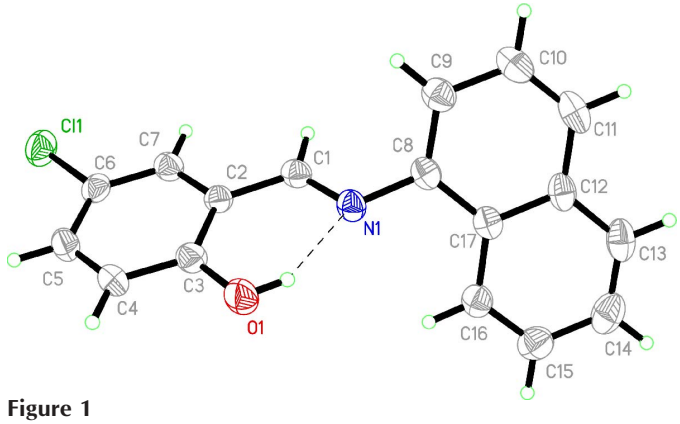



**Figure 1**
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The dashed line indicates the intramolecular hydrogen bond.

*et al.*, 1987). The C1═N1 bond length of 1.283 (3) Å conforms to the value for a double bond. The dihedral angle between the benzene ring and the naphthalene system is 57.5 (3)°. As expected, the molecular structure adopts a *trans* configuration about the C1═N1 bond. In the molecule, there exists an intramolecular O—H···N hydrogen bond involving hydroxyl atom O1 and imine atom N1 (Table 1).

The crystal packing is shown in Fig. 2 and it can be seen that the molecules stack along the *b* axis.

## Experimental

5-Chlorosalicylaldehyde (0.1 mmol, 15.7 mg) and 1-naphthylamine (0.1 mmol, 14.3 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for 10 min and then filtered. The filtrate was allowed to stand in air for 3 d, after which time yellow block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

*Crystal data*

$C_{17}H_{12}ClNO$
$M_r = 281.73$
Monoclinic, $P2_1/c$
$a = 24.733$ (9) Å
$b = 4.420$ (2) Å
$c = 12.376$ (4) Å
$\beta = 90.720$ (6)°
$V = 1352.8$ (9) Å$^3$
$Z = 4$
$D_x = 1.383$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 1012 reflections
$\theta = 2.2$–22.4°
$\mu = 0.28$ mm$^{-1}$
$T = 298$ (2) K
Block, yellow
0.48 × 0.32 × 0.12 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.879$, $T_{max} = 0.968$
5273 measured reflections
2391 independent reflections
1522 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 25.0°$
$h = -29 \rightarrow 23$
$k = -4 \rightarrow 5$
$l = -9 \rightarrow 14$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.125$
$S = 1.00$
2391 reflections
182 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å$^{-3}$
$\Delta\rho_{min} = -0.16$ e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···N1 | 0.82 | 1.90 | 2.629 (3) | 147 |

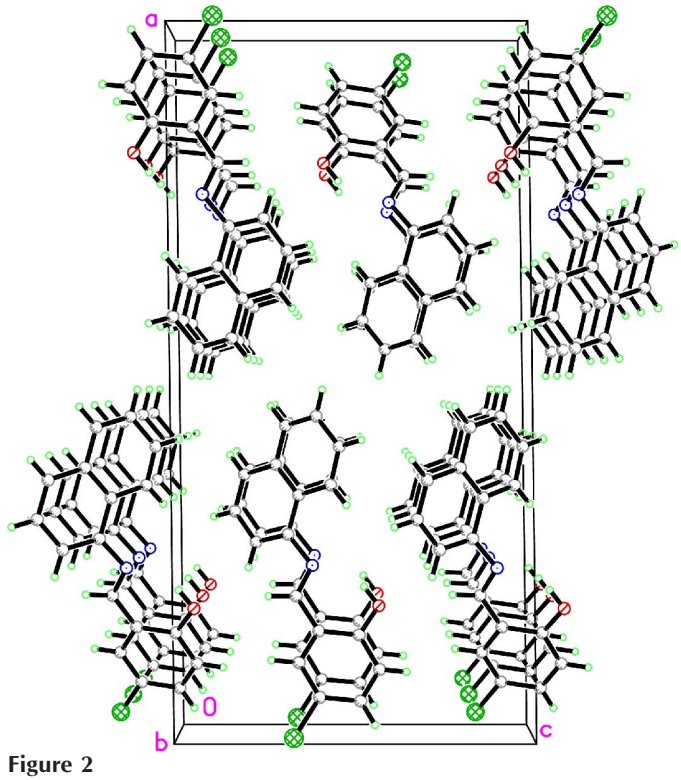



**Figure 2**
The crystal packing of (I), viewed along the *b* axis.

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms: C—H = 0.93 Å with $U_{iso}(H) = 1.2U_{eq}(C)$, and O—H = 0.82 Å with $U_{iso}(H) = 1.5U_{eq}(O)$.

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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## References

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