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# *N*,*N*′-Bis(4-chlorobenzylidene)propane-1,2-diamine

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The title compound, $C_{17}H_{16}Cl_2N_2$, adopts a 'vault' conformation. The molecules are linked by a pair of C—H···N hydrogen bonds into a centrosymmetric dimer with an $R_2^2(18)$ ring. These dimers are linked by a weak centrosymmetric $\pi$–$\pi$ interaction into a chain along the [001] direction, and these chains are connected by van der Waals interactions, resulting in a three-dimensional network structure.

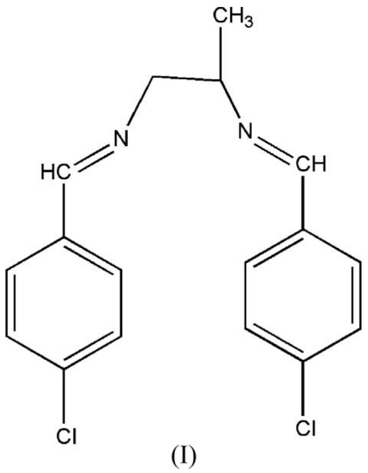
**Key indicators**

Single-crystal X-ray study
$T$ = 298 K
Mean $\sigma$(C–C) = 0.004 Å
$R$ factor = 0.045
$wR$ factor = 0.115
Data-to-parameter ratio = 14.6

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

## Comment

Schiff bases are ligands of significant importance because they are potentially capable of forming stable complexes with metal ions (Johnson *et al.*, 1996; Alizadeh *et al.*, 1999), and some diamine Schiff bases have shown good anti-inflammatory activity and good analgesic activity (Sondhi *et al.*, 2006). The crystal structures of some diamine Schiff bases have been reported (Xiao & Wang, 2006; Sun *et al.*, 2004). Here, we report the crystal structure of the title diamine Schiff base, (I).



(I)

Compound (I) (Fig.1), adopts a 'vault' conformation, with the two 4-chlorobenzyl rings located on the same side of the molecule. The two benzene rings enclose a dihedral angle of 80.77 (8)°.

In the crystal structure of (I), the molecules are linked by a pair of C—H···N hydrogen bonds into a centrosymmetric dimer with an $R_2^2(18)$ ring (Bernstein *et al.*, 1995), centred at ($\frac{1}{2}$, $\frac{1}{2}$, 1) (Fig. 2 and Table 1). These dimers are then linked by a weak centrosymmetric $\pi$–$\pi$ interaction into a chain along the [001] direction, centred at ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$) (Fig. 3) [$Cg1\cdots Cg1^{ii}$ = 4.163 Å; $Cg1$ is the centroid of ring C2–C7; symmetry code: (ii) $1 - x, 1 - y, 1 - z$]. These chains are connected by van der Waals interactions, resulting in a three-dimensional network structure.

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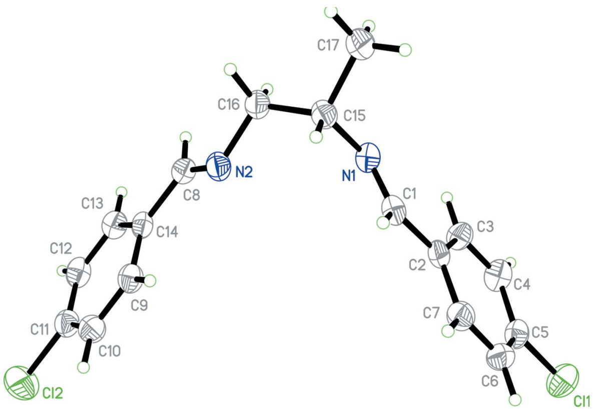

**Figure 1**
The molecular structure of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

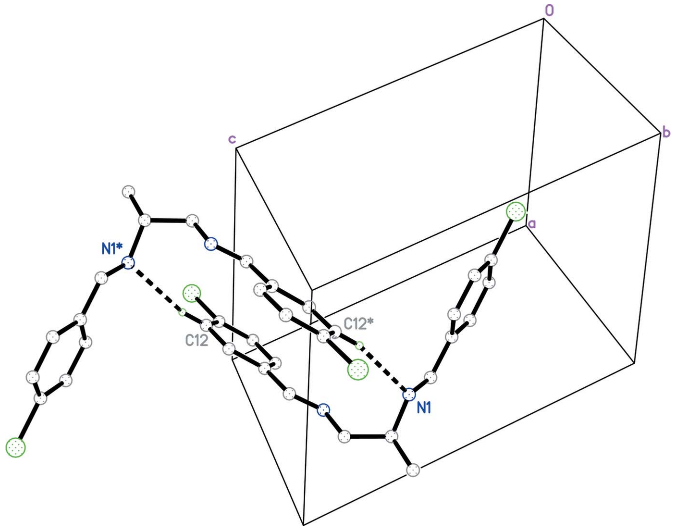

**Figure 2**
Part of the crystal structure of (I), showing the formation of the centrosymmetric hydrogen-bonded $R_2^2(18)$ dimer centred at ($\frac{1}{2}$, $\frac{1}{2}$, 1). For clarity, H atoms have been omitted. [Symmetry code: (*) 1 − *x*,1 − *y*, 2 − *z*]. Dashed lines indicate hydrogen bonds.

## Experimental

A mixture of propane-1,2-diamine (1.48 g, 20 mmol) and 4-chlorobenzaldehyde (1.40 g, 10 mmol) was refluxed for about 2 h in ethanol (20 ml), and then the mixture was cooled and the products were filtered off, washed with methanol and dried. Colourless crystals of (I) suitable for X-ray structure analysis were obtained by recrystallizing the crude product from ethanol (m.p. 350–352 K).

*Crystal data*

$C_{17}H_{16}Cl_2N_2$
$M_r$ = 319.22
Triclinic, $P\bar{1}$
*a* = 7.731 (3) Å
*b* = 9.301 (3) Å
*c* = 11.970 (3) Å
α = 81.031 (3)°
β = 72.354 (2)°
γ = 82.339 (3)°
*V* = 806.8 (5) Å$^3$
*Z* = 2
$D_x$ = 1.314 Mg m$^{-3}$
Mo *K*α radiation
μ = 0.40 mm$^{-1}$
*T* = 298 (2) K
Block, colourless
0.58 × 0.52 × 0.19 mm

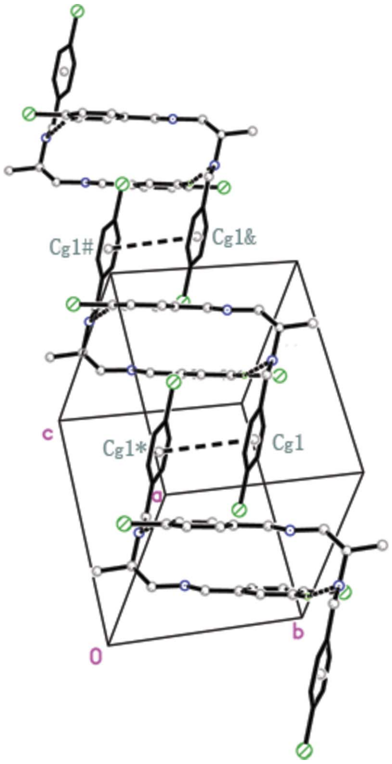

**Figure 3**
A view of part of the crystal structure of (I), showing the formation of a π-stacked chain of hydrogen-bonded dimers along the [001] direction. For clarity, H atoms not involved in the motif shown have been omitted. [Symmetry codes: (*) 1 − *x*, 1 − *y*, 1 − *z*; (#) 1 − *x*, 1 − *y*, 2 − *z*; (&) *x*, *y*, 1 + *z*].

*Data collection*

Siemens SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.803, $T_{max}$ = 0.928
4174 measured reflections
2794 independent reflections
1704 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020
$\theta_{max}$ = 25.0°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.115
*S* = 1.06
2794 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0349P)^2 + 0.2563P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C12—H12···N1$^i$ | 0.93 | 2.72 | 3.613 (4) | 161 |

Symmetry code: (i) −*x* + 1, −*y* + 1, −*z* + 2.

All H atoms were positioned geometrically and refined as riding on their parent atoms, with C—H = 0.96 Å and $U_{iso}$(H)= 1.5$U_{eq}$(C) for methyl H atoms, and C—H = 0.93–0.98 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) for all other H atoms.

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*); software used to prepare material for publication: *SHELXTL*.

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