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(*E*,*E*)-*N*,*N*′-Bis(4-chlorophenyl)ethylenediamine

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.028
wR factor = 0.074
Data-to-parameter ratio = 22.5

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

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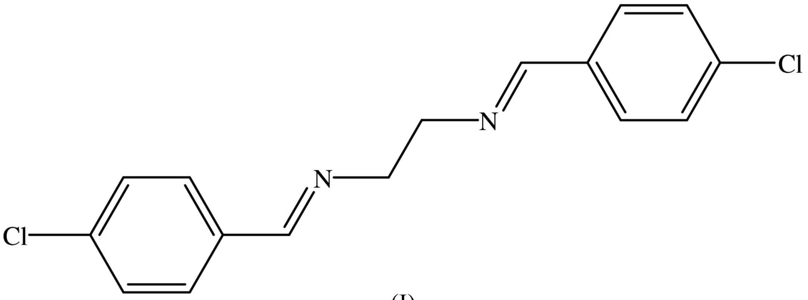
There are two crystallographically independent molecules in the asymmetric unit of the title compound, $C_{16}H_{14}Cl_2N_2$, each possessing an *E* configuration about each azomethine C═N bond. The molecules also adopt a staggered conformation about the ethylene bridge. Weak C—H⋯π interactions link the molecules into ribbons along the *b* axis.

Comment

Schiff bases have found extensive application in coordination chemistry as ligands. They can be designed to be multidentate, offering several binding sites for most metals, leaving vacant coordination sites for potential catalytic (Drozdzak *et al.*, 2005) or enzymatic (Zhang *et al.*, 2005) activities. Aromatic rings that are commonly designed into the structure of Schiff bases offer an infinite number of possibilities of introducing functional groups at various positions, fine-tuning the properties of the ligands and hence their metal complexes. This may enhance the applicability of the ligands and complexes as antimicrobial agents (Coombs *et al.*, 2005), antitumor agents (Kandemirli *et al.*, 2005), corrosion inhibitors (Emregul *et al.*, 2006), coating materials (Atta *et al.*, 2006), sensors (Ganjali *et al.*, 2006) and many more physical and biological applications. The title compound, (I), is similar to (*E*,*E*)-*N*,*N*′-bis(4-tolylmethylidene)ethylenediamine, (II) (Kassim *et al.*, 2006) except that the chloro group attached to the 4-position of the benzene is replaced by a methyl group.



(I)

The asymmetric unit of (I) contains two independent molecules, *A* and *B*, which are almost identical (Fig. 1). The corresponding bond lengths and angles of these two molecules agree with each other (Table 1) and are within normal ranges (Allen *et al.*, 1987), and comparable to those in (II) (Kassim *et al.*, 2006). In both molecules *A* and *B*, the two benzene rings are parallel to each other, as indicated by the dihedral angle between the two rings of 0.74 (7)° in molecule *A* and 1.88 (8)° in molecule *B*. The molecule has a staggered conformation about the C8–C9 bond. The dihedral angle between the planar

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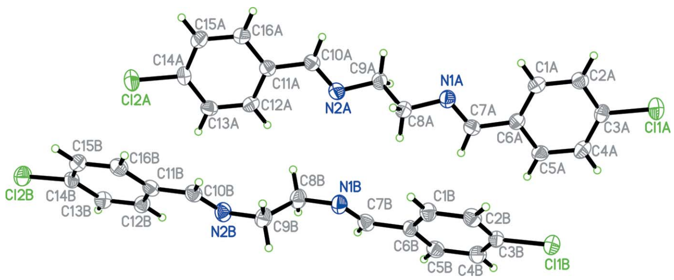

Figure 1
The asymmetric unit of (I), showing 80% probability displacement ellipsoids and the atomic numbering.

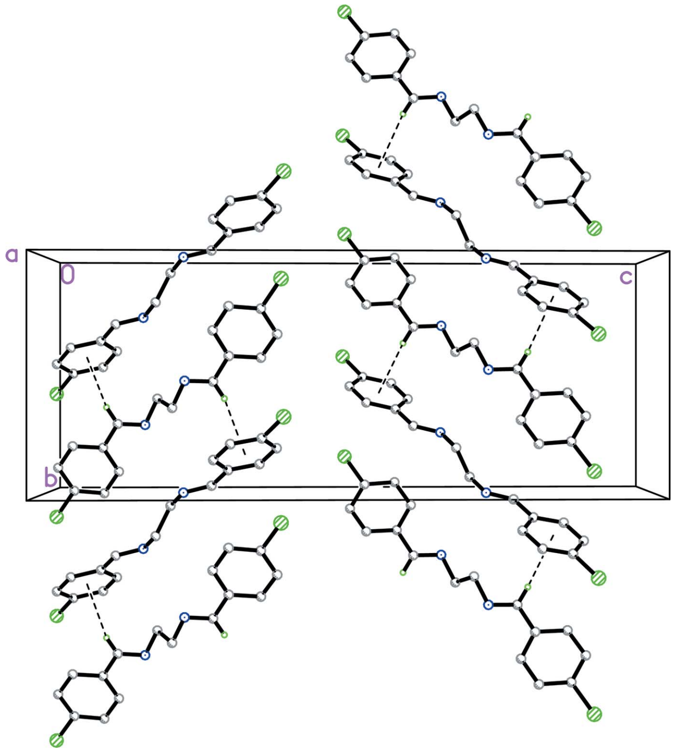

Figure 2
The crystal packing of (I), viewed down the *a* axis. C—H$\cdots\pi$ interactions are shown as dashed lines.

N1/C8/C9/N2 bridge and the chloromethylbenzene (Cl/C1–C7) fragment is 61.67 (7)° in molecule *A* [59.04 (7)° in molecule *B* and 61.65 (17)° in (II)]. The dihedral angle between the C1*A*–C6*A* and C1*B*–C6*B* rings is 37.60 (6)°, and that between the C11*A*–C16*A* and C11*B*–C16*B* rings is 38.74 (6)°.

In the crystal structure of (I), *A*- and *B*-type molecules are stacked alternately along the *b* axis with weak C—H $\cdots\pi$ interactions between them (Table 2). These interactions lead to the formation of ribbons along the *b* axis (Fig. 2).

Experimental

Ethylenediamine (1.80 g, 0.03 mmol) was added dropwise into a solution of 4-chlorobenzaldehyde (8.43 g, 0.06 mmol) in absolute ethanol (200 ml). The resulting mixture containing white crystals in a yellowish solution was then stirred and heated in a water bath at 323 K for 3 h before being cooled to room temperature and left in a refrigerator overnight. The solid was filtered off, washed with cold absolute ethanol and dried in air. Plate-shaped colourless single crystals suitable for X-ray investigations were obtained by recrystallization from a mixture of chloroform and ethanol (1:1) (yield 7.69 g, 84%; m.p. 398–399 K).

Crystal data

$C_{16}H_{14}Cl_2N_2$
$M_r = 305.19$
Monoclinic, *Cc*
$a = 10.1657$ (3) Å
$b = 10.3602$ (3) Å
$c = 26.6975$ (7) Å
$\beta = 92.115$ (2)°
$V = 2809.83$ (14) Å^3

$Z = 8$
$D_x = 1.443$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.45$ mm^{-1}
$T = 100.0$ (1) K
Plate, colourless
0.59 × 0.52 × 0.15 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{\min} = 0.775$, $T_{\max} = 0.935$

26237 measured reflections
8157 independent reflections
7884 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.025$
$\theta_{\max} = 30.0$°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.074$
$S = 1.06$
8157 reflections
362 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2 + 1.1133P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.35$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}
Absolute structure: Flack (1983); 4063 Friedel pairs
Flack parameter: 0.15 (3)

Table 1
Selected bond lengths (Å).

Cl1*A*—C3*A*	1.7439 (14)	Cl1*B*—C3*B*	1.7403 (15)
Cl2*A*—C14*A*	1.7392 (15)	Cl2*B*—C14*B*	1.7398 (14)
N1*A*—C7*A*	1.2751 (19)	N1*B*—C7*B*	1.271 (2)
N1*A*—C8*A*	1.464 (2)	N1*B*—C8*B*	1.4598 (18)
N2*A*—C10*A*	1.2721 (19)	N2*B*—C10*B*	1.271 (2)
N2*A*—C9*A*	1.4617 (19)	N2*B*—C9*B*	1.4643 (18)
C8*A*—C9*A*	1.5260 (16)	C8*B*—C9*B*	1.5229 (18)

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
C7*A*—H7*A*$\cdots$*Cg*1	0.93	2.96	3.656 (2)	132
C10*A*—H10*A*$\cdots$*Cg*2$^{\rm i}$	0.93	2.95	3.618 (2)	130

Symmetry code: (i) *x*, *y* − 1, *z*. *Cg*1 and *Cg*2 denote the C1*B*–C6*B* and C11*B*–C16*B* ring centroids, respectively.

H atoms were placed in calculated positions [C—H = 0.93 Å (aromatic) or 0.97 Å (aliphatic)] and constrained to ride on their parent atoms, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The structure involves some degree of inversion twinning.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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