organic compounds

N-(2-Chloroquinolin-3-ylmethylene)-aniline

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The title compound, $C_{16}H_{11}ClN_2$, displays a *trans* configuration across the C=N bond and a transoid arrangement across the quinoline ring and the azomethine C atom. This arrangement facilitates C—H···Cl interactions. The packing in the crystal structure is due to intermolecular C—H···π and Cl···π (3.52 and 3.84 Å) interactions. The dihedral angle between the least-squares planes of 2-chloroquinoline and phenylamine is 16.61 (2)°.

Related literature

For the importance of chloro-substituted quinolines, see: Meth-Cohn *et al.* (1981); Rajendran & Karavembu (2002); Dutta *et al.* (2002). For chloro-substituted benzylidine anilines see: Prasanna & Guru Row (2000).

For related literature, see: Meth-Cohn & Narine (1978); Umezawa *et al.* (1998, 1999).
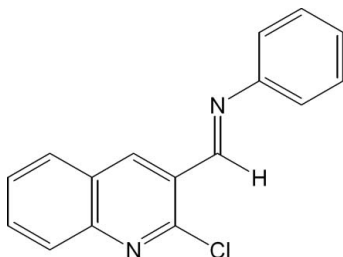
Experimental

Crystal data

$C_{16}H_{11}ClN_2$	V = 1289.67 (11) Å^3
M_r = 266.72	Z = 4
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
a = 6.0069 (3) Å	μ = 0.28 mm^{-1}
b = 11.6812 (6) Å	T = 273 (2) K
c = 18.3798 (9) Å	0.40 × 0.11 × 0.09 mm

Data collection

Bruker SMART CCD area-detector diffractometer	13778 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2272 independent reflections
T_{min} = 0.880, T_{max} = 0.975	1984 reflections with $I > 2\sigma(I)$
	R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024	$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$wR(F^2)$ = 0.060	$\Delta\rho_{min}$ = −0.13 e Å^{-3}
S = 1.01	Absolute structure: Flack (1983),
2272 reflections	929 Friedel pairs
217 parameters	Flack parameter: −0.05 (5)
H atoms treated by a mixture of independent and constrained refinement	

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

*Cg*2 is the centroid of the C2–C7 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···Cl1	0.997 (17)	2.68	3.0667	104
C6—H6···$Cg2^i$	0.956 (19)	2.96	3.755 (1)	142

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2018).

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supporting information

N-(2-Chloroquinolin-3-ylmethylene)aniline

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S1. Comment

2-chloro substituted quinolines are vital synthetic intermediates in the construction of a large number of linearly fused tri- and tetra - cyclic quinolines studied for the DNA intercalating properties (Meth-Cohn *et al.*, 1981; Rajendran & Karavembu, 2002; Dutta *et al.*, 2002). Several interesting structural features associated with chloro substituted Benzilidine anilines, like polymorphism, twisting of aryl moieties, presence of weak Cl⋯π interactions have come to light through their diffraction studies (Prasanna & Guru Row, 2000).

Many schiff bases have been synthesized from 2-chloro-3-formyl-quinoline (Meth-Cohn & Narine, 1978), for studying nonlinear Optical phenomenon arising due to the extended conjugation within the molecule. It is of interest to know the conformation around the azomethine double bond which restricts the free rotation and causes changes in dipole moment manifestations.

The prefered *trans* conformer is stabilized due to C—H⋯Cl (2.676 Å) intramolecular interaction (Fig. 1). Molecular packing formed along *a* axis organizes the molecules in a Zigzag pattern due to C—H..π (2.962 Å) and Cl⋯π (3.521°, 3.845°) intermolecular interactions.(Fig.2) The dihedral angle between the least squares planes of 2-chloro-quinoline and the phenylamine is 16.61 (2)°.

S2. Experimental

A mixture of 2-chloro-3-formyl-quinoline (1.064 g, 0.004 mol) and aniline (0.37 ml,0.004 mol) in ethanol-acetic acid mixture (20 ml, 2:1) was stirred at room temperature for 6 h. After the completion of the reaction (6 h), the separated solid was filtered and washed with excess of cold alcohol.It was dried and crystallized from ethanol (yield = 92%, M.P=435 K). Colourless rectangular crystals were grown from benzene and etyl acetate solvents (1:1, *v/v*) by slow evaporation method at room temperature.

S3. Refinement

All H atoms atoms were located in difference fourier map and refined isotropically, with $U_{iso}(H)=1.2U_{eq}(C)$.
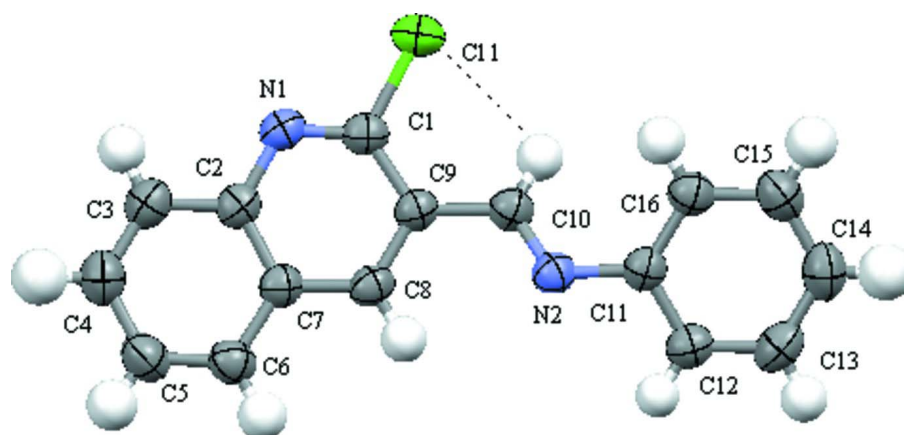
Figure 1

ORTEP diagram of the molecule in asymmetric unit with 50% probability displacement ellipsoids showing the atom-numbering scheme and C—H⋯Cl interaction.
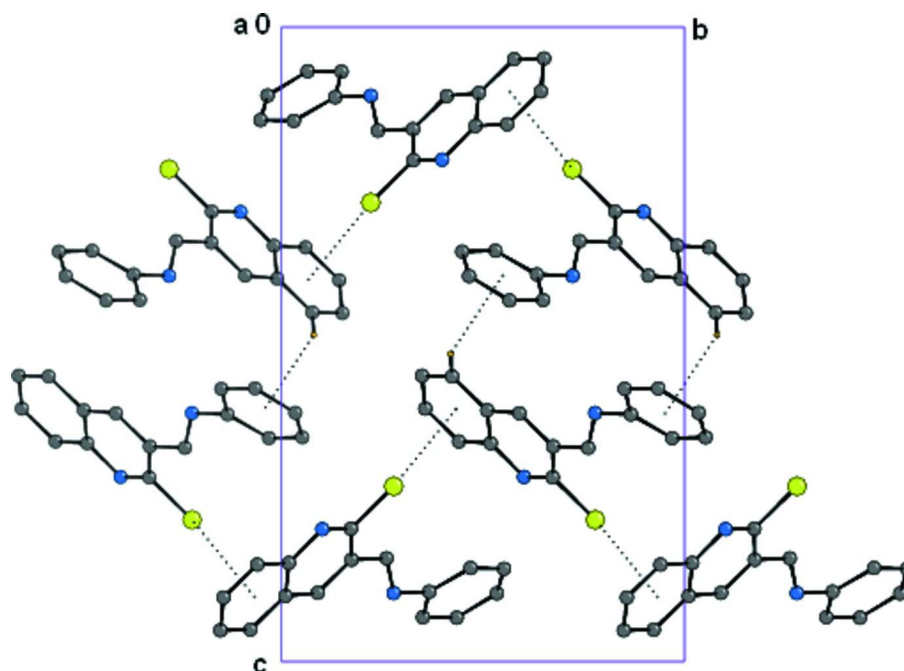
Figure 2

Molecular packing due to C—H⋯π and Cl⋯π interactions along *a* axis.

N-(2-Chloroquinolin-3-ylmethylene)aniline

Crystal data

$C_{16}H_{11}ClN_2$	$Z = 4$
$M_r = 266.72$	$F(000) = 552$
Orthorhombic, $P2_12_12_1$	$D_x = 1.374$ Mg m^{-3}
Hall symbol: P2ac2ab	Melting point: 162 K
$a = 6.0069$ (3) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 11.6812$ (6) Å	Cell parameters from 3933 reflections
$c = 18.3798$ (9) Å	$\theta = 2.2–22.3°$
$V = 1289.67$ (11) Å^3	$\mu = 0.28$ mm^{-1}

T = 273 K

Rectangular, colourless

$0.40 \times 0.11 \times 0.09$ mm

Data collection

CCD area-detector diffractometer	13778 measured reflections
Radiation source: fine-focus sealed tube	2272 independent reflections
Graphite monochromator	1984 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.031$
Absorption correction: multi-scan	$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
(*SADABS*; Sheldrick, 1996)	$h = -7\rightarrow7$
$T_{min} = 0.880$, $T_{max} = 0.975$	$k = -13\rightarrow13$
	$l = -21\rightarrow21$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.024$	$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2 + 0.1031P]$
$wR(F^2) = 0.060$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
2272 reflections	$\Delta\rho_{max} = 0.10$ e Å⁻³
217 parameters	$\Delta\rho_{min} = -0.13$ e Å⁻³
0 restraints	Extinction correction: *SHELXL*,
Primary atom site location: structure-invariant direct methods	$Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.0221 (13)
Secondary atom site location: difference Fourier map	Absolute structure: Flack (1983), 929 Friedel pairs
Hydrogen site location: inferred from neighbouring sites	Absolute structure parameter: −0.05 (5)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cl1	−0.09134 (8)	0.27844 (4)	0.72352 (2)	0.06349 (15)
N1	−0.2433 (2)	0.10138 (11)	0.79120 (7)	0.0480 (3)
N2	0.4029 (2)	0.27821 (11)	0.89186 (6)	0.0485 (3)
C1	−0.0786 (3)	0.17247 (13)	0.79054 (8)	0.0460 (4)
C2	−0.2429 (3)	0.01865 (13)	0.84434 (8)	0.0457 (4)
C3	−0.4204 (3)	−0.05994 (15)	0.84716 (10)	0.0560 (4)
H3	−0.533 (3)	−0.0514 (14)	0.8119 (10)	0.059 (5)*
C4	−0.4242 (4)	−0.14343 (16)	0.89875 (10)	0.0626 (5)
H4	−0.552 (4)	−0.1966 (17)	0.9029 (11)	0.082 (6)*
C5	−0.2529 (4)	−0.15120 (16)	0.95073 (11)	0.0640 (5)
H5	−0.266 (3)	−0.2075 (15)	0.9847 (10)	0.067 (5)*

C6	−0.0802 (4)	−0.07688 (14)	0.94957 (10)	0.0559 (4)
H6	0.036 (3)	−0.0804 (14)	0.9851 (10)	0.062 (5)*
C7	−0.0705 (3)	0.01022 (13)	0.89623 (8)	0.0456 (4)
C8	0.1042 (3)	0.09005 (13)	0.89156 (9)	0.0475 (4)
H8	0.228 (3)	0.0865 (14)	0.9251 (9)	0.055 (5)*
C9	0.1048 (3)	0.17368 (13)	0.83936 (8)	0.0441 (4)
C10	0.2813 (3)	0.26074 (14)	0.83700 (9)	0.0481 (4)
H10	0.300 (3)	0.3049 (14)	0.7910 (10)	0.057 (5)*
C11	0.5640 (3)	0.36654 (13)	0.88976 (8)	0.0454 (4)
C12	0.7579 (3)	0.35109 (15)	0.93006 (9)	0.0505 (4)
H12	0.773 (3)	0.2826 (14)	0.9550 (9)	0.049 (4)*
C13	0.9205 (4)	0.43458 (17)	0.93071 (10)	0.0602 (5)
H13	1.044 (3)	0.4184 (14)	0.9571 (10)	0.057 (5)*
C14	0.8916 (4)	0.53449 (17)	0.89224 (11)	0.0662 (5)
H14	1.005 (4)	0.5924 (17)	0.8927 (11)	0.082 (7)*
C15	0.6971 (4)	0.55175 (17)	0.85356 (11)	0.0630 (5)
H15	0.672 (3)	0.6234 (17)	0.8277 (11)	0.070 (6)*
C16	0.5336 (3)	0.46919 (15)	0.85239 (9)	0.0522 (4)
H16	0.395 (3)	0.4831 (15)	0.8266 (9)	0.060 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0701 (3)	0.0640 (3)	0.0564 (2)	0.0052 (3)	−0.0084 (2)	0.0134 (2)
N1	0.0461 (7)	0.0535 (7)	0.0446 (7)	0.0035 (7)	−0.0045 (6)	−0.0039 (6)
N2	0.0494 (7)	0.0496 (7)	0.0464 (7)	−0.0009 (8)	−0.0015 (7)	−0.0011 (6)
C1	0.0509 (9)	0.0476 (8)	0.0396 (8)	0.0064 (8)	0.0009 (8)	−0.0037 (6)
C2	0.0476 (9)	0.0468 (9)	0.0428 (8)	0.0038 (8)	0.0015 (8)	−0.0092 (7)
C3	0.0501 (10)	0.0625 (11)	0.0553 (10)	−0.0012 (10)	−0.0003 (10)	−0.0078 (9)
C4	0.0606 (11)	0.0603 (11)	0.0668 (11)	−0.0096 (11)	0.0063 (11)	−0.0058 (9)
C5	0.0800 (14)	0.0523 (10)	0.0598 (11)	−0.0048 (12)	0.0020 (11)	0.0055 (9)
C6	0.0668 (12)	0.0505 (10)	0.0503 (10)	0.0018 (10)	−0.0044 (10)	−0.0004 (7)
C7	0.0518 (10)	0.0433 (8)	0.0417 (8)	0.0036 (8)	−0.0019 (9)	−0.0070 (7)
C8	0.0490 (9)	0.0496 (9)	0.0440 (9)	0.0044 (9)	−0.0068 (9)	−0.0065 (7)
C9	0.0471 (9)	0.0458 (8)	0.0394 (7)	0.0024 (8)	−0.0004 (8)	−0.0054 (6)
C10	0.0519 (10)	0.0512 (9)	0.0413 (8)	0.0005 (8)	0.0015 (8)	−0.0021 (7)
C11	0.0475 (9)	0.0502 (9)	0.0386 (7)	−0.0010 (8)	0.0040 (7)	−0.0056 (7)
C12	0.0526 (10)	0.0528 (10)	0.0461 (9)	0.0046 (9)	−0.0005 (8)	−0.0050 (8)
C13	0.0459 (10)	0.0762 (13)	0.0583 (10)	0.0014 (11)	−0.0034 (10)	−0.0122 (9)
C14	0.0656 (13)	0.0665 (12)	0.0664 (12)	−0.0156 (12)	0.0120 (12)	−0.0075 (10)
C15	0.0779 (14)	0.0535 (11)	0.0575 (11)	−0.0070 (10)	0.0076 (10)	0.0027 (9)
C16	0.0572 (12)	0.0543 (10)	0.0451 (9)	0.0017 (9)	0.0005 (8)	−0.0006 (8)

Geometric parameters (Å, º)

Cl1—C1	1.7479 (16)	C7—C8	1.406 (3)
N1—C1	1.291 (2)	C8—C9	1.369 (2)
N1—C2	1.374 (2)	C8—H8	0.968 (18)

N2—C10	1.261 (2)	C9—C10	1.470 (2)
N2—C11	1.415 (2)	C10—H10	0.997 (17)
C1—C9	1.421 (2)	C11—C12	1.392 (2)
C2—C3	1.408 (3)	C11—C16	1.394 (2)
C2—C7	1.411 (2)	C12—C13	1.380 (3)
C3—C4	1.360 (3)	C12—H12	0.926 (16)
C3—H3	0.940 (19)	C13—C14	1.375 (3)
C4—C5	1.407 (3)	C13—H13	0.906 (19)
C4—H4	0.99 (2)	C14—C15	1.383 (3)
C5—C6	1.353 (3)	C14—H14	0.96 (2)
C5—H5	0.910 (18)	C15—C16	1.377 (3)
C6—C7	1.414 (2)	C15—H15	0.97 (2)
C6—H6	0.956 (19)	C16—H16	0.972 (19)
C1—N1—C2	117.24 (14)	C7—C8—H8	120.4 (10)
C10—N2—C11	119.48 (13)	C8—C9—C1	115.67 (15)
N1—C1—C9	126.46 (14)	C8—C9—C10	121.10 (15)
N1—C1—Cl1	115.37 (12)	C1—C9—C10	123.19 (14)
C9—C1—Cl1	118.16 (12)	N2—C10—C9	120.39 (15)
N1—C2—C3	118.91 (16)	N2—C10—H10	122.0 (10)
N1—C2—C7	122.05 (15)	C9—C10—H10	117.7 (10)
C3—C2—C7	119.04 (16)	C12—C11—C16	118.91 (17)
C4—C3—C2	120.39 (19)	C12—C11—N2	117.60 (14)
C4—C3—H3	123.0 (11)	C16—C11—N2	123.42 (15)
C2—C3—H3	116.6 (11)	C13—C12—C11	120.33 (17)
C3—C4—C5	120.5 (2)	C13—C12—H12	122.6 (11)
C3—C4—H4	121.1 (12)	C11—C12—H12	117.1 (11)
C5—C4—H4	118.3 (12)	C14—C13—C12	120.4 (2)
C6—C5—C4	120.57 (18)	C14—C13—H13	123.8 (11)
C6—C5—H5	122.9 (13)	C12—C13—H13	115.8 (11)
C4—C5—H5	116.6 (13)	C13—C14—C15	119.7 (2)
C5—C6—C7	120.28 (19)	C13—C14—H14	120.1 (13)
C5—C6—H6	121.4 (11)	C15—C14—H14	120.2 (13)
C7—C6—H6	118.3 (11)	C16—C15—C14	120.6 (2)
C8—C7—C2	117.38 (14)	C16—C15—H15	118.8 (12)
C8—C7—C6	123.38 (17)	C14—C15—H15	120.6 (12)
C2—C7—C6	119.24 (18)	C15—C16—C11	120.08 (18)
C9—C8—C7	121.20 (16)	C15—C16—H16	120.1 (11)
C9—C8—H8	118.4 (10)	C11—C16—H16	119.8 (11)

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···Cl1	0.997 (17)	2.68	3.0667	104
C6—H6···*Cg*2[i]	0.956 (19)	2.96	3.755 (1)	142

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