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# *N*-[(*E*)-2,4-Dichlorobenzylidene]-4-methylaniline

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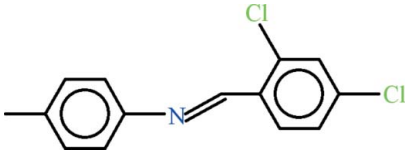
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.030; $wR$ factor = 0.079; data-to-parameter ratio = 13.4.

In the title compound, $C_{14}H_{11}Cl_2N$, the dihedral angle between the 4-methylanilinic and 2,4-dichlorobenzaldehyde moieties is 7.37 (8)°. In the crystal, C—H$\cdots\pi$ interactions between the terminal methyl group and a symmetry-related ring of the anilinic group help to establish the packing.

## Related literature

For background to our project to synthesize various Schiff bases of 2,4-dichlorobenzaldehyde as possible ligands for complexing metals, see: Hayat *et al.* (2010). For related structures, see: Hayat *et al.* (2010); Bernstein (1972). For graph-set notation, see: Bernstein *et al.* (1995).




## Experimental

### *Crystal data*

$C_{14}H_{11}Cl_2N$
$M_r$ = 264.14
Monoclinic, $P2_1$
$a$ = 10.1069 (3) Å
$b$ = 4.7469 (2) Å
$c$ = 12.9922 (4) Å
$\beta$ = 95.668 (2)°
$V$ = 620.27 (4) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.50 mm$^{-1}$
$T$ = 296 K
0.32 × 0.20 × 0.18 mm

### *Data collection*

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.886, $T_{max}$ = 0.916
5221 measured reflections
2082 independent reflections
1937 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.079
$S$ = 1.06
2082 reflections
155 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$
Absolute structure: Flack (1983), 807 Friedel pairs
Flack parameter: 0.10 (7)

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

*Cg*1 is the centroid of the C1–C6 ring.

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C7—H7*C*$\cdots$*Cg*1$^{i}$ | 0.96 | 2.71 | 3.565 (2) | 148 |

Symmetry code: (i) $x, y-1, z$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

The authors acknowledge the provision of funds for the purchase of the diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Vice Chancellor, University of Sargodha, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2602).

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# supporting information

*Acta Cryst.* (2010). E**66**, o2583 [doi:10.1107/S1600536810036640]

## *N*-[(*E*)-2,4-Dichlorobenzylidene]-4-methylaniline

**M. Nawaz Tahir, Hazoor Ahmad Shad, Muhammad Ilyas Tariq and Riaz H. Tariq**

### S1. Comment

As a part of our on going project related to synthesize various Schiff bases of 2,4-dichlorobenzaldehyde as possible ligands for complexing metals (Hayat *et al.*, 2010), we report here the title compound.

In the title compound, the 4-methylanilinic group A (C1—C7/N1) and 2,4-dichlorobenzaldehyde moiety B (C8—C14/CL1/CL2) are planar with r. m. s. deviation of 0.0114 and 0.0209 Å, respectively. The dihedral angle between A/B is 7.37 (8)°. The title compound essentially consists of monomers (Fig. 1). There exist weak intramolecular C—H···Cl hydrogen bonds (Table 1, Fig. 1) forming an S(5) ring motif (Bernstein *et al.*, 1995). There also exists a C—H···$\pi$ interaction (Table 1) which helps in consolidating the crystal packing. Bond distances and bond angles agree with related compounds already published as the 4-chloro-*N*-[(*E*)-2,4-dichlorobenzylidene]aniline (Hayat *et al.*, 2010) and the *N*-(2,4-dichlorobenzylidene)aniline (Bernstein, 1972).

### S2. Experimental

Equimolar quantities of 4-methylaniline and 2,4-dichlorobanzaldehyde were refluxed in methanol for 30 min resulting in yellow solution. The solution was kept at room temperature which affoarded light yellow needles after 72 h.

### S3. Refinement

The H-atoms were positioned geometrically (C–H = 0.93–0.96 Å) and were included in the refinement in the riding model approximation, with $U_{iso}$(H) = $xU_{eq}$(C), where $x$ = 1.5 for methyl H-atoms and $x$ = 1.2 for aryl H-atoms.

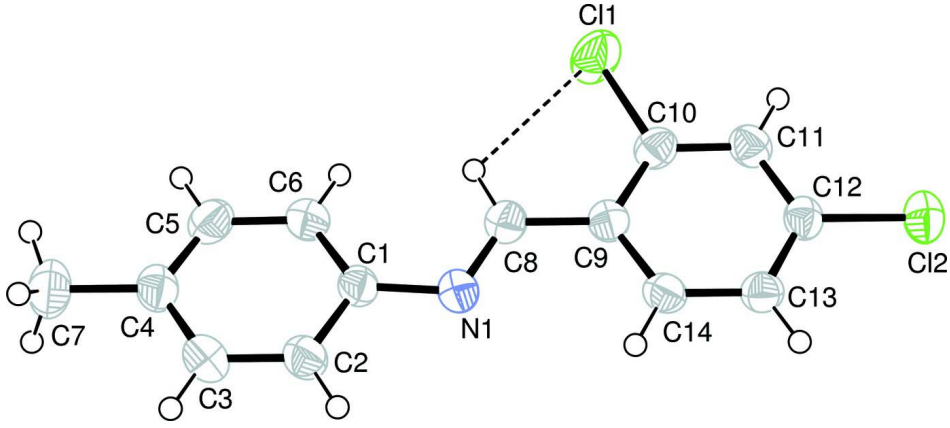


**Figure 1**

View of the title compound with the atom numbering scheme. The thermal ellipsoids are drawn at the 50% probability level. H-atoms are shown as small circles of arbitrary radii. The dotted line represents the intramolecular H-bonding.

## *N*-[(*E*)-2,4-Dichlorobenzylidene]-4-methylaniline

*Crystal data*

$C_{14}H_{11}Cl_2N$
$M_r = 264.14$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 10.1069$ (3) Å
$b = 4.7469$ (2) Å
$c = 12.9922$ (4) Å
$\beta = 95.668$ (2)°
$V = 620.27$ (4) Å$^3$
$Z = 2$
$F(000) = 272$
$D_x = 1.414$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1937 reflections
$\theta = 1.6$–25.2°
$\mu = 0.50$ mm$^{-1}$
$T = 296$ K
Needles, colorless
0.32 × 0.20 × 0.18 mm

*Data collection*

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.20 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.886$, $T_{max} = 0.916$
5221 measured reflections
2082 independent reflections
1937 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 25.2°$, $\theta_{min} = 1.6°$
$h = -12 \rightarrow 12$
$k = -5 \rightarrow 4$
$l = -15 \rightarrow 15$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.079$
$S = 1.06$
2082 reflections
155 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 0.0661P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å$^{-3}$
$\Delta\rho_{min} = -0.15$ e Å$^{-3}$
Absolute structure: Flack (1983), 807 Friedel pairs
Absolute structure parameter: 0.10 (7)

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | −0.16693 (6) | 0.51040 (18) | 0.89821 (4) | 0.0670 (3) |
| Cl2 | −0.39799 (5) | 1.07125 (13) | 0.57256 (4) | 0.0492 (2) |
| N1 | 0.08154 (17) | 0.0949 (5) | 0.69281 (13) | 0.0393 (6) |

| | | | | |
|---|---|---|---|---|
| C1 | 0.1724 (2) | −0.1021 (5) | 0.74152 (15) | 0.0359 (7) |
| C2 | 0.2670 (2) | −0.2162 (5) | 0.68218 (17) | 0.0436 (8) |
| C3 | 0.3592 (2) | −0.4089 (6) | 0.72278 (18) | 0.0488 (8) |
| C4 | 0.3619 (2) | −0.4993 (5) | 0.82462 (16) | 0.0422 (8) |
| C5 | 0.2663 (2) | −0.3948 (6) | 0.88216 (16) | 0.0478 (8) |
| C6 | 0.1728 (2) | −0.1997 (6) | 0.84251 (16) | 0.0450 (8) |
| C7 | 0.4635 (3) | −0.7104 (6) | 0.8693 (2) | 0.0601 (10) |
| C8 | 0.0090 (2) | 0.2361 (5) | 0.74719 (16) | 0.0396 (7) |
| C9 | −0.08867 (19) | 0.4437 (5) | 0.70395 (15) | 0.0354 (6) |
| C10 | −0.17493 (19) | 0.5787 (6) | 0.76574 (14) | 0.0394 (6) |
| C11 | −0.2697 (2) | 0.7695 (5) | 0.72713 (16) | 0.0408 (7) |
| C12 | −0.2778 (2) | 0.8341 (5) | 0.62295 (16) | 0.0359 (7) |
| C13 | −0.1920 (2) | 0.7130 (5) | 0.55900 (15) | 0.0376 (7) |
| C14 | −0.10045 (19) | 0.5191 (5) | 0.59983 (14) | 0.0378 (7) |
| H2 | 0.26757 | −0.16057 | 0.61359 | 0.0523* |
| H3 | 0.42111 | −0.48034 | 0.68121 | 0.0586* |
| H5 | 0.26408 | −0.45686 | 0.94987 | 0.0574* |
| H6 | 0.10958 | −0.13313 | 0.88390 | 0.0540* |
| H7A | 0.45868 | −0.72613 | 0.94246 | 0.0901* |
| H7B | 0.55083 | −0.64872 | 0.85642 | 0.0901* |
| H7C | 0.44563 | −0.89053 | 0.83730 | 0.0901* |
| H8 | 0.01785 | 0.20723 | 0.81833 | 0.0475* |
| H11 | −0.32689 | 0.85279 | 0.77004 | 0.0490* |
| H13 | −0.19621 | 0.76212 | 0.48946 | 0.0452* |
| H14 | −0.04426 | 0.43496 | 0.55632 | 0.0453* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0692 (4) | 0.0965 (7) | 0.0371 (3) | 0.0234 (4) | 0.0140 (3) | 0.0138 (3) |
| Cl2 | 0.0445 (3) | 0.0449 (4) | 0.0571 (3) | 0.0089 (3) | −0.0002 (2) | 0.0058 (3) |
| N1 | 0.0421 (9) | 0.0365 (12) | 0.0392 (8) | 0.0048 (9) | 0.0034 (7) | 0.0005 (9) |
| C1 | 0.0374 (11) | 0.0300 (13) | 0.0394 (11) | 0.0005 (9) | −0.0007 (8) | −0.0031 (9) |
| C2 | 0.0509 (13) | 0.0423 (15) | 0.0388 (11) | 0.0090 (12) | 0.0108 (10) | 0.0015 (10) |
| C3 | 0.0487 (12) | 0.0460 (15) | 0.0524 (12) | 0.0099 (14) | 0.0083 (10) | −0.0053 (13) |
| C4 | 0.0413 (12) | 0.0301 (15) | 0.0529 (12) | −0.0007 (10) | −0.0063 (9) | −0.0033 (11) |
| C5 | 0.0565 (13) | 0.0481 (17) | 0.0373 (10) | 0.0021 (13) | −0.0029 (9) | 0.0031 (11) |
| C6 | 0.0497 (13) | 0.0473 (15) | 0.0384 (11) | 0.0087 (12) | 0.0062 (9) | −0.0025 (10) |
| C7 | 0.0529 (15) | 0.0483 (17) | 0.0748 (18) | 0.0085 (13) | −0.0145 (12) | 0.0017 (14) |
| C8 | 0.0419 (12) | 0.0385 (14) | 0.0380 (10) | 0.0012 (10) | 0.0026 (9) | 0.0012 (10) |
| C9 | 0.0330 (10) | 0.0335 (12) | 0.0394 (10) | −0.0025 (10) | 0.0016 (8) | −0.0012 (10) |
| C10 | 0.0415 (10) | 0.0443 (14) | 0.0328 (9) | −0.0009 (12) | 0.0057 (8) | 0.0030 (11) |
| C11 | 0.0399 (11) | 0.0410 (15) | 0.0424 (11) | 0.0039 (10) | 0.0089 (9) | −0.0022 (10) |
| C12 | 0.0352 (11) | 0.0290 (12) | 0.0426 (11) | −0.0022 (9) | −0.0004 (8) | 0.0011 (9) |
| C13 | 0.0419 (12) | 0.0360 (13) | 0.0348 (10) | −0.0011 (10) | 0.0027 (9) | −0.0014 (10) |
| C14 | 0.0370 (10) | 0.0388 (15) | 0.0378 (10) | 0.0020 (10) | 0.0055 (8) | −0.0060 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C10 | 1.7454 (19) | C11—C12 | 1.382 (3) |
| Cl2—C12 | 1.736 (2) | C12—C13 | 1.384 (3) |
| N1—C1 | 1.415 (3) | C13—C14 | 1.374 (3) |
| N1—C8 | 1.260 (3) | C2—H2 | 0.9300 |
| C1—C2 | 1.396 (3) | C3—H3 | 0.9300 |
| C1—C6 | 1.391 (3) | C5—H5 | 0.9300 |
| C2—C3 | 1.373 (3) | C6—H6 | 0.9300 |
| C3—C4 | 1.389 (3) | C7—H7A | 0.9600 |
| C4—C5 | 1.372 (3) | C7—H7B | 0.9600 |
| C4—C7 | 1.509 (4) | C7—H7C | 0.9600 |
| C5—C6 | 1.386 (3) | C8—H8 | 0.9300 |
| C8—C9 | 1.467 (3) | C11—H11 | 0.9300 |
| C9—C10 | 1.398 (3) | C13—H13 | 0.9300 |
| C9—C14 | 1.393 (3) | C14—H14 | 0.9300 |
| C10—C11 | 1.376 (3) | | |
| | | | |
| Cl1···C6$^{i}$ | 3.519 (2) | C1···H7C$^{viii}$ | 3.0800 |
| Cl2···Cl2$^{ii}$ | 3.5598 (8) | C2···H7C$^{viii}$ | 3.0000 |
| Cl2···Cl2$^{iii}$ | 3.5598 (8) | C3···H7C$^{viii}$ | 2.9600 |
| Cl1···H7B$^{iv}$ | 2.9500 | C4···H7C$^{viii}$ | 3.0100 |
| Cl1···H6$^{i}$ | 2.9100 | C5···H7C$^{viii}$ | 3.0900 |
| Cl1···H8 | 2.6500 | C6···H8 | 2.4900 |
| Cl2···H2$^{v}$ | 3.1400 | C8···H6 | 2.6300 |
| N1···C14$^{vi}$ | 3.446 (3) | C13···H2$^{x}$ | 2.9000 |
| N1···H14 | 2.6300 | H2···Cl2$^{xi}$ | 3.1400 |
| N1···H13$^{vii}$ | 2.8500 | H2···C13$^{vii}$ | 2.9000 |
| C1···C4$^{viii}$ | 3.552 (3) | H2···H13$^{vii}$ | 2.4800 |
| C1···C8$^{vi}$ | 3.553 (3) | H5···H7A | 2.3600 |
| C1···C9$^{vi}$ | 3.405 (3) | H6···C8 | 2.6300 |
| C4···C1$^{vi}$ | 3.552 (3) | H6···H8 | 2.0100 |
| C5···C8$^{vi}$ | 3.465 (3) | H6···Cl1$^{ix}$ | 2.9100 |
| C6···C9$^{vi}$ | 3.486 (3) | H7A···H5 | 2.3600 |
| C6···C8$^{vi}$ | 3.323 (3) | H7B···Cl1$^{xii}$ | 2.9500 |
| C6···Cl1$^{ix}$ | 3.519 (2) | H7C···C1$^{vi}$ | 3.0800 |
| C8···C6$^{viii}$ | 3.323 (3) | H7C···C2$^{vi}$ | 3.0000 |
| C8···C1$^{viii}$ | 3.553 (3) | H7C···C3$^{vi}$ | 2.9600 |
| C8···C5$^{viii}$ | 3.465 (3) | H7C···C4$^{vi}$ | 3.0100 |
| C8···C11$^{vi}$ | 3.573 (3) | H7C···C5$^{vi}$ | 3.0900 |
| C9···C6$^{viii}$ | 3.486 (3) | H8···Cl1 | 2.6500 |
| C9···C1$^{viii}$ | 3.405 (3) | H8···C6 | 2.4900 |
| C9···C12$^{vi}$ | 3.569 (3) | H8···H6 | 2.0100 |
| C11···C8$^{viii}$ | 3.573 (3) | H13···N1$^{x}$ | 2.8500 |
| C12···C9$^{viii}$ | 3.569 (3) | H13···H2$^{x}$ | 2.4800 |
| C14···N1$^{viii}$ | 3.446 (3) | H14···N1 | 2.6300 |
| | | | |
| C1—N1—C8 | 119.23 (18) | C9—C14—C13 | 122.46 (19) |

| | | | |
|---|---|---|---|
| N1—C1—C2 | 117.33 (18) | C1—C2—H2 | 119.00 |
| N1—C1—C6 | 125.67 (19) | C3—C2—H2 | 119.00 |
| C2—C1—C6 | 117.0 (2) | C2—C3—H3 | 119.00 |
| C1—C2—C3 | 121.5 (2) | C4—C3—H3 | 119.00 |
| C2—C3—C4 | 121.4 (2) | C4—C5—H5 | 119.00 |
| C3—C4—C5 | 117.3 (2) | C6—C5—H5 | 119.00 |
| C3—C4—C7 | 121.4 (2) | C1—C6—H6 | 120.00 |
| C5—C4—C7 | 121.3 (2) | C5—C6—H6 | 120.00 |
| C4—C5—C6 | 122.0 (2) | C4—C7—H7A | 109.00 |
| C1—C6—C5 | 120.8 (2) | C4—C7—H7B | 109.00 |
| N1—C8—C9 | 123.32 (19) | C4—C7—H7C | 109.00 |
| C8—C9—C10 | 121.49 (18) | H7A—C7—H7B | 110.00 |
| C8—C9—C14 | 122.30 (19) | H7A—C7—H7C | 110.00 |
| C10—C9—C14 | 116.21 (19) | H7B—C7—H7C | 109.00 |
| Cl1—C10—C9 | 120.69 (17) | N1—C8—H8 | 118.00 |
| Cl1—C10—C11 | 116.39 (16) | C9—C8—H8 | 118.00 |
| C9—C10—C11 | 122.92 (18) | C10—C11—H11 | 121.00 |
| C10—C11—C12 | 118.33 (19) | C12—C11—H11 | 121.00 |
| Cl2—C12—C11 | 118.99 (16) | C12—C13—H13 | 121.00 |
| Cl2—C12—C13 | 119.97 (16) | C14—C13—H13 | 120.00 |
| C11—C12—C13 | 121.0 (2) | C9—C14—H14 | 119.00 |
| C12—C13—C14 | 118.98 (18) | C13—C14—H14 | 119.00 |

| | | | |
|---|---|---|---|
| C8—N1—C1—C2 | −168.7 (2) | N1—C8—C9—C14 | −5.9 (4) |
| C8—N1—C1—C6 | 13.7 (4) | C8—C9—C10—Cl1 | 1.5 (3) |
| C1—N1—C8—C9 | −179.6 (2) | C8—C9—C10—C11 | −178.5 (2) |
| N1—C1—C2—C3 | −180.0 (2) | C14—C9—C10—Cl1 | −178.14 (17) |
| C6—C1—C2—C3 | −2.2 (3) | C14—C9—C10—C11 | 2.0 (3) |
| N1—C1—C6—C5 | 179.6 (2) | C8—C9—C14—C13 | 179.9 (2) |
| C2—C1—C6—C5 | 2.0 (3) | C10—C9—C14—C13 | −0.6 (3) |
| C1—C2—C3—C4 | 0.2 (4) | Cl1—C10—C11—C12 | 178.75 (18) |
| C2—C3—C4—C5 | 1.9 (4) | C9—C10—C11—C12 | −1.3 (4) |
| C2—C3—C4—C7 | −179.8 (2) | C10—C11—C12—Cl2 | 179.26 (18) |
| C3—C4—C5—C6 | −2.1 (4) | C10—C11—C12—C13 | −0.7 (3) |
| C7—C4—C5—C6 | 179.6 (2) | Cl2—C12—C13—C14 | −177.94 (17) |
| C4—C5—C6—C1 | 0.2 (4) | C11—C12—C13—C14 | 2.1 (3) |
| N1—C8—C9—C10 | 174.6 (2) | C12—C13—C14—C9 | −1.4 (3) |

Symmetry codes: (i) −*x*, *y*+1/2, −*z*+2; (ii) −*x*−1, *y*−1/2, −*z*+1; (iii) −*x*−1, *y*+1/2, −*z*+1; (iv) *x*−1, *y*+1, *z*; (v) −*x*, *y*+3/2, −*z*+1; (vi) *x*, *y*−1, *z*; (vii) −*x*, *y*−1/2, −*z*+1; (viii) *x*, *y*+1, *z*; (ix) −*x*, *y*−1/2, −*z*+2; (x) −*x*, *y*+1/2, −*z*+1; (xi) −*x*, *y*−3/2, −*z*+1; (xii) *x*+1, *y*−1, *z*.

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the C1–C6 phenyl ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8—H8···Cl1 | 0.93 | 2.65 | 3.065 (2) | 108 |
| C7—H7*C*···*Cg*1$^{vi}$ | 0.96 | 2.71 | 3.565 (2) | 148 |

Symmetry code: (vi) *x*, *y*−1, *z*.