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# (*E*)-1-(6-Chloro-2-methyl-4-phenyl-3-quinolyl)-3-(2-methoxyphenyl)prop-2-en-1-one

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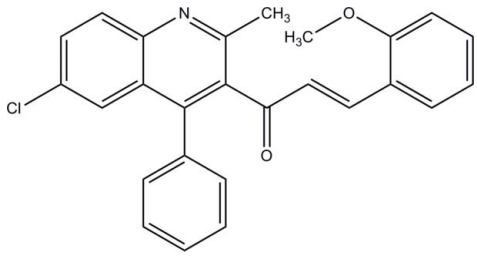
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.053; $wR$ factor = 0.136; data-to-parameter ratio = 30.0.

In the title compound, $C_{26}H_{20}ClNO_2$, the quinoline ring system and the methoxyphenyl ring form dihedral angles of 69.97 (6) and 22.10 (10)°, respectively, with the propenone linkage. The 4-phenyl ring substituent on the quinoline ring system is oriented at a dihedral angle of 66.47 (3)°. In the crystal, molecules exist as C—H···O hydrogen-bonded dimers. The structure is further stabilized by C—H···$\pi$ interactions.

## Related literature

For background details and the biological activity of quinolines, see: Michael (1997); Markees *et al.* (1970); Kalluraya & Sreenivasa (1998); Chen *et al.* (2001). For the biological activity of chalcones, see: Dimmock *et al.* (1999); Zi & Simoneau (2005). For related structures, see: Loh *et al.* (2009*a*,*b*). For bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).




## Experimental

### Crystal data

$C_{26}H_{20}ClNO_2$
$M_r$ = 413.88
Monoclinic, $C2/c$
$a$ = 15.1154 (2) Å
$b$ = 15.4655 (2) Å
$c$ = 17.2400 (2) Å
$\beta$ = 104.418 (1)°
$V$ = 3903.22 (9) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.22 mm$^{-1}$
$T$ = 100 K
0.39 × 0.25 × 0.19 mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.919, $T_{max}$ = 0.960
30753 measured reflections
8197 independent reflections
5864 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.136
$S$ = 1.06
8197 reflections
273 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

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

*Cg*1 and *Cg*2 are the centroids of the C2–C7 and N1/C1/C2/C7–C9 rings, respectively.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C12—H12*A*···O1$^{i}$ | 0.93 | 2.59 | 3.2963 (16) | 133 |
| C17—H17*A*···*Cg*1$^{ii}$ | 0.93 | 2.96 | 3.6617 (14) | 134 |
| C20—H20*A*···*Cg*2$^{ii}$ | 0.93 | 2.85 | 3.6353 (14) | 143 |

Symmetry codes: (i) $-x+\frac{1}{2}, -y+\frac{3}{2}, -z+2$; (ii) $x, -y-1, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5015).

## References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, Y.-L., Fang, K.-C., Sheu, J.-Y., Hsu, S.-L. & Tzeng, C.-C. (2001). *J. Med. Chem.* **44**, 2374–2377.
Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
Dimmock, J. R., Elias, D. W., Beazely, M. A. & Kandepu, N. M. (1999). *Curr. Med. Chem.* **6**, 1125–1149.

‡ Thomson Reuters ResearcherID: C-7581-2009.
§ Thomson Reuters ResearcherID: A-3561-2009.

Kalluraya, B. & Sreenivasa, S. (1998). *Il Farmaco*, **53**, 399–404.
Loh, W.-S., Fun, H.-K., Sarveswari, S., Vijayakumar, V. & Reddy, B. P. (2009*a*). *Acta Cryst.* E**65**, o3144–o3145.
Loh, W.-S., Fun, H.-K., Sarveswari, S., Vijayakumar, V. & Reddy, B. P. (2009*b*). *Acta Cryst.* E**65**, o3237–o3238.
Markees, D. G., Dewey, V. C. & Kidder, G. W. (1970). *J. Med. Chem.* **13**, 324–326.
Michael, J. P. (1997). *Nat. Prod. Rep.* **14**, 605–608.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Zi, X. & Simoneau, A. R. (2005). *Cancer Res.* **65**, 3479–3486.

# supplementary materials

*Acta Cryst.* (2010). E**66**, o353-o354 [ **doi:10.1107/S1600536810000784** ]

# (*E*)-1-(6-Chloro-2-methyl-4-phenyl-3-quinolyl)-3-(2-methoxyphenyl)prop-2-en-1-one

**W.-S. Loh, H.-K. Fun, S. Sarveswari, V. Vijayakumar and B. P. Reddy**

## Comment

Quinoline and its derivatives are very important compounds because of their wide occurrence in natural products (Michael, 1997) and biologically active compounds (Markees *et al.*, 1970). A large variety of quinolines have interesting physiological activities and found attractive applications as pharmaceuticals, agrochemicals and as synthetic building blocks (Kalluraya & Sreenivasa, 1998; Chen *et al.*, 2001). The chalcones are open chain flavonoids, possessing a variety of biological activities, including antioxidant, anti-inflammation, antimicrobial, antiprotozoal, antiulcer, as well as other activities (Dimmock *et al.*, 1999). More importantly, chalcones have shown several anticancer activities as inhibitors of cancer cell proliferation, carcinogenesis and metastasis (Zi & Simoneau, 2005).

In the molecule of the title compound (Fig. 1), the quinoline ring system (C1–C9/N1) is approximately planar with a maximum deviation of 0.065 (1) Å for atom C9. The mean plane of the quinoline ring system forms a dihedral angle of 66.47 (3)° with the C10-C15 phenyl ring. The C1–C9/N1 and C19-C24 planes form dihedral angles of 69.97 (6) and 22.10 (10)°, respectively, with the O1/C16-C18 plane. Bond lengths (Allen *et al.*, 1987) and angles are within the normal range and are comparable to closely related structures (Loh *et al.*, 2009*a*; Loh *et al.*, 2009*b*).

In the crystal (Fig. 2), pairs of neighbouring molecules are arranged into dimers by pairs of intermolecular C12—H12A···O1 hydrogen bonds. The crystal structure is further stabilized by C—H···π interactions (Table 1), involving C2–C7 (centroid *Cg*1) and N1/C1/C2/C7-C9 (centroid *Cg*2) rings.

## Experimental

A mixture of 3-acetyl-6-chloro-2-methyl-4-phenylquinoline (2.95 g, 0.01 mol), 2-methoxybenzaldehyde (1.36 g, 0.01 mol) and a catalytic amount of KOH in distilled ethanol was stirred for 12 h. The resulting mixture was concentrated to remove the ethanol and then poured onto ice and neutralized with diluted acetic acid. The resultant solid was filtered, dried and purified by column chromatography using a 1:1 mixture of ethyl acetate and petroleum ether (m.p. 403–405 K, yield: 68%).

## Refinement

H atoms were positioned geometrically [C–H = 0.93 or 0.96 Å] and were refined using a riding model, with $U_{iso}$(H) = 1.2-1.5$U_{eq}$(C). A rotating group model was applied to the methyl groups.

## Figures

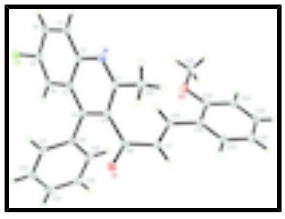

Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

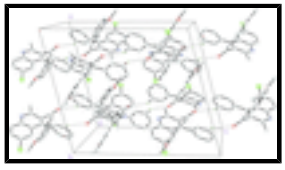

Fig. 2. The crystal packing of the title compound, viewed approximately along the *b* axis, showing the dimers. H atoms not involved in the intermolecular interactions (dashed lines) have been omitted for clarity.

## (*E*)-1-(6-Chloro-2-methyl-4-phenyl-3-quinolyl)-3-(2-methoxyphenyl)prop- 2-en-1-one

*Crystal data*

| | |
|---|---|
| $C_{26}H_{20}ClNO_2$ | $F(000) = 1728$ |
| $M_r = 413.88$ | $D_x = 1.409$ Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation, λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 7486 reflections |
| *a* = 15.1154 (2) Å | θ = 2.4–31.5° |
| *b* = 15.4655 (2) Å | μ = 0.22 mm$^{-1}$ |
| *c* = 17.2400 (2) Å | *T* = 100 K |
| β = 104.418 (1)° | Block, yellow |
| *V* = 3903.22 (9) Å$^3$ | 0.39 × 0.25 × 0.19 mm |
| *Z* = 8 | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII CCD area-detector diffractometer | 8197 independent reflections |
| Radiation source: fine-focus sealed tube | 5864 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.039$ |
| φ and ω scans | $\theta_{max} = 34.5°$, $\theta_{min} = 2.4°$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | $h = -20\rightarrow24$ |
| $T_{min} = 0.919$, $T_{max} = 0.960$ | $k = -24\rightarrow19$ |
| 30753 measured reflections | $l = -27\rightarrow27$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.053$ | Hydrogen site location: inferred from neighbouring sites |

| | |
|---|---|
| $wR(F^2) = 0.136$ | H-atom parameters constrained |
| $S = 1.06$ | $w = 1/[\sigma^2(F_o^2) + (0.0625P)^2 + 0.7227P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 8197 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 273 parameters | $\Delta\rho_{max} = 0.54$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.31$ e Å$^{-3}$ |

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.02177 (2) | 1.01758 (2) | 0.635395 (19) | 0.01901 (8) |
| O1 | 0.27571 (6) | 0.58953 (6) | 0.86651 (5) | 0.0176 (2) |
| O2 | −0.04599 (6) | 0.49228 (6) | 0.58651 (5) | 0.0182 (2) |
| N1 | 0.23373 (7) | 0.70354 (7) | 0.61280 (6) | 0.0132 (2) |
| C1 | 0.24441 (8) | 0.64331 (8) | 0.66867 (7) | 0.0119 (2) |
| C2 | 0.18686 (8) | 0.77723 (8) | 0.62237 (7) | 0.0118 (2) |
| C3 | 0.17164 (9) | 0.83936 (8) | 0.55976 (7) | 0.0140 (2) |
| H3A | 0.1948 | 0.8299 | 0.5153 | 0.017* |
| C4 | 0.12304 (9) | 0.91308 (8) | 0.56457 (7) | 0.0147 (2) |
| H4A | 0.1130 | 0.9538 | 0.5236 | 0.018* |
| C5 | 0.08838 (8) | 0.92650 (8) | 0.63233 (7) | 0.0137 (2) |
| C6 | 0.10437 (8) | 0.87006 (8) | 0.69522 (7) | 0.0130 (2) |
| H6A | 0.0826 | 0.8818 | 0.7400 | 0.016* |
| C7 | 0.15466 (8) | 0.79326 (8) | 0.69143 (7) | 0.0114 (2) |
| C8 | 0.17037 (8) | 0.72900 (8) | 0.75300 (7) | 0.0113 (2) |
| C9 | 0.21100 (8) | 0.65250 (8) | 0.73916 (7) | 0.0117 (2) |
| C10 | 0.14444 (8) | 0.74686 (8) | 0.82932 (7) | 0.0126 (2) |
| C11 | 0.18819 (9) | 0.81414 (9) | 0.87804 (8) | 0.0184 (3) |
| H11A | 0.2323 | 0.8468 | 0.8622 | 0.022* |
| C12 | 0.16655 (11) | 0.83282 (10) | 0.94971 (8) | 0.0234 (3) |
| H12A | 0.1966 | 0.8774 | 0.9819 | 0.028* |
| C13 | 0.10036 (10) | 0.78525 (10) | 0.97343 (8) | 0.0236 (3) |
| H13A | 0.0853 | 0.7983 | 1.0212 | 0.028* |

| | | | | |
|---|---|---|---|---|
| C14 | 0.05658 (9) | 0.71812 (10) | 0.92586 (8) | 0.0213 (3) |
| H14A | 0.0122 | 0.6860 | 0.9419 | 0.026* |
| C15 | 0.07867 (9) | 0.69836 (9) | 0.85395 (7) | 0.0166 (2) |
| H15A | 0.0495 | 0.6528 | 0.8225 | 0.020* |
| C16 | 0.22442 (8) | 0.57996 (8) | 0.79974 (7) | 0.0125 (2) |
| C17 | 0.17554 (9) | 0.49843 (8) | 0.77583 (7) | 0.0144 (2) |
| H17A | 0.1908 | 0.4509 | 0.8095 | 0.017* |
| C18 | 0.10990 (9) | 0.48907 (8) | 0.70786 (7) | 0.0137 (2) |
| H18A | 0.0929 | 0.5384 | 0.6769 | 0.016* |
| C19 | 0.06258 (8) | 0.40889 (8) | 0.67781 (7) | 0.0135 (2) |
| C20 | 0.09598 (9) | 0.32817 (8) | 0.70747 (8) | 0.0161 (2) |
| H20A | 0.1493 | 0.3253 | 0.7484 | 0.019* |
| C21 | 0.05186 (9) | 0.25228 (9) | 0.67757 (8) | 0.0186 (3) |
| H21A | 0.0758 | 0.1990 | 0.6974 | 0.022* |
| C22 | −0.02865 (9) | 0.25684 (9) | 0.61751 (8) | 0.0193 (3) |
| H22A | −0.0595 | 0.2062 | 0.5983 | 0.023* |
| C23 | −0.06371 (9) | 0.33563 (9) | 0.58583 (8) | 0.0171 (3) |
| H23A | −0.1175 | 0.3377 | 0.5454 | 0.021* |
| C24 | −0.01789 (9) | 0.41163 (8) | 0.61490 (7) | 0.0148 (2) |
| C25 | 0.29908 (9) | 0.56529 (8) | 0.65696 (8) | 0.0170 (2) |
| H25A | 0.3273 | 0.5758 | 0.6137 | 0.026* |
| H25B | 0.2594 | 0.5160 | 0.6445 | 0.026* |
| H25C | 0.3454 | 0.5542 | 0.7052 | 0.026* |
| C26 | −0.12419 (10) | 0.49727 (10) | 0.51992 (8) | 0.0213 (3) |
| H26A | −0.1348 | 0.5564 | 0.5034 | 0.032* |
| H26B | −0.1767 | 0.4752 | 0.5353 | 0.032* |
| H26C | −0.1136 | 0.4636 | 0.4763 | 0.032* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.01956 (16) | 0.01561 (16) | 0.02069 (15) | 0.00653 (12) | 0.00279 (12) | 0.00098 (11) |
| O1 | 0.0204 (5) | 0.0172 (5) | 0.0129 (4) | 0.0012 (4) | −0.0004 (3) | −0.0009 (3) |
| O2 | 0.0176 (5) | 0.0162 (5) | 0.0172 (4) | 0.0006 (4) | −0.0022 (4) | 0.0005 (3) |
| N1 | 0.0144 (5) | 0.0130 (5) | 0.0124 (4) | 0.0001 (4) | 0.0039 (4) | −0.0009 (4) |
| C1 | 0.0120 (5) | 0.0122 (6) | 0.0117 (5) | −0.0003 (4) | 0.0030 (4) | −0.0017 (4) |
| C2 | 0.0109 (5) | 0.0123 (5) | 0.0119 (5) | −0.0004 (4) | 0.0026 (4) | −0.0004 (4) |
| C3 | 0.0148 (6) | 0.0156 (6) | 0.0112 (5) | −0.0014 (4) | 0.0025 (4) | 0.0004 (4) |
| C4 | 0.0158 (6) | 0.0147 (6) | 0.0125 (5) | −0.0006 (5) | 0.0013 (4) | 0.0014 (4) |
| C5 | 0.0130 (6) | 0.0110 (5) | 0.0155 (5) | 0.0003 (4) | 0.0008 (4) | −0.0005 (4) |
| C6 | 0.0139 (5) | 0.0135 (6) | 0.0118 (5) | 0.0002 (4) | 0.0034 (4) | −0.0010 (4) |
| C7 | 0.0108 (5) | 0.0120 (6) | 0.0111 (5) | −0.0003 (4) | 0.0021 (4) | −0.0001 (4) |
| C8 | 0.0113 (5) | 0.0121 (5) | 0.0106 (5) | −0.0017 (4) | 0.0028 (4) | −0.0001 (4) |
| C9 | 0.0120 (5) | 0.0116 (5) | 0.0111 (5) | −0.0007 (4) | 0.0022 (4) | −0.0005 (4) |
| C10 | 0.0152 (6) | 0.0121 (5) | 0.0107 (5) | 0.0031 (4) | 0.0038 (4) | 0.0011 (4) |
| C11 | 0.0228 (7) | 0.0180 (6) | 0.0154 (5) | −0.0025 (5) | 0.0069 (5) | −0.0022 (5) |
| C12 | 0.0329 (8) | 0.0227 (7) | 0.0153 (6) | 0.0010 (6) | 0.0073 (6) | −0.0046 (5) |
| C13 | 0.0293 (8) | 0.0305 (8) | 0.0135 (5) | 0.0091 (6) | 0.0103 (5) | 0.0023 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C14 | 0.0206 (7) | 0.0282 (8) | 0.0186 (6) | 0.0042 (6) | 0.0116 (5) | 0.0059 (5) |
| C15 | 0.0170 (6) | 0.0179 (6) | 0.0157 (5) | 0.0009 (5) | 0.0054 (5) | 0.0019 (5) |
| C16 | 0.0132 (5) | 0.0132 (6) | 0.0116 (5) | 0.0015 (4) | 0.0042 (4) | −0.0001 (4) |
| C17 | 0.0180 (6) | 0.0119 (6) | 0.0139 (5) | 0.0003 (4) | 0.0052 (5) | 0.0012 (4) |
| C18 | 0.0152 (6) | 0.0129 (6) | 0.0136 (5) | −0.0001 (4) | 0.0047 (4) | −0.0003 (4) |
| C19 | 0.0126 (5) | 0.0155 (6) | 0.0132 (5) | −0.0009 (4) | 0.0047 (4) | −0.0006 (4) |
| C20 | 0.0140 (6) | 0.0166 (6) | 0.0170 (6) | 0.0000 (5) | 0.0026 (5) | −0.0017 (5) |
| C21 | 0.0200 (6) | 0.0130 (6) | 0.0218 (6) | 0.0005 (5) | 0.0036 (5) | −0.0012 (5) |
| C22 | 0.0215 (7) | 0.0163 (6) | 0.0201 (6) | −0.0037 (5) | 0.0052 (5) | −0.0041 (5) |
| C23 | 0.0156 (6) | 0.0204 (6) | 0.0150 (5) | −0.0024 (5) | 0.0032 (5) | −0.0031 (5) |
| C24 | 0.0144 (6) | 0.0167 (6) | 0.0140 (5) | 0.0004 (5) | 0.0048 (4) | −0.0016 (4) |
| C25 | 0.0193 (6) | 0.0160 (6) | 0.0168 (6) | 0.0046 (5) | 0.0065 (5) | 0.0005 (5) |
| C26 | 0.0179 (7) | 0.0245 (7) | 0.0178 (6) | 0.0014 (5) | −0.0025 (5) | 0.0019 (5) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cl1—C5 | 1.7397 (13) | C13—C14 | 1.385 (2) |
| O1—C16 | 1.2262 (14) | C13—H13A | 0.93 |
| O2—C24 | 1.3683 (15) | C14—C15 | 1.3956 (17) |
| O2—C26 | 1.4302 (16) | C14—H14A | 0.93 |
| N1—C1 | 1.3207 (15) | C15—H15A | 0.93 |
| N1—C2 | 1.3733 (15) | C16—C17 | 1.4678 (18) |
| C1—C9 | 1.4344 (16) | C17—C18 | 1.3414 (17) |
| C1—C25 | 1.5042 (17) | C17—H17A | 0.93 |
| C2—C7 | 1.4158 (16) | C18—C19 | 1.4606 (18) |
| C2—C3 | 1.4205 (17) | C18—H18A | 0.93 |
| C3—C4 | 1.3700 (18) | C19—C20 | 1.3951 (18) |
| C3—H3A | 0.93 | C19—C24 | 1.4144 (18) |
| C4—C5 | 1.4098 (17) | C20—C21 | 1.3845 (18) |
| C4—H4A | 0.93 | C20—H20A | 0.93 |
| C5—C6 | 1.3657 (16) | C21—C22 | 1.3895 (18) |
| C6—C7 | 1.4204 (17) | C21—H21A | 0.93 |
| C6—H6A | 0.93 | C22—C23 | 1.3855 (19) |
| C7—C8 | 1.4302 (16) | C22—H22A | 0.93 |
| C8—C9 | 1.3808 (17) | C23—C24 | 1.3926 (18) |
| C8—C10 | 1.4893 (16) | C23—H23A | 0.93 |
| C9—C16 | 1.5116 (17) | C25—H25A | 0.96 |
| C10—C15 | 1.3934 (18) | C25—H25B | 0.96 |
| C10—C11 | 1.3960 (18) | C25—H25C | 0.96 |
| C11—C12 | 1.3851 (18) | C26—H26A | 0.96 |
| C11—H11A | 0.93 | C26—H26B | 0.96 |
| C12—C13 | 1.383 (2) | C26—H26C | 0.96 |
| C12—H12A | 0.93 | | |
| C24—O2—C26 | 117.21 (10) | C15—C14—H14A | 119.8 |
| C1—N1—C2 | 118.08 (10) | C10—C15—C14 | 119.97 (12) |
| N1—C1—C9 | 122.90 (11) | C10—C15—H15A | 120.0 |
| N1—C1—C25 | 116.07 (10) | C14—C15—H15A | 120.0 |
| C9—C1—C25 | 120.94 (10) | O1—C16—C17 | 121.58 (11) |
| N1—C2—C7 | 122.82 (11) | O1—C16—C9 | 120.26 (11) |

| | | | |
|---|---|---|---|
| N1—C2—C3 | 117.44 (10) | C17—C16—C9 | 118.16 (10) |
| C7—C2—C3 | 119.74 (11) | C18—C17—C16 | 123.30 (11) |
| C4—C3—C2 | 120.32 (11) | C18—C17—H17A | 118.3 |
| C4—C3—H3A | 119.8 | C16—C17—H17A | 118.3 |
| C2—C3—H3A | 119.8 | C17—C18—C19 | 126.29 (12) |
| C3—C4—C5 | 119.23 (11) | C17—C18—H18A | 116.9 |
| C3—C4—H4A | 120.4 | C19—C18—H18A | 116.9 |
| C5—C4—H4A | 120.4 | C20—C19—C24 | 118.13 (11) |
| C6—C5—C4 | 122.34 (11) | C20—C19—C18 | 121.94 (11) |
| C6—C5—Cl1 | 118.87 (10) | C24—C19—C18 | 119.89 (11) |
| C4—C5—Cl1 | 118.79 (9) | C21—C20—C19 | 121.69 (12) |
| C5—C6—C7 | 119.27 (11) | C21—C20—H20A | 119.2 |
| C5—C6—H6A | 120.4 | C19—C20—H20A | 119.2 |
| C7—C6—H6A | 120.4 | C20—C21—C22 | 119.06 (12) |
| C2—C7—C6 | 119.02 (10) | C20—C21—H21A | 120.5 |
| C2—C7—C8 | 118.30 (11) | C22—C21—H21A | 120.5 |
| C6—C7—C8 | 122.60 (11) | C23—C22—C21 | 121.09 (12) |
| C9—C8—C7 | 117.77 (10) | C23—C22—H22A | 119.5 |
| C9—C8—C10 | 122.53 (10) | C21—C22—H22A | 119.5 |
| C7—C8—C10 | 119.68 (11) | C22—C23—C24 | 119.56 (12) |
| C8—C9—C1 | 119.79 (10) | C22—C23—H23A | 120.2 |
| C8—C9—C16 | 120.36 (10) | C24—C23—H23A | 120.2 |
| C1—C9—C16 | 119.79 (10) | O2—C24—C23 | 123.95 (11) |
| C15—C10—C11 | 119.01 (11) | O2—C24—C19 | 115.63 (11) |
| C15—C10—C8 | 122.28 (11) | C23—C24—C19 | 120.42 (12) |
| C11—C10—C8 | 118.71 (11) | C1—C25—H25A | 109.5 |
| C12—C11—C10 | 120.69 (13) | C1—C25—H25B | 109.5 |
| C12—C11—H11A | 119.7 | H25A—C25—H25B | 109.5 |
| C10—C11—H11A | 119.7 | C1—C25—H25C | 109.5 |
| C13—C12—C11 | 120.11 (13) | H25A—C25—H25C | 109.5 |
| C13—C12—H12A | 119.9 | H25B—C25—H25C | 109.5 |
| C11—C12—H12A | 119.9 | O2—C26—H26A | 109.5 |
| C12—C13—C14 | 119.85 (12) | O2—C26—H26B | 109.5 |
| C12—C13—H13A | 120.1 | H26A—C26—H26B | 109.5 |
| C14—C13—H13A | 120.1 | O2—C26—H26C | 109.5 |
| C13—C14—C15 | 120.36 (13) | H26A—C26—H26C | 109.5 |
| C13—C14—H14A | 119.8 | H26B—C26—H26C | 109.5 |
| C2—N1—C1—C9 | −1.36 (17) | C7—C8—C10—C11 | −63.24 (16) |
| C2—N1—C1—C25 | −177.88 (10) | C15—C10—C11—C12 | −0.21 (19) |
| C1—N1—C2—C7 | 3.89 (17) | C8—C10—C11—C12 | −179.71 (12) |
| C1—N1—C2—C3 | −176.69 (11) | C10—C11—C12—C13 | −0.6 (2) |
| N1—C2—C3—C4 | 178.10 (11) | C11—C12—C13—C14 | 0.9 (2) |
| C7—C2—C3—C4 | −2.46 (18) | C12—C13—C14—C15 | −0.2 (2) |
| C2—C3—C4—C5 | 0.00 (18) | C11—C10—C15—C14 | 0.85 (19) |
| C3—C4—C5—C6 | 2.54 (19) | C8—C10—C15—C14 | −179.67 (11) |
| C3—C4—C5—Cl1 | −176.70 (10) | C13—C14—C15—C10 | −0.6 (2) |
| C4—C5—C6—C7 | −2.50 (18) | C8—C9—C16—O1 | −64.94 (16) |
| Cl1—C5—C6—C7 | 176.75 (9) | C1—C9—C16—O1 | 112.20 (13) |
| N1—C2—C7—C6 | −178.11 (11) | C8—C9—C16—C17 | 115.85 (13) |

| | | | |
|---|---|---|---|
| C3—C2—C7—C6 | 2.48 (17) | C1—C9—C16—C17 | −67.02 (15) |
| N1—C2—C7—C8 | −1.18 (17) | O1—C16—C17—C18 | 170.75 (12) |
| C3—C2—C7—C8 | 179.42 (11) | C9—C16—C17—C18 | −10.04 (18) |
| C5—C6—C7—C2 | −0.04 (17) | C16—C17—C18—C19 | 175.84 (12) |
| C5—C6—C7—C8 | −176.84 (11) | C17—C18—C19—C20 | −15.8 (2) |
| C2—C7—C8—C9 | −4.05 (17) | C17—C18—C19—C24 | 166.47 (12) |
| C6—C7—C8—C9 | 172.77 (11) | C24—C19—C20—C21 | −0.80 (18) |
| C2—C7—C8—C10 | 174.87 (11) | C18—C19—C20—C21 | −178.61 (12) |
| C6—C7—C8—C10 | −8.31 (17) | C19—C20—C21—C22 | −1.21 (19) |
| C7—C8—C9—C1 | 6.47 (17) | C20—C21—C22—C23 | 1.8 (2) |
| C10—C8—C9—C1 | −172.42 (11) | C21—C22—C23—C24 | −0.39 (19) |
| C7—C8—C9—C16 | −176.40 (10) | C26—O2—C24—C23 | −3.77 (18) |
| C10—C8—C9—C16 | 4.71 (18) | C26—O2—C24—C19 | 176.59 (11) |
| N1—C1—C9—C8 | −3.94 (18) | C22—C23—C24—O2 | 178.69 (12) |
| C25—C1—C9—C8 | 172.42 (11) | C22—C23—C24—C19 | −1.69 (19) |
| N1—C1—C9—C16 | 178.91 (11) | C20—C19—C24—O2 | −178.09 (11) |
| C25—C1—C9—C16 | −4.73 (17) | C18—C19—C24—O2 | −0.24 (17) |
| C9—C8—C10—C15 | −63.86 (17) | C20—C19—C24—C23 | 2.26 (18) |
| C7—C8—C10—C15 | 117.28 (13) | C18—C19—C24—C23 | −179.89 (11) |
| C9—C8—C10—C11 | 115.63 (14) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C12—H12A···O1$^{i}$ | 0.93 | 2.59 | 3.2963 (16) | 133 |
| C17—H17A···Cg1$^{ii}$ | 0.93 | 2.96 | 3.6617 (14) | 134 |
| C20—H20A···Cg2$^{ii}$ | 0.93 | 2.85 | 3.6353 (14) | 143 |

Symmetry codes: (i) −*x*+1/2, −*y*+3/2, −*z*+2; (ii) *x*, −*y*−1, *z*+1/2.

**Fig. 1**

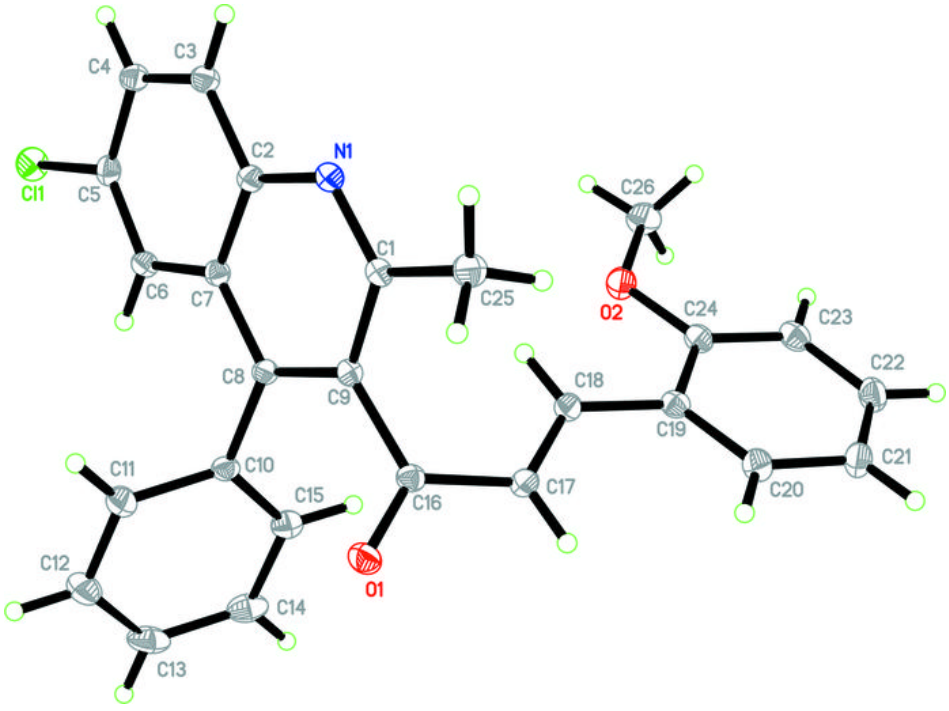
C4
C3
C2
N1
Cl1
C5
C1
C26
C6
C7
C25
O2
C24
C23
C8
C9
C18
C22
C19
C11
C10
C15
C16
C17
C21
C20
C12
O1
C14
C13

**Fig. 2**