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2-(4-Chlorophenyl)-6-methyl-4-(3-methylphenyl)quinoline

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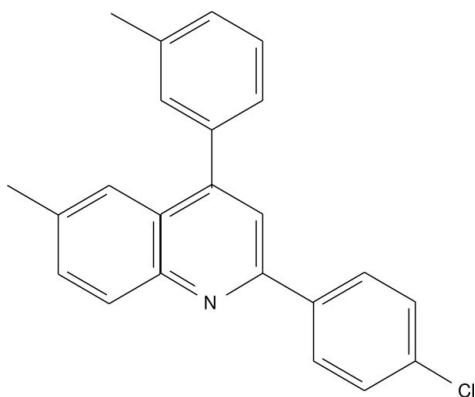
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.057; wR factor = 0.168; data-to-parameter ratio = 14.9.

In the title compound, $\text{C}_{23}\text{H}_{18}\text{ClN}$, the dihedral angles between the quinoline unit and the chlorobenzene and methylbenzene rings are 2.57 (9) and 56.06 (9)°, respectively. The crystal structure is stabilized by $\pi-\pi$ interactions [minimum ring centroid separation = 3.733 (2) Å].

Related literature

For quinolines, see: Michael (1997); Balasubramanian *et al.* (1996). For a related structure, see: Asiri *et al.* (2011).



Experimental

Crystal data

| | |
|--|---|
| $\text{C}_{23}\text{H}_{18}\text{ClN}$ | $V = 1783.1 (11) \text{ \AA}^3$ |
| $M_r = 343.83$ | $Z = 4$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a = 7.982 (3) \text{ \AA}$ | $\mu = 0.22 \text{ mm}^{-1}$ |
| $b = 17.921 (6) \text{ \AA}$ | $T = 293 \text{ K}$ |
| $c = 12.478 (4) \text{ \AA}$ | $0.23 \times 0.22 \times 0.22 \text{ mm}$ |
| $\beta = 92.581 (6)^\circ$ | |

Data collection

| | |
|--|--|
| Oxford Diffraction Xcalibur CCD diffractometer | 3392 independent reflections |
| 16998 measured reflections | 2508 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.044$ |

Refinement

| | |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.057$ | 228 parameters |
| $wR(F^2) = 0.168$ | H-atom parameters constrained |
| $S = 1.04$ | $\Delta\rho_{\text{max}} = 0.49 \text{ e \AA}^{-3}$ |
| 3392 reflections | $\Delta\rho_{\text{min}} = -0.45 \text{ e \AA}^{-3}$ |

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2238).

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supporting information

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2-(4-Chlorophenyl)-6-methyl-4-(3-methylphenyl)quinoline

M Prabhuswamy, T. R. Swaroop, S. Madan Kumar, K. S. Rangappa and N. K. Lokanath

S1. Comment

Quinolines and their derivatives occur in numerous natural products (Michael, 1997) and may exhibit interesting physiochemical activities, finding applications as pharmaceuticals and agrochemicals as well as being general synthetic platforms (Balasubramanian *et al.*, 1996).

In the title molecule, C₂₃ H₁₈ Cl N, (Fig. 1), dihedral angles between the quinoline moiety and the chlorobenzene and methylbenzene rings are 2.57 (9) and 56.06 (9)°, respectively, with the conformation of the chlorobenzene ring influenced by the presence of an intramolecular C5—H···N1 interaction [2.764 (3) Å]. The overall geometry of the title compound is similar to 4-(4-chlorophenyl)-8-methyl-2-oxo-1,2,5,6,7,8-hexahydroquinoline-3-carbonitrile (Asiri *et al.*, 2011).

The crystal structure (Fig. 2) is stabilized by aromatic ring $\pi \cdots \pi$ interactions with the ring centroids defined as follows: Cg(1), N1/C7/C8/C9/C10/C15; Cg(2), C1/C2/C3/C4/C5/C6 and Cg(3), C10/C11/C12/C13/C14/C15. The distance between Cg(1) and Cg(1) is 3.7427 (18) Å [-x+3, -y+2, -z+1], Cg(1) and Cg(2) is 3.7679 (19) Å [-x+2, -y+2, 1 -z], Cg(1) and Cg(3) is 3.7635 (18) Å [-x+3, -y+2, -z+1], Cg(2) and Cg(3) is 3.733 (2) Å [-x+2, -y+2, -z+1].

S2. Experimental

The enaminone [3-(4-chlorophenyl)-1-m-tolyl-3-(p-tolyamino)prop-2-en-1-one] (5 mmol) was taken in polyphosphoric acid (5 mL) and heated at 140 °C for 5 h. After completion of the reaction (monitored by TLC), the reaction mixture was diluted with water (50 mL). The aqueous layer was extracted with ethyl acetate (3 x 20 mL), the combined ethyl acetate layer was washed with 0.1 N NaOH (2 x 25 mL), followed by brine solution (25 mL). The organic layer was then dried over anhydrous sodium sulfate and concentrated under reduced pressure to afford the crude product which was purified by column chromatography over silica gel (60–120 mesh) using a hexane:ethyl acetate mixture (9.5:0.5) as eluent. The pure title compound was crystallized in an ethyl acetate–hexane mixture to obtain pale yellow single crystals. ¹H NMR (CDCl₃, 300 MHz): 8.49 (d, 2H, J=8.4 Hz), 7.92 (d, 1H, J=7.2 Hz), 7.79 (s, 1H), 7.55–7.66 (m, 5H), 7.19 (d, 1H), 2.34 (s, 3H), 2.35 (s, 3H). Mass: Calc. 343.2 found 344.2 (M⁺+1): m.p. 98–100 °C (uncorrected).

S3. Refinement

All hydrogen atoms were located geometrically with C—H = 0.93–0.97) Å and allowed to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{aromatic C})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

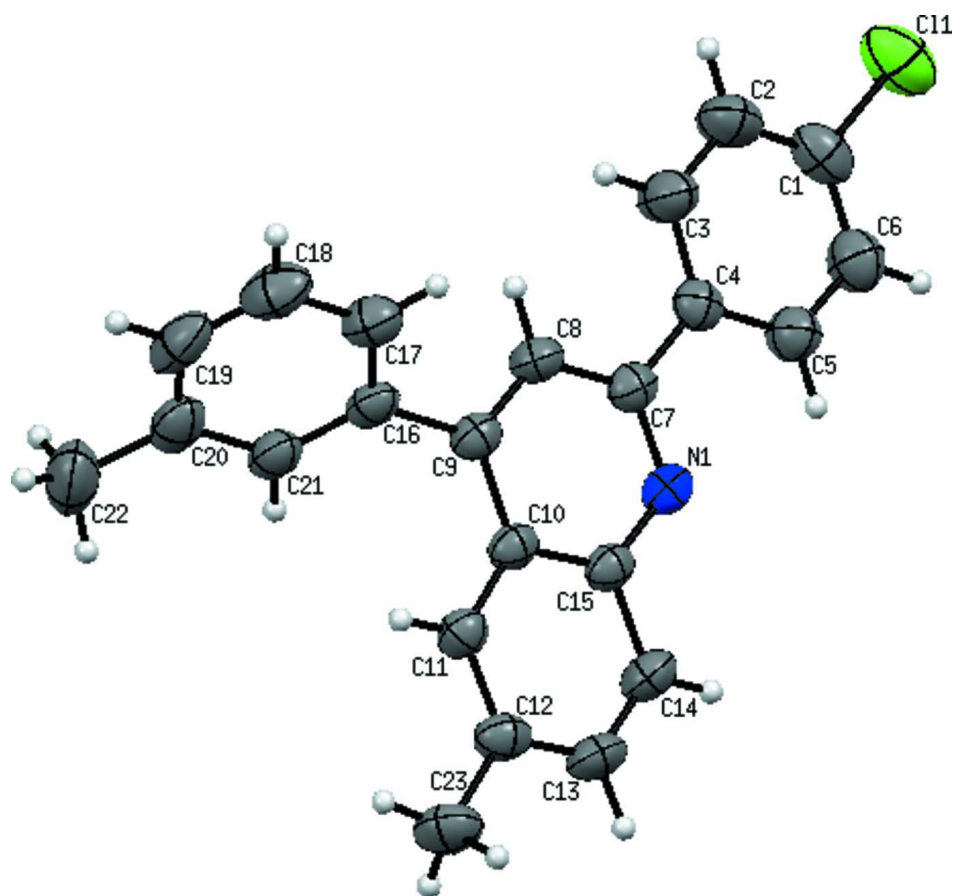
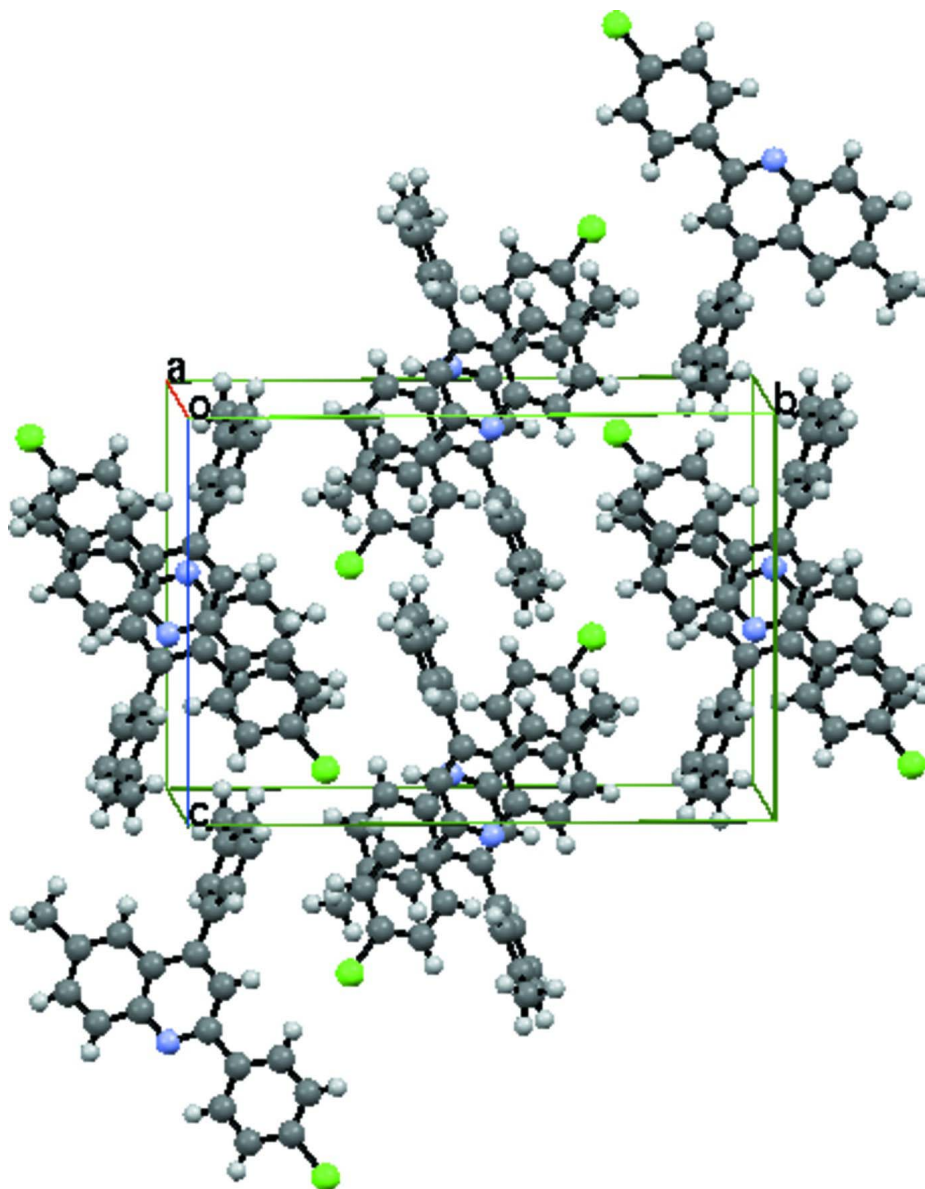


Figure 1

ORTEP diagram of the title compound showing 50% probability ellipsoids.

**Figure 2**

A packing diagram of the title compound, viewed along the crystallographic *a* axis.

2-(4-Chlorophenyl)-6-methyl-4-(3-methylphenyl)quinoline

Crystal data

$C_{23}H_{18}ClN$

$M_r = 343.83$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 7.982\ (3)\ \text{\AA}$

$b = 17.921\ (6)\ \text{\AA}$

$c = 12.478\ (4)\ \text{\AA}$

$\beta = 92.581\ (6)^\circ$

$V = 1783.1\ (11)\ \text{\AA}^3$

$Z = 4$

$F(000) = 720$

$D_x = 1.281\ \text{Mg m}^{-3}$

Melting point = 371–373 K

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3392 reflections

$\theta = 2.0\text{--}25.7^\circ$

$\mu = 0.22\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Block, yellow

$0.23 \times 0.22 \times 0.22\ \text{mm}$

Data collection

Oxford Diffraction Xcalibur CCD
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.0839 pixels mm⁻¹
 ω scans
16998 measured reflections

3392 independent reflections
2508 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$
 $\theta_{\text{max}} = 25.7^\circ$, $\theta_{\text{min}} = 2.0^\circ$
 $h = -9 \rightarrow 9$
 $k = -21 \rightarrow 21$
 $l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.168$
 $S = 1.04$
3392 reflections
228 parameters
0 restraints
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
 $w = 1/[\sigma^2(F_o^2) + (0.0922P)^2 + 0.5751P]$ $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.49 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.45 \text{ e } \text{\AA}^{-3}$

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 on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating $-R$ -factor-obs *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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| C11 | 0.89231 (10) | 1.22893 (5) | 0.85463 (6) | 0.0816 (3) |
| N1 | 1.2557 (2) | 0.97450 (10) | 0.55301 (13) | 0.0406 (6) |
| C1 | 0.9786 (3) | 1.17421 (15) | 0.7563 (2) | 0.0542 (8) |
| C2 | 0.9969 (4) | 1.20263 (15) | 0.6569 (2) | 0.0640 (9) |
| C3 | 1.0682 (4) | 1.15951 (14) | 0.5796 (2) | 0.0607 (9) |
| C4 | 1.1224 (3) | 1.08789 (12) | 0.60147 (17) | 0.0404 (7) |
| C5 | 1.0989 (3) | 1.06052 (14) | 0.70260 (18) | 0.0510 (8) |
| C6 | 1.0278 (3) | 1.10238 (15) | 0.7802 (2) | 0.0590 (9) |
| C7 | 1.2017 (2) | 1.04084 (11) | 0.52008 (17) | 0.0387 (6) |
| C8 | 1.2226 (3) | 1.06583 (11) | 0.41476 (17) | 0.0411 (6) |
| C9 | 1.2984 (3) | 1.02293 (11) | 0.34173 (16) | 0.0380 (6) |
| C10 | 1.3536 (2) | 0.95017 (11) | 0.37377 (16) | 0.0369 (6) |
| C11 | 1.4245 (3) | 0.89791 (11) | 0.30488 (18) | 0.0413 (7) |
| C12 | 1.4739 (3) | 0.82860 (11) | 0.33979 (19) | 0.0451 (7) |
| C13 | 1.4533 (3) | 0.81027 (12) | 0.44755 (19) | 0.0512 (8) |
| C14 | 1.3836 (3) | 0.85844 (12) | 0.51636 (19) | 0.0486 (7) |
| C15 | 1.3289 (2) | 0.92982 (11) | 0.48076 (16) | 0.0379 (6) |

| | | | | |
|------|------------|--------------|--------------|-------------|
| C16 | 1.3247 (3) | 1.05256 (11) | 0.23256 (16) | 0.0417 (7) |
| C17 | 1.1911 (3) | 1.08107 (13) | 0.17090 (18) | 0.0523 (8) |
| C18 | 1.2162 (4) | 1.10960 (14) | 0.0705 (2) | 0.0630 (10) |
| C19 | 1.3729 (4) | 1.11009 (13) | 0.03096 (19) | 0.0639 (9) |
| C20 | 1.5098 (4) | 1.08379 (13) | 0.0910 (2) | 0.0555 (8) |
| C21 | 1.4827 (3) | 1.05492 (11) | 0.19201 (18) | 0.0467 (7) |
| C22 | 1.6837 (4) | 1.08762 (18) | 0.0504 (3) | 0.0827 (11) |
| C23 | 1.5477 (4) | 0.77324 (13) | 0.2648 (2) | 0.0612 (9) |
| H2 | 0.96150 | 1.25100 | 0.64090 | 0.0770* |
| H3 | 1.07990 | 1.17910 | 0.51130 | 0.0730* |
| H5 | 1.13240 | 1.01200 | 0.71880 | 0.0610* |
| H6 | 1.01310 | 1.08260 | 0.84800 | 0.0710* |
| H8 | 1.18350 | 1.11290 | 0.39470 | 0.0490* |
| H11 | 1.43820 | 0.91080 | 0.23360 | 0.0500* |
| H13 | 1.48850 | 0.76370 | 0.47260 | 0.0610* |
| H14 | 1.37150 | 0.84460 | 0.58740 | 0.0580* |
| H17 | 1.08400 | 1.08090 | 0.19740 | 0.0630* |
| H18 | 1.12600 | 1.12860 | 0.02940 | 0.0750* |
| H19 | 1.38760 | 1.12850 | -0.03770 | 0.0770* |
| H21 | 1.57340 | 1.03670 | 0.23350 | 0.0560* |
| H22A | 1.75030 | 1.04790 | 0.08160 | 0.1240* |
| H22B | 1.73340 | 1.13470 | 0.06980 | 0.1240* |
| H22C | 1.67850 | 1.08260 | -0.02630 | 0.1240* |
| H23A | 1.47600 | 0.73030 | 0.25820 | 0.0920* |
| H23B | 1.65660 | 0.75820 | 0.29280 | 0.0920* |
| H23C | 1.55780 | 0.79580 | 0.19560 | 0.0920* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C11 | 0.0855 (6) | 0.0839 (6) | 0.0764 (5) | 0.0060 (4) | 0.0149 (4) | -0.0363 (4) |
| N1 | 0.0447 (10) | 0.0354 (9) | 0.0415 (10) | -0.0025 (8) | 0.0002 (8) | 0.0039 (7) |
| C1 | 0.0449 (13) | 0.0615 (16) | 0.0562 (14) | -0.0035 (11) | 0.0027 (11) | -0.0205 (12) |
| C2 | 0.0766 (18) | 0.0471 (14) | 0.0690 (17) | 0.0126 (13) | 0.0111 (14) | -0.0059 (13) |
| C3 | 0.0819 (19) | 0.0481 (14) | 0.0527 (14) | 0.0151 (13) | 0.0097 (13) | 0.0048 (11) |
| C4 | 0.0347 (11) | 0.0415 (12) | 0.0448 (12) | -0.0022 (9) | -0.0009 (9) | -0.0023 (9) |
| C5 | 0.0576 (14) | 0.0497 (13) | 0.0457 (13) | 0.0044 (11) | 0.0039 (10) | 0.0013 (10) |
| C6 | 0.0653 (16) | 0.0642 (16) | 0.0477 (13) | 0.0006 (13) | 0.0060 (12) | -0.0022 (11) |
| C7 | 0.0359 (11) | 0.0364 (11) | 0.0433 (11) | -0.0029 (8) | -0.0032 (9) | 0.0012 (9) |
| C8 | 0.0463 (12) | 0.0325 (10) | 0.0441 (11) | 0.0039 (9) | -0.0012 (9) | 0.0032 (9) |
| C9 | 0.0396 (11) | 0.0340 (10) | 0.0401 (11) | -0.0022 (9) | -0.0026 (9) | 0.0023 (8) |
| C10 | 0.0356 (11) | 0.0307 (10) | 0.0438 (11) | -0.0037 (8) | -0.0036 (8) | 0.0026 (8) |
| C11 | 0.0454 (12) | 0.0345 (11) | 0.0440 (11) | -0.0031 (9) | 0.0015 (9) | 0.0000 (9) |
| C12 | 0.0448 (13) | 0.0326 (11) | 0.0576 (13) | -0.0005 (9) | -0.0018 (10) | -0.0033 (10) |
| C13 | 0.0620 (15) | 0.0300 (11) | 0.0612 (15) | 0.0031 (10) | -0.0007 (12) | 0.0081 (10) |
| C14 | 0.0601 (14) | 0.0359 (11) | 0.0496 (13) | -0.0009 (10) | -0.0005 (11) | 0.0109 (9) |
| C15 | 0.0370 (11) | 0.0322 (10) | 0.0441 (11) | -0.0042 (8) | -0.0016 (9) | 0.0030 (8) |
| C16 | 0.0567 (13) | 0.0268 (10) | 0.0415 (11) | 0.0019 (9) | 0.0021 (10) | 0.0002 (8) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C17 | 0.0626 (16) | 0.0441 (13) | 0.0495 (13) | 0.0051 (11) | -0.0037 (11) | 0.0025 (10) |
| C18 | 0.089 (2) | 0.0514 (15) | 0.0472 (14) | 0.0086 (13) | -0.0120 (14) | 0.0055 (11) |
| C19 | 0.112 (2) | 0.0409 (13) | 0.0391 (12) | -0.0041 (14) | 0.0070 (14) | 0.0062 (10) |
| C20 | 0.0813 (18) | 0.0334 (11) | 0.0529 (14) | -0.0071 (11) | 0.0155 (13) | -0.0022 (10) |
| C21 | 0.0614 (14) | 0.0315 (11) | 0.0476 (12) | 0.0009 (10) | 0.0061 (10) | 0.0026 (9) |
| C22 | 0.102 (2) | 0.0675 (18) | 0.082 (2) | -0.0143 (17) | 0.0404 (18) | 0.0048 (16) |
| C23 | 0.0752 (18) | 0.0396 (13) | 0.0686 (17) | 0.0096 (12) | 0.0006 (14) | -0.0068 (11) |

Geometric parameters (Å, °)

| | | | |
|-----------|-------------|-------------|-----------|
| C11—C1 | 1.737 (3) | C17—C18 | 1.376 (3) |
| N1—C7 | 1.324 (3) | C18—C19 | 1.365 (4) |
| N1—C15 | 1.358 (3) | C19—C20 | 1.380 (4) |
| C1—C2 | 1.355 (4) | C20—C21 | 1.388 (3) |
| C1—C6 | 1.375 (4) | C20—C22 | 1.501 (5) |
| C2—C3 | 1.379 (4) | C2—H2 | 0.9300 |
| C3—C4 | 1.378 (3) | C3—H3 | 0.9300 |
| C4—C5 | 1.375 (3) | C5—H5 | 0.9300 |
| C4—C7 | 1.484 (3) | C6—H6 | 0.9300 |
| C5—C6 | 1.368 (3) | C8—H8 | 0.9300 |
| C7—C8 | 1.405 (3) | C11—H11 | 0.9300 |
| C8—C9 | 1.355 (3) | C13—H13 | 0.9300 |
| C9—C10 | 1.428 (3) | C14—H14 | 0.9300 |
| C9—C16 | 1.486 (3) | C17—H17 | 0.9300 |
| C10—C11 | 1.407 (3) | C18—H18 | 0.9300 |
| C10—C15 | 1.406 (3) | C19—H19 | 0.9300 |
| C11—C12 | 1.368 (3) | C21—H21 | 0.9300 |
| C12—C13 | 1.401 (3) | C22—H22A | 0.9600 |
| C12—C23 | 1.502 (3) | C22—H22B | 0.9600 |
| C13—C14 | 1.355 (3) | C22—H22C | 0.9600 |
| C14—C15 | 1.417 (3) | C23—H23A | 0.9600 |
| C16—C17 | 1.384 (3) | C23—H23B | 0.9600 |
| C16—C21 | 1.381 (3) | C23—H23C | 0.9600 |
| C7—N1—C15 | 117.87 (17) | C21—C20—C22 | 120.5 (3) |
| C11—C1—C2 | 119.8 (2) | C16—C21—C20 | 121.8 (2) |
| C11—C1—C6 | 119.60 (19) | C1—C2—H2 | 120.00 |
| C2—C1—C6 | 120.6 (2) | C3—C2—H2 | 120.00 |
| C1—C2—C3 | 119.7 (2) | C2—C3—H3 | 119.00 |
| C2—C3—C4 | 121.3 (2) | C4—C3—H3 | 119.00 |
| C3—C4—C5 | 117.4 (2) | C4—C5—H5 | 119.00 |
| C3—C4—C7 | 122.3 (2) | C6—C5—H5 | 119.00 |
| C5—C4—C7 | 120.4 (2) | C1—C6—H6 | 121.00 |
| C4—C5—C6 | 122.2 (2) | C5—C6—H6 | 121.00 |
| C1—C6—C5 | 118.9 (2) | C7—C8—H8 | 119.00 |
| N1—C7—C4 | 116.17 (18) | C9—C8—H8 | 119.00 |
| N1—C7—C8 | 121.72 (18) | C10—C11—H11 | 119.00 |
| C4—C7—C8 | 122.09 (18) | C12—C11—H11 | 119.00 |

| | | | |
|---------------|--------------|-----------------|--------------|
| C7—C8—C9 | 121.55 (19) | C12—C13—H13 | 119.00 |
| C8—C9—C10 | 118.12 (18) | C14—C13—H13 | 119.00 |
| C8—C9—C16 | 119.97 (18) | C13—C14—H14 | 120.00 |
| C10—C9—C16 | 121.91 (18) | C15—C14—H14 | 120.00 |
| C9—C10—C11 | 124.36 (19) | C16—C17—H17 | 120.00 |
| C9—C10—C15 | 116.61 (17) | C18—C17—H17 | 120.00 |
| C11—C10—C15 | 119.00 (18) | C17—C18—H18 | 120.00 |
| C10—C11—C12 | 121.9 (2) | C19—C18—H18 | 120.00 |
| C11—C12—C13 | 118.3 (2) | C18—C19—H19 | 119.00 |
| C11—C12—C23 | 121.1 (2) | C20—C19—H19 | 119.00 |
| C13—C12—C23 | 120.61 (19) | C16—C21—H21 | 119.00 |
| C12—C13—C14 | 121.9 (2) | C20—C21—H21 | 119.00 |
| C13—C14—C15 | 120.4 (2) | C20—C22—H22A | 109.00 |
| N1—C15—C10 | 124.08 (18) | C20—C22—H22B | 109.00 |
| N1—C15—C14 | 117.40 (18) | C20—C22—H22C | 109.00 |
| C10—C15—C14 | 118.52 (18) | H22A—C22—H22B | 110.00 |
| C9—C16—C17 | 120.3 (2) | H22A—C22—H22C | 109.00 |
| C9—C16—C21 | 121.1 (2) | H22B—C22—H22C | 109.00 |
| C17—C16—C21 | 118.6 (2) | C12—C23—H23A | 109.00 |
| C16—C17—C18 | 120.2 (2) | C12—C23—H23B | 109.00 |
| C17—C18—C19 | 120.3 (3) | C12—C23—H23C | 109.00 |
| C18—C19—C20 | 121.2 (2) | H23A—C23—H23B | 109.00 |
| C19—C20—C21 | 117.9 (3) | H23A—C23—H23C | 110.00 |
| C19—C20—C22 | 121.5 (2) | H23B—C23—H23C | 110.00 |
| | | | |
| C15—N1—C7—C8 | -1.7 (3) | C8—C9—C10—C11 | 175.9 (2) |
| C7—N1—C15—C14 | -178.93 (18) | C10—C9—C16—C21 | -54.9 (3) |
| C7—N1—C15—C10 | 1.2 (3) | C10—C9—C16—C17 | 127.5 (2) |
| C15—N1—C7—C4 | 179.95 (17) | C15—C10—C11—C12 | -1.7 (3) |
| C11—C1—C6—C5 | -178.59 (19) | C9—C10—C15—N1 | 0.6 (3) |
| C11—C1—C2—C3 | 178.8 (2) | C11—C10—C15—N1 | -177.30 (18) |
| C6—C1—C2—C3 | -1.1 (4) | C11—C10—C15—C14 | 2.8 (3) |
| C2—C1—C6—C5 | 1.4 (4) | C9—C10—C15—C14 | -179.27 (19) |
| C1—C2—C3—C4 | -0.4 (5) | C9—C10—C11—C12 | -179.4 (2) |
| C2—C3—C4—C7 | -179.1 (2) | C10—C11—C12—C23 | 179.4 (2) |
| C2—C3—C4—C5 | 1.5 (4) | C10—C11—C12—C13 | -0.4 (3) |
| C3—C4—C7—N1 | 176.7 (2) | C23—C12—C13—C14 | -178.5 (2) |
| C5—C4—C7—C8 | 177.7 (2) | C11—C12—C13—C14 | 1.3 (4) |
| C5—C4—C7—N1 | -3.9 (3) | C12—C13—C14—C15 | -0.1 (4) |
| C3—C4—C5—C6 | -1.3 (4) | C13—C14—C15—C10 | -2.0 (3) |
| C7—C4—C5—C6 | 179.3 (2) | C13—C14—C15—N1 | 178.1 (2) |
| C3—C4—C7—C8 | -1.6 (3) | C9—C16—C17—C18 | 178.9 (2) |
| C4—C5—C6—C1 | -0.1 (4) | C21—C16—C17—C18 | 1.3 (3) |
| N1—C7—C8—C9 | 0.3 (3) | C9—C16—C21—C20 | -178.7 (2) |
| C4—C7—C8—C9 | 178.6 (2) | C17—C16—C21—C20 | -1.1 (3) |
| C7—C8—C9—C10 | 1.5 (3) | C16—C17—C18—C19 | -0.1 (4) |
| C7—C8—C9—C16 | -177.4 (2) | C17—C18—C19—C20 | -1.5 (4) |
| C8—C9—C10—C15 | -1.9 (3) | C18—C19—C20—C21 | 1.7 (4) |

| | | | |
|----------------|-------------|-----------------|------------|
| C16—C9—C10—C11 | −5.3 (3) | C18—C19—C20—C22 | −176.9 (2) |
| C8—C9—C16—C17 | −53.6 (3) | C19—C20—C21—C16 | −0.4 (3) |
| C8—C9—C16—C21 | 123.9 (2) | C22—C20—C21—C16 | 178.2 (2) |
| C16—C9—C10—C15 | 176.97 (19) | | |

Hydrogen-bond geometry (Å, °)

| <i>D—H⋯A</i> | <i>D—H</i> | <i>H⋯A</i> | <i>D⋯A</i> | <i>D—H⋯A</i> |
|--------------|------------|------------|------------|--------------|
| C5—H5⋯N1 | 0.93 | 2.43 | 2.764 (3) | 101 |