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N-[(2-Chloro-3-quinoly)methyl]-4-fluoroaniline

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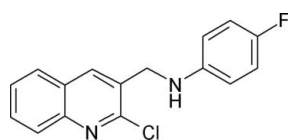
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.034; wR factor = 0.094; data-to-parameter ratio = 21.7.

In the title compound, $\text{C}_{16}\text{H}_{12}\text{ClFN}_2$, the dihedral angle between the quinoline ring system and the fluoro-phenyl ring is $86.70(4)^\circ$. In the crystal, molecules are linked into chains along the a axis by $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds. In addition, $\text{C}-\text{H}\cdots\pi$ interactions involving the two benzene rings are observed.

Related literature

For general background, properties and the biological activity of quinolines, see: Campbell *et al.* (1988); Dutta *et al.* (2002); Markees *et al.* (1970); Meth-Cohn *et al.* (1981); Michael *et al.* (1997); Morimoto *et al.* (1991); Padwa *et al.* (1999); Rajendran & Karavembu (2002); Robert & Meunier *et al.* (1998). For the synthesis of quinolines, see: Kouznetsov *et al.* (2005). For related structures, see: Butcher *et al.* (2007); Lynch *et al.* (2001); Subashini *et al.* (2009); Yathirajan *et al.* (2007); Wu *et al.* (2009); Khan *et al.* (2010). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_{16}\text{H}_{12}\text{ClFN}_2$
 $M_r = 286.73$
 Triclinic, $P\bar{1}$
 $a = 7.3661(8)$ Å
 $b = 8.8967(9)$ Å
 $c = 11.5129(12)$ Å
 $\alpha = 68.704(1)^\circ$
 $\beta = 74.468(1)^\circ$

$\gamma = 75.445(1)^\circ$
 $V = 667.25(12)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.29$ mm⁻¹
 $T = 100$ K
 $0.55 \times 0.50 \times 0.25$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2008)
 $T_{\min} = 0.858$, $T_{\max} = 0.932$
 8162 measured reflections
 3930 independent reflections
 3633 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.014$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.094$
 $S = 1.03$
 3930 reflections
 181 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.49$ e Å⁻³
 $\Delta\rho_{\min} = -0.30$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 and Cg2 are the centroids of the C1–C6 and C11–C16 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N2}-\text{H18}\cdots\text{N1}^{\text{i}}$	0.86	2.30	3.1353 (12)	165
$\text{C4}-\text{H4}\cdots\text{Cg2}^{\text{ii}}$	0.93	2.91	3.7494 (13)	151
$\text{C10}-\text{H10A}\cdots\text{Cg1}^{\text{iii}}$	0.97	2.62	3.5365 (12)	157
$\text{C10}-\text{H10B}\cdots\text{Cg2}^{\text{iv}}$	0.97	2.98	3.8083 (11)	145

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+2, -y+1, -z+1$; (iii) $-x+2, -y, -z+1$; (iv) $-x+1, -y, -z+2$.

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); 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: CI5158).

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supporting information

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***N*-[(2-Chloro-3-quinoly)methyl]-4-fluoroaniline**

Jerry P. Jasinski, Albert E. Pek, C. S. Chidan Kumar, H. S. Yathirajan and Suresh Kumar

S1. Comment

Quinoline derivatives represent a major class of heterocycles, and a number of preparations using them have been known since the late 1800s. Quinolines are found in natural products (Morimoto *et al.*, 1991; Michael *et al.*, 1997), numerous commercial products, including fragrances, dyes (Padwa *et al.*, 1999) and biologically active compounds (Markees *et al.*, 1970; Campbell *et al.*, 1988). Quinoline alkaloids such as quinine, chloroquin, mefloquine and amodiaquine are used as efficient drugs for the treatment of malaria (Robert & Meunier, 1998). Several quinoline derivatives have been evaluated *in vitro* against a number of parasites of HTLV-1 transformed cells. 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). A review on recent progress in the synthesis of quinolines (Kouznetsov *et al.* 2005) has been described. The crystal structure studies of 8-chloro-2-methylquinoline (Wu *et al.*, 2009), 2-chloro-4-methylquinoline (Lynch *et al.*, 2001), 4-chloro-8-(trifluoromethyl)quinoline (Yathirajan *et al.*, 2007), 1-(quinolin-2-yl)ethanone (Butcher *et al.*, 2007) and 2-chloro-7-methylquinoline-3-carbaldehyde (Subashini *et al.*, 2009) have been reported. In view of the importance of quinolines, the paper reports the synthesis and crystal structure of the title compound.

In the title molecule (Fig. 1), the 2-chloroquinoline ring system and 4-fluoroaniline ring are bonded to a methane carbon, C10. The dihedral angle between the mean planes of the planar chloroquinoline ring system (dihedral angle between rings = 0.92 (5)°) and the fluoroaniline ring is 86.70 (4)°. Bond distances (Allen *et al.*, 1987) and angles are in normal ranges.

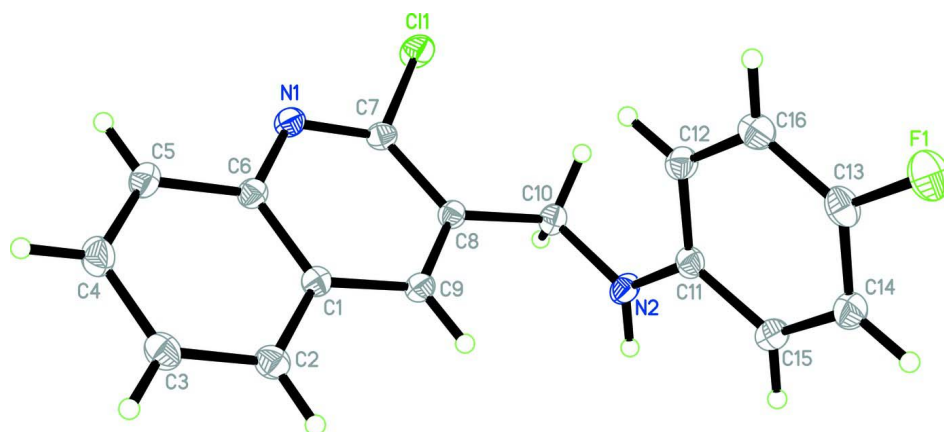
The molecules are linked into chains along the *a* axis by N—H···N hydrogen bonds (Fig. 2). In addition, C—H··· π interactions involving the two benzene rings (Table 1) influence crystal packing in the unit cell.

S2. Experimental

In a mixture of 3-(chloromethyl)-2-chloroquinoline (0.003 mol) and substituted phenyl amine (0.003 mol) in 20 ml of absolute ethanol, 1 ml of triethylamine (TEA) was added and refluxed for 12–15 hrs (Fig. 3). After completion of the reaction, content of the flask was reduced to half and left overnight. The crystalline mass obtained was filtered off, washed with water, dried and re-crystallized from ethanol to give *N*-[(2-chloroquinolin-3-yl)methyl]-4-fluoroaniline. X-ray quality crystals were obtained by slow evaporation of a methanol solution (m.p. 413–415 K).

S3. Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with atom—H lengths of 0.93 Å (CH), 0.97 Å (CH₂) or 0.86 Å (NH). Isotropic displacement parameters for these atoms were set to 1.2 times U_{eq} of the parent atom.

**Figure 1**

Molecular structure of the title compound, showing the atom-labeling scheme and 50% probability displacement ellipsoids.

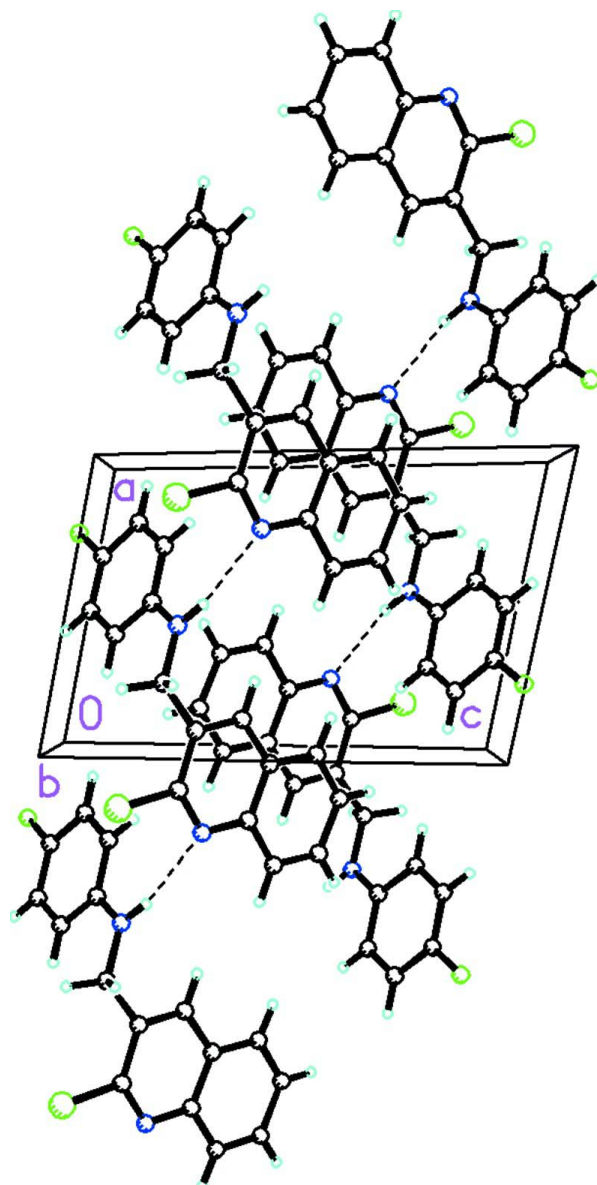


Figure 2

Packing diagram of the title compound, viewed down the *b* axis. Dashed lines indicate weak N—H...N hydrogen bonds.

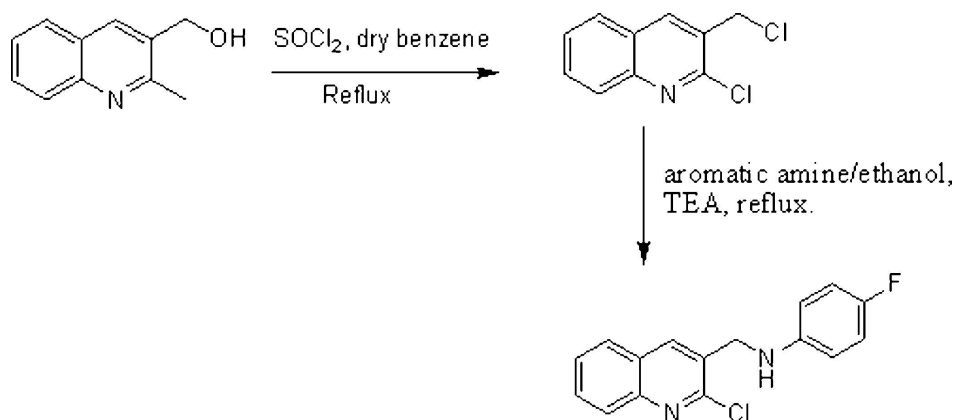


Figure 3

Reaction scheme for the title compound.

N-[(2-Chloro-3-quinolyl)methyl]-4-fluoroaniline

Crystal data

$\text{C}_{16}\text{H}_{12}\text{ClFN}_2$
 $M_r = 286.73$
 Triclinic, $P\bar{1}$
 Hall symbol: -P 1
 $a = 7.3661$ (8) Å
 $b = 8.8967$ (9) Å
 $c = 11.5129$ (12) Å
 $\alpha = 68.704$ (1)°
 $\beta = 74.468$ (1)°
 $\gamma = 75.445$ (1)°
 $V = 667.25$ (12) Å³

$Z = 2$
 $F(000) = 296$
 $D_x = 1.427$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 5222 reflections
 $\theta = 2.5\text{--}31.0^\circ$
 $\mu = 0.29$ mm⁻¹
 $T = 100$ K
 Plate, colourless
 $0.55 \times 0.50 \times 0.25$ mm

Data collection

Bruker APEXII CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2008)
 $T_{\min} = 0.858$, $T_{\max} = 0.932$

8162 measured reflections
 3930 independent reflections
 3633 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.014$
 $\theta_{\max} = 31.4^\circ$, $\theta_{\min} = 1.9^\circ$
 $h = -10 \rightarrow 10$
 $k = -12 \rightarrow 12$
 $l = -16 \rightarrow 16$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.094$
 $S = 1.03$
 3930 reflections
 181 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
 $w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.2404P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.49$ e Å⁻³
 $\Delta\rho_{\min} = -0.30$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	1.15120 (4)	-0.21591 (3)	0.79554 (2)	0.02245 (8)
N1	1.24567 (12)	0.03932 (10)	0.60973 (8)	0.01634 (16)
N2	0.55793 (12)	0.03799 (11)	0.74940 (8)	0.01744 (17)
H18	0.4905	0.0291	0.7025	0.021*
F1	0.24347 (10)	0.46529 (9)	1.02706 (7)	0.02663 (16)
C7	1.09918 (14)	-0.03020 (11)	0.67819 (9)	0.01494 (17)
C1	1.02460 (14)	0.25805 (11)	0.49326 (9)	0.01455 (17)
C10	0.74539 (14)	-0.05999 (12)	0.75411 (9)	0.01625 (18)
H10A	0.7513	-0.1557	0.7308	0.020*
H10B	0.7657	-0.0977	0.8407	0.020*
C8	0.90473 (13)	0.03112 (11)	0.66692 (9)	0.01406 (17)
C5	1.36831 (15)	0.26375 (13)	0.44050 (10)	0.01949 (19)
H5	1.4913	0.2165	0.4552	0.023*
C6	1.21153 (14)	0.18553 (12)	0.51570 (9)	0.01520 (17)
C9	0.87191 (13)	0.17731 (12)	0.57294 (9)	0.01522 (17)
H9	0.7474	0.2240	0.5615	0.018*
C14	0.21346 (15)	0.33659 (13)	0.88812 (10)	0.0206 (2)
H14	0.0879	0.3910	0.8882	0.025*
C11	0.48346 (14)	0.14581 (12)	0.81816 (9)	0.01552 (18)
C2	0.99836 (15)	0.40819 (12)	0.39406 (9)	0.01792 (19)
H17	0.8764	0.4568	0.3777	0.022*
C13	0.32377 (16)	0.36116 (12)	0.95720 (10)	0.01941 (19)
C3	1.15214 (16)	0.48201 (13)	0.32212 (10)	0.01972 (19)
H3	1.1338	0.5806	0.2572	0.024*
C12	0.59034 (14)	0.17592 (12)	0.88891 (9)	0.01760 (18)
H12	0.7166	0.1235	0.8889	0.021*
C4	1.33828 (16)	0.40979 (13)	0.34565 (10)	0.0210 (2)
H4	1.4413	0.4616	0.2965	0.025*
C15	0.29365 (14)	0.22899 (13)	0.81854 (10)	0.01916 (19)
H15	0.2208	0.2116	0.7714	0.023*
C16	0.50987 (15)	0.28339 (13)	0.95926 (10)	0.01933 (19)
H16	0.5809	0.3021	1.0068	0.023*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.01931 (13)	0.01748 (12)	0.02433 (13)	-0.00220 (9)	-0.00775 (9)	0.00240 (9)
N1	0.0150 (4)	0.0161 (4)	0.0176 (4)	-0.0027 (3)	-0.0047 (3)	-0.0039 (3)
N2	0.0128 (4)	0.0214 (4)	0.0208 (4)	-0.0023 (3)	-0.0036 (3)	-0.0099 (3)
F1	0.0308 (4)	0.0241 (3)	0.0268 (3)	-0.0030 (3)	-0.0011 (3)	-0.0146 (3)
C7	0.0154 (4)	0.0129 (4)	0.0162 (4)	-0.0015 (3)	-0.0049 (3)	-0.0037 (3)
C1	0.0149 (4)	0.0143 (4)	0.0149 (4)	-0.0024 (3)	-0.0030 (3)	-0.0052 (3)
C10	0.0139 (4)	0.0152 (4)	0.0183 (4)	-0.0028 (3)	-0.0019 (3)	-0.0045 (3)
C8	0.0137 (4)	0.0142 (4)	0.0148 (4)	-0.0028 (3)	-0.0028 (3)	-0.0049 (3)
C5	0.0159 (4)	0.0216 (5)	0.0208 (5)	-0.0063 (4)	-0.0028 (3)	-0.0050 (4)
C6	0.0147 (4)	0.0157 (4)	0.0161 (4)	-0.0033 (3)	-0.0033 (3)	-0.0054 (3)
C9	0.0134 (4)	0.0156 (4)	0.0164 (4)	-0.0016 (3)	-0.0037 (3)	-0.0049 (3)
C14	0.0181 (4)	0.0211 (5)	0.0200 (5)	-0.0001 (4)	-0.0030 (4)	-0.0063 (4)
C11	0.0152 (4)	0.0152 (4)	0.0143 (4)	-0.0044 (3)	-0.0012 (3)	-0.0025 (3)
C2	0.0197 (4)	0.0159 (4)	0.0169 (4)	-0.0022 (3)	-0.0044 (3)	-0.0035 (3)
C13	0.0242 (5)	0.0161 (4)	0.0165 (4)	-0.0047 (4)	-0.0001 (4)	-0.0054 (3)
C3	0.0239 (5)	0.0166 (4)	0.0174 (4)	-0.0054 (4)	-0.0037 (4)	-0.0029 (3)
C12	0.0165 (4)	0.0180 (4)	0.0180 (4)	-0.0051 (3)	-0.0030 (3)	-0.0043 (3)
C4	0.0210 (5)	0.0212 (5)	0.0202 (5)	-0.0088 (4)	-0.0012 (4)	-0.0043 (4)
C15	0.0165 (4)	0.0220 (5)	0.0196 (4)	-0.0016 (4)	-0.0051 (3)	-0.0073 (4)
C16	0.0221 (5)	0.0199 (4)	0.0175 (4)	-0.0077 (4)	-0.0037 (4)	-0.0050 (4)

Geometric parameters (Å, °)

Cl1—C7	1.7434 (10)	C5—H5	0.93
N1—C7	1.3016 (13)	C9—H9	0.93
N1—C6	1.3732 (12)	C14—C13	1.3792 (15)
N2—C11	1.3792 (12)	C14—C15	1.3878 (14)
N2—C10	1.4388 (13)	C14—H14	0.93
N2—H18	0.86	C11—C12	1.4011 (14)
F1—C13	1.3661 (12)	C11—C15	1.4077 (14)
C7—C8	1.4217 (13)	C2—C3	1.3700 (14)
C1—C9	1.4133 (13)	C2—H17	0.93
C1—C6	1.4149 (13)	C13—C16	1.3737 (15)
C1—C2	1.4164 (13)	C3—C4	1.4128 (15)
C10—C8	1.5161 (13)	C3—H3	0.93
C10—H10A	0.97	C12—C16	1.3936 (14)
C10—H10B	0.97	C12—H12	0.93
C8—C9	1.3714 (13)	C4—H4	0.93
C5—C4	1.3726 (15)	C15—H15	0.93
C5—C6	1.4136 (13)	C16—H16	0.93
C7—N1—C6	117.48 (8)	C13—C14—C15	118.66 (10)
C11—N2—C10	121.76 (8)	C13—C14—H14	120.7
C11—N2—H18	119.1	C15—C14—H14	120.7
C10—N2—H18	119.1	N2—C11—C12	122.23 (9)

N1—C7—C8	126.51 (9)	N2—C11—C15	119.59 (9)
N1—C7—C11	115.47 (7)	C12—C11—C15	118.18 (9)
C8—C7—C11	118.01 (7)	C3—C2—C1	120.15 (9)
C9—C1—C6	117.92 (9)	C3—C2—H17	119.9
C9—C1—C2	123.09 (9)	C1—C2—H17	119.9
C6—C1—C2	118.98 (9)	F1—C13—C16	119.13 (9)
N2—C10—C8	113.32 (8)	F1—C13—C14	118.49 (9)
N2—C10—H10A	108.9	C16—C13—C14	122.38 (10)
C8—C10—H10A	108.9	C2—C3—C4	120.64 (9)
N2—C10—H10B	108.9	C2—C3—H3	119.7
C8—C10—H10B	108.9	C4—C3—H3	119.7
H10A—C10—H10B	107.7	C16—C12—C11	120.86 (9)
C9—C8—C7	115.61 (8)	C16—C12—H12	119.6
C9—C8—C10	122.70 (8)	C11—C12—H12	119.6
C7—C8—C10	121.69 (8)	C5—C4—C3	120.52 (9)
C4—C5—C6	119.71 (9)	C5—C4—H4	119.7
C4—C5—H5	120.1	C3—C4—H4	119.7
C6—C5—H5	120.1	C14—C15—C11	121.05 (9)
N1—C6—C5	118.51 (9)	C14—C15—H15	119.5
N1—C6—C1	121.50 (9)	C11—C15—H15	119.5
C5—C6—C1	119.99 (9)	C13—C16—C12	118.87 (9)
C8—C9—C1	120.95 (9)	C13—C16—H16	120.6
C8—C9—H9	119.5	C12—C16—H16	120.6
C1—C9—H9	119.5		
C6—N1—C7—C8	-0.94 (15)	C6—C1—C9—C8	-1.63 (14)
C6—N1—C7—C11	179.70 (7)	C2—C1—C9—C8	179.30 (9)
C11—N2—C10—C8	-82.06 (11)	C10—N2—C11—C12	4.96 (14)
N1—C7—C8—C9	0.82 (15)	C10—N2—C11—C15	-174.83 (9)
C11—C7—C8—C9	-179.83 (7)	C9—C1—C2—C3	178.48 (9)
N1—C7—C8—C10	-178.91 (9)	C6—C1—C2—C3	-0.58 (15)
C11—C7—C8—C10	0.43 (13)	C15—C14—C13—F1	-179.04 (9)
N2—C10—C8—C9	-14.02 (13)	C15—C14—C13—C16	0.18 (16)
N2—C10—C8—C7	165.69 (9)	C1—C2—C3—C4	0.04 (16)
C7—N1—C6—C5	179.69 (9)	N2—C11—C12—C16	-178.83 (9)
C7—N1—C6—C1	-0.29 (14)	C15—C11—C12—C16	0.96 (14)
C4—C5—C6—N1	179.83 (9)	C6—C5—C4—C3	-0.37 (16)
C4—C5—C6—C1	-0.19 (15)	C2—C3—C4—C5	0.44 (16)
C9—C1—C6—N1	1.53 (14)	C13—C14—C15—C11	0.14 (16)
C2—C1—C6—N1	-179.36 (9)	N2—C11—C15—C14	179.10 (9)
C9—C1—C6—C5	-178.45 (9)	C12—C11—C15—C14	-0.70 (15)
C2—C1—C6—C5	0.65 (14)	F1—C13—C16—C12	179.30 (9)
C7—C8—C9—C1	0.55 (14)	C14—C13—C16—C12	0.08 (16)
C10—C8—C9—C1	-179.73 (8)	C11—C12—C16—C13	-0.67 (15)

Hydrogen-bond geometry (Å, °)

Cg1 and Cg2 are the centroids of the C1–C6 and C11–C16 rings, respectively.

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N2—H18 \cdots N1 ⁱ	0.86	2.30	3.1353 (12)	165
C4—H4 \cdots Cg2 ⁱⁱ	0.93	2.91	3.7494 (13)	151
C10—H10 <i>A</i> \cdots Cg1 ⁱⁱⁱ	0.97	2.62	3.5365 (12)	157
C10—H10 <i>B</i> \cdots Cg2 ^{iv}	0.97	2.98	3.8083 (11)	145

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+2, -y+1, -z+1$; (iii) $-x+2, -y, -z+1$; (iv) $-x+1, -y, -z+2$.