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## 2-(2-Chloro-8-methylquinolin-3-yl)-4-phenyl-1,2-dihydroquinazoline

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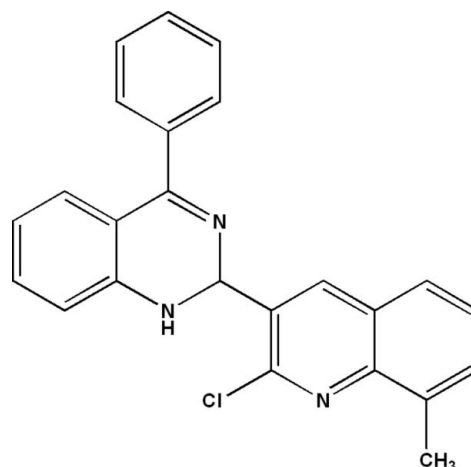
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Key indicators: single-crystal X-ray study;  $T = 150$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.031;  $wR$  factor = 0.082; data-to-parameter ratio = 12.9.

In the title compound,  $\text{C}_{24}\text{H}_{18}\text{ClN}_3$ , the dihydroquinazoline and methyl-substituted quinoline benzene rings make a dihedral angle of  $78.18(4)^\circ$  and form dihedral angles of  $45.91(5)$  and  $79.80(4)^\circ$ , respectively, with the phenyl ring. The dihedral angle between the phenyl ring of dihydroquinazoline and the methyl-substituted benzene ring of quinoline is  $78.18(4)^\circ$ . The crystal packing can be described as crossed layers parallel to the (011) and (0 $\bar{1}$ 1) planes. The structure features  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds and  $\pi-\pi$  interactions [centroid-centroid distance between phenyl rings =  $3.7301(9)$  Å].

### Related literature

For the preparation and applications of quinazoline and quinoline derivatives, see: Jenekhe *et al.* (2001); Hoemann *et al.* (2000); Connolly *et al.* (2005); Besson *et al.* (2007); Roma *et al.* (2000); Chen *et al.* (2001); Debache *et al.* (2008, 2009); Nemouchi *et al.* (2012).



### Experimental

#### Crystal data

$\text{C}_{24}\text{H}_{18}\text{ClN}_3$   
 $M_r = 383.86$   
 Monoclinic,  $P2_1/c$   
 $a = 14.4553(13)$  Å  
 $b = 8.7501(9)$  Å  
 $c = 16.8630(16)$  Å  
 $\beta = 119.696(6)^\circ$   
 $V = 1852.8(3)$  Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.22$  mm<sup>-1</sup>  
 $T = 150$  K  
 $0.12 \times 0.04 \times 0.02$  mm

#### Data collection

Bruker APEXII CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 2002)  
 $T_{\min} = 0.959$ ,  $T_{\max} = 1.000$   
 10282 measured reflections  
 3276 independent reflections  
 2894 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.082$   
 $S = 1.06$   
 3276 reflections  
 254 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.26$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.26$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N3}-\text{H3N}\cdots\text{N2}^i$	0.86	2.26	3.0998 (18)	165

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

Data collection: APEX2 (Bruker, 2011); cell refinement: SAINT (Bruker, 2011); data reduction: SAINT; program(s) used to solve structure: SIR2002 (Burla *et al.*, 2003); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012) and DIAMOND (Brandenburg & Berndt, 2001); software used to prepare material for publication: WinGX (Farrugia, 2012).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5353).

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## supporting information

*Acta Cryst.* (2013). E69, o1719–o1720 [doi:10.1107/S1600536813029334]

## 2-(2-Chloro-8-methylquinolin-3-yl)-4-phenyl-1,2-dihydroquinazoline

Chamseddine Derabli, Raouf Boulcina, Sofiane Bouacida, Hocine Merazig and Abdelmadjid Debache

### S1. Comment

It is well known that the quinoline ring system is an important structural unit widely existing in alkaloids, therapeutics and synthetic analogues with interesting biological activities (Roma *et al.*, 2000; Chen *et al.*, 2001). In addition quinolines are valuable synthons for the preparation of nano- and *meso*-structures with enhanced electronic and photonic functions (Jenekhe *et al.*, 2001). Due to their importance as substructures in a broad range of natural and designed products, significant efforts continue to be directed into the development of new quinoline-based structures (Hoemann *et al.*, 2000). In the other hand, the quinazoline unit represents a useful natural product scaffold with demonstrated activities against numerous disorders. The transferable nature of its properties provides a strong rationale for the development of synthetic methods. Not surprisingly, considerable progress in synthetic methodology applicable to quinazoline alkaloids has been made during the past decade (Connolly *et al.*, 2005; Besson *et al.*, 2007). As part of our research in developing new efficient methods for heterocycles synthesis and also multicomponent reactions (Debache *et al.*, 2008; Debache *et al.*, 2009; Nemouchi *et al.*, 2012), we decided to design some new molecules containing reactive fonctionnalities. As a result of this investigation we report herein a fast and efficient protocol for the synthesis of 2-(2-Chloro-8-methylquinolin-3-yl)-4-phenyl-1,2-dihydroquinazoline *via* a three-component reaction between 2-aminobenzophenone, 2-chloro-8-methylquinoline-3-carbaldehyde, and ammonium acetate, completed by the X-ray structure analysis.

The molecular geometry and the atom-numbering scheme of (I) are shown in Fig. 1. The benzene ring of dihydroquinazoline and methyl-substituted benzene rings of quinoline form a dihedral angles of 45.91 (5) and 79.80 (4)° respectively with a phenyl ring group. The dihedral angle between the phenyl ring of dihydroquinazoline and methyl-substituted benzene rings of quinoline is 78.18 (4)°. The crystal packing can be described as crossed layers parallel to the (011) and (0–11) planes. (Fig. 2). It is stabilized by a N—H⋯N hydrogen bond (Table 1, Fig. 2) and  $\pi$ - $\pi$  interactions. however the centroid to centroid small distance between the phenyl rings is 3.7301 (9) Å. These interactions link the molecules within the layers and also link the layers together and reinforcing the cohesion of the structure.

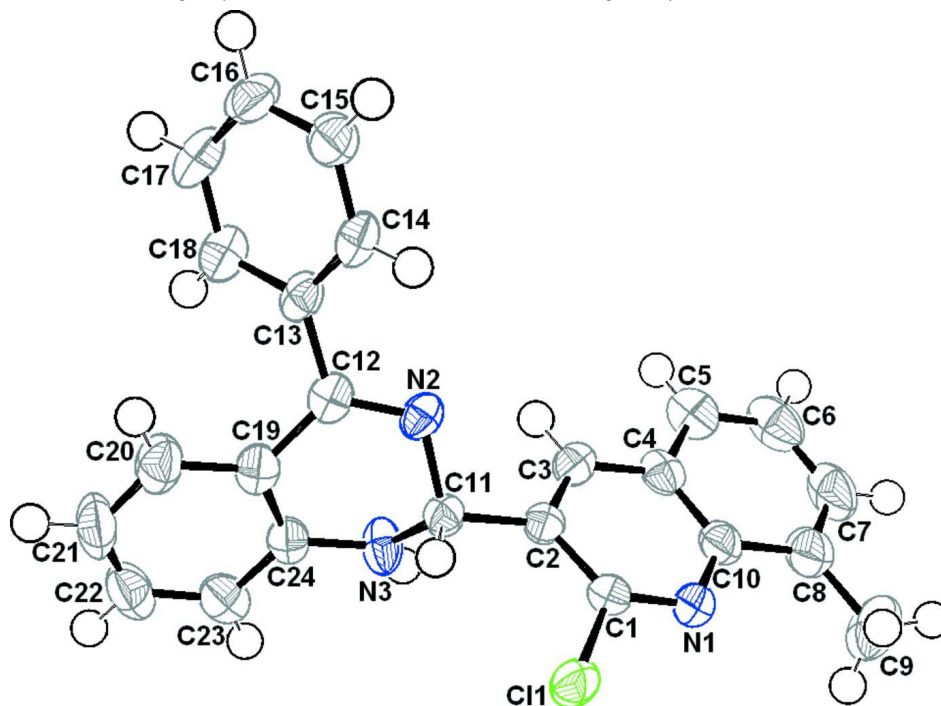
### S2. Experimental

A mixture of 2-chloro-8-methylquinoline-3-carbaldehyde (1.0 equiv), 2-aminobenzophenone (1.0 equiv), ammonium acetate (2.0 equiv), and 4-(*N,N*-dimethylamino)pyridine (0.2 equiv.) in 5 ml of absolute ethanol was stirred at 40°C. After completion of the reaction as monitored by TLC, the reaction mixture was poured into ice cold water; solid product was filtered, washed with water (3–5 ml) and dried. The crude product was recrystallized from ethyl acetate to give pure dihydroquinazoline as a yellow solid; m.p. 182–184 °C; IR (KBr)  $\nu$  3329, 1605, 1551, 1470, 1315, 1080, 756, 698 cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 250 MHz)  $\delta$  8.52 (s, 1H, arom.), 7.74–7.41 (m, 8H, arom.), 7.34–7.26 (m, 2H, arom.), 6.83–6.74 (m, 2H, arom.), 6.48 (s, 1H, CH), 4.79 (s, 1H, NH), 2.81 (s, 3H, CH<sub>3</sub>); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 62.5 MHz)  $\delta$  167.4, 148.2, 146.8, 146.6, 139.3, 138.0, 136.4, 133.2, 132.6, 130.9, 129.9, 129.3, 123.0, 128.4, 127.5, 127.1, 126.1, 120.4, 118.9, 117.9,

114.8, 68.8, 18.0. Anal. calcd for  $C_{24}H_{18}N_3Cl$ : C, 75.09; H, 4.73; N, 10.95; Found: C, 75.18; H, 4.94; N, 11.37. HRMS calcd f or  $C_{24}H_{19}N_3Cl$  (MH<sup>+</sup>) 384.1189; found 384.1162.

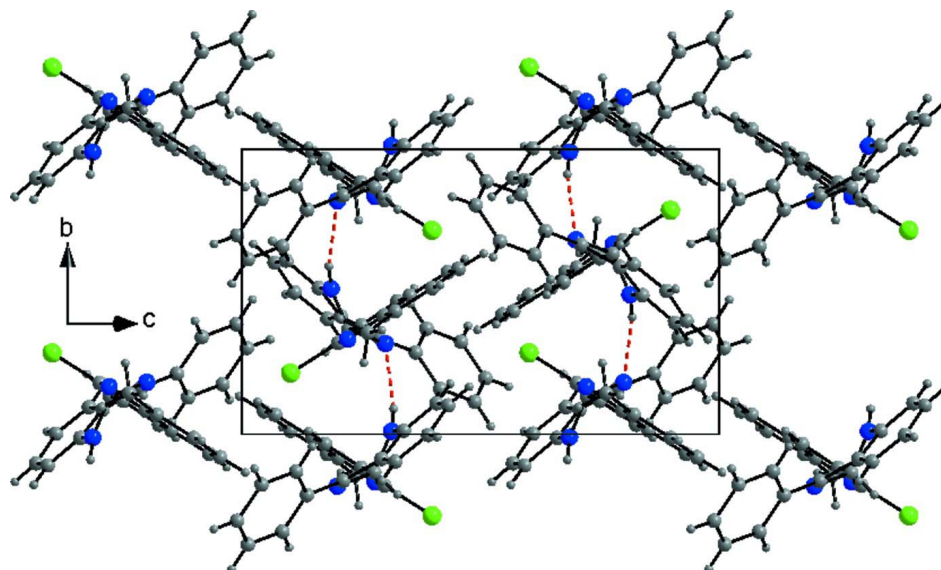
### S3. Refinement

Hydrogen atoms were localized on Fourier maps but introduced in calculated positions and treated as riding on their parent atoms (C and N) with C—H = 0.96 Å (methyl); C—H = 0.93 Å (aromatic) or C—H = 0.98 Å (methine); N—H = 0.86 Å and with  $U_{iso}(H) = 1.2 U_{eq}(C_{aryl}; C_{methine} \text{ or } N)$  and  $U_{iso}(H) = 1.5 U_{eq}(C_{methyl})$ .



**Figure 1**

The title molecule (Farrugia, 2012) with the atomic labelling scheme. The displacement parameters are drawn at the 50% probability level.

**Figure 2**

(Brandenburg & Berndt, 2001) Part of the crystal structure viewed down the *b* axis showing the hydrogen bonds N—H...N as dashed red lines.

### 2-(2-Chloro-8-methylquinolin-3-yl)-4-phenyl-1,2-dihydroquinazoline

#### Crystal data

$C_{24}H_{18}ClN_3$

$M_r = 383.86$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2ybc$

$a = 14.4553\ (13)\ \text{\AA}$

$b = 8.7501\ (9)\ \text{\AA}$

$c = 16.8630\ (16)\ \text{\AA}$

$\beta = 119.696\ (6)^\circ$

$V = 1852.8\ (3)\ \text{\AA}^3$

$Z = 4$

$F(000) = 800$

$D_x = 1.376\ \text{Mg m}^{-3}$

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

Cell parameters from 4868 reflections

$\theta = 2.4\text{--}25.1^\circ$

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

$T = 150\ \text{K}$

Stick, colourless

$0.12 \times 0.04 \times 0.02\ \text{mm}$

#### Data collection

Bruker APEXII CCD area-detector  
diffractometer

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Sheldrick, 2002)

$T_{\min} = 0.959$ ,  $T_{\max} = 1.000$

10282 measured reflections

3276 independent reflections

2894 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 25.1^\circ$ ,  $\theta_{\min} = 2.7^\circ$

$h = -17 \rightarrow 17$

$k = -10 \rightarrow 10$

$l = -20 \rightarrow 20$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.082$

$S = 1.06$

3276 reflections

254 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0364P)^2 + 0.8263P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.26 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$

#### 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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.69552 (11)	0.67980 (16)	0.79870 (9)	0.0147 (3)
C2	0.59188 (11)	0.61713 (15)	0.74927 (9)	0.0127 (3)
C3	0.57150 (11)	0.53348 (16)	0.67390 (9)	0.0146 (3)
H3	0.5049	0.4887	0.6391	0.018*
C4	0.64981 (11)	0.51388 (16)	0.64785 (9)	0.0159 (3)
C5	0.63045 (12)	0.43142 (17)	0.56897 (10)	0.0209 (3)
H5	0.5646	0.3853	0.5328	0.025*
C6	0.70818 (13)	0.41953 (19)	0.54594 (11)	0.0254 (4)
H6	0.6951	0.3665	0.4936	0.031*
C7	0.80782 (13)	0.4873 (2)	0.60120 (11)	0.0282 (4)
H7	0.8602	0.4765	0.5849	0.034*
C8	0.83123 (12)	0.5691 (2)	0.67858 (11)	0.0269 (4)
C9	0.93732 (14)	0.6438 (3)	0.73654 (13)	0.0489 (6)
H9A	0.9794	0.6349	0.7071	0.073*
H9B	0.9734	0.5944	0.795	0.073*
H9C	0.927	0.7498	0.7446	0.073*
C10	0.74979 (11)	0.58353 (17)	0.70258 (10)	0.0178 (3)
C11	0.50792 (11)	0.63352 (16)	0.77731 (9)	0.0131 (3)
H11	0.5314	0.7111	0.8254	0.016*
C12	0.32475 (11)	0.66315 (15)	0.71152 (9)	0.0138 (3)
C13	0.21909 (11)	0.71284 (16)	0.63629 (10)	0.0146 (3)
C14	0.21119 (11)	0.84104 (17)	0.58439 (10)	0.0167 (3)
H14	0.2721	0.8973	0.5986	0.02*
C15	0.11447 (11)	0.88597 (18)	0.51219 (10)	0.0202 (3)
H15	0.1106	0.9722	0.4785	0.024*
C16	0.02306 (12)	0.80291 (18)	0.48979 (10)	0.0217 (3)
H16	-0.0421	0.8325	0.4409	0.026*
C17	0.02994 (12)	0.67590 (18)	0.54081 (11)	0.0223 (3)
H17	-0.0313	0.6204	0.5264	0.027*
C18	0.12673 (11)	0.62970 (17)	0.61323 (10)	0.0193 (3)
H18	0.1302	0.5431	0.6466	0.023*
C19	0.33313 (11)	0.58635 (16)	0.79269 (10)	0.0158 (3)

C20	0.25708 (12)	0.59518 (18)	0.82105 (10)	0.0215 (3)
H20	0.2009	0.6641	0.7931	0.026*
C21	0.26503 (13)	0.5023 (2)	0.89021 (11)	0.0261 (4)
H21	0.2146	0.5094	0.909	0.031*
C22	0.34775 (13)	0.39837 (19)	0.93189 (10)	0.0237 (4)
H22	0.3507	0.333	0.9765	0.028*
C23	0.42583 (12)	0.39113 (17)	0.90769 (10)	0.0192 (3)
H23	0.482	0.3226	0.9367	0.023*
C24	0.41994 (11)	0.48728 (16)	0.83933 (9)	0.0145 (3)
N1	0.77105 (9)	0.66658 (15)	0.77866 (8)	0.0185 (3)
N2	0.40582 (9)	0.68184 (13)	0.69974 (8)	0.0136 (3)
N3	0.49626 (9)	0.48955 (14)	0.81327 (8)	0.0177 (3)
H3N	0.5343	0.4108	0.818	0.021*
Cl1	0.72959 (3)	0.78522 (4)	0.89821 (2)	0.02018 (12)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0142 (7)	0.0167 (7)	0.0124 (7)	0.0004 (6)	0.0059 (6)	0.0021 (6)
C2	0.0125 (7)	0.0110 (7)	0.0142 (7)	0.0021 (5)	0.0064 (6)	0.0036 (5)
C3	0.0134 (7)	0.0122 (7)	0.0170 (7)	-0.0001 (6)	0.0064 (6)	0.0020 (6)
C4	0.0191 (7)	0.0134 (7)	0.0168 (7)	0.0053 (6)	0.0100 (6)	0.0053 (6)
C5	0.0259 (8)	0.0171 (7)	0.0212 (8)	0.0033 (6)	0.0129 (7)	-0.0001 (6)
C6	0.0348 (9)	0.0253 (9)	0.0221 (8)	0.0093 (7)	0.0186 (7)	0.0019 (7)
C7	0.0273 (9)	0.0406 (10)	0.0267 (8)	0.0135 (8)	0.0209 (8)	0.0093 (8)
C8	0.0184 (8)	0.0441 (10)	0.0214 (8)	0.0068 (7)	0.0122 (7)	0.0075 (7)
C9	0.0188 (9)	0.1013 (19)	0.0341 (10)	-0.0071 (10)	0.0188 (8)	-0.0086 (11)
C10	0.0157 (7)	0.0236 (8)	0.0155 (7)	0.0050 (6)	0.0089 (6)	0.0058 (6)
C11	0.0124 (7)	0.0129 (7)	0.0138 (7)	-0.0008 (5)	0.0064 (6)	-0.0002 (6)
C12	0.0146 (7)	0.0101 (7)	0.0176 (7)	-0.0012 (5)	0.0088 (6)	-0.0041 (5)
C13	0.0124 (7)	0.0160 (7)	0.0173 (7)	0.0009 (6)	0.0087 (6)	-0.0039 (6)
C14	0.0129 (7)	0.0180 (7)	0.0215 (7)	-0.0008 (6)	0.0102 (6)	-0.0027 (6)
C15	0.0188 (7)	0.0232 (8)	0.0211 (7)	0.0056 (6)	0.0118 (6)	0.0041 (6)
C16	0.0125 (7)	0.0302 (9)	0.0201 (8)	0.0047 (6)	0.0064 (6)	-0.0008 (7)
C17	0.0122 (7)	0.0241 (8)	0.0299 (8)	-0.0023 (6)	0.0098 (7)	-0.0041 (7)
C18	0.0162 (7)	0.0179 (7)	0.0251 (8)	0.0001 (6)	0.0112 (6)	0.0003 (6)
C19	0.0166 (7)	0.0146 (7)	0.0179 (7)	-0.0029 (6)	0.0099 (6)	-0.0041 (6)
C20	0.0195 (8)	0.0251 (8)	0.0243 (8)	-0.0009 (6)	0.0142 (7)	-0.0052 (7)
C21	0.0265 (8)	0.0354 (10)	0.0268 (8)	-0.0073 (7)	0.0210 (7)	-0.0067 (7)
C22	0.0304 (9)	0.0258 (8)	0.0198 (8)	-0.0097 (7)	0.0160 (7)	-0.0023 (7)
C23	0.0229 (8)	0.0172 (7)	0.0176 (7)	-0.0027 (6)	0.0102 (6)	-0.0012 (6)
C24	0.0164 (7)	0.0139 (7)	0.0149 (7)	-0.0037 (6)	0.0090 (6)	-0.0045 (6)
N1	0.0126 (6)	0.0272 (7)	0.0156 (6)	0.0003 (5)	0.0071 (5)	0.0034 (5)
N2	0.0113 (6)	0.0122 (6)	0.0172 (6)	0.0008 (5)	0.0069 (5)	0.0003 (5)
N3	0.0198 (6)	0.0148 (6)	0.0255 (7)	0.0062 (5)	0.0166 (6)	0.0058 (5)
Cl1	0.01497 (19)	0.0289 (2)	0.01610 (19)	-0.00583 (15)	0.00722 (15)	-0.00646 (15)

*Geometric parameters (Å, °)*

C1—N1	1.2981 (18)	C12—C19	1.475 (2)
C1—C2	1.4151 (19)	C12—C13	1.487 (2)
C1—C11	1.7580 (14)	C13—C14	1.392 (2)
C2—C3	1.366 (2)	C13—C18	1.396 (2)
C2—C11	1.5118 (18)	C14—C15	1.380 (2)
C3—C4	1.4129 (19)	C14—H14	0.93
C3—H3	0.93	C15—C16	1.386 (2)
C4—C10	1.411 (2)	C15—H15	0.93
C4—C5	1.414 (2)	C16—C17	1.379 (2)
C5—C6	1.363 (2)	C16—H16	0.93
C5—H5	0.93	C17—C18	1.385 (2)
C6—C7	1.402 (2)	C17—H17	0.93
C6—H6	0.93	C18—H18	0.93
C7—C8	1.376 (2)	C19—C20	1.4017 (19)
C7—H7	0.93	C19—C24	1.402 (2)
C8—C10	1.427 (2)	C20—C21	1.379 (2)
C8—C9	1.500 (3)	C20—H20	0.93
C9—H9A	0.96	C21—C22	1.385 (2)
C9—H9B	0.96	C21—H21	0.93
C9—H9C	0.96	C22—C23	1.379 (2)
C10—N1	1.3704 (19)	C22—H22	0.93
C11—N3	1.4437 (18)	C23—C24	1.395 (2)
C11—N2	1.4681 (18)	C23—H23	0.93
C11—H11	0.98	C24—N3	1.3753 (17)
C12—N2	1.2924 (17)	N3—H3N	0.86
N1—C1—C2	126.42 (13)	C14—C13—C18	118.39 (13)
N1—C1—C11	114.91 (11)	C14—C13—C12	120.11 (12)
C2—C1—C11	118.67 (10)	C18—C13—C12	121.44 (13)
C3—C2—C1	115.65 (12)	C15—C14—C13	121.05 (13)
C3—C2—C11	120.34 (12)	C15—C14—H14	119.5
C1—C2—C11	123.96 (12)	C13—C14—H14	119.5
C2—C3—C4	121.16 (13)	C14—C15—C16	120.21 (14)
C2—C3—H3	119.4	C14—C15—H15	119.9
C4—C3—H3	119.4	C16—C15—H15	119.9
C10—C4—C3	117.58 (13)	C17—C16—C15	119.22 (14)
C10—C4—C5	119.81 (13)	C17—C16—H16	120.4
C3—C4—C5	122.59 (14)	C15—C16—H16	120.4
C6—C5—C4	120.01 (15)	C16—C17—C18	120.96 (14)
C6—C5—H5	120	C16—C17—H17	119.5
C4—C5—H5	120	C18—C17—H17	119.5
C5—C6—C7	119.94 (14)	C17—C18—C13	120.16 (14)
C5—C6—H6	120	C17—C18—H18	119.9
C7—C6—H6	120	C13—C18—H18	119.9
C8—C7—C6	122.67 (14)	C20—C19—C24	118.54 (13)
C8—C7—H7	118.7	C20—C19—C12	125.02 (13)



C6—C7—H7	118.7	C24—C19—C12	116.21 (12)
C7—C8—C10	117.71 (15)	C21—C20—C19	120.35 (15)
C7—C8—C9	122.46 (14)	C21—C20—H20	119.8
C10—C8—C9	119.83 (15)	C19—C20—H20	119.8
C8—C9—H9A	109.5	C20—C21—C22	120.36 (13)
C8—C9—H9B	109.5	C20—C21—H21	119.8
H9A—C9—H9B	109.5	C22—C21—H21	119.8
C8—C9—H9C	109.5	C23—C22—C21	120.51 (14)
H9A—C9—H9C	109.5	C23—C22—H22	119.7
H9B—C9—H9C	109.5	C21—C22—H22	119.7
N1—C10—C4	121.56 (12)	C22—C23—C24	119.53 (14)
N1—C10—C8	118.58 (14)	C22—C23—H23	120.2
C4—C10—C8	119.85 (14)	C24—C23—H23	120.2
N3—C11—N2	110.52 (11)	N3—C24—C23	122.85 (13)
N3—C11—C2	109.11 (11)	N3—C24—C19	116.63 (12)
N2—C11—C2	110.92 (11)	C23—C24—C19	120.51 (13)
N3—C11—H11	108.7	C1—N1—C10	117.61 (12)
N2—C11—H11	108.7	C12—N2—C11	114.49 (11)
C2—C11—H11	108.7	C24—N3—C11	115.21 (11)
N2—C12—C19	122.44 (13)	C24—N3—H3N	122.4
N2—C12—C13	117.27 (12)	C11—N3—H3N	122.4
C19—C12—C13	120.16 (12)		
N1—C1—C2—C3	0.8 (2)	C14—C15—C16—C17	0.4 (2)
C11—C1—C2—C3	-178.49 (10)	C15—C16—C17—C18	-0.6 (2)
N1—C1—C2—C11	178.55 (13)	C16—C17—C18—C13	0.7 (2)
C11—C1—C2—C11	-0.74 (19)	C14—C13—C18—C17	-0.6 (2)
C1—C2—C3—C4	-0.7 (2)	C12—C13—C18—C17	-177.81 (13)
C11—C2—C3—C4	-178.50 (12)	N2—C12—C19—C20	163.29 (14)
C2—C3—C4—C10	0.1 (2)	C13—C12—C19—C20	-21.0 (2)
C2—C3—C4—C5	-178.31 (13)	N2—C12—C19—C24	-22.4 (2)
C10—C4—C5—C6	-0.1 (2)	C13—C12—C19—C24	153.26 (13)
C3—C4—C5—C6	178.33 (14)	C24—C19—C20—C21	-3.3 (2)
C4—C5—C6—C7	0.9 (2)	C12—C19—C20—C21	170.81 (14)
C5—C6—C7—C8	-1.0 (3)	C19—C20—C21—C22	-0.5 (2)
C6—C7—C8—C10	0.3 (3)	C20—C21—C22—C23	2.9 (2)
C6—C7—C8—C9	-178.86 (18)	C21—C22—C23—C24	-1.3 (2)
C3—C4—C10—N1	0.4 (2)	C22—C23—C24—N3	178.18 (14)
C5—C4—C10—N1	178.87 (13)	C22—C23—C24—C19	-2.6 (2)
C3—C4—C10—C8	-179.12 (14)	C20—C19—C24—N3	-175.84 (13)
C5—C4—C10—C8	-0.6 (2)	C12—C19—C24—N3	9.50 (19)
C7—C8—C10—N1	-179.01 (14)	C20—C19—C24—C23	4.9 (2)
C9—C8—C10—N1	0.2 (2)	C12—C19—C24—C23	-169.73 (13)
C7—C8—C10—C4	0.5 (2)	C2—C1—N1—C10	-0.3 (2)
C9—C8—C10—C4	179.71 (17)	C11—C1—N1—C10	178.99 (10)
C3—C2—C11—N3	71.53 (16)	C4—C10—N1—C1	-0.3 (2)
C1—C2—C11—N3	-106.12 (15)	C8—C10—N1—C1	179.22 (14)
C3—C2—C11—N2	-50.45 (17)	C19—C12—N2—C11	-5.44 (19)

C1—C2—C11—N2	131.90 (14)	C13—C12—N2—C11	178.74 (12)
N2—C12—C13—C14	-34.96 (19)	N3—C11—N2—C12	42.97 (16)
C19—C12—C13—C14	149.12 (13)	C2—C11—N2—C12	164.12 (12)
N2—C12—C13—C18	142.19 (14)	C23—C24—N3—C11	-151.84 (13)
C19—C12—C13—C18	-33.73 (19)	C19—C24—N3—C11	28.95 (18)
C18—C13—C14—C15	0.4 (2)	N2—C11—N3—C24	-56.16 (15)
C12—C13—C14—C15	177.67 (13)	C2—C11—N3—C24	-178.38 (12)
C13—C14—C15—C16	-0.4 (2)		

*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>
N3—H3N...N2 <sup>i</sup>	0.86	2.26	3.0998 (18)	165
C11—H11...C11	0.98	2.58	3.1166 (16)	115

Symmetry code: (i)  $-x+1, y-1/2, -z+3/2$ .