

2-(4-Chlorophenyl)-4-phenyl-1,2-dihydroquinazoline

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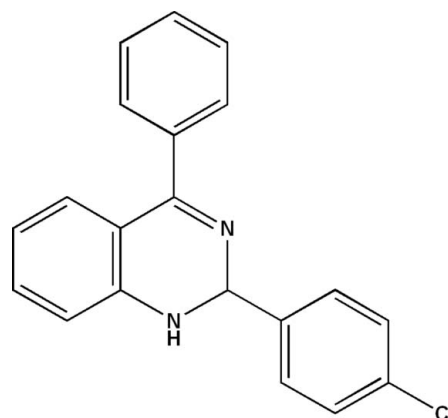
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Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.031; wR factor = 0.081; data-to-parameter ratio = 12.8.

In the title compound, $\text{C}_{20}\text{H}_{15}\text{ClN}_2$, the pyrimidine ring is in a flattened half-chair conformation. The phenyl and chloro-substituted benzene rings form dihedral angles of 84.97 (5) and 80.23 (4)°, respectively, with the benzene ring of the dihydroquinazoline group. The dihedral angle between the phenyl and chloro-substituted benzene rings is 61.71 (5)°. In the crystal, molecules are arranged in intersecting layers parallel to (101) and ($\bar{1}02$), with $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds linking molecules along [010]. In addition, a weak $\text{C}-\text{H}\cdots\pi$ interaction is observed.

Related literature

For the preparation and applications of quinazoline derivatives, see: Gundla *et al.* (2008); Luth & Lowe (2008); Fry *et al.* (1994); Kunes *et al.* (2000); Michael (2002); Frère *et al.* (2003); Langer & Bodtke (2003).



Experimental

Crystal data

$\text{C}_{20}\text{H}_{15}\text{ClN}_2$
 $M_r = 318.79$
 Monoclinic, $P2_1/c$
 $a = 9.2563$ (10) Å
 $b = 10.6283$ (11) Å
 $c = 17.6230$ (19) Å
 $\beta = 116.775$ (7)°
 $V = 1547.8$ (3) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.25$ mm⁻¹
 $T = 150$ K
 $0.18 \times 0.04 \times 0.03$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2002)
 $T_{\min} = 0.948$, $T_{\max} = 1.000$
 8914 measured reflections
 2724 independent reflections
 2462 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.081$
 $S = 1.05$
 2724 reflections
 212 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.22$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.26$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

C_g is the centroid of the C15–C20 ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1N}\cdots\text{N2}^i$	0.830 (19)	2.316 (19)	3.1234 (18)	164.3 (19)
$\text{C11}-\text{H11}\cdots\text{Cg}^{\text{ii}}$	0.93	2.76	3.666 (2)	165

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

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).

We are grateful to all the personnel of the LSMIB laboratory and UR-CHEMS, Université Constantine 1, Algeria, for their assistance. Thanks are due to the MESRS (Ministère de l'Enseignement Supérieur et de la Recherche Scientifique, Algeria) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5660).

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supporting information

Acta Cryst. (2013). E69, o1653–o1654 [doi:10.1107/S1600536813027839]

2-(4-Chlorophenyl)-4-phenyl-1,2-dihydroquinazoline

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S1. Comment

Heterocyclic chemistry is a potential part of the synthetic organic chemistry, covering a wide variety of bioactive molecules. Among six-membered heterocycles, quinazoline occupies significant position and is commonly found in a wide variety of natural products, synthetic pharmaceutical molecules, and other functional materials (Gundla *et al.*, 2008; Luth & Lowe, 2008). Quinazoline derivatives are among the most potent tyrosine kinase and cellular phosphorylation inhibitors (Fry *et al.*, 1994), and they also show remarkable activity as antitubercular, antiviral, and anticancer agents (Kunes *et al.*, 2000). The growing medicinal importance of these heterocycles perpetuates to provide strong rationale for the development of synthetic methods for their preparation. These efforts have led to several reviews emphasizing the synthesis (Michael, 2002; Frère *et al.*, 2003; Langer & Bodtke, 2003), and biological evaluation of quinazolines.

In the course of a program directed toward the synthesis of new heterocyclic systems for pharmacological evaluation, we report herein the crystallographic study and the synthesis of the title compound. The molecular structure is shown in Fig. 1. The phenyl ring and chloro-substituted benzene rings form a dihedral angles of 84.97 (5) and 80.23 (4)° respectively with the benzene ring of dihydroquinazoline group. The dihedral angle between the phenyl ring and chloro-substituted benzene ring is 61.71 (5)°. In the crystal, molecules are arranged in intersecting layers parallel to (101) and (-102) (see, Fig. 2) with N—H···N hydrogen bonds linking molecules along [010] (Fig. 3). In addition, a weak C—H··· π interaction is observed (Table 1).

S2. Experimental

The title compound was prepared by condensation of 4-chlorobenzaldehyde (1.0 equiv), 2-aminobenzophenone (1.0 equiv), ammonium acetate (2.0 equiv), and dimethylaminopyridine (0.2 equiv.) in 5 ml of absolute ethanol at 313 K. After completion of the reaction as monitored by TLC, the reaction was poured into ice cold water; solid product was filtered, washed with water and dried. The crude product was recrystallized from ethyl acetate to give the title compound as a yellow solid (m.p. 415–417 K). X-ray quality crystals were grown from a solution of the title compound in ethyl acetate.

S3. Refinement

H atoms bonded to C atoms were initially located in a difference Fourier map. However, they were subsequently placed in idealized positions and refined in a riding-model approximation. The applied constraints were as follows: $C_{\text{aryl}}-H_{\text{aryl}} = 0.93 \text{ \AA}$; $C_{\text{methine}}-H_{\text{methine}} = 0.98 \text{ \AA}$; $U_{\text{iso}}(H_{\text{aryl}}H_{\text{methine}}) = 1.2U_{\text{eq}}(C_{\text{aryl}}/C_{\text{methine}})$. Atom H1N was located in a difference Fourier map and refined isotropically.

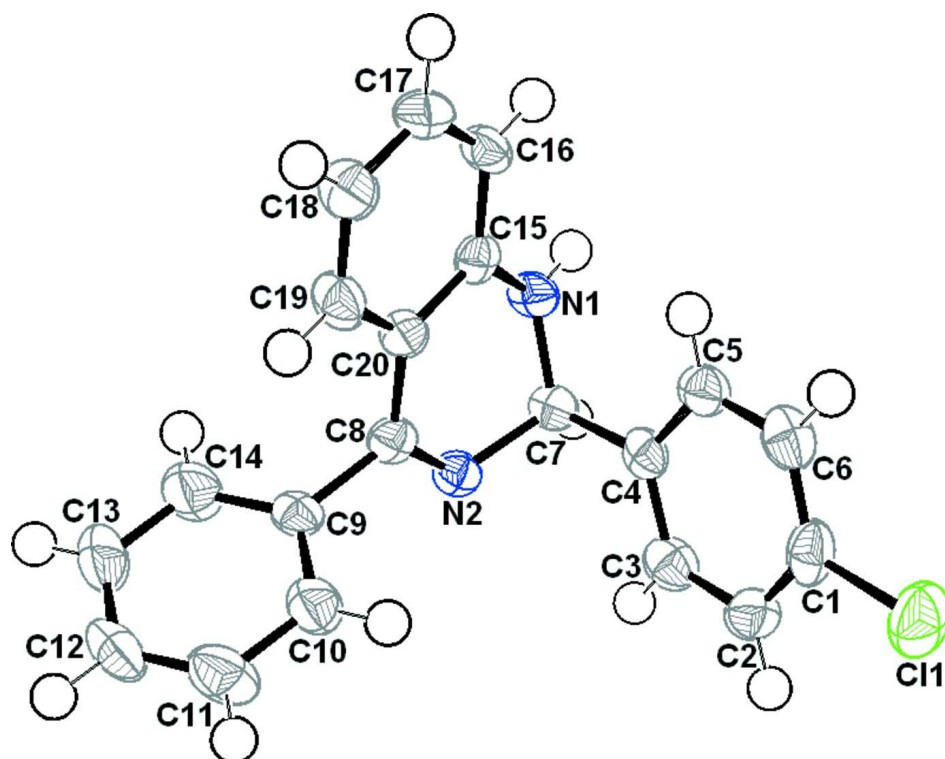


Figure 1

The molecular structure with displacement ellipsoids drawn at the 50% probability level.

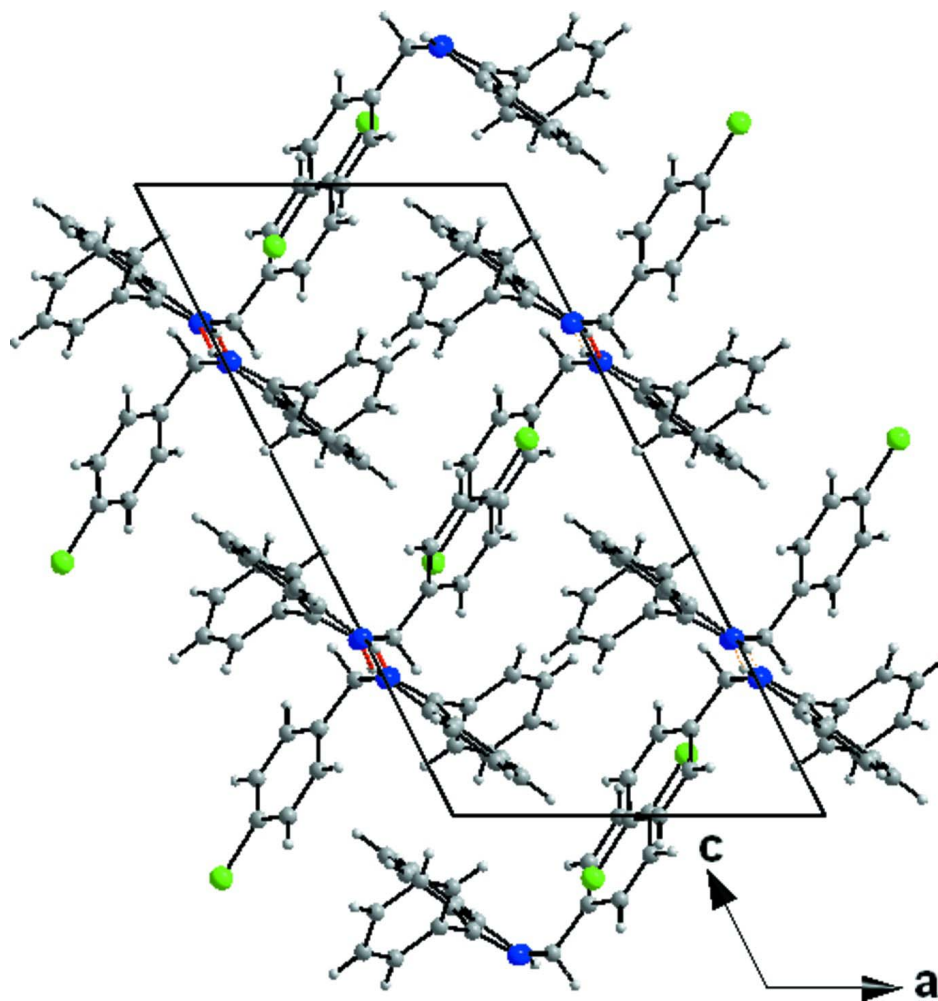
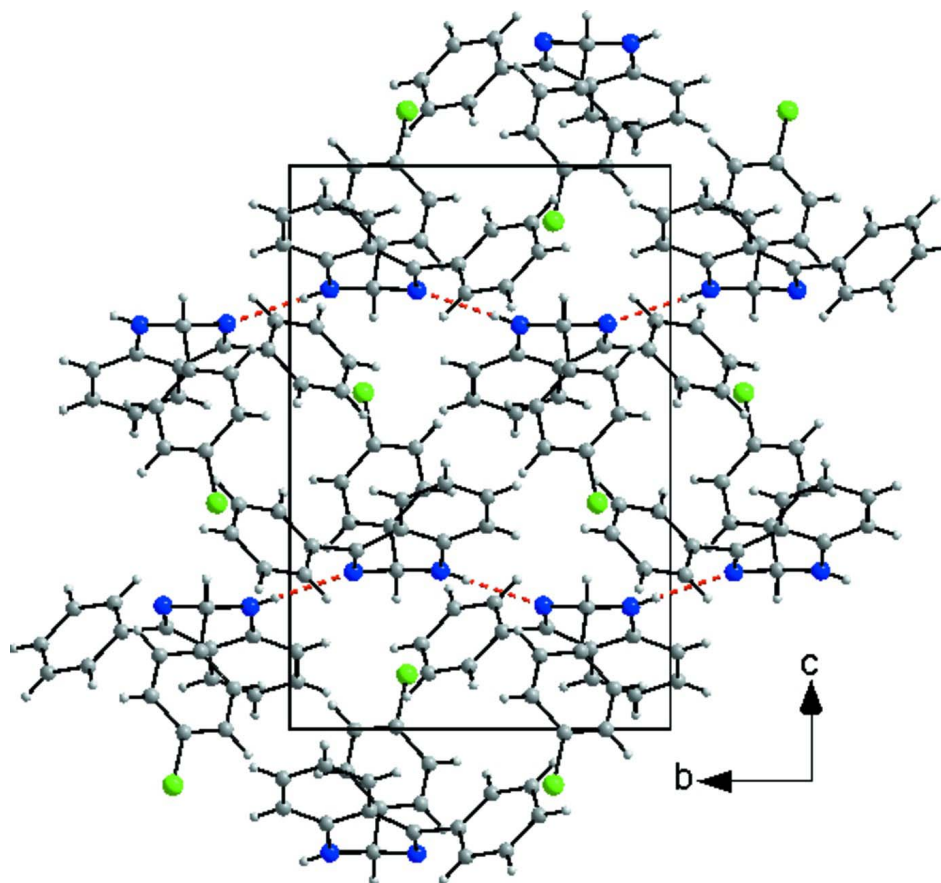


Figure 2

Part of the crystal structure viewed along the *b* axis. Cl is shown in green, N in blue and C in grey. Red lines indicate hydrogen bonds.

**Figure 3**

Part of the crystal structure showing the hydrogen bonds N—H...N as dashed red lines.

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Crystal data

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$b = 10.6283$ (11) Å

$c = 17.6230$ (19) Å

$\beta = 116.775$ (7)°

$V = 1547.8$ (3) Å³

$Z = 4$

$F(000) = 664$

$D_x = 1.368$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4726 reflections

$\theta = 2.5$ – 25.1 °

$\mu = 0.25$ mm⁻¹

$T = 150$ K

Needle, colourless

$0.18 \times 0.04 \times 0.03$ mm

Data collection

Bruker APEXII CCD area-detector
diffractometer

Graphite monochromator

φ and ω scans

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

$T_{\min} = 0.948$, $T_{\max} = 1.000$

8914 measured reflections

2724 independent reflections

2462 reflections with $I > 2\sigma(I)$

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

$\theta_{\max} = 25.1$ °, $\theta_{\min} = 2.3$ °

$h = -10 \rightarrow 11$

$k = -12 \rightarrow 12$

$l = -17 \rightarrow 21$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.081$
 $S = 1.05$
 2724 reflections
 212 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 atoms treated by a mixture of independent
 and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.033P)^2 + 0.9522P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.22 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. Spectroscopic data: IR (KBr) ν 3320, 2364 1620, 1537, 1486, 1321, 1263, 1155, 1015, 964, 805, 741, 697 cm^{-1} ; ^1H NMR (CDCl_3 , 400 MHz) δ 7.72–7.61 (m, 5H, arom.), 7.49–7.36 (m, 4H, arom.), 7.32–7.21 (m, 2H, arom.), 6.77 (td, $J=8.0, 1.0$ Hz, 1H, arom.), 6.72 (d, $J=8.0$ Hz, 1H), 6.02 (s, 1H, CH), 4.38 (s, 1H, NH); ^{13}C NMR (CDCl_3 , 100 MHz) δ 165.8, 146.9, 141.5, 141.4, 140.9, 138.1, 132.9, 130.2, 129.4, 129.3, 129.1, 128.1, 127.8, 127.5, 127.3, 127.2, 118.3, 117.9, 114.3, 72.4. Anal. calcd for $\text{C}_{20}\text{H}_{15}\text{N}_2\text{Cl}$: C, 75.35; H, 4.74; N, 8.79; Found: C, 75.75; H, 4.95; N, 9.42. HRMS calcd for $\text{C}_{20}\text{H}_{16}\text{N}_2\text{Cl}$ (MH⁺) 319.0924; found 319.0863.

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.53121 (17)	0.77886 (14)	0.50548 (10)	0.0165 (3)
C2	0.44580 (18)	0.66972 (14)	0.49960 (9)	0.0168 (3)
H2	0.4841	0.6114	0.5437	0.02*
C3	0.30186 (17)	0.64835 (14)	0.42695 (10)	0.0153 (3)
H3	0.244	0.5748	0.4223	0.018*
C4	0.24323 (17)	0.73546 (13)	0.36111 (9)	0.0130 (3)
C5	0.33457 (18)	0.84305 (14)	0.36800 (10)	0.0161 (3)
H5	0.2981	0.9009	0.3237	0.019*
C6	0.47870 (18)	0.86503 (14)	0.43980 (10)	0.0177 (3)
H6	0.5393	0.9367	0.4438	0.021*
C7	0.07957 (17)	0.71954 (13)	0.28323 (9)	0.0131 (3)
H7	0.0982	0.72	0.2327	0.016*
C8	-0.10527 (16)	0.82529 (13)	0.31836 (9)	0.0124 (3)
C9	-0.18848 (17)	0.94230 (13)	0.32554 (9)	0.0129 (3)
C10	-0.35237 (19)	0.96183 (15)	0.27479 (11)	0.0239 (4)
H10	-0.4123	0.903	0.2334	0.029*
C11	-0.42727 (19)	1.06843 (15)	0.28539 (11)	0.0258 (4)
H11	-0.5367	1.0821	0.2503	0.031*
C12	-0.33965 (19)	1.15455 (14)	0.34810 (10)	0.0208 (3)

H12	-0.3906	1.2252	0.356	0.025*
C13	-0.1764 (2)	1.13562 (15)	0.39897 (10)	0.0228 (4)
H13	-0.1174	1.1936	0.4412	0.027*
C14	-0.10031 (18)	1.03001 (14)	0.38718 (10)	0.0188 (3)
H14	0.0101	1.0182	0.4208	0.023*
C15	-0.08004 (16)	0.59670 (13)	0.33333 (9)	0.0119 (3)
C16	-0.12929 (16)	0.70970 (13)	0.35624 (9)	0.0129 (3)
C17	-0.20595 (17)	0.70602 (14)	0.40861 (9)	0.0160 (3)
H17	-0.2382	0.7806	0.424	0.019*
C18	-0.23427 (18)	0.59305 (14)	0.43764 (10)	0.0180 (3)
H18	-0.2842	0.5913	0.4731	0.022*
C19	-0.18758 (18)	0.48132 (14)	0.41355 (10)	0.0171 (3)
H19	-0.2075	0.405	0.4329	0.021*
C20	-0.11248 (17)	0.48210 (13)	0.36158 (9)	0.0140 (3)
H20	-0.0834	0.4068	0.3453	0.017*
N1	-0.00529 (14)	0.60480 (12)	0.28194 (8)	0.0135 (3)
N2	-0.01662 (14)	0.83324 (11)	0.27983 (7)	0.0129 (3)
Cl1	0.70928 (4)	0.80771 (4)	0.59784 (2)	0.02398 (13)
H1N	0.018 (2)	0.5377 (18)	0.2660 (11)	0.023 (5)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0120 (7)	0.0221 (8)	0.0148 (7)	0.0023 (6)	0.0053 (6)	-0.0041 (6)
C2	0.0180 (7)	0.0189 (8)	0.0154 (7)	0.0047 (6)	0.0093 (6)	0.0039 (6)
C3	0.0161 (7)	0.0135 (7)	0.0193 (8)	0.0010 (6)	0.0107 (6)	0.0008 (6)
C4	0.0143 (7)	0.0136 (7)	0.0146 (7)	0.0027 (5)	0.0095 (6)	-0.0015 (5)
C5	0.0191 (8)	0.0151 (7)	0.0161 (7)	0.0019 (6)	0.0095 (6)	0.0024 (6)
C6	0.0168 (8)	0.0150 (7)	0.0221 (8)	-0.0014 (6)	0.0096 (6)	-0.0028 (6)
C7	0.0158 (7)	0.0122 (7)	0.0137 (7)	0.0001 (5)	0.0088 (6)	0.0001 (5)
C8	0.0122 (7)	0.0127 (7)	0.0098 (7)	-0.0014 (5)	0.0027 (6)	-0.0017 (5)
C9	0.0166 (7)	0.0106 (7)	0.0137 (7)	0.0001 (5)	0.0090 (6)	0.0029 (5)
C10	0.0194 (8)	0.0181 (8)	0.0263 (9)	0.0000 (6)	0.0034 (7)	-0.0073 (7)
C11	0.0157 (8)	0.0223 (8)	0.0329 (9)	0.0061 (6)	0.0050 (7)	0.0001 (7)
C12	0.0269 (9)	0.0144 (7)	0.0254 (9)	0.0071 (6)	0.0156 (7)	0.0023 (6)
C13	0.0283 (9)	0.0155 (8)	0.0203 (8)	0.0015 (6)	0.0073 (7)	-0.0045 (6)
C14	0.0169 (8)	0.0157 (8)	0.0197 (8)	0.0022 (6)	0.0047 (6)	-0.0002 (6)
C15	0.0101 (7)	0.0142 (7)	0.0097 (7)	-0.0006 (5)	0.0029 (5)	-0.0016 (5)
C16	0.0124 (7)	0.0125 (7)	0.0131 (7)	-0.0002 (5)	0.0051 (6)	-0.0005 (5)
C17	0.0184 (8)	0.0143 (7)	0.0184 (8)	0.0031 (6)	0.0109 (6)	-0.0007 (6)
C18	0.0217 (8)	0.0176 (8)	0.0219 (8)	0.0020 (6)	0.0162 (7)	0.0021 (6)
C19	0.0192 (8)	0.0129 (7)	0.0210 (8)	-0.0008 (6)	0.0105 (6)	0.0034 (6)
C20	0.0158 (7)	0.0100 (7)	0.0156 (7)	0.0012 (5)	0.0066 (6)	-0.0019 (5)
N1	0.0171 (6)	0.0115 (6)	0.0155 (6)	-0.0005 (5)	0.0104 (5)	-0.0031 (5)
N2	0.0139 (6)	0.0122 (6)	0.0118 (6)	-0.0003 (5)	0.0052 (5)	-0.0007 (5)
Cl1	0.0168 (2)	0.0295 (2)	0.0186 (2)	-0.00015 (15)	0.00177 (16)	-0.00224 (15)

Geometric parameters (Å, °)

C1—C2	1.381 (2)	C10—H10	0.93
C1—C6	1.381 (2)	C11—C12	1.382 (2)
C1—C11	1.7443 (15)	C11—H11	0.93
C2—C3	1.389 (2)	C12—C13	1.381 (2)
C2—H2	0.93	C12—H12	0.93
C3—C4	1.389 (2)	C13—C14	1.390 (2)
C3—H3	0.93	C13—H13	0.93
C4—C5	1.395 (2)	C14—H14	0.93
C4—C7	1.528 (2)	C15—N1	1.3678 (19)
C5—C6	1.384 (2)	C15—C20	1.399 (2)
C5—H5	0.93	C15—C16	1.407 (2)
C6—H6	0.93	C16—C17	1.395 (2)
C7—N1	1.4452 (18)	C17—C18	1.376 (2)
C7—N2	1.4861 (18)	C17—H17	0.93
C7—H7	0.98	C18—C19	1.394 (2)
C8—N2	1.2820 (19)	C18—H18	0.93
C8—C16	1.462 (2)	C19—C20	1.377 (2)
C8—C9	1.4979 (19)	C19—H19	0.93
C9—C14	1.384 (2)	C20—H20	0.93
C9—C10	1.386 (2)	N1—H1N	0.831 (19)
C10—C11	1.384 (2)		
C2—C1—C6	121.37 (14)	C12—C11—H11	120
C2—C1—C11	119.08 (12)	C10—C11—H11	120
C6—C1—C11	119.56 (12)	C13—C12—C11	119.94 (14)
C1—C2—C3	119.04 (13)	C13—C12—H12	120
C1—C2—H2	120.5	C11—C12—H12	120
C3—C2—H2	120.5	C12—C13—C14	120.04 (15)
C2—C3—C4	120.82 (14)	C12—C13—H13	120
C2—C3—H3	119.6	C14—C13—H13	120
C4—C3—H3	119.6	C9—C14—C13	120.12 (14)
C3—C4—C5	118.71 (14)	C9—C14—H14	119.9
C3—C4—C7	122.18 (13)	C13—C14—H14	119.9
C5—C4—C7	119.07 (13)	N1—C15—C20	122.97 (13)
C6—C5—C4	121.00 (14)	N1—C15—C16	117.54 (12)
C6—C5—H5	119.5	C20—C15—C16	119.47 (13)
C4—C5—H5	119.5	C17—C16—C15	119.54 (13)
C1—C6—C5	119.00 (14)	C17—C16—C8	123.56 (13)
C1—C6—H6	120.5	C15—C16—C8	116.78 (13)
C5—C6—H6	120.5	C18—C17—C16	120.62 (13)
N1—C7—N2	111.97 (11)	C18—C17—H17	119.7
N1—C7—C4	114.81 (12)	C16—C17—H17	119.7
N2—C7—C4	106.24 (11)	C17—C18—C19	119.54 (14)
N1—C7—H7	107.9	C17—C18—H18	120.2
N2—C7—H7	107.9	C19—C18—H18	120.2
C4—C7—H7	107.9	C20—C19—C18	121.08 (13)

N2—C8—C16	124.23 (13)	C20—C19—H19	119.5
N2—C8—C9	117.79 (12)	C18—C19—H19	119.5
C16—C8—C9	117.99 (12)	C19—C20—C15	119.72 (13)
C14—C9—C10	119.50 (14)	C19—C20—H20	120.1
C14—C9—C8	118.79 (13)	C15—C20—H20	120.1
C10—C9—C8	121.65 (13)	C15—N1—C7	118.43 (12)
C11—C10—C9	120.30 (14)	C15—N1—H1N	117.2 (13)
C11—C10—H10	119.8	C7—N1—H1N	120.4 (13)
C9—C10—H10	119.8	C8—N2—C7	116.09 (12)
C12—C11—C10	120.06 (15)		
C6—C1—C2—C3	-1.8 (2)	C12—C13—C14—C9	-1.2 (2)
C11—C1—C2—C3	178.36 (11)	N1—C15—C16—C17	-179.97 (12)
C1—C2—C3—C4	-0.5 (2)	C20—C15—C16—C17	1.7 (2)
C2—C3—C4—C5	2.2 (2)	N1—C15—C16—C8	3.85 (19)
C2—C3—C4—C7	-175.49 (13)	C20—C15—C16—C8	-174.52 (12)
C3—C4—C5—C6	-1.8 (2)	N2—C8—C16—C17	170.14 (14)
C7—C4—C5—C6	176.00 (13)	C9—C8—C16—C17	-9.4 (2)
C2—C1—C6—C5	2.2 (2)	N2—C8—C16—C15	-13.8 (2)
C11—C1—C6—C5	-177.93 (11)	C9—C8—C16—C15	166.65 (12)
C4—C5—C6—C1	-0.4 (2)	C15—C16—C17—C18	-0.3 (2)
C3—C4—C7—N1	-2.54 (19)	C8—C16—C17—C18	175.64 (14)
C5—C4—C7—N1	179.78 (12)	C16—C17—C18—C19	-0.8 (2)
C3—C4—C7—N2	121.79 (14)	C17—C18—C19—C20	0.4 (2)
C5—C4—C7—N2	-55.89 (16)	C18—C19—C20—C15	1.0 (2)
N2—C8—C9—C14	-79.22 (17)	N1—C15—C20—C19	179.72 (13)
C16—C8—C9—C14	100.32 (16)	C16—C15—C20—C19	-2.0 (2)
N2—C8—C9—C10	103.78 (17)	C20—C15—N1—C7	-155.71 (13)
C16—C8—C9—C10	-76.68 (18)	C16—C15—N1—C7	25.99 (18)
C14—C9—C10—C11	0.3 (2)	N2—C7—N1—C15	-45.39 (17)
C8—C9—C10—C11	177.24 (15)	C4—C7—N1—C15	75.86 (16)
C9—C10—C11—C12	-1.6 (3)	C16—C8—N2—C7	-6.74 (19)
C10—C11—C12—C13	1.5 (3)	C9—C8—N2—C7	172.77 (12)
C11—C12—C13—C14	-0.1 (2)	N1—C7—N2—C8	34.69 (16)
C10—C9—C14—C13	1.1 (2)	C4—C7—N2—C8	-91.38 (14)
C8—C9—C14—C13	-175.93 (14)		

Hydrogen-bond geometry (Å, °)

Cg is the centroid of the C15–C20 ring.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H1N···N2 ⁱ	0.830 (19)	2.316 (19)	3.1234 (18)	164.3 (19)
C3—H3···N1	0.93	2.53	2.878 (2)	102
C11—H11···Cg ⁱⁱ	0.93	2.76	3.666 (2)	165

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