Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

7-(2-Chlorophenyl)-2,6,9-trimethyldibenzo[*b*,*h*][1,6]naphthyridine

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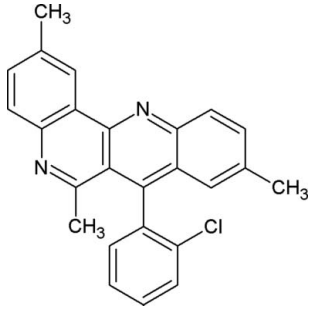
Received 13 July 2010; accepted 30 July 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.143; data-to-parameter ratio = 18.7.

In the title compound, $C_{25}H_{19}ClN_2$, the dibenzo[*b*,*h*][1,6]-naphthyridine system is planar to within 0.16 (2) Å, and the chlorophenyl ring is inclined to it by 82.53 (7)°. In the crystal, molecules are linked by C—H···N hydrogen bonds, forming chains propagating in [100]. There are also a number of weak π–π stacking interactions present [centroid–centroid distances = 3.8531 (1) and 3.7631 (1) Å].

Related literature

For the biological properties of [1,6]naphthyridine derivatives, see: Zhuang *et al.* (2003); Bedard *et al.* (2003); Hinschberger *et al.* (2003); Naik *et al.* (2006). For the synthesis of the precursor of the title compound, see: Nandha Kumar *et al.* (2007). For the crystal structures of other naphthrydine derivatives, see: Sivakumar *et al.* (2003); Fun *et al.* (2009); Vennila *et al.* (2010). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{25}H_{19}ClN_2$
M_r = 382.87
Triclinic, $P\overline{1}$
a = 6.5575 (4) Å
b = 10.6538 (7) Å
c = 14.3522 (9) Å
α = 93.755 (3)°
β = 103.099 (3)°
γ = 102.074 (3)°
V = 948.25 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 293 K
0.27 × 0.25 × 0.23 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.944, T_{max} = 0.952
17317 measured reflections
4771 independent reflections
3514 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.143
S = 1.00
4771 reflections
255 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C22—H22···N7^{i}	0.93	2.42	3.318 (2)	162

Symmetry code: (i) $x-1, y, z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

KNV thanks the CSIR for providing a Senior Research Fellowship. DV acknowledges the Department of Science and Technology (DST) for providing data collection facilities under major research projects and is also thankful for the financial support to the Department under UGC–SAP and DST–FIST programs.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2198).

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supporting information

Acta Cryst. (2010). E**66**, o2426–o2427 [https://doi.org/10.1107/S1600536810030576]

7-(2-Chlorophenyl)-2,6,9-trimethyldibenzo[*b*,*h*][1,6]naphthyridine

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S1. Comment

[1,6]naphthyridine derivatives are reported to be a good class of HIV integrase inhibitors (Zhuang *et al.*, 2003). Their antiviral properties have also been reported by (Bedard *et al.*, 2003), and they were proved to be selective antagonists of 5-HT4 receptors (Hinschberger *et al.*, 2003). The planar fused heterocyclic system in the title compound may lead to its DNA intercalating property (Naik *et al.*, 2006). Due to this biological importance, the title compound was chosen for structural studies.

The title compound, illustrated in Fig. 1, consists of a dibenzo[*b*,*h*][1,6]naphthyridine core with chlorophenyl and methyl group substitutions. The bond lengths are in normal ranges (Allen *et al.*, 1987), and are similar to those observed for other naphthrydine derivatives (Sivakumar *et al.*, 2003; Fun *et al.*, 2009; Vennila *et al.*, 2010), as are the bond angles. The dihedral angle between the fused ring dibenzo[*b*,*h*][1,6]naphthyridine system (N1/N2/C1/C6/C8-C10/C12-C14; planar to within 0.16 (2) Å) and the chlorophenyl ring was found to be 82.53 (7)°. There is an apparent steric clash between the methyl group attached to C8 and the chlorophenyl ring attached to C14. The C9-C8-C19 bond angle of 123.05 (13)° and the C9-C14-C21 bond angle of 124.24 (12)°, suggests that these groups are being forced apart.

The crystal packing is stabilized by C—H···N hydrogen bonds forming chain like patterns propagating along [100] (Table 1, Fig. 2). A number of weak π–π stacking interactions may also stablize the crystal packing (see Table 2 for details).

S2. Experimental

The precursor of the title compoud, 2,6,4′-trimethyl-4-(*N*-phenylamino) quinoline, was prepared following the procedure of (Nandha Kumar *et al.*., 2007). 4-Chloro-2,6-dimethylquinoline (0.002 mol) was reacted with *p*-toluidine (0.002 mol) under neat conditions at 433 K for 30 mins. The product obtained was washed with water, dried, and purified by column chromatography over silica gel using an ethyl acetate:methanol (95:5) mixture to obtain the product as a white solid. A mixture of 2,6,4′-trimethyl-4-(*N*-phenylamino) quinoline (0.001 mol) and *o*-chlorobenzoic acid (0.0011 mol) was added to polyphosphoric acid (1 g of P_2O_5 and 0.5 ml H_3PO_4) and heated at 433 k for 5 h. The reaction mixture was poured into ice water, neutralized with saturated sodium bicarbonate solution to remove the excess of *o*-chlorobenzoic acid, extracted with ethyl acetate. It was then purified using silica gel column chromatography and the product was eluted with a petroleum ether:ethyl acetate (99:1) mixture to get the final product as a pale yellow solid. Recrystallization using ethanol gave yellow block-like crystals of the title compound suitable for X-ray diffraction analysis.

S3. Refinement

The H-atoms of methyl group C20 were disordered over two positions and were placed in calculated positions and treated as riding atoms, each with an occupancy of 0.5. The remaining H-atoms were positioned geometrically and treated as riding on their parent atoms; N—H = 0.86 Å, C—H = 0.93, 0.96 and 0.97 Å, for CH(aromatic), methyl and

methylene H-atoms, respectively, with U_{iso} = k × U_{eq}(parent N, or C atom), where k = 1.5 for methyl H-atoms and 1.2 for all other H-atoms.

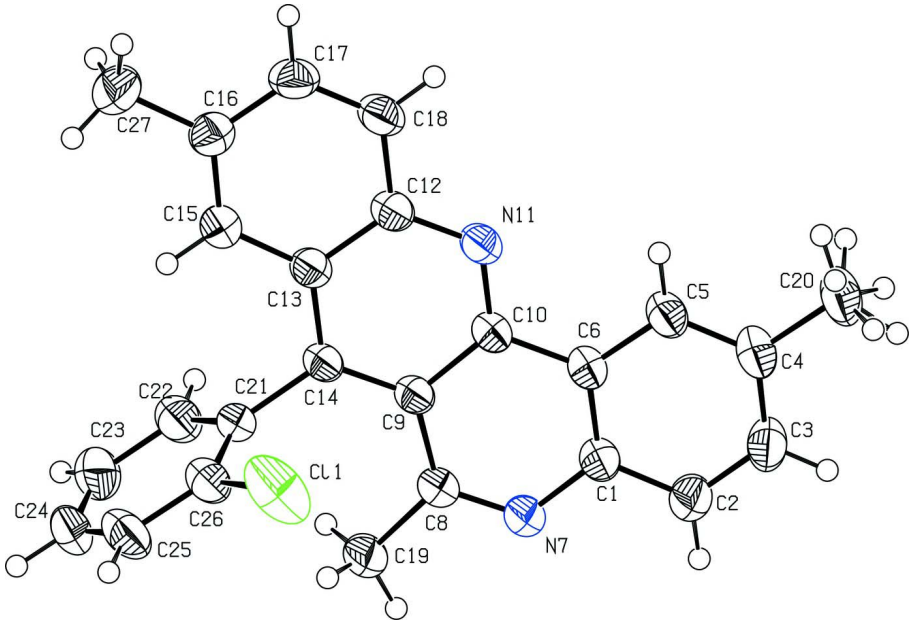

Figure 1

View of the title molecule showing the displacement ellipsoids drawn at 50% probability level.

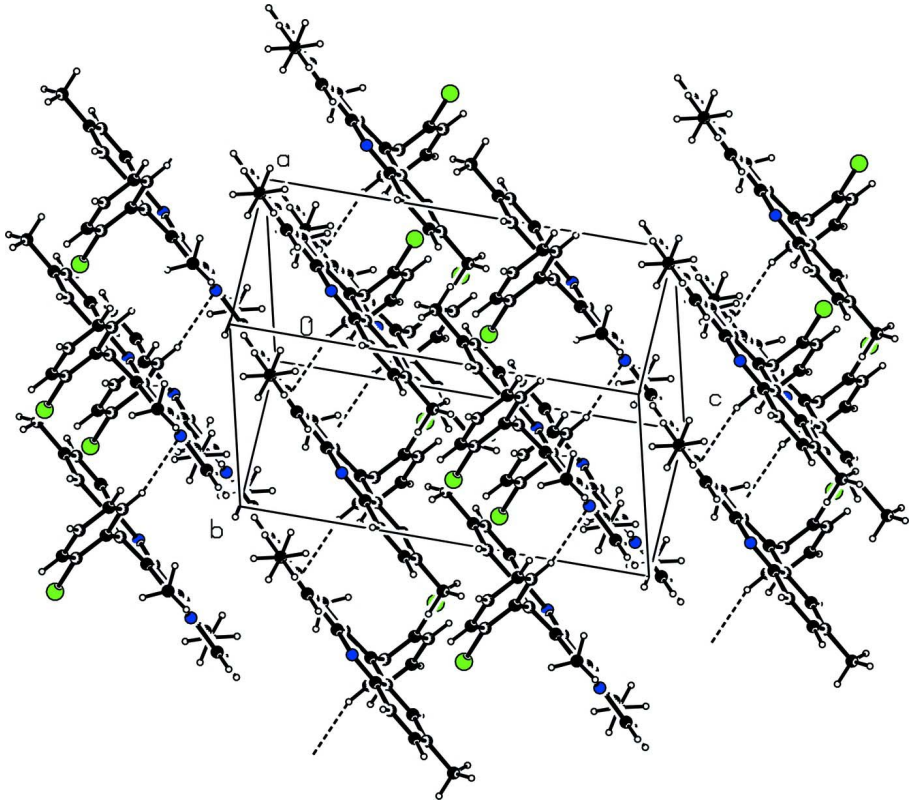

Figure 2

The crystal packing of the title compound illustrating the formation of the C-H···N hydrogen bonded (dashed lines) chain propagating along [100], and the π–π interactions (dashed lines); see Tables 1 and 2 for details.

12-(2-chlorophenyl)-2,7,11-trimethyl-5,10-diazatetraphene

Crystal data

$C_{25}H_{19}ClN_2$
$M_r = 382.87$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.5575$ (4) Å
$b = 10.6538$ (7) Å
$c = 14.3522$ (9) Å
$\alpha = 93.755$ (3)°
$\beta = 103.099$ (3)°
$\gamma = 102.074$ (3)°
$V = 948.25$ (10) Å^3
$Z = 2$
$F(000) = 400$
$D_x = 1.341$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4797 reflections
$\theta = 1.5$–$28.5°$
$\mu = 0.21$ mm^{-1}
$T = 293$ K
Block, yellow
0.27 × 0.25 × 0.23 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.944$, $T_{max} = 0.952$
17317 measured reflections
4771 independent reflections
3514 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 28.5°$, $\theta_{min} = 1.5°$
$h = -8 \rightarrow 8$
$k = -14 \rightarrow 14$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.143$
$S = 1.00$
4771 reflections
255 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
$w = 1/[\sigma^2(F_o^2) + (0.0694P)^2 + 0.2763P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.51$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	0.22259 (9)	0.49217 (5)	0.41457 (4)	0.0809 (2)	
C9	0.1060 (2)	0.63949 (13)	0.20011 (10)	0.0345 (3)	
C14	−0.0361 (2)	0.61889 (13)	0.25997 (11)	0.0354 (3)	
N11	0.1756 (2)	0.87266 (11)	0.24184 (9)	0.0396 (3)	
C10	0.2149 (2)	0.77063 (13)	0.19709 (10)	0.0353 (3)	
C13	−0.0816 (2)	0.72702 (14)	0.30668 (11)	0.0371 (3)	
C6	0.3810 (2)	0.79371 (14)	0.14465 (10)	0.0367 (3)	
C1	0.4188 (2)	0.68758 (14)	0.09475 (11)	0.0382 (3)	
C12	0.0265 (2)	0.85236 (14)	0.29330 (11)	0.0379 (3)	
N7	0.2977 (2)	0.56271 (12)	0.09035 (9)	0.0405 (3)	
C5	0.5087 (3)	0.91727 (15)	0.14455 (12)	0.0427 (3)	
H5	0.4829	0.9885	0.1770	0.051*	
C21	−0.1424 (2)	0.48827 (13)	0.28004 (11)	0.0383 (3)	
C15	−0.2299 (3)	0.71701 (15)	0.36619 (12)	0.0426 (3)	
H15	−0.2983	0.6356	0.3770	0.051*	
C2	0.5826 (3)	0.70513 (17)	0.04574 (13)	0.0478 (4)	
H2	0.6075	0.6347	0.0119	0.057*	
C18	−0.0219 (3)	0.96186 (15)	0.33756 (12)	0.0459 (4)	
H18	0.0465	1.0444	0.3289	0.055*	
C8	0.1537 (2)	0.53873 (14)	0.13957 (11)	0.0376 (3)	
C16	−0.2740 (3)	0.82394 (16)	0.40769 (12)	0.0435 (4)	
C4	0.6710 (3)	0.93469 (16)	0.09730 (12)	0.0463 (4)	
C26	−0.0401 (3)	0.42446 (15)	0.35054 (12)	0.0450 (4)	
C17	−0.1666 (3)	0.94743 (16)	0.39226 (12)	0.0471 (4)	
H17	−0.1960	1.0206	0.4204	0.057*	

C22	−0.3525 (3)	0.42820 (16)	0.23021 (15)	0.0529 (4)	
H22	−0.4273	0.4693	0.1833	0.063*	
C3	0.7064 (3)	0.82702 (17)	0.04798 (13)	0.0512 (4)	
H3	0.8162	0.8381	0.0160	0.061*	
C23	−0.4512 (3)	0.30820 (18)	0.24972 (17)	0.0622 (5)	
H23	−0.5900	0.2684	0.2146	0.075*	
C19	0.0335 (3)	0.39954 (15)	0.12548 (14)	0.0502 (4)	
H19A	0.0790	0.3520	0.0779	0.075*	
H19B	−0.1181	0.3942	0.1043	0.075*	
H19C	0.0630	0.3635	0.1853	0.075*	
C25	−0.1401 (3)	0.30526 (16)	0.37131 (14)	0.0563 (5)	
H25	−0.0683	0.2646	0.4195	0.068*	
C24	−0.3463 (3)	0.24775 (17)	0.32009 (15)	0.0583 (5)	
H24	−0.4144	0.1676	0.3334	0.070*	
C20	0.8124 (3)	1.06674 (18)	0.10020 (15)	0.0613 (5)	
H20A	0.9161	1.0606	0.0635	0.092*	0.50
H20B	0.8857	1.0999	0.1658	0.092*	0.50
H20C	0.7254	1.1239	0.0732	0.092*	0.50
H20D	0.7687	1.1290	0.1382	0.092*	0.50
H20E	0.7992	1.0897	0.0359	0.092*	0.50
H20F	0.9594	1.0657	0.1284	0.092*	0.50
C27	−0.4337 (3)	0.81378 (19)	0.46916 (15)	0.0603 (5)	
H27A	−0.5716	0.8179	0.4303	0.090*	
H27B	−0.3858	0.8839	0.5203	0.090*	
H27C	−0.4454	0.7331	0.4960	0.090*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0751 (4)	0.0620 (3)	0.0805 (4)	−0.0032 (2)	−0.0189 (3)	0.0237 (3)
C9	0.0369 (7)	0.0290 (6)	0.0383 (7)	0.0081 (5)	0.0095 (6)	0.0067 (5)
C14	0.0374 (7)	0.0284 (7)	0.0415 (8)	0.0080 (5)	0.0105 (6)	0.0080 (6)
N11	0.0477 (7)	0.0294 (6)	0.0430 (7)	0.0072 (5)	0.0149 (6)	0.0055 (5)
C10	0.0388 (7)	0.0309 (7)	0.0359 (7)	0.0069 (6)	0.0089 (6)	0.0071 (5)
C13	0.0415 (8)	0.0318 (7)	0.0391 (8)	0.0092 (6)	0.0111 (6)	0.0063 (6)
C6	0.0393 (7)	0.0333 (7)	0.0366 (7)	0.0048 (6)	0.0098 (6)	0.0074 (6)
C1	0.0400 (8)	0.0353 (7)	0.0388 (8)	0.0057 (6)	0.0110 (6)	0.0062 (6)
C12	0.0451 (8)	0.0318 (7)	0.0372 (7)	0.0093 (6)	0.0103 (6)	0.0051 (6)
N7	0.0450 (7)	0.0326 (6)	0.0461 (7)	0.0072 (5)	0.0171 (6)	0.0044 (5)
C5	0.0490 (9)	0.0339 (7)	0.0428 (8)	0.0014 (6)	0.0137 (7)	0.0050 (6)
C21	0.0423 (8)	0.0293 (7)	0.0478 (8)	0.0088 (6)	0.0194 (6)	0.0061 (6)
C15	0.0464 (8)	0.0366 (8)	0.0481 (9)	0.0089 (6)	0.0180 (7)	0.0078 (6)
C2	0.0514 (9)	0.0449 (9)	0.0506 (9)	0.0080 (7)	0.0230 (7)	0.0033 (7)
C18	0.0616 (10)	0.0308 (7)	0.0475 (9)	0.0104 (7)	0.0181 (8)	0.0046 (6)
C8	0.0411 (8)	0.0308 (7)	0.0416 (8)	0.0083 (6)	0.0114 (6)	0.0057 (6)
C16	0.0455 (8)	0.0433 (8)	0.0435 (8)	0.0122 (7)	0.0131 (7)	0.0031 (7)
C4	0.0469 (9)	0.0426 (8)	0.0446 (9)	−0.0026 (7)	0.0128 (7)	0.0081 (7)
C26	0.0552 (9)	0.0343 (7)	0.0445 (9)	0.0064 (7)	0.0134 (7)	0.0069 (6)

C17	0.0599 (10)	0.0380 (8)	0.0470 (9)	0.0170 (7)	0.0165 (8)	0.0001 (7)
C22	0.0446 (9)	0.0416 (9)	0.0728 (12)	0.0090 (7)	0.0142 (8)	0.0142 (8)
C3	0.0487 (9)	0.0539 (10)	0.0520 (10)	0.0013 (7)	0.0239 (8)	0.0071 (8)
C23	0.0433 (9)	0.0473 (10)	0.0937 (15)	−0.0002 (8)	0.0221 (10)	0.0087 (10)
C19	0.0589 (10)	0.0321 (7)	0.0617 (11)	0.0036 (7)	0.0268 (8)	−0.0009 (7)
C25	0.0803 (13)	0.0368 (8)	0.0536 (10)	0.0088 (8)	0.0216 (9)	0.0145 (7)
C24	0.0701 (12)	0.0359 (8)	0.0749 (13)	0.0029 (8)	0.0367 (10)	0.0121 (8)
C20	0.0643 (12)	0.0476 (10)	0.0667 (12)	−0.0099 (8)	0.0265 (10)	0.0076 (9)
C27	0.0630 (11)	0.0554 (11)	0.0694 (12)	0.0128 (9)	0.0334 (10)	−0.0011 (9)

Geometric parameters (Å, º)

Cl1—C26	1.7342 (18)	C8—C19	1.504 (2)
C9—C14	1.399 (2)	C16—C17	1.413 (2)
C9—C10	1.4381 (19)	C16—C27	1.507 (2)
C9—C8	1.465 (2)	C4—C3	1.397 (2)
C14—C13	1.414 (2)	C4—C20	1.507 (2)
C14—C21	1.4978 (19)	C26—C25	1.386 (2)
N11—C10	1.3272 (18)	C17—H17	0.9300
N11—C12	1.3449 (19)	C22—C23	1.384 (2)
C10—C6	1.448 (2)	C22—H22	0.9300
C13—C12	1.422 (2)	C3—H3	0.9300
C13—C15	1.425 (2)	C23—C24	1.365 (3)
C6—C1	1.395 (2)	C23—H23	0.9300
C6—C5	1.405 (2)	C19—H19A	0.9600
C1—N7	1.3888 (19)	C19—H19B	0.9600
C1—C2	1.399 (2)	C19—H19C	0.9600
C12—C18	1.419 (2)	C25—C24	1.374 (3)
N7—C8	1.2966 (19)	C25—H25	0.9300
C5—C4	1.374 (2)	C24—H24	0.9300
C5—H5	0.9300	C20—H20A	0.9600
C21—C26	1.382 (2)	C20—H20B	0.9600
C21—C22	1.394 (2)	C20—H20C	0.9600
C15—C16	1.365 (2)	C20—H20D	0.9600
C15—H15	0.9300	C20—H20E	0.9600
C2—C3	1.374 (2)	C20—H20F	0.9600
C2—H2	0.9300	C27—H27A	0.9600
C18—C17	1.353 (2)	C27—H27B	0.9600
C18—H18	0.9300	C27—H27C	0.9600
C14—C9—C10	117.59 (12)	C18—C17—H17	119.2
C14—C9—C8	125.62 (13)	C16—C17—H17	119.2
C10—C9—C8	116.79 (13)	C23—C22—C21	120.83 (17)
C9—C14—C13	118.93 (13)	C23—C22—H22	119.6
C9—C14—C21	124.24 (12)	C21—C22—H22	119.6
C13—C14—C21	116.82 (13)	C2—C3—C4	121.42 (15)
C10—N11—C12	118.23 (12)	C2—C3—H3	119.3
N11—C10—C9	123.65 (13)	C4—C3—H3	119.3

N11—C10—C6	117.60 (13)	C24—C23—C22	120.50 (18)
C9—C10—C6	118.73 (12)	C24—C23—H23	119.8
C14—C13—C12	118.07 (13)	C22—C23—H23	119.8
C14—C13—C15	123.54 (13)	C8—C19—H19A	109.5
C12—C13—C15	118.39 (13)	C8—C19—H19B	109.5
C1—C6—C5	119.07 (14)	H19A—C19—H19B	109.5
C1—C6—C10	118.10 (13)	C8—C19—H19C	109.5
C5—C6—C10	122.80 (14)	H19A—C19—H19C	109.5
N7—C1—C6	122.51 (13)	H19B—C19—H19C	109.5
N7—C1—C2	117.55 (13)	C24—C25—C26	119.42 (17)
C6—C1—C2	119.94 (14)	C24—C25—H25	120.3
N11—C12—C18	118.06 (13)	C26—C25—H25	120.3
N11—C12—C13	123.19 (13)	C23—C24—C25	120.02 (16)
C18—C12—C13	118.73 (14)	C23—C24—H24	120.0
C8—N7—C1	120.50 (13)	C25—C24—H24	120.0
C4—C5—C6	121.15 (15)	C4—C20—H20A	109.5
C4—C5—H5	119.4	C4—C20—H20B	109.5
C6—C5—H5	119.4	H20A—C20—H20B	109.5
C26—C21—C22	117.31 (14)	C4—C20—H20C	109.5
C26—C21—C14	121.67 (14)	H20A—C20—H20C	109.5
C22—C21—C14	120.98 (14)	H20B—C20—H20C	109.5
C16—C15—C13	121.68 (15)	C4—C20—H20D	109.5
C16—C15—H15	119.2	H20A—C20—H20D	141.1
C13—C15—H15	119.2	H20B—C20—H20D	56.3
C3—C2—C1	119.59 (15)	H20C—C20—H20D	56.3
C3—C2—H2	120.2	C4—C20—H20E	109.5
C1—C2—H2	120.2	H20A—C20—H20E	56.3
C17—C18—C12	120.70 (15)	H20B—C20—H20E	141.1
C17—C18—H18	119.6	H20C—C20—H20E	56.3
C12—C18—H18	119.6	H20D—C20—H20E	109.5
N7—C8—C9	122.88 (13)	C4—C20—H20F	109.5
N7—C8—C19	114.02 (13)	H20A—C20—H20F	56.3
C9—C8—C19	123.05 (13)	H20B—C20—H20F	56.3
C15—C16—C17	118.83 (15)	H20C—C20—H20F	141.1
C15—C16—C27	121.87 (15)	H20D—C20—H20F	109.5
C17—C16—C27	119.31 (14)	H20E—C20—H20F	109.5
C5—C4—C3	118.82 (15)	C16—C27—H27A	109.5
C5—C4—C20	120.96 (16)	C16—C27—H27B	109.5
C3—C4—C20	120.20 (15)	H27A—C27—H27B	109.5
C21—C26—C25	121.90 (16)	C16—C27—H27C	109.5
C21—C26—Cl1	119.98 (12)	H27A—C27—H27C	109.5
C25—C26—Cl1	118.11 (14)	H27B—C27—H27C	109.5
C18—C17—C16	121.65 (14)		

C10—C9—C14—C13	6.1 (2)	C13—C14—C21—C22	82.85 (19)
C8—C9—C14—C13	−173.70 (13)	C14—C13—C15—C16	−178.02 (15)
C10—C9—C14—C21	−172.70 (13)	C12—C13—C15—C16	1.9 (2)
C8—C9—C14—C21	7.5 (2)	N7—C1—C2—C3	179.93 (16)

C12—N11—C10—C9	0.4 (2)	C6—C1—C2—C3	0.6 (3)
C12—N11—C10—C6	−177.97 (13)	N11—C12—C18—C17	−178.30 (15)
C14—C9—C10—N11	−5.4 (2)	C13—C12—C18—C17	0.6 (2)
C8—C9—C10—N11	174.47 (13)	C1—N7—C8—C9	1.4 (2)
C14—C9—C10—C6	172.95 (13)	C1—N7—C8—C19	178.83 (14)
C8—C9—C10—C6	−7.2 (2)	C14—C9—C8—N7	−175.27 (14)
C9—C14—C13—C12	−2.4 (2)	C10—C9—C8—N7	4.9 (2)
C21—C14—C13—C12	176.51 (13)	C14—C9—C8—C19	7.5 (2)
C9—C14—C13—C15	177.54 (14)	C10—C9—C8—C19	−172.28 (14)
C21—C14—C13—C15	−3.6 (2)	C13—C15—C16—C17	−1.1 (2)
N11—C10—C6—C1	−177.95 (13)	C13—C15—C16—C27	178.85 (16)
C9—C10—C6—C1	3.6 (2)	C6—C5—C4—C3	0.6 (3)
N11—C10—C6—C5	4.1 (2)	C6—C5—C4—C20	−177.91 (16)
C9—C10—C6—C5	−174.35 (14)	C22—C21—C26—C25	0.3 (2)
C5—C6—C1—N7	−179.11 (14)	C14—C21—C26—C25	178.09 (15)
C10—C6—C1—N7	2.8 (2)	C22—C21—C26—Cl1	179.19 (13)
C5—C6—C1—C2	0.1 (2)	C14—C21—C26—Cl1	−3.0 (2)
C10—C6—C1—C2	−177.91 (14)	C12—C18—C17—C16	0.2 (3)
C10—N11—C12—C18	−177.28 (14)	C15—C16—C17—C18	0.0 (3)
C10—N11—C12—C13	3.8 (2)	C27—C16—C17—C18	−179.91 (17)
C14—C13—C12—N11	−2.8 (2)	C26—C21—C22—C23	−1.4 (3)
C15—C13—C12—N11	177.25 (14)	C14—C21—C22—C23	−179.24 (16)
C14—C13—C12—C18	178.29 (14)	C1—C2—C3—C4	−0.8 (3)
C15—C13—C12—C18	−1.6 (2)	C5—C4—C3—C2	0.2 (3)
C6—C1—N7—C8	−5.5 (2)	C20—C4—C3—C2	178.72 (18)
C2—C1—N7—C8	175.23 (15)	C21—C22—C23—C24	1.7 (3)
C1—C6—C5—C4	−0.8 (2)	C21—C26—C25—C24	0.6 (3)
C10—C6—C5—C4	177.17 (14)	Cl1—C26—C25—C24	−178.38 (14)
C9—C14—C21—C26	83.9 (2)	C22—C23—C24—C25	−0.9 (3)
C13—C14—C21—C26	−94.89 (17)	C26—C25—C24—C23	−0.3 (3)
C9—C14—C21—C22	−98.31 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C22—H22···N7^{i}	0.93	2.42	3.318 (2)	162

Symmetry code: (i) *x*−1, *y*, *z*.