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6-Fluoro-4-methyl-2-(3-pyridyl)-1,2,3,4-tetrahydroquinoline

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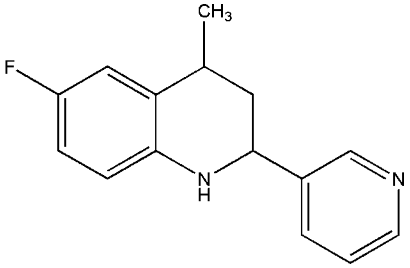
Key indicators: single-crystal synchrotron study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.063; wR factor = 0.178; data-to-parameter ratio = 24.5.

In the title compound, $C_{15}H_{15}FN_2$, the tetrahydropyridine ring adopts a half-chair conformation. Hydrogen bonds of the type N—H···N form extended zigzag chains related by 2_1 screw axes running along [010]. Additionally, C—H···π hydrogen bonds contribute to the stabilization of the crystal structure, which packs with an efficiency of 68.2%.

Related literature

For related literature, see: Allen *et al.* (1987); Cremer & Pople (1975); Obodovskaya *et al.* (1985); Rybakov *et al.* (2004); Vargas-Méndez *et al.* (2003); Zavalishin *et al.* (1977).



Experimental

Crystal data

$C_{15}H_{15}FN_2$
M_r = 242.29
Orthorhombic, *Pbca*
a = 16.2219 (7) Å
b = 8.5208 (2) Å
c = 18.1612 (7) Å
V = 2510.31 (16) Å^3
Z = 8
Synchrotron radiation
λ = 0.50915 Å
μ = 0.04 mm^{-1}
T = 120 K
0.20 × 0.05 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
23667 measured reflections
4099 independent reflections
3706 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.178
S = 1.13
4099 reflections
167 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\rm max}$ = 0.39 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.39 e Å^{-3}

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

Cg is the centroid of the C16/C5–C8/C17 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2$^{\rm i}$	0.90 (2)	2.15 (2)	3.0300 (18)	165.5 (18)
C4—H4···$Cg^{\rm ii}$	1.00	2.87	3.7421 (16)	146

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *PLATON* (Spek, 2003) and *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2006).

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supplementary materials

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6-Fluoro-4-methyl-2-(3-pyridyl)-1,2,3,4-tetrahydroquinoline

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Comment

In this work, the structure of the compound 6-fluoro-4-methyl-2-(3'-pyridil)-1,2,3,4-tetrahydroquinoline (I) is presented, which was prepared from the related homoallylamine derivative by mixing with H_2SO_4 (85%),$CHCl_3$ at 363 K for 10–12 hrs (Vargas *et al.*, 2003). There is a binary axis bisecting the C2—C3 and C6—C17 bonds (Cs = +8.2 (2)°) (Cremer & Pople,1975) in the pyridine ring; therefore, this ring adopts the half-chair conformation (Fig. 1), as seen in the related structures DISHIW (Obodovskaya *etal.*, 1985) and IXAHOE (Rybakov *et al.*, 2004) (Cambridge Structural Database, 2006). C2 and C3 are out of the pyridine ring mean plane by 0.302 (1)Å and −0.314 (1) Å, respectively. The methyl group in position 4 and the pyridyl group in position 2 are bisectorial and equatorial to the pyridine ring, respectively. The N1—C17 distance is shorter than the N1—C2 distance by 0.0604 (2)Å (Table 1). The asymmetry in the N—C distances have also been observed in three 1,2,3,4-tetrahydroquinoline compounds substituted in positions 2,4,6 reported in the CSD [DISHIW, IXAHOE, MHXHQV] (Obodovskaya *et al.*, 1985; Rybakov *et al.*, 2004; Zavalishin *et al.*, 1977), and have been attributed to resonance effects between the benzene ring and the electron pair of N1, awarding a pseudo double character to the N1—C17 bond.

The crystal structure is essentially lamellar, with layers of molecules bonded by hydrogen bonds packing in a sinusoidal way along the [001] direction (Fig.2 & Table 2). This interaction by hydrogen bond forms extended zigzag chains along [010]. In the chain depicted in Fig. 2, pairs of molecules are related by 2_1 screw axis. Non-conventional C—H···aromatic hydrogen bonds between benzene rings (C5—C8/C16—C17) and hydrogen atoms of neighboring layers link every two layer. Between these hydrogen-bonded double-layers there are intercalated H···H hydrophophic interactions; all these attractive and disruptive interactions contribute to the stabilization of the crystal structure, which packs with an efficiency of 68.2% of filled space.

Experimental

The synthesis of the fluoro tetrahydroquinoline derivative is explained elsewhere (Vargas *et al.*, 2003). Single crystals were obtained from the slow evaporation of 50 mg of $C_{15}H_{15}FN_2$ from chloroform.

Refinement

The H atom of N1 refined freely. The other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å for aromatic H atoms and C—H = 0.99 Å for methylene H atoms, both with $U_{iso}(H) = 1.2U_{eq}(C)$, and C—H = 0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms.

Figures

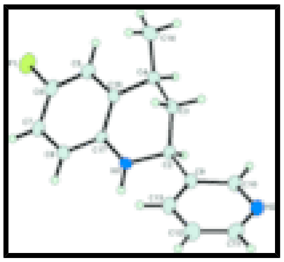

Fig. 1. Asymmetric unit and labeling of atoms in (I), showing thermal ellipsoids with 50% probability.

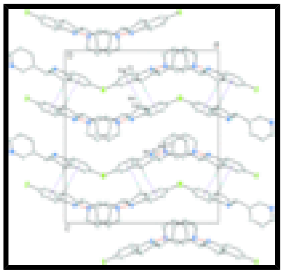

Fig. 2. Layer packing of (I) seen down *b*. [Symmetry codes: (i) −*x* + 3/2, *y* + 1/2, *z*; (ii) −*x* + 1, *y* − 1/2, −*z* + 1/2.]

6-Fluoro-4-methyl-2-(3-pyridyl)-1,2,3,4-tetrahydroquinoline

Crystal data

$C_{15}H_{15}FN_2$	D_x = 1.282 Mg m^{-3}
M_r = 242.29	Melting point: 387-388 K
Orthorhombic, *Pbca*	Synchrotron radiation λ = 0.50915 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 3048 reflections
a = 16.2219 (7) Å	θ = 9.1–42.7°
b = 8.5208 (2) Å	μ = 0.04 mm^{-1}
c = 18.1612 (7) Å	*T* = 120 K
V = 2510.31 (16) Å^3	Needle, colourless
Z = 8	0.20 × 0.05 × 0.05 mm
F_{000} = 1024	

Data collection

Bruker SMART CCD area-detector diffractometer	4099 independent reflections
Radiation source: Beam line ID-11 ESRF	3706 reflections with $I > 2\sigma(I)$
Monochromator: double crystal Si	R_{int} = 0.033
Detector resolution: 8.0 pixels mm^{-1}	θ_{max} = 22.1°
T = 120 K	θ_{min} = 1.6°
oscillation scans	$h = -22 \rightarrow 23$
Absorption correction: none	$k = -12 \rightarrow 12$
23667 measured reflections	$l = -26 \rightarrow 26$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.063$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.178$	$w = 1/[\sigma^2(F_o^2) + (0.0761P)^2 + 1.7041P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{max} < 0.001$
4099 reflections	$\Delta\rho_{max} = 0.39$ e Å^{-3}
167 parameters	$\Delta\rho_{min} = -0.39$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.25209 (6)	0.89015 (15)	0.22468 (6)	0.0409 (3)
N1	0.56467 (7)	0.87020 (14)	0.10281 (7)	0.0219 (3)
N2	0.84577 (8)	0.68002 (16)	0.08529 (8)	0.0274 (3)
C2	0.62185 (8)	0.75116 (16)	0.13001 (7)	0.0205 (3)
C3	0.57922 (9)	0.59195 (16)	0.12436 (8)	0.0239 (3)
C4	0.50292 (9)	0.58544 (17)	0.17442 (8)	0.0246 (3)
C5	0.37335 (8)	0.74564 (19)	0.19852 (8)	0.0259 (4)
C6	0.32926 (8)	0.8843 (2)	0.19385 (8)	0.0272 (4)
C7	0.35906 (8)	1.01602 (18)	0.15868 (8)	0.0253 (4)
C8	0.43766 (8)	1.00741 (17)	0.12804 (8)	0.0225 (3)
C9	0.70204 (8)	0.75541 (16)	0.08748 (7)	0.0203 (3)
C10	0.77139 (8)	0.68369 (18)	0.11756 (8)	0.0239 (3)
C11	0.85312 (9)	0.75054 (19)	0.01961 (9)	0.0278 (4)
C12	0.78812 (10)	0.8257 (2)	−0.01530 (8)	0.0301 (4)
C13	0.71109 (9)	0.82767 (19)	0.01895 (8)	0.0265 (4)
C14	0.45329 (11)	0.4364 (2)	0.15721 (13)	0.0403 (5)
C16	0.45266 (8)	0.73577 (16)	0.16809 (7)	0.0202 (3)

C17	0.48560 (7)	0.87039 (15)	0.13369 (7)	0.0186 (3)
H1	0.5849 (12)	0.968 (3)	0.1038 (11)	0.025 (5)*
H2	0.63390	0.77310	0.18300	0.0250*
H3A	0.61830	0.50820	0.13880	0.0290*
H3B	0.56240	0.57300	0.07270	0.0290*
H4	0.52270	0.57720	0.22640	0.0290*
H5	0.34990	0.65700	0.22240	0.0310*
H7	0.32710	1.10930	0.15550	0.0300*
H8	0.45930	1.09590	0.10280	0.0270*
H10	0.76570	0.63400	0.16410	0.0290*
H11	0.90530	0.74890	−0.00410	0.0330*
H12	0.79590	0.87500	−0.06170	0.0360*
H13	0.66550	0.87750	−0.00400	0.0320*
H14A	0.48900	0.34430	0.16230	0.0480*
H14B	0.43230	0.44200	0.10670	0.0480*
H14C	0.40700	0.42800	0.19160	0.0480*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0180 (4)	0.0536 (7)	0.0512 (6)	0.0078 (4)	0.0113 (4)	0.0115 (5)
N1	0.0157 (5)	0.0172 (5)	0.0327 (6)	0.0014 (4)	0.0026 (4)	0.0051 (4)
N2	0.0198 (5)	0.0270 (6)	0.0353 (6)	0.0051 (4)	0.0010 (4)	0.0001 (5)
C2	0.0170 (5)	0.0225 (6)	0.0221 (5)	0.0032 (4)	−0.0001 (4)	0.0019 (4)
C3	0.0226 (6)	0.0186 (6)	0.0306 (6)	0.0024 (5)	0.0001 (5)	0.0034 (5)
C4	0.0212 (6)	0.0218 (6)	0.0307 (6)	0.0010 (5)	−0.0004 (5)	0.0085 (5)
C5	0.0192 (6)	0.0302 (7)	0.0284 (6)	−0.0006 (5)	0.0014 (5)	0.0072 (5)
C6	0.0141 (5)	0.0384 (8)	0.0290 (6)	0.0030 (5)	0.0021 (5)	0.0033 (6)
C7	0.0181 (6)	0.0277 (7)	0.0300 (6)	0.0055 (5)	−0.0024 (5)	0.0009 (5)
C8	0.0186 (5)	0.0208 (6)	0.0280 (6)	0.0019 (4)	−0.0016 (4)	0.0019 (5)
C9	0.0176 (5)	0.0213 (6)	0.0221 (5)	0.0028 (4)	0.0009 (4)	0.0003 (4)
C10	0.0199 (6)	0.0255 (6)	0.0264 (6)	0.0047 (5)	0.0000 (4)	0.0023 (5)
C11	0.0210 (6)	0.0293 (7)	0.0330 (7)	0.0025 (5)	0.0061 (5)	−0.0047 (6)
C12	0.0269 (7)	0.0384 (8)	0.0250 (6)	0.0036 (6)	0.0060 (5)	0.0028 (6)
C13	0.0227 (6)	0.0330 (7)	0.0238 (6)	0.0054 (5)	0.0013 (5)	0.0044 (5)
C14	0.0312 (8)	0.0226 (7)	0.0671 (12)	−0.0030 (6)	0.0017 (8)	0.0094 (7)
C16	0.0172 (5)	0.0219 (6)	0.0216 (5)	0.0004 (4)	−0.0019 (4)	0.0041 (4)
C17	0.0149 (5)	0.0191 (6)	0.0218 (5)	0.0001 (4)	−0.0016 (4)	0.0013 (4)

Geometric parameters (Å, °)

F1—C6	1.3723 (17)	C11—C12	1.387 (2)
N1—C2	1.4606 (18)	C12—C13	1.396 (2)
N1—C17	1.3999 (16)	C16—C17	1.4112 (18)
N2—C10	1.3418 (19)	C2—H2	1.0000
N2—C11	1.341 (2)	C3—H3A	0.9900
N1—H1	0.90 (2)	C3—H3B	0.9900
C2—C9	1.5133 (18)	C4—H4	1.0000
C2—C3	1.5261 (19)	C5—H5	0.9500

C3—C4	1.537 (2)	C7—H7	0.9500
C4—C14	1.536 (2)	C8—H8	0.9500
C4—C16	1.523 (2)	C10—H10	0.9500
C5—C16	1.4028 (19)	C11—H11	0.9500
C5—C6	1.384 (2)	C12—H12	0.9500
C6—C7	1.379 (2)	C13—H13	0.9500
C7—C8	1.3931 (19)	C14—H14A	0.9800
C8—C17	1.4066 (19)	C14—H14B	0.9800
C9—C10	1.3919 (19)	C14—H14C	0.9800
C9—C13	1.396 (2)		
F1···H2^{i}	2.7400	H2···C16	2.9700
F1···H5^{ii}	2.8100	H2···H4	2.5800
F1···H14C^{ii}	2.6700	H2···H10	2.4700
N1···N2^{iii}	3.0300 (18)	H2···F1^{x}	2.7400
N2···C13^{iv}	3.364 (2)	H3A···C10	2.9200
N2···N1^{iv}	3.0300 (18)	H3A···H14A	2.5600
N1···H13	2.5400	H3B···C17	3.0300
N2···H1^{iv}	2.15 (2)	H3B···H14B	2.4700
C10···C13^{iv}	3.534 (2)	H4···H2	2.5800
C13···C10^{iii}	3.534 (2)	H4···C7^{xi}	2.8800
C13···N2^{iii}	3.364 (2)	H4···C8^{xi}	2.7800
C5···H14C	2.7600	H4···C17^{xi}	3.1000
C5···H12^{v}	2.9700	H5···C14	2.7800
C7···H13^{vi}	2.9800	H5···H14C	2.2300
C7···H4^{vii}	2.8800	H5···H10^{i}	2.4800
C8···H14A^{viii}	3.0500	H5···F1^{xii}	2.8100
C8···H13^{vi}	2.9700	H8···C14^{viii}	3.0700
C8···H4^{vii}	2.7800	H8···H1	2.3100
C10···H3A	2.9200	H8···H14A^{viii}	2.4200
C10···H1^{iv}	2.98 (2)	H10···H2	2.4700
C11···H1^{iv}	3.02 (2)	H10···H5^{x}	2.4800
C13···H1	2.83 (2)	H11···C16^{xiii}	3.0800
C14···H5	2.7800	H11···C17^{xiii}	2.8800
C14···H8^{ix}	3.0700	H12···C5^{xiii}	2.9700
C16···H2	2.9700	H13···N1	2.5400
C16···H11^{v}	3.0800	H13···H1	2.4800
C17···H3B	3.0300	H13···C7^{vi}	2.9800
C17···H11^{v}	2.8800	H13···C8^{vi}	2.9700
C17···H4^{vii}	3.1000	H14A···C8^{ix}	3.0500
H1···C13	2.83 (2)	H14A···H3A	2.5600
H1···H8	2.3100	H14A···H8^{ix}	2.4200
H1···H13	2.4800	H14B···H3B	2.4700
H1···N2^{iii}	2.15 (2)	H14C···C5	2.7600

H1···C10^{iii}	2.98 (2)	H14C···H5	2.2300
H1···C11^{iii}	3.02 (2)	H14C···F1^{xii}	2.6700

C2—N1—C17	116.56 (11)	C3—C2—H2	109.00
C10—N2—C11	117.26 (13)	C9—C2—H2	109.00
C2—N1—H1	114.0 (13)	C2—C3—H3A	109.00
C17—N1—H1	109.1 (13)	C2—C3—H3B	109.00
N1—C2—C3	107.87 (11)	C4—C3—H3A	109.00
N1—C2—C9	110.90 (11)	C4—C3—H3B	109.00
C3—C2—C9	112.12 (11)	H3A—C3—H3B	108.00
C2—C3—C4	110.93 (11)	C3—C4—H4	108.00
C14—C4—C16	113.55 (12)	C14—C4—H4	108.00
C3—C4—C14	109.37 (13)	C16—C4—H4	108.00
C3—C4—C16	110.87 (11)	C6—C5—H5	120.00
C6—C5—C16	120.07 (14)	C16—C5—H5	120.00
C5—C6—C7	122.83 (13)	C6—C7—H7	121.00
F1—C6—C5	118.53 (14)	C8—C7—H7	121.00
F1—C6—C7	118.64 (14)	C7—C8—H8	119.00
C6—C7—C8	117.58 (13)	C17—C8—H8	119.00
C7—C8—C17	121.37 (13)	N2—C10—H10	118.00
C2—C9—C13	123.77 (12)	C9—C10—H10	118.00
C10—C9—C13	117.29 (12)	N2—C11—H11	118.00
C2—C9—C10	118.94 (12)	C12—C11—H11	118.00
N2—C10—C9	124.44 (14)	C11—C12—H12	121.00
N2—C11—C12	123.09 (14)	C13—C12—H12	121.00
C11—C12—C13	118.84 (14)	C9—C13—H13	120.00
C9—C13—C12	119.08 (13)	C12—C13—H13	120.00
C4—C16—C17	120.96 (11)	C4—C14—H14A	109.00
C5—C16—C17	118.23 (12)	C4—C14—H14B	109.00
C4—C16—C5	120.78 (12)	C4—C14—H14C	109.00
C8—C17—C16	119.84 (11)	H14A—C14—H14B	109.00
N1—C17—C8	118.58 (12)	H14A—C14—H14C	110.00
N1—C17—C16	121.56 (11)	H14B—C14—H14C	110.00
N1—C2—H2	109.00		

C17—N1—C2—C3	51.97 (15)	C16—C5—C6—C7	1.4 (2)
C17—N1—C2—C9	175.10 (11)	C6—C5—C16—C4	178.44 (13)
C2—N1—C17—C8	160.05 (12)	C6—C5—C16—C17	0.5 (2)
C2—N1—C17—C16	−21.78 (18)	F1—C6—C7—C8	179.78 (13)
C11—N2—C10—C9	0.0 (2)	C5—C6—C7—C8	−1.2 (2)
C10—N2—C11—C12	0.1 (2)	C6—C7—C8—C17	−1.0 (2)
N1—C2—C3—C4	−63.55 (14)	C7—C8—C17—N1	−178.91 (13)
C9—C2—C3—C4	174.07 (11)	C7—C8—C17—C16	2.9 (2)
N1—C2—C9—C10	162.18 (12)	C2—C9—C10—N2	−179.82 (14)
N1—C2—C9—C13	−17.85 (18)	C13—C9—C10—N2	0.2 (2)
C3—C2—C9—C10	−77.19 (16)	C2—C9—C13—C12	179.53 (14)
C3—C2—C9—C13	102.79 (16)	C10—C9—C13—C12	−0.5 (2)
C2—C3—C4—C14	170.01 (13)	N2—C11—C12—C13	−0.4 (2)
C2—C3—C4—C16	44.05 (15)	C11—C12—C13—C9	0.6 (2)
C3—C4—C16—C5	168.74 (12)	C4—C16—C17—N1	1.35 (19)

C3—C4—C16—C17	−13.41 (18)	C4—C16—C17—C8	179.50 (12)
C14—C4—C16—C5	45.14 (19)	C5—C16—C17—N1	179.26 (12)
C14—C4—C16—C17	−137.01 (15)	C5—C16—C17—C8	−2.59 (19)
C16—C5—C6—F1	−179.54 (13)		

Symmetry codes: (i) *x*−1/2, *y*, −*z*+1/2; (ii) −*x*+1/2, *y*+1/2, *z*; (iii) −*x*+3/2, *y*+1/2, *z*; (iv) −*x*+3/2, *y*−1/2, *z*; (v) *x*−1/2, −*y*+3/2, −*z*; (vi) −*x*+1, −*y*+2, −*z*; (vii) −*x*+1, *y*+1/2, −*z*+1/2; (viii) *x*, *y*+1, *z*; (ix) *x*, *y*−1, *z*; (x) *x*+1/2, *y*, −*z*+1/2; (xi) −*x*+1, *y*−1/2, −*z*+1/2; (xii) −*x*+1/2, *y*−1/2, *z*; (xiii) *x*+1/2, −*y*+3/2, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2^{iii}	0.90 (2)	2.15 (2)	3.0300 (18)	165.5 (18)
C4—H4···Cg^{xi}	1.00	2.87	3.7421 (16)	146

Symmetry codes: (iii) −*x*+3/2, *y*+1/2, *z*; (xi) −*x*+1, *y*−1/2, −*z*+1/2.

Fig. 1

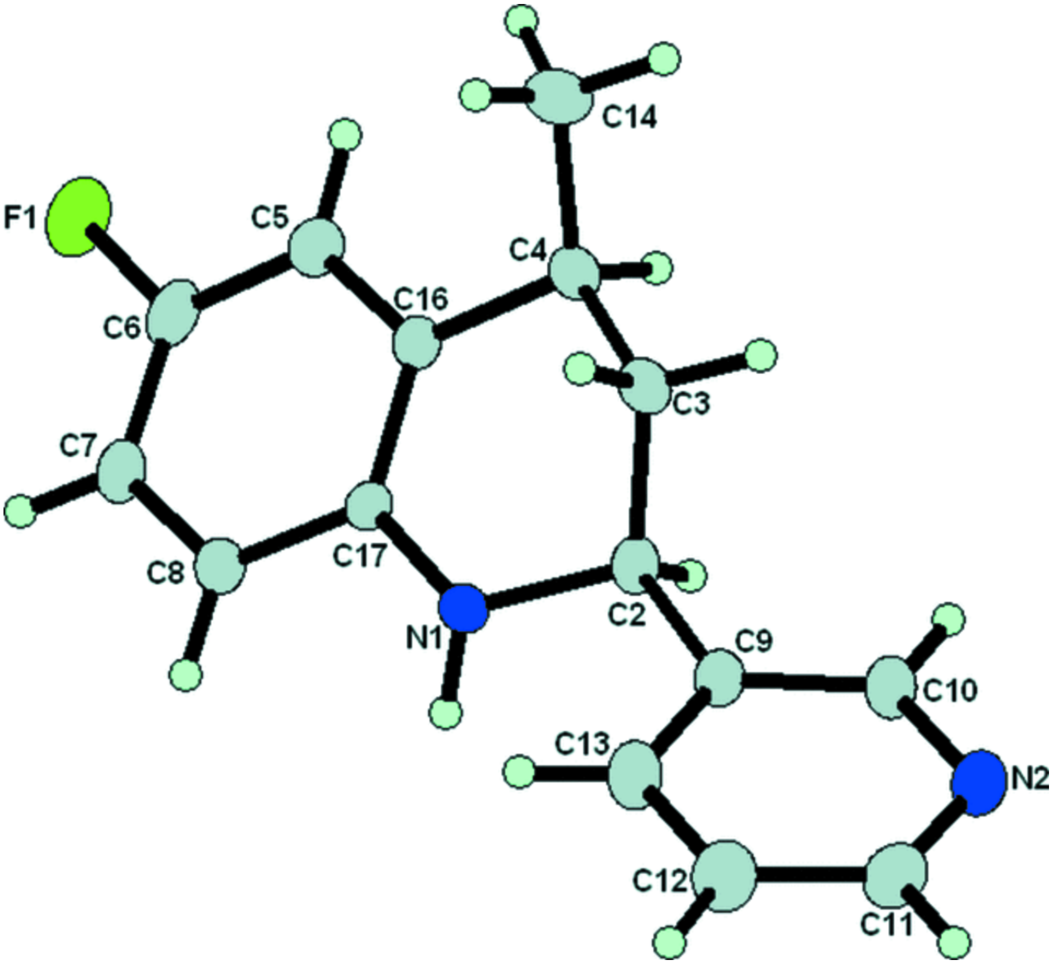

Fig. 2