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1-(2-Chlorophenyl)-6-fluoro-2-methyl-1*H*-indole-3-carbonitrile

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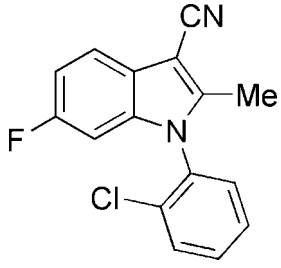
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.113; data-to-parameter ratio = 21.4.

In the title compound, $C_{16}H_{10}ClFN_2$, the dihedral angle between the indole ring system and the benzyl ring is 80.91 (5)°. The crystal packing features C—H···Cl, C—H···F and C—H···π interactions.

Related literature

For the synthesis of the title compound, see: Du *et al.* (2006). For its precursor, see: Jin *et al.* (2009). For related structures, see: Li & Huang (2009); Li *et al.* (2009, 2010*a*,*b*).



Experimental

Crystal data

$C_{16}H_{10}ClFN_2$
M_r = 284.71
Orthorhombic, *Pbca*
a = 7.4581 (9) Å
b = 16.8480 (15) Å
c = 21.356 (2) Å
V = 2683.5 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 113 K
0.26 × 0.22 × 0.20 mm

Data collection

Rigaku Saturn724 CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2009)
T_{min} = 0.929, T_{max} = 0.945
28426 measured reflections
3893 independent reflections
3219 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.113
S = 1.11
3893 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

*Cg*1 is the centroid of the C3–C8 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···F1^{i}	0.95	2.54	3.1638 (16)	123
C7—H7···Cl1^{ii}	0.95	2.73	3.5296 (14)	142
C15—H15···*Cg*1^{iii}	0.95	2.92	3.7246 (14)	143

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

Data collection: *CrystalClear* (Rigaku, 2009); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2009); software used to prepare material for publication: *CrystalStructure*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5823).

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supplementary materials

Acta Cryst. (2011). E**67**, o1041 [**doi:10.1107/S1600536811011214**]

1-(2-Chlorophenyl)-6-fluoro-2-methyl-1*H*-indole-3-carbonitrile

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Comment

Indoles are an important compound possessing pharmaceutical properties. Extensive investigation on the crystal structures of indoles helps disclose their structure-activity relationship. For continuing our reseach, herein, we reported the crystal structure of the title indole derivative.

In the molecular structure, (I) (Fig. 1), the indole ring system is almost planar with a dihedral angle of 0.85 (6)° between its pyrrole ring and fused benzene ring. The indole ring forms an angle of 80.91 (5)° with the chlorobenzene ring.

Experimental

The title compound was prepared according to the method of the literature (Du, *et al.*, 2006). Colourless prisms were grown from a mixture of ethyl actate and petroleum ether.

Refinement

All H atoms were positioned geometrically (C—H = 0.95 and 0.98 Å)and refined as riding with U_{iso}(H) = 1.2U_{eq}(CH) or 1.5U_{eq}(CH_3).

Figures

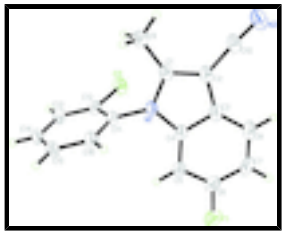

Fig. 1. The molecular structure of (I) with 50% probability displacement ellipsoids.

1-(2-Chlorophenyl)-6-fluoro-2-methyl-1*H*-indole-3-carbonitrile

Crystal data

$C_{16}H_{10}ClFN_2$	$F(000)$ = 1168
M_r = 284.71	D_x = 1.409 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation, λ = 0.71075 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 10281 reflections
a = 7.4581 (9) Å	θ = 1.5–31.4°
b = 16.8480 (15) Å	μ = 0.29 mm^{-1}

c = 21.356 (2) Å	T = 113 K
V = 2683.5 (5) Å^3	Prism, colorless
Z = 8	0.26 × 0.22 × 0.20 mm

Data collection

Rigaku Saturn724 CCD diffractometer	3893 independent reflections
Radiation source: rotating anode	3219 reflections with $I > 2\sigma(I)$
multilayer	R_{int} = 0.034
Detector resolution: 14.222 pixels mm^{-1}	θ_{max} = 30.0°, θ_{min} = 1.9°
ω scans	h = −10→9
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2009)	k = −23→23
T_{min} = 0.929, T_{max} = 0.945	l = −30→30
28426 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.041	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.113	H-atom parameters constrained
S = 1.11	$w = 1/[\sigma^2(F_o^2) + (0.0644P)^2 + 0.1004P]$ where $P = (F_o^2 + 2F_c^2)/3$
3893 reflections	$(\Delta/\sigma)_{max}$ = 0.001
182 parameters	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
0 restraints	$\Delta\rho_{min}$ = −0.20 e Å^{-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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.50520 (4)	0.220294 (19)	0.641958 (16)	0.03226 (11)
F1	0.61121 (11)	0.54670 (5)	0.76153 (4)	0.0480 (2)

N1	0.39260 (12)	0.37712 (5)	0.59488 (4)	0.0236 (2)
N2	0.79477 (16)	0.43384 (7)	0.42798 (6)	0.0420 (3)
C1	0.45553 (17)	0.36559 (7)	0.53489 (5)	0.0258 (2)
C2	0.60108 (16)	0.41469 (7)	0.52619 (6)	0.0271 (3)
C3	0.63160 (15)	0.45816 (7)	0.58328 (6)	0.0265 (3)
C4	0.49938 (14)	0.43272 (7)	0.62558 (6)	0.0237 (2)
C5	0.48747 (16)	0.46061 (7)	0.68659 (6)	0.0280 (3)
H5	0.3986	0.4427	0.7151	0.034*
C6	0.61408 (17)	0.51607 (7)	0.70243 (6)	0.0337 (3)
C7	0.74735 (17)	0.54359 (8)	0.66235 (7)	0.0361 (3)
H7	0.8315	0.5819	0.6765	0.043*
C8	0.75667 (16)	0.51503 (7)	0.60210 (7)	0.0318 (3)
H8	0.8460	0.5336	0.5740	0.038*
C9	0.36953 (19)	0.30813 (8)	0.49124 (6)	0.0333 (3)
H9A	0.3812	0.2543	0.5081	0.040*
H9B	0.4286	0.3109	0.4503	0.040*
H9C	0.2423	0.3213	0.4866	0.040*
C10	0.70533 (17)	0.42350 (7)	0.47083 (6)	0.0317 (3)
C11	0.25337 (16)	0.33290 (7)	0.62467 (5)	0.0223 (2)
C12	0.28935 (15)	0.25756 (7)	0.64802 (5)	0.0230 (2)
C13	0.15588 (16)	0.21330 (7)	0.67690 (5)	0.0271 (3)
H13	0.1800	0.1612	0.6918	0.032*
C14	−0.01309 (16)	0.24642 (8)	0.68363 (6)	0.0277 (3)
H14	−0.1052	0.2169	0.7037	0.033*
C15	−0.04958 (18)	0.32238 (7)	0.66141 (6)	0.0295 (3)
H15	−0.1658	0.3446	0.6664	0.035*
C16	0.08411 (16)	0.36557 (7)	0.63194 (6)	0.0276 (3)
H16	0.0598	0.4175	0.6167	0.033*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.02051 (19)	0.02941 (18)	0.0468 (2)	0.00492 (11)	0.00001 (12)	0.00824 (12)
F1	0.0450 (5)	0.0454 (5)	0.0535 (5)	−0.0100 (4)	−0.0018 (4)	−0.0201 (4)
N1	0.0198 (5)	0.0213 (4)	0.0298 (5)	−0.0031 (4)	0.0030 (4)	0.0022 (4)
N2	0.0363 (7)	0.0436 (7)	0.0461 (6)	0.0006 (5)	0.0128 (5)	0.0089 (5)
C1	0.0240 (6)	0.0243 (5)	0.0290 (5)	0.0016 (5)	0.0019 (5)	0.0054 (4)
C2	0.0218 (6)	0.0250 (5)	0.0344 (6)	0.0014 (4)	0.0040 (5)	0.0079 (5)
C3	0.0199 (6)	0.0210 (5)	0.0385 (6)	0.0020 (4)	0.0007 (5)	0.0081 (4)
C4	0.0178 (6)	0.0181 (5)	0.0353 (6)	0.0001 (4)	−0.0013 (4)	0.0036 (4)
C5	0.0234 (6)	0.0230 (6)	0.0376 (6)	−0.0001 (4)	0.0013 (5)	0.0006 (5)
C6	0.0311 (7)	0.0253 (6)	0.0446 (7)	0.0007 (5)	−0.0046 (6)	−0.0057 (5)
C7	0.0267 (7)	0.0220 (6)	0.0597 (8)	−0.0050 (5)	−0.0061 (6)	0.0016 (6)
C8	0.0199 (6)	0.0225 (6)	0.0528 (7)	−0.0007 (4)	0.0011 (6)	0.0100 (5)
C9	0.0349 (7)	0.0345 (7)	0.0304 (6)	−0.0037 (6)	0.0011 (5)	0.0007 (5)
C10	0.0259 (7)	0.0291 (6)	0.0402 (6)	0.0026 (5)	0.0047 (5)	0.0088 (5)
C11	0.0194 (6)	0.0216 (5)	0.0259 (5)	−0.0029 (4)	0.0004 (4)	0.0022 (4)
C12	0.0188 (6)	0.0235 (5)	0.0267 (5)	0.0008 (4)	−0.0021 (4)	0.0014 (4)

C13	0.0263 (6)	0.0255 (5)	0.0295 (5)	−0.0022 (5)	−0.0015 (5)	0.0070 (4)
C14	0.0230 (6)	0.0324 (6)	0.0275 (5)	−0.0069 (5)	0.0020 (5)	0.0031 (5)
C15	0.0199 (6)	0.0318 (6)	0.0369 (6)	0.0006 (5)	0.0032 (5)	−0.0002 (5)
C16	0.0229 (6)	0.0241 (6)	0.0358 (6)	0.0015 (5)	0.0009 (5)	0.0041 (5)

Geometric parameters (Å, °)

Cl1—C12	1.7328 (12)	C7—C8	1.375 (2)
F1—C6	1.3636 (15)	C7—H7	0.9500
N1—C1	1.3780 (15)	C8—H8	0.9500
N1—C4	1.3934 (14)	C9—H9A	0.9800
N1—C11	1.4276 (14)	C9—H9B	0.9800
N2—C10	1.1457 (16)	C9—H9C	0.9800
C1—C2	1.3775 (16)	C11—C16	1.3857 (16)
C1—C9	1.4892 (17)	C11—C12	1.3900 (15)
C2—C10	1.4227 (17)	C12—C13	1.3883 (16)
C2—C3	1.4404 (18)	C13—C14	1.3857 (17)
C3—C8	1.3963 (17)	C13—H13	0.9500
C3—C4	1.4045 (16)	C14—C15	1.3918 (18)
C4—C5	1.3879 (18)	C14—H14	0.9500
C5—C6	1.3708 (17)	C15—C16	1.3855 (17)
C5—H5	0.9500	C15—H15	0.9500
C6—C7	1.3914 (19)	C16—H16	0.9500
C1—N1—C4	109.73 (9)	C3—C8—H8	120.8
C1—N1—C11	126.05 (10)	C1—C9—H9A	109.5
C4—N1—C11	123.83 (9)	C1—C9—H9B	109.5
C2—C1—N1	108.01 (10)	H9A—C9—H9B	109.5
C2—C1—C9	130.19 (11)	C1—C9—H9C	109.5
N1—C1—C9	121.80 (11)	H9A—C9—H9C	109.5
C1—C2—C10	127.27 (12)	H9B—C9—H9C	109.5
C1—C2—C3	108.40 (10)	N2—C10—C2	176.12 (15)
C10—C2—C3	124.33 (11)	C16—C11—C12	119.89 (10)
C8—C3—C4	119.56 (12)	C16—C11—N1	120.35 (10)
C8—C3—C2	134.28 (11)	C12—C11—N1	119.73 (10)
C4—C3—C2	106.16 (10)	C13—C12—C11	120.76 (11)
C5—C4—N1	129.26 (11)	C13—C12—Cl1	120.31 (9)
C5—C4—C3	123.06 (11)	C11—C12—Cl1	118.91 (9)
N1—C4—C3	107.68 (11)	C14—C13—C12	118.81 (11)
C6—C5—C4	114.73 (11)	C14—C13—H13	120.6
C6—C5—H5	122.6	C12—C13—H13	120.6
C4—C5—H5	122.6	C13—C14—C15	120.85 (11)
F1—C6—C5	118.39 (12)	C13—C14—H14	119.6
F1—C6—C7	117.04 (11)	C15—C14—H14	119.6
C5—C6—C7	124.57 (13)	C16—C15—C14	119.80 (12)
C8—C7—C6	119.68 (12)	C16—C15—H15	120.1
C8—C7—H7	120.2	C14—C15—H15	120.1
C6—C7—H7	120.2	C15—C16—C11	119.86 (11)
C7—C8—C3	118.39 (12)	C15—C16—H16	120.1
C7—C8—H8	120.8	C11—C16—H16	120.1

C4—N1—C1—C2	−1.08 (13)	C4—C5—C6—C7	−0.48 (18)
C11—N1—C1—C2	−174.11 (10)	F1—C6—C7—C8	−179.81 (11)
C4—N1—C1—C9	178.91 (11)	C5—C6—C7—C8	0.4 (2)
C11—N1—C1—C9	5.89 (17)	C6—C7—C8—C3	−0.63 (18)
N1—C1—C2—C10	−178.61 (11)	C4—C3—C8—C7	0.91 (17)
C9—C1—C2—C10	1.4 (2)	C2—C3—C8—C7	−178.87 (13)
N1—C1—C2—C3	0.59 (13)	C1—C2—C10—N2	177 (100)
C9—C1—C2—C3	−179.40 (12)	C3—C2—C10—N2	−2(2)
C1—C2—C3—C8	179.90 (13)	C1—N1—C11—C16	−104.36 (13)
C10—C2—C3—C8	−0.9 (2)	C4—N1—C11—C16	83.56 (14)
C1—C2—C3—C4	0.10 (13)	C1—N1—C11—C12	77.42 (15)
C10—C2—C3—C4	179.33 (11)	C4—N1—C11—C12	−94.66 (13)
C1—N1—C4—C5	−178.37 (12)	C16—C11—C12—C13	2.09 (17)
C11—N1—C4—C5	−5.16 (18)	N1—C11—C12—C13	−179.69 (10)
C1—N1—C4—C3	1.15 (13)	C16—C11—C12—Cl1	−176.62 (9)
C11—N1—C4—C3	174.36 (10)	N1—C11—C12—Cl1	1.61 (15)
C8—C3—C4—C5	−1.03 (17)	C11—C12—C13—C14	−1.76 (17)
C2—C3—C4—C5	178.81 (11)	Cl1—C12—C13—C14	176.93 (9)
C8—C3—C4—N1	179.41 (10)	C12—C13—C14—C15	0.59 (18)
C2—C3—C4—N1	−0.75 (12)	C13—C14—C15—C16	0.24 (19)
N1—C4—C5—C6	−179.77 (11)	C14—C15—C16—C11	0.07 (19)
C3—C4—C5—C6	0.78 (17)	C12—C11—C16—C15	−1.22 (17)
C4—C5—C6—F1	179.77 (11)	N1—C11—C16—C15	−179.44 (11)

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the C3–C8 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···F1^{i}	0.95	2.54	3.1638 (16)	123
C7—H7···Cl1^{ii}	0.95	2.73	3.5296 (14)	142
C15—H15···Cg1^{iii}	0.95	2.92	3.7246 (14)	143

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

Fig. 1