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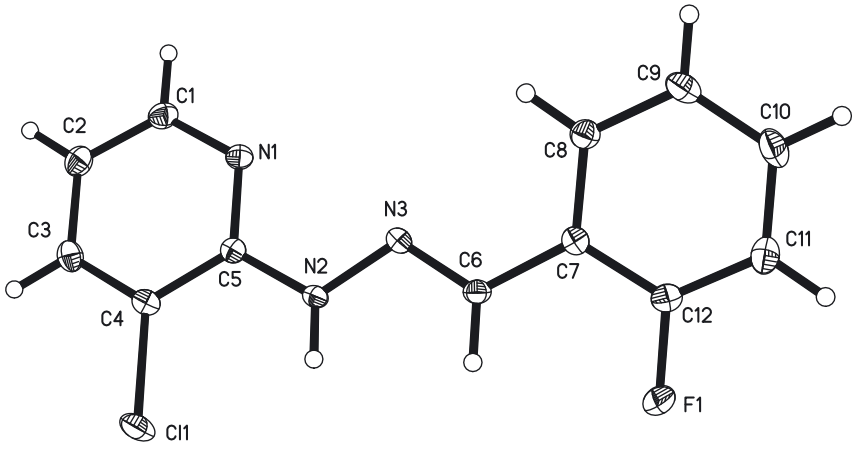
The crystal structure of (*E*)-3-chloro-2-(2-(2-fluorobenzylidene)hydrazinyl)pyridine, $C_{12}H_9ClFN_3$



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Abstract

$C_{12}H_9ClFN_3$, monoclinic, *C*2/*c* (no. 15), a = 24.713(13) Å, b = 15.459(13) Å, c = 17.507(12) Å, β = 17.515(11)°, V = 4742(6) Å^3, Z = 16, $R_{gt}(F)$ = 0.0530, $wR_{ref}(F^2)$ = 0.1161, T = 113(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

Crystal:	Colourless plate
Size:	0.20 × 0.20 × 0.20 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.31 mm^{-1}
Diffractometer, scan mode:	Rigaku Saturn, ω
θ_{max}, completeness:	27.9°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	23,772, 2832, 0.056
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 2622
$N(param)_{refined}$:	154
Programs:	XSCANS [1], Olex2 [2], Shelx [3, 4]

Source of material

According to the literature methods [5], 3-chloro-2-hydrazinylpyridine and 2-fluorobenzaldehyde was added into the round bottom in EtOH. The mixture was stirred at room temperature overnight. Then the mixture was filtered and dried with 85% yield. The title compound was recrystallized from ethanol at room temperature to obtain colorless block crystals.

Experimental details

The structure was solved by direct methods with the SHELXS program. Hydrogen atoms were positioned geometrically (C–H = 0.93–0.98 Å). Their U_{iso} values were set to 1.2 U_{eq} or 1.5 U_{eq} of the parent atoms.

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cl1	−0.92004 (3)	−0.11885 (3)	−0.60976 (3)	0.03474 (17)
F1	−0.57434 (7)	0.08219 (7)	−0.61849 (7)	0.0368 (3)
N1	−0.87759 (8)	−0.01892 (8)	−0.38450 (9)	0.0225 (3)
N2	−0.80485 (8)	−0.02867 (8)	−0.51000 (9)	0.0222 (3)
H2	−0.7941	−0.0502	−0.5609	0.027*
N3	−0.74479 (8)	0.00490 (8)	−0.46704 (10)	0.0207 (3)
C1	−0.94229 (11)	−0.03331 (11)	−0.34138 (12)	0.0274 (4)
H1	−0.9463	−0.0157	−0.2848	0.033*
C2	−1.00338 (11)	−0.07264 (11)	−0.37587 (12)	0.0297 (4)
H2A	−1.0475	−0.0812	−0.3439	0.036*
C3	−0.99637 (10)	−0.09895 (11)	−0.46004 (13)	0.0278 (4)
H3	−1.0362	−0.1257	−0.4858	0.033*
C4	−0.93059 (10)	−0.08534 (10)	−0.50494 (12)	0.0223 (4)
C5	−0.87071 (9)	−0.04435 (9)	−0.46563 (11)	0.0192 (3)
C6	−0.68606 (10)	0.01864 (10)	−0.51451 (11)	0.0217 (4)
H6	−0.6874	0.0068	−0.5731	0.026*
C7	−0.61711 (9)	0.05274 (9)	−0.47727 (11)	0.0212 (4)
C8	−0.60253 (10)	0.05541 (10)	−0.38852 (12)	0.0253 (4)
H8	−0.6381	0.0354	−0.3500	0.030*
C9	−0.53572 (11)	0.08746 (11)	−0.35719(13)	0.0306 (4)
H9	−0.5268	0.0887	−0.2979	0.037*
C10	−0.48232 (11)	0.11750 (12)	−0.41319 (14)	0.0359 (5)
H10	−0.4377	0.1390	−0.3916	0.043*
C11	−0.49508 (11)	0.11575 (12)	−0.50152 (14)	0.0351 (5)
H11	−0.4595	0.1360	−0.5398	0.042*
C12	−0.56143 (10)	0.08347 (11)	−0.53132 (12)	0.0263 (4)

Comment

Nowadays, nitrogen-linked heterocycles have received important attentions because of their divers bioactivities [6–8]. The pyridine derivatives often possess excellent biological activities, such as herbicidal activity [9], antifungal activity [10], anti-HIV [11], insecticidal [12] and so on. On the other hand, the hydrazone group is an active group in many bioactive molecules [13].

Generally, the average bond lengths and bond angles of ring systems (phenyl and pyridine) are normal. The C6=N2 bond [1.285(2) Å] is a little bit longer than the general C=N double bond length of 1.27 Å [14]. The torsion angle of N(2)–N(3)–C(6)–C(7) is −178.60(15)° similar to related structures [15]. More importantly, the target compound is in an E configuration. In the crystal structure, there are two intermolecular N–H···N hydrogen bonds that lead to a chain structure.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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