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The crystal structure of (*E*)-4-amino-*N*′-(1-(4-fluorophenyl)propylidene)benzohydrazide, $C_{16}H_{16}FN_3O$

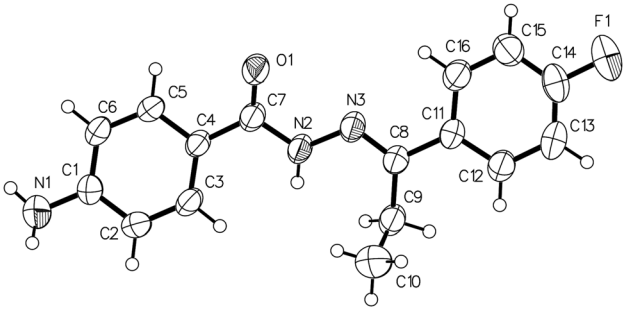

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.46 × 0.38 × 0.31 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.09 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	29.1°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	10,068, 3345, 0.046
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 1870
$N(param)_{refined}$:	192
Programs:	Bruker [1], SHELX [2, 3], Olex2 [4]

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Abstract

$C_{16}H_{16}FN_3O$, orthorhombic, *Pbca* (no. 61), a = 12.5936(10) Å, b = 7.7308(9) Å, c = 29.568(3) Å, V = 2878.7(5) Å^3, Z = 8, $R_{gt}(F)$ = 0.0872, $wR_{ref}(F^2)$ = 0.1893, T = 293 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.

1 Source of materials

In a 50 mL round-bottom flask equipped with a stopper, 1 mmol of 4-aminobenzohydrazide and 1 mmol of 4′-fluoropropiophenone were added, along with 25 mL of anhydrous ethanol. The mixture was stirred at room temperature for 10 min. Subsequently, 3 drops of concentrated acetic acid were added, and the mixture was heated to 50 °C with stirring for 3 h. The solvent was evaporated using a rotary evaporator to obtain the crude product. Afterwards, 80 mg of the crude product was dissolved in a solvent mixture of ethanol and water (v:v = 3:1). Once dissolved, the system was left open at room temperature, allowing the solvent to evaporate. During the evaporation process, the formation of crystalline particles was observed.

2 Experimental details

The C–H bond distances were constrained to be between 0.90 and 0.97 Å with an isotropic displacement parameter (U_{iso}) of 1.5 times the equivalent isotropic displacement parameter (U_{eq}) of carbon for methyl hydrogen atoms, and 1.2 times U_{eq}(C) for all other hydrogen atoms.

3 Comment

Acylhydrazine is a derivative of hydrazine obtained through acylation. Its pharmacological activities, including anti-inflammatory, anti-tumor, and anti-tuberculosis properties [5]. This is attributed to the presence of the methyleneimino group (–NH–N=CH–) connected to the carbonyl group [6–9], and many similar crystal structures were reported [10–13]. This article presents the crystal structure of (*E*)-4-amino-*N*′-(1-(4-fluorophenyl)propylidene)benzohydrazide, belonging to the acylhydrazine derivative class.

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
F1	0.33490 (19)	0.0102 (3)	0.60032 (7)	0.0838 (7)
O1	0.08465 (18)	0.2963 (4)	0.35338 (8)	0.0730 (8)
N1	0.1478 (2)	0.7258 (5)	0.17172 (9)	0.0739 (10)
H1A	0.199532	0.688745	0.155122	0.089*
H1B	0.088463	0.703150	0.158303	0.089*
N2	0.2473 (2)	0.4070 (3)	0.36772 (8)	0.0492 (7)
H2	0.299115	0.471114	0.358925	0.059*
N3	0.2524 (2)	0.3209 (3)	0.40856 (8)	0.0490 (7)
C1	0.1520 (2)	0.6445 (4)	0.21330 (10)	0.0483 (8)
C2	0.2485 (2)	0.6062 (5)	0.23368 (10)	0.0564 (9)
H2A	0.311557	0.634849	0.219103	0.068*
C3	0.2517 (2)	0.5263 (4)	0.27524 (10)	0.0508 (9)
H3	0.317246	0.501212	0.288202	0.061*
C4	0.1599 (2)	0.4823 (4)	0.29822 (10)	0.0410 (7)
C5	0.0637 (2)	0.5199 (5)	0.27737 (10)	0.0517 (9)
H5	0.000710	0.490012	0.291793	0.062*
C6	0.0595 (2)	0.6001 (5)	0.23604 (10)	0.0536 (9)
H6	−0.006070	0.624990	0.223107	0.064*
C7	0.1588 (2)	0.3891 (4)	0.34149 (11)	0.0477 (8)
C8	0.3394 (2)	0.3380 (4)	0.43131 (10)	0.0421 (7)
C9	0.4344 (2)	0.4372 (5)	0.41529 (11)	0.0556 (9)
H9A	0.479404	0.463822	0.441001	0.067*
H9B	0.411058	0.545816	0.402213	0.067*
C10	0.4992 (3)	0.3381 (6)	0.38027 (13)	0.0853 (13)
H10A	0.455147	0.311835	0.354663	0.128*
H10B	0.524802	0.232423	0.393390	0.128*
H10C	0.558252	0.407441	0.370716	0.128*
C11	0.3403 (2)	0.2490 (4)	0.47574 (10)	0.0421 (7)
C12	0.4326 (3)	0.2249 (5)	0.50035 (11)	0.0572 (9)
H12	0.496848	0.263047	0.488454	0.069*
C13	0.4314 (3)	0.1448 (5)	0.54256 (12)	0.0639 (10)
H13	0.493723	0.128966	0.558896	0.077*
C14	0.3367 (3)	0.0907 (5)	0.55914 (11)	0.0575 (9)
C15	0.2445 (3)	0.1094 (5)	0.53635 (11)	0.0616 (10)
H15	0.181014	0.068901	0.548469	0.074*
C16	0.2463 (3)	0.1896 (4)	0.49494 (10)	0.0544 (9)
H16	0.182967	0.204596	0.479280	0.065*

In the title compound, the dihedral angle between the planes of the 4-fluorophenyl and 4-aminophenyl rings is 7.3°. These rings make dihedral angles of 32.4° and 25.1°, respectively, with the central hydrazide group.

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

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