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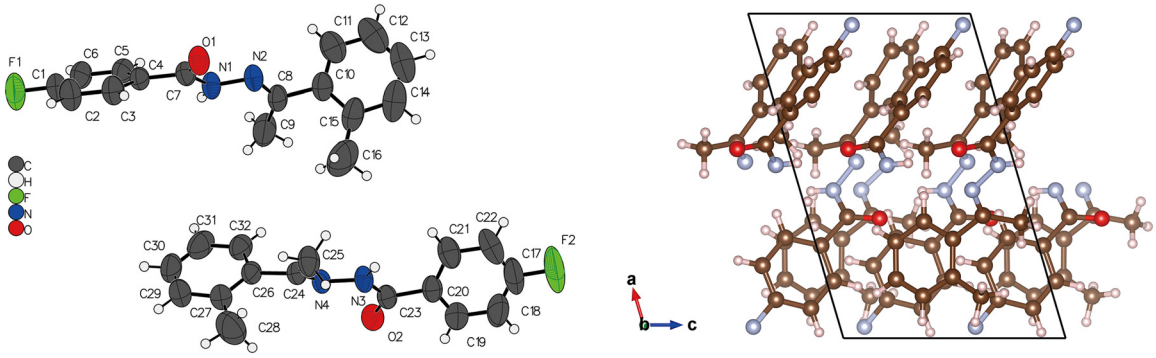
The crystal structure of (*E*)-4-fluoro-*N*′-(1-(*o*-tolyl) ethylidene)benzohydrazide, $C_{16}H_{15}FN_2O$



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Abstract

$C_{16}H_{15}FN_2O$, monoclinic, *Pc* (no. 7), a = 12.3610(11) Å, b = 15.1269(17) Å, c = 8.1382(6) Å, β = 106.411(9)°, V = 1459.7(2) Å^3, Z = 4, $R_{gt}(F)$ = 0.0565, $wR_{ref}(F^2)$ = 0.1315, T = 293 K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.42 × 0.38 × 0.33 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.09 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	29.3°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	12,312, 5772, 0.024
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 3966
$N(param)_{refined}$:	365
Programs:	Bruker [1], SHELX [2, 3], Olex2 [4]

1 Source of materials

A 50 mL round-bottom flask, equipped with a stirring bar and a rubber membrane, was prepared. Then 1 mmol 4-fluorobenzoyl hydrazine and 1 mmol 2′-methyl-acetophenone were mixed with 3 drops of ice-cold acetic acid to serve as the starting materials for the reaction. Subsequently, 25 mL of anhydrous alcohol was added to the mixture, and stirring was performed at room temperature for 10 min to facilitate the reaction progress. The mixture was continuously stirred and maintained at 50 °C for 5 h to ensure completion of the desired reaction. To obtain the crude product, solvent evaporation was carried out using a rotary evaporator until complete dryness, leaving behind the solid product. The crude product was dissolved in a minimum quantity of hot ethanol under controlled heating conditions to ensure complete dissolution. Then, during the cooling and volatilization process of ethanol, the formation of crystals of the targeted compound was observed.

2 Experimental details

The obtained diffraction data were processed using the SHELXT software [2] to solve the crystal structure, which was further refined using full-matrix least-squares procedures in SHELXL [3]. Anisotropic refinement was applied to

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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	0.0349 (2)	0.6781 (3)	−0.3906 (4)	0.1095 (11)
F2	0.9653 (3)	−0.1591 (4)	0.9521 (5)	0.1581 (18)
O1	0.3686 (3)	0.5823 (2)	0.3206 (3)	0.0677 (8)
O2	0.5830 (2)	−0.1018 (2)	0.2715 (3)	0.0634 (8)
N1	0.4556 (3)	0.5101 (2)	0.1501 (4)	0.0565 (9)
H1	0.452821	0.491639	0.049060	0.068*
N2	0.5438 (3)	0.4877 (3)	0.2906 (4)	0.0570 (9)
N3	0.5337 (3)	0.0074 (2)	0.4245 (3)	0.0539 (8)
H3A	0.539566	0.031121	0.522577	0.065*
N4	0.4568 (3)	0.0376 (2)	0.2760 (3)	0.0507 (8)
C1	0.1190 (4)	0.6507 (3)	−0.2528 (6)	0.0705 (13)
C2	0.0923 (4)	0.6297 (4)	−0.1073 (6)	0.0788 (14)
H2	0.018501	0.634645	−0.101548	0.095*
C3	0.1764 (4)	0.6011 (3)	0.0312 (5)	0.0689 (12)
H3	0.159730	0.586959	0.132554	0.083*
C4	0.2851 (3)	0.5930 (3)	0.0217 (4)	0.0528 (10)
C5	0.3090 (4)	0.6156 (3)	−0.1290 (5)	0.0595 (10)
H5	0.382444	0.611237	−0.136514	0.071*
C6	0.2237 (4)	0.6449 (3)	−0.2689 (5)	0.0708 (13)
H6	0.238793	0.659953	−0.371019	0.085*
C7	0.3735 (3)	0.5625 (3)	0.1779 (5)	0.0534 (10)
C8	0.6033 (3)	0.4220 (3)	0.2778 (5)	0.0562 (11)
C9	0.5839 (6)	0.3638 (4)	0.1235 (7)	0.102 (2)
H9A	0.507178	0.343550	0.090546	0.152*
H9B	0.633802	0.313873	0.150107	0.152*
H9C	0.598340	0.396558	0.030888	0.152*
C10	0.7043 (4)	0.4045 (3)	0.4279 (5)	0.0621 (12)
C11	0.7880 (4)	0.4677 (4)	0.4673 (6)	0.0825 (15)
H11	0.778559	0.520050	0.404845	0.099*
C12	0.8850 (5)	0.4545 (6)	0.5973 (8)	0.108 (2)
H12	0.941603	0.497016	0.622900	0.130*
C13	0.8965 (6)	0.3786 (7)	0.6873 (7)	0.109 (2)
H13	0.962311	0.369278	0.775290	0.131*
C14	0.8165 (6)	0.3163 (6)	0.6544 (8)	0.113 (2)
H14	0.827163	0.264983	0.720075	0.136*
C15	0.7164 (5)	0.3276 (4)	0.5212 (7)	0.0872 (16)
C16	0.6244 (7)	0.2584 (5)	0.4860 (11)	0.147 (3)
H16A	0.566605	0.276430	0.536613	0.221*
H16B	0.655661	0.202981	0.534432	0.221*
H16C	0.592652	0.251895	0.364522	0.221*
C17	0.8749 (5)	−0.1344 (6)	0.8192 (8)	0.100 (2)
C18	0.8265 (5)	−0.1956 (5)	0.7016 (10)	0.113 (2)
H18	0.852992	−0.253459	0.709692	0.135*
C19	0.7353 (4)	−0.1688 (4)	0.5673 (7)	0.0809 (14)
H19	0.701079	−0.209114	0.482176	0.097*
C20	0.6954 (3)	−0.0846 (3)	0.5587 (5)	0.0548 (10)
C21	0.7501 (4)	−0.0231 (4)	0.6789 (5)	0.0753 (14)
H21	0.725473	0.035270	0.670888	0.090*
C22	0.8418 (4)	−0.0492 (5)	0.8116 (6)	0.0929 (18)
H22	0.879906	−0.008816	0.893778	0.112*
C23	0.5981 (3)	−0.0606 (3)	0.4065 (4)	0.0499 (9)
C24	0.3779 (3)	0.0884 (3)	0.2899 (4)	0.0496 (9)
C25	0.3566 (4)	0.1193 (3)	0.4528 (5)	0.0713 (13)
H25A	0.344015	0.069094	0.517186	0.107*
H25B	0.291364	0.156794	0.426409	0.107*
H25C	0.420934	0.151711	0.519132	0.107*
C26	0.3053 (4)	0.1236 (3)	0.1234 (4)	0.0551 (10)
C27	0.1896 (4)	0.1141 (3)	0.0724 (6)	0.0717 (13)
C28	0.1294 (5)	0.0638 (5)	0.1748 (8)	0.121 (2)
H28A	0.159096	0.004808	0.192855	0.182*
H28B	0.050496	0.061437	0.114779	0.182*
H28C	0.139373	0.092333	0.283457	0.182*
C29	0.1307 (5)	0.1511 (4)	−0.0856 (7)	0.0897 (17)
H29	0.052601	0.145751	−0.122145	0.108*
C30	0.1823 (6)	0.1934 (4)	−0.1848 (6)	0.0918 (18)
H30	0.139721	0.217234	−0.288190	0.110*
C31	0.2972 (6)	0.2026 (3)	−0.1375 (6)	0.0894 (16)
H31	0.332722	0.232378	−0.207820	0.107*
C32	0.3594 (4)	0.1670 (3)	0.0164 (5)	0.0663 (12)
H32	0.437610	0.171866	0.049224	0.080*

non-hydrogen atoms, while hydrogen atoms were refined isotropically. The resulting crystal structure was visually represented using the OLEX2 [4] and VESTA [5] software package.

3 Comment

Hydrazine derivatives have evoked a profound interest due to their diverse biological activities, making them promising candidates for the development of highly effective anti-infective agents [6]. The precise determination of crystal structures for hydrazine derivatives holds pivotal importance in the pursuit of novel drug discovery. A considerable number of crystal structures of hydrazine derivatives have been successfully elucidated and reported in the existing scientific literature [7–15]. In this study, we present the crystal structure of a novel hydrazine derivative, namely (*E*)-4-fluoro-*N*′-(1-(o-tolyl)ethylidene)benzohydrazide, and engage in a thorough structural discussion. These findings provide substantial support for the development of innovative pharmaceutical agents.

In the compound delineated in the title, a 4-fluorophenyl moiety replaces a hydrogen atom on the acyl carbon, resulting in the fluorine atom. Furthermore, in the molecular structure, the substituents on both sides of the C=N double bond adopt an configuration, wherein the larger substituent resides on either side of the double bond to facilitate favorable spatial orientation. The two phenyl rings exhibit discernible torsion, with a dihedral angle of 45°, akin to comparable crystal structures documented in previous literature [16–20].

The molecules within the crystal lattice are arranged in a stacked manner along the c-axis direction. Significantly, no conspicuous intermolecular hydrogen bonding or $\pi\cdots\pi$ interactions are detected. The molecular arrangement within the crystal primarily stems from the maximization of spatial utilization.

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Competing interests: The authors declare no conflicts of interest regarding this article.

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