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The crystal structure of (*Z*)-4-amino-*N*′-(1-(*o*-tolyl) ethylidene)benzohydrazide, $C_{16}H_{17}N_3O$

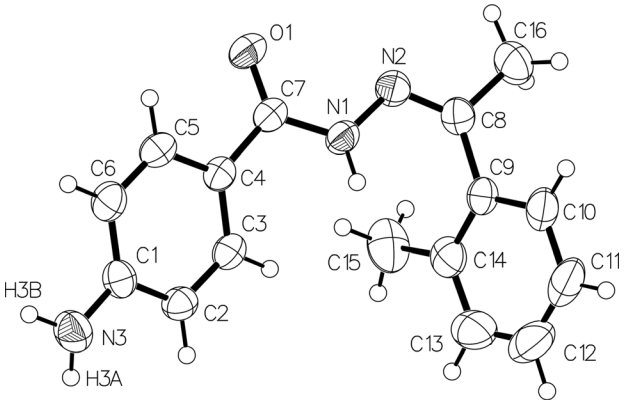

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.32 × 0.30 × 0.27 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.08 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	29.4°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	12,434, 3475, 0.026
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 2710
$N(param)_{refined}$:	191
Programs:	CrysAlis^{PRO} [1], SHELX [2, 3], Olex2 [4]

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Abstract

$C_{16}H_{17}N_3O$, monoclinic, $P2_1/n$ (no. 14), a = 8.2818(6) Å, b = 17.0495(10) Å, c = 10.2429(7) Å, β = 98.980(6)°, V = 1428.58(17) $Å^3$, Z = 4, $R_{gt}(F)$ = 0.0629, $wR_{ref}(F^2)$ = 0.1461, 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 this experimental procedure, 4-aminobenzohydrazide (0.17 g, 1 mmol) and 2′-methylacetophenone (0.13 g, 1 mmol) were added to a 50 mL round-bottom flask along with 25 mL absolute alcohol and 3 drops of glacial acetic acid. The mixture was stirred at 50 °C for 10 min resulting in a yellow solution. Subsequently, the mixture was left to stir for additional 5 h. The solvent was evaporated to dryness utilizing a rotary evaporator. The product was then dissolved in a minimal quantity of hot ethanol and cooled slowly to room temperature.

2 Experimental details

The crystal structure was elucidated through SHELXT [2] and afterward refined using the SHELXL software [3]. Anisotropic refinement was conducted for all non-hydrogen atoms, while hydrogen atoms were situated at calculated positions and refined isotropically.

3 Comment

The *N*-acylhydrazone moiety has demonstrated versatility in facilitating the development of biologically active compounds, which underscores its potential as a significant structural motif for drug discovery [5, 6]. Research involving single crystal structures has provided insight into the conformation of these compounds in relation to the C=N double bond, showcasing cis or trans arrangements, as well as intramolecular hydrogen bonds [7–10].

The compound denoted by the title is found to crystallize in the monoclinic space group $P2_1/n$, containing two molecules within a unit cell. Through analysis of the bond lengths in the aromatic ring, it was found that these bond lengths were typical for similar compounds [11]. The molecule

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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}
C1	1.1080 (2)	0.47452 (11)	0.70030 (18)	0.0413 (4)
C2	1.0699 (2)	0.42276 (11)	0.59507 (18)	0.0405 (4)
H2	1.152267	0.403886	0.551306	0.049*
C3	0.9107 (2)	0.39939 (10)	0.55551 (17)	0.0386 (4)
H3	0.886549	0.365403	0.484110	0.046*
C4	0.7847 (2)	0.42568 (10)	0.62044 (17)	0.0367 (4)
C5	0.8250 (2)	0.47533 (12)	0.72764 (19)	0.0465 (5)
H5	0.743536	0.492480	0.773846	0.056*
C6	0.9835 (2)	0.49973 (12)	0.76696 (19)	0.0487 (5)
H6	1.007552	0.533393	0.838797	0.058*
C7	0.6109 (2)	0.40197 (10)	0.58340 (17)	0.0389 (4)
C8	0.3796 (2)	0.32998 (11)	0.29338 (18)	0.0412 (4)
C9	0.4996 (2)	0.32793 (11)	0.19883 (18)	0.0401 (4)
C10	0.4704 (3)	0.37472 (13)	0.08604 (19)	0.0514 (5)
H10	0.376659	0.405516	0.070957	0.062*
C11	0.5785 (3)	0.37599 (16)	−0.0035 (2)	0.0670 (7)
H11	0.558854	0.407820	−0.077996	0.080*
C12	0.7153 (4)	0.32982 (18)	0.0187 (3)	0.0775 (8)
H12	0.789872	0.331197	−0.040361	0.093*
C13	0.7438 (3)	0.28139 (16)	0.1274 (3)	0.0693 (7)
H13	0.836249	0.249654	0.139492	0.083*
C14	0.6368 (3)	0.27902 (12)	0.2195 (2)	0.0495 (5)
C15	0.6665 (3)	0.22317 (14)	0.3334 (3)	0.0710 (7)
H15A	0.692902	0.252108	0.414274	0.106*
H15B	0.755697	0.189042	0.322754	0.106*
H15C	0.569829	0.192505	0.336128	0.106*
C16	0.2093 (3)	0.30150 (14)	0.2451 (2)	0.0589 (6)
H16A	0.212469	0.246902	0.222724	0.088*
H16B	0.163322	0.330923	0.168313	0.088*
H16C	0.143227	0.308460	0.313318	0.088*
N1	0.56549 (18)	0.38279 (9)	0.45519 (14)	0.0419 (4)
H1	0.633360	0.387774	0.400168	0.050*
N2	0.40905 (19)	0.35505 (10)	0.41259 (16)	0.0438 (4)
N3	1.2664 (2)	0.50226 (13)	0.7339 (2)	0.0563 (5)
H3A	1.345 (3)	0.4703 (15)	0.712 (3)	0.072 (8)*
H3B	1.291 (3)	0.5234 (16)	0.813 (3)	0.073 (8)*
O1	0.51690 (17)	0.39851 (10)	0.66467 (13)	0.0567 (4)

exhibits a Z-configuration with respect to the C=N double bond, which is similar to other N-acylhydrazone derivatives. Moreover, it was observed that the molecular structure adopts a non-planar conformation with a dihedral angle of 47.1° between the two aromatic rings. Additionally, it was determined that the dihedral angle between the amino-phenyl and the acylhydrazone group is 27.9°, while the dihedral angle between the (*o*-tolyl)ethylidene and the acylhydrazone group is 66.4°.

The crystal packing of this compound is primarily stabilized by intermolecular hydrogen bonding interactions N3–H3A···O1 involving the azyl group and the oxygen atom of the acylhydrazone group. The hydrogen bond length is 1.99(3) Å, and the bond angle is 179(3)°, forming a network within the crystal structure similar as other acylhydrazone derivatives [12–14].

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

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