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2-Fluoro-*N'*-(2-methoxybenzylidene)-benzohydrazide

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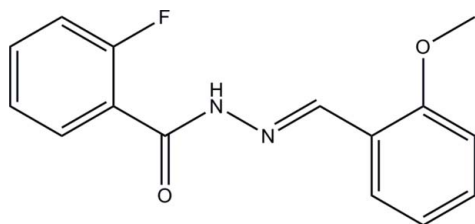
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Key indicators: single-crystal X-ray study; *T* = 298 K; mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$; *R* factor = 0.058; *wR* factor = 0.164; data-to-parameter ratio = 15.5.

The molecule of the title compound, $\text{C}_{15}\text{H}_{13}\text{FN}_2\text{O}_2$, exists in a *trans* configuration with respect to the methyldene unit. The two benzene rings form a dihedral angle of $64.7(2)^\circ$. In the crystal, molecules are linked through $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds into chains propagating along the *c* axis.

Related literature

For the reference bond lengths, see: Allen *et al.* (1987). For structural studies of hydrazone compounds, see: Han & Zhao (2010); Zhou & Yang (2010); Huang & Wu (2010); Shalash *et al.* (2010). For a related structure, see: Xu *et al.* (2011).



Experimental

Crystal data

$\text{C}_{15}\text{H}_{13}\text{FN}_2\text{O}_2$

$M_r = 272.27$

Monoclinic, $P2_1/c$
a = 13.612 (2) Å
b = 12.278 (2) Å
c = 7.925 (1) Å
 $\beta = 92.802(3)^\circ$
V = 1322.9 (3) Å^3

Z = 4
Mo $K\alpha$ radiation
 $\mu = 0.10 \text{ mm}^{-1}$
T = 298 K
 $0.17 \times 0.13 \times 0.12 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.983, T_{\text{max}} = 0.988$

10047 measured reflections
2821 independent reflections
1643 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.047$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.058$
 $wR(F^2) = 0.164$
S = 1.03
2821 reflections

182 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.47 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry ($\text{Å}, ^\circ$).

<i>D</i> — <i>H</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i> ⋯ <i>A</i>
$\text{N1}-\text{H1}\cdots\text{O1}^{\text{i}}$	0.86	2.08	2.866 (2)	152

Symmetry code: (i) $x, -y + \frac{1}{2}, z - \frac{1}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1998); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5011).

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supplementary materials

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2-Fluoro-*N'*-(2-methoxybenzylidene)benzohydrazide

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Comment

As a contribution to a structural study of hydrazone compounds (Han & Zhao, 2010; Zhou & Yang, 2010; Huang & Wu, 2010; Shalash *et al.*, 2010), we present here the crystal structure of the title compound.

The molecule of the title compound exists in a *trans* configuration with respect to the methylenidene unit (Fig. 1). The molecule is twisted, with the dihedral angle between the two benzene rings of $64.7(2)^\circ$. The torsion angle C7—N1—N2—C8 is $8.6(2)^\circ$. The bond lengths are within normal ranges (Allen *et al.*, 1987) and are comparable with those observed in the similar compound (Xu *et al.*, 2011).

In the crystal structure, molecules are linked through intermolecular N—H \cdots O hydrogen bonds (Table 1), to form chains down the *c* axis (Fig. 2).

Experimental

2-Methoxybenzaldehyde (0.1 mmol, 13.6 mg) and 2-fluorobenzohydrazide (0.1 mmol, 15.4 mg) were mixed in ethanol (20 ml). The mixture was stirred at room temperature to give a clear colorless solution. Colourless well shaped crystals of the title compound were formed by gradual evaporation of the solvent over a period of five days at room temperature.

Refinement

All H atoms were placed in geometrically idealized positions, with C—H = 0.93–0.96 Å, N—H = 0.86 Å, and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$ and $1.5U_{\text{eq}}(\text{C15})$.

Figures

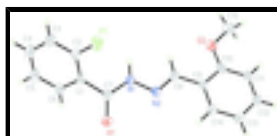


Fig. 1. The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

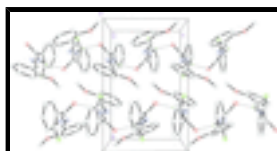


Fig. 2. A portion of the crystal packing showing the hydrogen-bonded (dashed lines) chains of the molecules. H atoms omitted for clarity/

2-Fluoro-*N'*-(2-methoxybenzylidene)benzohydrazide

Crystal data

$C_{15}H_{13}FN_2O_2$	$F(000) = 568$
$M_r = 272.27$	$D_x = 1.367 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -P 2ybc	Cell parameters from 1625 reflections
$a = 13.612 (2) \text{ \AA}$	$\theta = 2.2\text{--}26.4^\circ$
$b = 12.278 (2) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$c = 7.925 (1) \text{ \AA}$	$T = 298 \text{ K}$
$\beta = 92.802 (3)^\circ$	Block, colorless
$V = 1322.9 (3) \text{ \AA}^3$	$0.17 \times 0.13 \times 0.12 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	2821 independent reflections
Radiation source: fine-focus sealed tube graphite	1643 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.047$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{\text{max}} = 27.0^\circ$, $\theta_{\text{min}} = 1.5^\circ$
$T_{\text{min}} = 0.983$, $T_{\text{max}} = 0.988$	$h = -17 \rightarrow 16$
10047 measured reflections	$k = -15 \rightarrow 15$
	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.058$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.164$	H-atom parameters constrained
$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.0839P)^2]$
2821 reflections	where $P = (F_o^2 + 2F_c^2)/3$
182 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.47 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds

in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	0.89639 (10)	0.58503 (11)	0.9614 (2)	0.0657 (5)
N1	0.72769 (12)	0.71726 (15)	0.9490 (2)	0.0409 (5)
H1	0.7427	0.6742	0.8687	0.049*
N2	0.63391 (12)	0.71379 (15)	1.0089 (2)	0.0392 (5)
O1	0.77942 (11)	0.85629 (12)	1.1218 (2)	0.0442 (4)
O2	0.43863 (11)	0.55230 (14)	0.7104 (2)	0.0561 (5)
C1	0.89489 (15)	0.77601 (18)	0.9435 (3)	0.0369 (5)
C2	0.94195 (16)	0.67840 (18)	0.9204 (3)	0.0414 (6)
C3	1.03448 (17)	0.6706 (2)	0.8625 (3)	0.0546 (7)
H3	1.0642	0.6030	0.8504	0.065*
C4	1.08295 (18)	0.7651 (3)	0.8224 (4)	0.0603 (8)
H4	1.1458	0.7614	0.7817	0.072*
C5	1.03917 (19)	0.8636 (2)	0.8423 (4)	0.0615 (8)
H5	1.0721	0.9269	0.8143	0.074*
C6	0.94636 (17)	0.8701 (2)	0.9034 (3)	0.0508 (7)
H6	0.9177	0.9379	0.9182	0.061*
C7	0.79557 (15)	0.78675 (18)	1.0143 (3)	0.0367 (6)
C8	0.57425 (15)	0.65389 (18)	0.9208 (3)	0.0384 (6)
H8	0.5954	0.6201	0.8240	0.046*
C9	0.47321 (15)	0.63784 (17)	0.9704 (3)	0.0376 (6)
C10	0.40509 (16)	0.58424 (17)	0.8620 (3)	0.0418 (6)
C11	0.31043 (16)	0.56584 (19)	0.9121 (4)	0.0504 (7)
H11	0.2652	0.5297	0.8403	0.061*
C12	0.28342 (17)	0.6008 (2)	1.0670 (4)	0.0591 (8)
H12	0.2197	0.5881	1.0996	0.071*
C13	0.34873 (18)	0.6544 (2)	1.1753 (4)	0.0607 (8)
H13	0.3295	0.6781	1.2801	0.073*
C14	0.44315 (17)	0.6725 (2)	1.1266 (3)	0.0500 (7)
H14	0.4876	0.7086	1.1998	0.060*
C15	0.3743 (2)	0.4906 (3)	0.6007 (4)	0.0838 (10)
H15A	0.3546	0.4257	0.6575	0.126*
H15B	0.4076	0.4711	0.5010	0.126*
H15C	0.3172	0.5333	0.5694	0.126*

Atomic displacement parameters (\AA^2)

U^{11} U^{22} U^{33} U^{12} U^{13} U^{23}

supplementary materials

F1	0.0498 (9)	0.0509 (9)	0.0966 (13)	-0.0034 (7)	0.0045 (8)	0.0114 (9)
N1	0.0280 (10)	0.0526 (12)	0.0425 (12)	-0.0043 (8)	0.0072 (9)	-0.0084 (9)
N2	0.0299 (10)	0.0461 (11)	0.0420 (12)	-0.0021 (8)	0.0045 (9)	0.0006 (9)
O1	0.0435 (9)	0.0482 (9)	0.0412 (10)	-0.0005 (7)	0.0046 (8)	-0.0040 (8)
O2	0.0504 (10)	0.0698 (12)	0.0480 (11)	-0.0142 (9)	0.0016 (9)	-0.0147 (9)
C1	0.0306 (11)	0.0478 (13)	0.0323 (13)	-0.0031 (10)	0.0004 (10)	0.0015 (11)
C2	0.0331 (13)	0.0460 (14)	0.0449 (15)	-0.0051 (11)	-0.0007 (11)	0.0034 (12)
C3	0.0377 (14)	0.0665 (17)	0.0593 (18)	0.0072 (12)	0.0019 (13)	-0.0005 (14)
C4	0.0358 (14)	0.083 (2)	0.0631 (19)	-0.0034 (14)	0.0111 (13)	0.0023 (16)
C5	0.0482 (16)	0.0693 (19)	0.068 (2)	-0.0163 (14)	0.0163 (14)	0.0086 (16)
C6	0.0441 (14)	0.0538 (15)	0.0550 (17)	-0.0073 (12)	0.0078 (13)	0.0024 (13)
C7	0.0349 (12)	0.0434 (13)	0.0319 (13)	-0.0011 (10)	0.0016 (10)	0.0050 (11)
C8	0.0322 (12)	0.0444 (13)	0.0387 (14)	0.0013 (10)	0.0029 (10)	0.0020 (11)
C9	0.0313 (12)	0.0347 (12)	0.0470 (15)	0.0000 (9)	0.0021 (11)	0.0021 (11)
C10	0.0393 (13)	0.0362 (13)	0.0497 (16)	-0.0007 (10)	0.0009 (12)	-0.0001 (11)
C11	0.0333 (13)	0.0487 (15)	0.069 (2)	-0.0054 (11)	-0.0012 (13)	-0.0069 (13)
C12	0.0325 (13)	0.0613 (16)	0.085 (2)	-0.0047 (12)	0.0172 (14)	-0.0060 (16)
C13	0.0435 (15)	0.0712 (18)	0.069 (2)	-0.0037 (13)	0.0179 (14)	-0.0168 (16)
C14	0.0390 (14)	0.0585 (16)	0.0531 (17)	-0.0051 (11)	0.0087 (12)	-0.0129 (13)
C15	0.080 (2)	0.112 (3)	0.059 (2)	-0.0263 (19)	-0.0072 (17)	-0.0299 (19)

Geometric parameters (\AA , $^\circ$)

F1—C2	1.351 (2)	C5—H5	0.9300
N1—C7	1.343 (3)	C6—H6	0.9300
N1—N2	1.384 (2)	C8—C9	1.462 (3)
N1—H1	0.8600	C8—H8	0.9300
N2—C8	1.278 (3)	C9—C14	1.390 (3)
O1—C7	1.234 (3)	C9—C10	1.397 (3)
O2—C10	1.364 (3)	C10—C11	1.385 (3)
O2—C15	1.422 (3)	C11—C12	1.368 (4)
C1—C2	1.375 (3)	C11—H11	0.9300
C1—C6	1.395 (3)	C12—C13	1.373 (4)
C1—C7	1.495 (3)	C12—H12	0.9300
C2—C3	1.365 (3)	C13—C14	1.378 (3)
C3—C4	1.379 (4)	C13—H13	0.9300
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.361 (4)	C15—H15A	0.9600
C4—H4	0.9300	C15—H15B	0.9600
C5—C6	1.377 (3)	C15—H15C	0.9600
C7—N1—N2	121.09 (19)	N2—C8—H8	119.6
C7—N1—H1	119.5	C9—C8—H8	119.6
N2—N1—H1	119.5	C14—C9—C10	118.4 (2)
C8—N2—N1	113.74 (19)	C14—C9—C8	121.3 (2)
C10—O2—C15	117.99 (19)	C10—C9—C8	120.2 (2)
C2—C1—C6	116.6 (2)	O2—C10—C11	124.2 (2)
C2—C1—C7	124.2 (2)	O2—C10—C9	115.86 (19)
C6—C1—C7	119.1 (2)	C11—C10—C9	120.0 (2)
F1—C2—C3	117.6 (2)	C12—C11—C10	120.0 (2)

F1—C2—C1	119.0 (2)	C12—C11—H11	120.0
C3—C2—C1	123.3 (2)	C10—C11—H11	120.0
C2—C3—C4	118.6 (2)	C11—C12—C13	121.1 (2)
C2—C3—H3	120.7	C11—C12—H12	119.4
C4—C3—H3	120.7	C13—C12—H12	119.4
C5—C4—C3	120.3 (2)	C12—C13—C14	119.1 (3)
C5—C4—H4	119.9	C12—C13—H13	120.4
C3—C4—H4	119.9	C14—C13—H13	120.4
C4—C5—C6	120.4 (2)	C13—C14—C9	121.3 (2)
C4—C5—H5	119.8	C13—C14—H14	119.4
C6—C5—H5	119.8	C9—C14—H14	119.4
C5—C6—C1	120.8 (2)	O2—C15—H15A	109.5
C5—C6—H6	119.6	O2—C15—H15B	109.5
C1—C6—H6	119.6	H15A—C15—H15B	109.5
O1—C7—N1	124.29 (19)	O2—C15—H15C	109.5
O1—C7—C1	121.0 (2)	H15A—C15—H15C	109.5
N1—C7—C1	114.7 (2)	H15B—C15—H15C	109.5
N2—C8—C9	120.8 (2)		

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1 \cdots O1 ⁱ	0.86	2.08	2.866 (2)	152

Symmetry codes: (i) $x, -y+3/2, z-1/2$.

Fig. 1

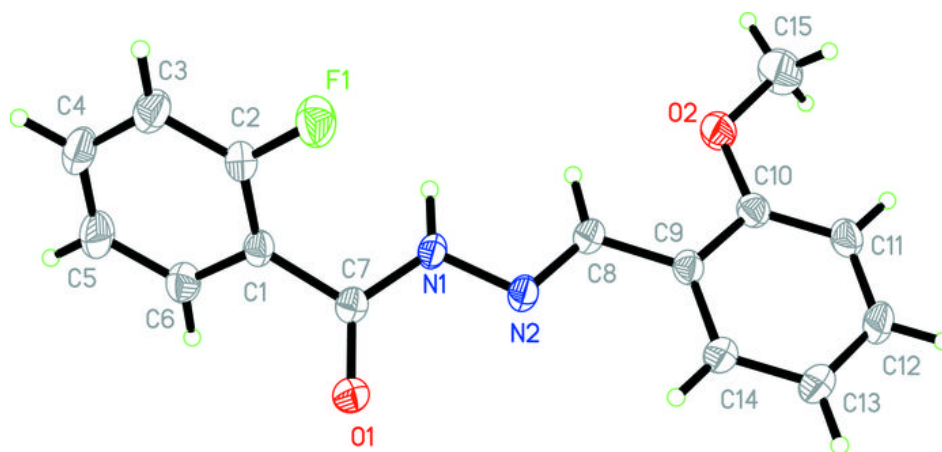


Fig. 2

