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1-(2,4-Difluorophenyl)-2-(1*H*-1,2,4-triazol-1-yl)ethanol

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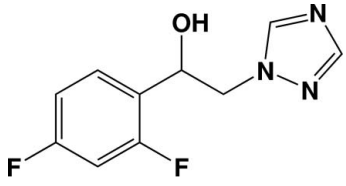
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.063; wR factor = 0.149; data-to-parameter ratio = 10.5.

In the title compound, $C_{10}H_9F_2N_3O$, the dihedral angle between the mean planes of the triazole and benzene rings is 20.6 (2)°. In the crystal, molecules are linked by strong O—H⋯N hydrogen bonds into chains with graph-set notation $C(9)$ along [100]. Weak C—H⋯N and C—H⋯F interactions are also observed.

Related literature

For phenacylazole derivatives, see: Emami *et al.* (2008, 2009). For their biological properties, see: Schiaffella *et al.* (2005). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{10}H_9F_2N_3O$
M_r = 225.20
Orthorhombic, $P2_12_12_1$
a = 5.3770 (11) Å
b = 12.598 (3) Å
c = 15.601 (3) Å
V = 1056.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 295 K
0.60 × 0.29 × 0.08 mm

Data collection

Nonius KappaCCD area-detector diffractometer
9658 measured reflections
1536 independent reflections
1344 reflections with $I > 2\sigma(I)$
R_{int} = 0.081

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.149
S = 1.16
1536 reflections
146 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1⋯N3^{i}	0.82	2.01	2.826 (4)	171
C3—H3⋯N2^{ii}	0.93	2.62	3.500 (5)	158
C8—H8B⋯F1^{iii}	0.97	2.45	3.340 (5)	153
C10—H10⋯F2^{iv}	0.93	2.48	3.270 (4)	142

Symmetry codes: (i) $x+\frac{1}{2}, -y-\frac{1}{2}, -z+1$; (ii) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x-1, y, z$; (iv) $x, y-1, z$.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2423).

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1-(2,4-Difluorophenyl)-2-(1*H*-1,2,4-triazol-1-yl)ethanol

Victor Kesternich, Ronald Nelson-González, Marcia Pérez-Fehrmann, Alejandro Cárdenas and Iván Brito

S1. Comment

Phenacyl azole derivatives (Emami *et al.*, 2008; Emami *et al.*, 2009) are very important due to their antifungal properties (Schiaffella *et al.*, 2005). We report herein on the synthesis and crystal structure of the title compound, a member of this important family of compounds.

In the title molecule, Fig. 1, the dihedral angle between the mean planes of the triazole and benzene rings is 20.6 (2)°.

In the crystal, molecules are linked by strong O—H··· N hydrogen bonds (Fig. 2 and Table 1) into chains propagating along [100] which have a C(9) graph-set notation (Bernstein *et al.*, 1995). There are also weak C-H···N and C-H···F interactions present (Table 1).

S2. Experimental

To a stirred solution of 1-(2,4-difluorophenyl)-2-(1*H*-1,2,4-triazol-1-yl)ethanone (6.00 g, 26.88 mmol) in methanol (50 ml), sodium borohydride (1.12 g, 29.57 mmol) dissolved in methanol (20 ml), was added drop wise. The reaction mixture was then stirred at room temperature for 30 min. After completion of the reaction, the solvent was removed under vacuum, and 25 ml of cold water was added. Extraction was performed with dichloromethane (3 × 40 ml), and the organic extracts were washed with water (3 × 30 ml). The organic phase was then dried over anhydrous sodium sulfate. After evaporation of the solvent under vacuum, the residue was purified by crystallization in ethanol to provide the title compound as colourless crystals [85% yield; M.p.: 391-393 K].

S3. Refinement

All of the H atoms could be located in difference Fourier maps. In the final cycles of refinement they were included in calculated positions and treated as riding atoms: O-H = 0.82 Å, C—H = 0.93 and 0.97 Å for CH and CH_2 H atoms, respectively, with U_{iso}(H) = k × U_{eq}(O,C), where k = 1.5 for the OH H atom, and = 1.2 for other H atoms. In the final cycles of refinement, in the absence of significant anomalous scattering effects, 1126 Friedel pairs were merged and Δf " set to zero.

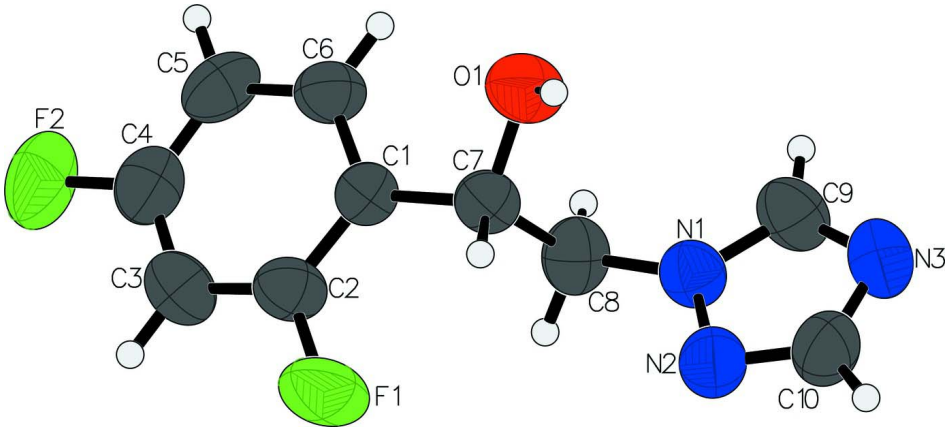

Figure 1

A view of the molecular structure of the title molecule, with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level.

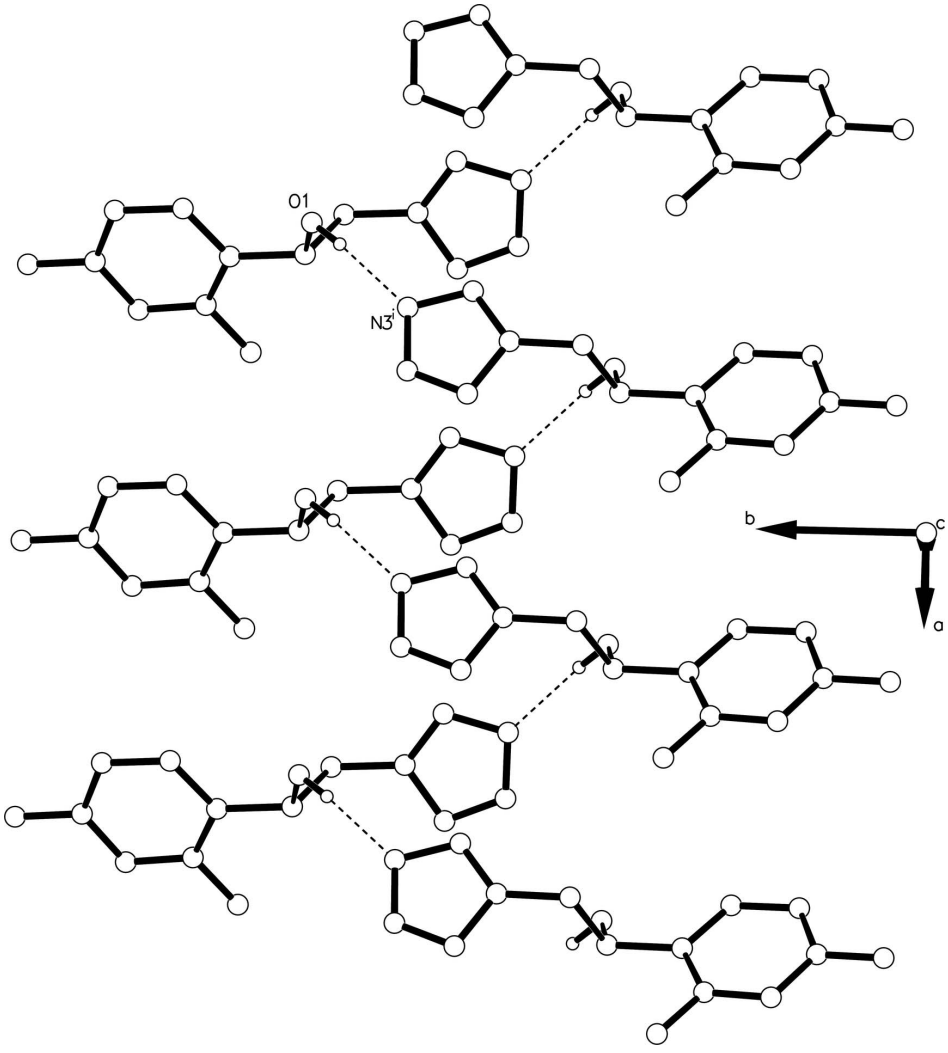

Figure 2

A partial view along the c axis of the crystal packing of the title compound, showing the formation of the O—H··· N hydrogen bonded chain [dashed lines; see Table 1 for details; the H-atoms not involved in hydrogen-bonding have been omitted for clarity]

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Crystal data

$C_{10}H_9F_2N_3O$
M_r = 225.20
Orthorhombic, $P2_12_12_1$
a = 5.3770 (11) Å
b = 12.598 (3) Å
c = 15.601 (3) Å
V = 1056.8 (3) Å^3
Z = 4
$F(000)$ = 464
D_x = 1.415 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
μ = 0.12 mm^{-1}
T = 295 K
Plate, colourless
0.60 × 0.29 × 0.08 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans with κ offsets
9658 measured reflections
1536 independent reflections
1344 reflections with $I > 2\sigma(I)$
$R_{int} = 0.081$
$\theta_{max} = 28.7°$, $\theta_{min} = 4.2°$
$h = 0 \rightarrow 7$
$k = 0 \rightarrow 16$
$l = 0 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.149$
$S = 1.16$
1536 reflections
146 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0491P)^2 + 0.3301P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	1.0193 (5)	0.0759 (2)	0.69521 (16)	0.0959 (9)
F2	0.7227 (6)	0.42266 (16)	0.67885 (15)	0.1001 (12)
O1	0.5799 (5)	−0.0141 (2)	0.49259 (14)	0.0733 (9)
N1	0.5125 (5)	−0.1766 (2)	0.62303 (17)	0.0583 (8)
N2	0.7087 (6)	−0.2399 (2)	0.6393 (2)	0.0725 (10)
N3	0.3927 (6)	−0.3347 (3)	0.5866 (2)	0.0716 (11)
C1	0.6906 (6)	0.1114 (2)	0.60153 (17)	0.0491 (8)
C2	0.8583 (6)	0.1469 (3)	0.6608 (2)	0.0615 (10)
C3	0.8761 (8)	0.2503 (3)	0.6881 (2)	0.0707 (11)
C4	0.7107 (8)	0.3195 (3)	0.6541 (2)	0.0686 (13)
C5	0.5350 (8)	0.2905 (3)	0.5961 (2)	0.0703 (13)
C6	0.5262 (7)	0.1855 (3)	0.5700 (2)	0.0614 (10)
C7	0.6804 (6)	−0.0045 (2)	0.57500 (18)	0.0528 (9)
C8	0.5227 (7)	−0.0634 (3)	0.6398 (2)	0.0655 (11)
C9	0.3289 (7)	−0.2346 (3)	0.5921 (2)	0.0699 (11)
C10	0.6262 (8)	−0.3331 (3)	0.6162 (3)	0.0744 (14)
H1	0.66000	−0.05800	0.46520	0.1100*
H3	0.99530	0.27150	0.72770	0.0850*

H5	0.42310	0.34000	0.57450	0.0840*
H6	0.40680	0.16460	0.53030	0.0740*
H7	0.84910	−0.03400	0.57530	0.0630*
H8A	0.59030	−0.05180	0.69660	0.0790*
H8B	0.35530	−0.03490	0.63880	0.0790*
H9	0.17440	−0.20790	0.57620	0.0840*
H10	0.72300	−0.39410	0.62000	0.0900*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0860 (16)	0.0923 (16)	0.1095 (16)	0.0289 (14)	−0.0421 (15)	−0.0148 (14)
F2	0.157 (3)	0.0540 (11)	0.0894 (14)	−0.0013 (15)	0.0206 (18)	−0.0154 (10)
O1	0.0848 (18)	0.0700 (15)	0.0650 (12)	0.0173 (14)	−0.0112 (13)	−0.0159 (11)
N1	0.0499 (13)	0.0594 (14)	0.0656 (14)	0.0022 (13)	−0.0011 (13)	−0.0030 (12)
N2	0.0575 (17)	0.0571 (16)	0.103 (2)	0.0034 (13)	−0.0163 (18)	0.0053 (15)
N3	0.0719 (19)	0.0660 (18)	0.0770 (18)	−0.0127 (16)	0.0007 (16)	−0.0090 (14)
C1	0.0462 (15)	0.0494 (14)	0.0517 (13)	0.0050 (12)	0.0040 (12)	−0.0018 (12)
C2	0.0571 (18)	0.0657 (19)	0.0616 (17)	0.0112 (16)	−0.0070 (15)	−0.0052 (15)
C3	0.072 (2)	0.075 (2)	0.0650 (18)	−0.0056 (19)	−0.0057 (19)	−0.0142 (17)
C4	0.091 (3)	0.0569 (17)	0.0578 (16)	0.001 (2)	0.016 (2)	−0.0059 (14)
C5	0.085 (3)	0.0578 (18)	0.0682 (19)	0.0215 (19)	0.007 (2)	0.0092 (15)
C6	0.0638 (19)	0.0613 (17)	0.0590 (16)	0.0096 (17)	−0.0086 (16)	−0.0008 (14)
C7	0.0481 (15)	0.0521 (15)	0.0581 (15)	0.0081 (14)	−0.0015 (14)	−0.0054 (13)
C8	0.0637 (19)	0.0569 (17)	0.076 (2)	0.0040 (17)	0.0088 (18)	−0.0080 (15)
C9	0.0487 (17)	0.080 (2)	0.081 (2)	−0.0026 (18)	−0.0050 (17)	−0.0055 (19)
C10	0.070 (2)	0.0563 (19)	0.097 (3)	0.0018 (18)	−0.008 (2)	0.0063 (18)

Geometric parameters (Å, º)

F1—C2	1.356 (4)	C2—C3	1.374 (5)
F2—C4	1.357 (4)	C3—C4	1.354 (6)
O1—C7	1.400 (4)	C4—C5	1.358 (5)
O1—H1	0.8200	C5—C6	1.385 (5)
N1—C8	1.451 (5)	C7—C8	1.514 (5)
N1—C9	1.320 (5)	C3—H3	0.9300
N1—N2	1.347 (4)	C5—H5	0.9300
N2—C10	1.306 (5)	C6—H6	0.9300
N3—C10	1.338 (5)	C7—H7	0.9800
N3—C9	1.310 (5)	C8—H8A	0.9700
C1—C2	1.367 (4)	C8—H8B	0.9700
C1—C7	1.519 (4)	C9—H9	0.9300
C1—C6	1.377 (5)	C10—H10	0.9300
C7—O1—H1	109.00	N1—C8—C7	112.5 (3)
N2—N1—C8	121.2 (3)	N1—C9—N3	111.2 (3)
C8—N1—C9	129.7 (3)	N2—C10—N3	115.3 (4)
N2—N1—C9	109.1 (3)	C2—C3—H3	122.00

N1—N2—C10	102.4 (3)	C4—C3—H3	122.00
C9—N3—C10	102.1 (3)	C4—C5—H5	121.00
C2—C1—C7	121.5 (3)	C6—C5—H5	121.00
C6—C1—C7	122.1 (3)	C1—C6—H6	119.00
C2—C1—C6	116.3 (3)	C5—C6—H6	119.00
F1—C2—C3	117.3 (3)	O1—C7—H7	109.00
C1—C2—C3	124.5 (3)	C1—C7—H7	109.00
F1—C2—C1	118.3 (3)	C8—C7—H7	109.00
C2—C3—C4	116.3 (3)	N1—C8—H8A	109.00
F2—C4—C3	118.3 (3)	N1—C8—H8B	109.00
C3—C4—C5	123.0 (4)	C7—C8—H8A	109.00
F2—C4—C5	118.7 (3)	C7—C8—H8B	109.00
C4—C5—C6	118.5 (4)	H8A—C8—H8B	108.00
C1—C6—C5	121.4 (3)	N1—C9—H9	124.00
O1—C7—C8	110.8 (3)	N3—C9—H9	124.00
C1—C7—C8	108.0 (2)	N2—C10—H10	122.00
O1—C7—C1	110.3 (2)	N3—C10—H10	122.00

C8—N1—N2—C10	179.9 (3)	C7—C1—C6—C5	178.8 (3)
C9—N1—N2—C10	0.1 (4)	C2—C1—C7—O1	−154.7 (3)
N2—N1—C8—C7	73.8 (4)	C2—C1—C7—C8	84.1 (4)
C9—N1—C8—C7	−106.5 (4)	C6—C1—C7—O1	27.9 (4)
N2—N1—C9—N3	−0.1 (4)	C6—C1—C7—C8	−93.3 (3)
C8—N1—C9—N3	−179.9 (3)	F1—C2—C3—C4	−178.8 (3)
N1—N2—C10—N3	−0.1 (5)	C1—C2—C3—C4	1.3 (5)
C10—N3—C9—N1	0.0 (4)	C2—C3—C4—F2	−179.6 (3)
C9—N3—C10—N2	0.1 (5)	C2—C3—C4—C5	0.0 (6)
C6—C1—C2—F1	178.3 (3)	F2—C4—C5—C6	179.0 (3)
C6—C1—C2—C3	−1.9 (5)	C3—C4—C5—C6	−0.6 (6)
C7—C1—C2—F1	0.7 (4)	C4—C5—C6—C1	0.0 (5)
C7—C1—C2—C3	−179.5 (3)	O1—C7—C8—N1	62.4 (3)
C2—C1—C6—C5	1.2 (5)	C1—C7—C8—N1	−176.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N3^{i}	0.82	2.01	2.826 (4)	171
C3—H3···N2^{ii}	0.93	2.62	3.500 (5)	158
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Symmetry codes: (i) *x*+1/2, −*y*−1/2, −*z*+1; (ii) −*x*+2, *y*+1/2, −*z*+3/2; (iii) *x*−1, *y*, *z*; (iv) *x*, *y*−1, *z*.