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2,4-Difluorobenzohydroxamic acid

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Key indicators

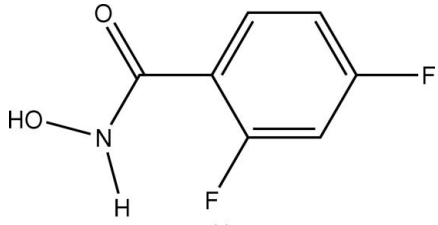
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.002 Å
R factor = 0.046
wR factor = 0.126
Data-to-parameter ratio = 14.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_7H_5F_2NO_2$, the hydroxyl group is *trans* to the difluorophenyl group with respect to the C—N bond. The molecules are linked into chains of rings parallel to [100] by a combination of O—H···O and N—H···O hydrogen bonds.

Comment

A range of aroylhydroxamic acids have been synthesized (Summers *et al.*, 1987) in the hope of developing an effective anticancer agent whose mode of action is directed against ribonucleotide reductase; difluorobenzohydroxamic acids have exhibited high potency both *in vitro* and *in vivo*.



(I)

The crystal structure of two substituted aroylhydroxamic acids have recently been reported (Shang *et al.*, 2005*a*,*b*), and here we describe the structure of another example, 2,4-difluorobenzohydroxamic acid, (I) (Fig. 1).

The mean deviation from the plane O1/C7/N1/O2 is 0.0292 Å, and the C—N bond length (Table 1) shows partial double-bond character. The dihedral angle between the O1/C7/C1 and benzene ring planes is 3.5 (1)°, indicating the possibility of conjugation between the carboxyl and benzene groups.

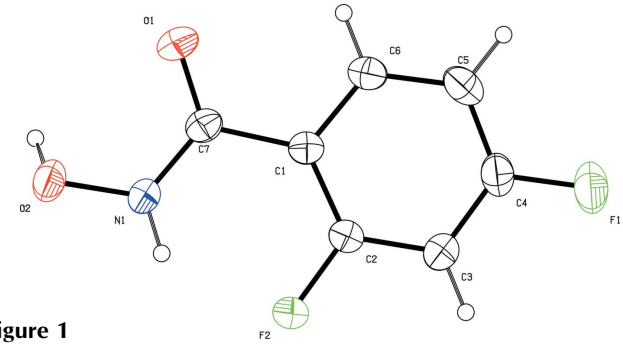


Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

There is a short intramolecular N—H···F contact and the molecules are linked by intermolecular O—H···O and N—H···O hydrogen bonds (Table 2), forming one-dimensional chains of rings running parallel to the [100] direction (Fig. 2).

Experimental

Methyl 2,4-difluorobenzoate (1.72 g, 10 mmol) was added to an aqueous solution (15 ml) of NH_2OH (16 mmol) under N_2 and the system was stirred at room temperature overnight. The pH of the solution was adjusted to about 7 using concentrated hydrochloric acid with ice cooling, and the resulting solid product was collected by filtration. Crystals suitable for single-crystal X-ray diffraction were obtained by recrystallization from methanol.

Crystal data

$C_7H_5F_2NO_2$
M_r = 173.12
Monoclinic, $P2_1/c$
a = 6.9266 (10) Å
b = 15.358 (2) Å
c = 7.0430 (11) Å
β = 111.795 (3)°
V = 695.68 (18) Å^3
Z = 4
D_x = 1.653 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.16 mm^{-1}
T = 292 (2) K
Block, colourless
0.30 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.955, T_{max} = 0.970
4297 measured reflections
1564 independent reflections
1091 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 27.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.126
S = 1.03
1564 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0664P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected bond lengths (Å).

C7—O1	1.2331 (17)	N1—O2	1.3903 (17)
C7—N1	1.324 (2)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···F2	0.85	2.03	2.6776 (17)	132
O2—H2A···O1^{i}	0.86	1.80	2.6129 (19)	158
N1—H1···O2^{ii}	0.85	2.28	2.935 (2)	134

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

All H atoms were placed in calculated positions and treated as riding atoms, with C—H = 0.93 Å, O—H = 0.82 Å, N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(C,N) or 1.5U_{eq}(O).

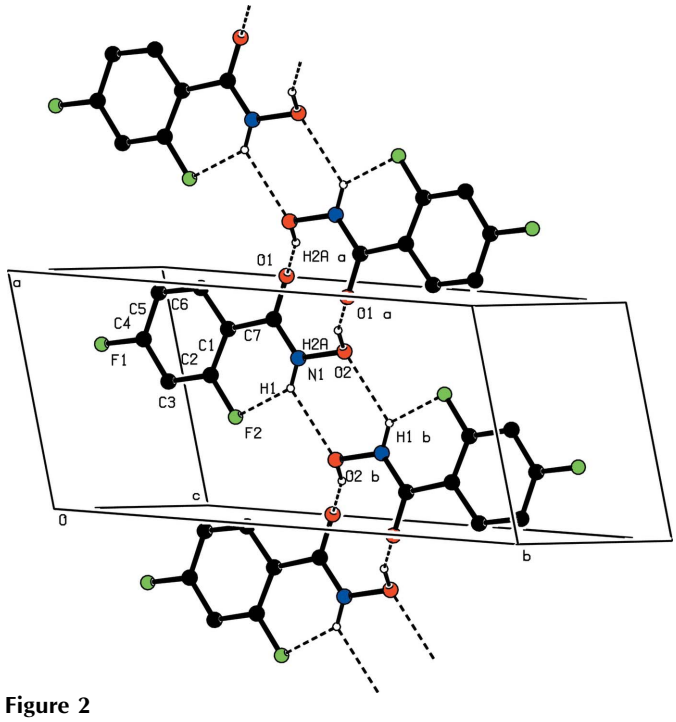


Figure 2
Packing diagram for the title compound, showing the hydrogen-bond interactions as dashed lines [symmetry codes: (*a*) $2-x, 1-y, 1-z$; (*b*) $1-x, 1-y, 1-z$].

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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References

Bruker (1997). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SAINT* (Version 6.45) and *SMART* (Version 5.628). Bruker AXS Inc., Madison, Wisconsin, USA.
Shang, X.-M., Meng, X.-G., Wu, J.-Z. & Li, Q.-S. (2005*a*). *Acta Cryst.* E**61**, o1961–o1962.
Shang, X.-M., Meng, X.-G., Wu, J.-Z. & Li, Q.-S. (2005*b*). *Acta Cryst.* E**61**, o2328–o2329.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Summers, J. B., Gunn, B. P., Mazdiyasni, H., Goetze, A. M., Young, P. R., Bouska, J. B., Dyer, R. D., Brooks, D. W. & Carter, G. W. (1987). *J. Med. Chem.* **30**, 2121–2126.