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2-Amino-5-fluorobenzoic acid

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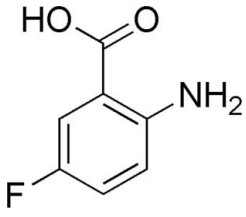
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.100; data-to-parameter ratio = 11.2.

In the title compound, $C_7H_6FNO_2$, the molecule is almost planar (r.m.s. deviation for the non-H atoms = 0.015 Å) and an intramolecular N—H···O hydrogen bond closes an $S(6)$ ring. In the crystal, inversion dimers linked by pairs of O—H···O hydrogen bonds generate $R_2^2(8)$ loops. Weak N—H···F hydrogen bonds, short F···F contacts [2.763 (2) Å] and aromatic π–π stacking interactions [centroid–centroid separation = 3.5570 (11) Å] are also observed in the crystal structure.

Related literature

For the applications of the title compound in the field of genetics, see: Toyn *et al.* (2000).



Experimental

Crystal data

$C_7H_6FNO_2$ M_r = 155.13
Monoclinic, $P2_1/c$
a = 4.9346 (2) Å
b = 11.7542 (6) Å
c = 11.9727 (5) Å
β = 96.782 (3)°
V = 689.58 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 293 K
0.43 × 0.37 × 0.25 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.947, T_{max} = 0.969
5184 measured reflections
1207 independent reflections
1057 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.100
S = 1.09
1207 reflections
108 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···O1	0.901 (19)	2.044 (19)	2.6959 (17)	128.2 (16)
N1—H1A···F1^{i}	0.91 (2)	2.55 (2)	3.3646 (17)	149.8 (14)
O2—H2···O1^{ii}	0.82	1.81	2.6279 (12)	175

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

Data collection: *APEX2* (Bruker, 2004);; cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7040).

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supporting information

Acta Cryst. (2013). E**69**, o387 [doi:10.1107/S160053681300408X]

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S1. Comment

2-Amino-5-fluorobenzoic acid is used for the counterselection of TRP1, a commonly used genetic marker in the yeast Saccharomyces cerevisiae (Toyn *et al.*, 2000). The ability to counterselect, as well as to select for, a genetic marker has numerous applications in microbial genetics. Keeping this in mind, the structure of the title compound is discussed here.

In the crystal structure of the title compound, $C_7H_6FNO_2$, the molecules are linked through O2—H2···O1 hydrogen bonds into inversion related dimers. N1—H1A···F1 hydrogen bonds and short F1···F1 contacts [2.763 (2) Å] are also observed in the crystal structure. Further, the structure features an intra molecular hydrogen bond between the amino proton and the adjacent carboxylic oxygen atom.

S2. Experimental

4-Fluoroaniline (0.01 mmol), aluminium chloride (0.05 mmol) and trichloroacetyl chloride(0.03 mmol) were taken in di-chloro methane (DCM) (20 ml) at 00 C under nitrogen atmosphere. The reaction mixture was refluxed for 16 h. The mixture was poured into ice-water carefully and the pH was adjusted to 2. The organic layer was separated and the aqueous layer was extracted with DCM. The combined extract was concentrated to get dark oily 1-(2-amino-5-fluoro-phenyl)-2,2,2-trichloroethanone. This compound (0.01 mmol) was dissolved in methanol. To this solution sodium methoxide (25% w/t in methanol) was added at 0 °C. The mixture was stirred for 1 h, the pH was adjusted to 6. The resulting solution was extracted with DCM and concentrated to get a brown solid methyl-2-amino-5-fluorobenzoate. To a solution of methyl-2-amino-5-fluorobenzoate (0.01 mmol) in tetrahydrofuran (10 ml),1 N Lithium hydroxide (0.03 mmol) was added at room temperature and stirred at 60 °C for 6 h. The reaction mixture was cooled to 0 °C and pH was adjusted to 5, the precipitate obtained was collected and dried in vacuum to get the title compound. Colourless prisms were obtained by slow evaporation of the solution of the compound in a mixture of DCM and methanol.

S3. Refinement

The H atoms were positioned with idealized geometry using a riding model with C—H = 0.93 Å. All H atoms were refined with isotropic displacement parameters (set to 1.2 times of the U_{eq} of the parent atom).

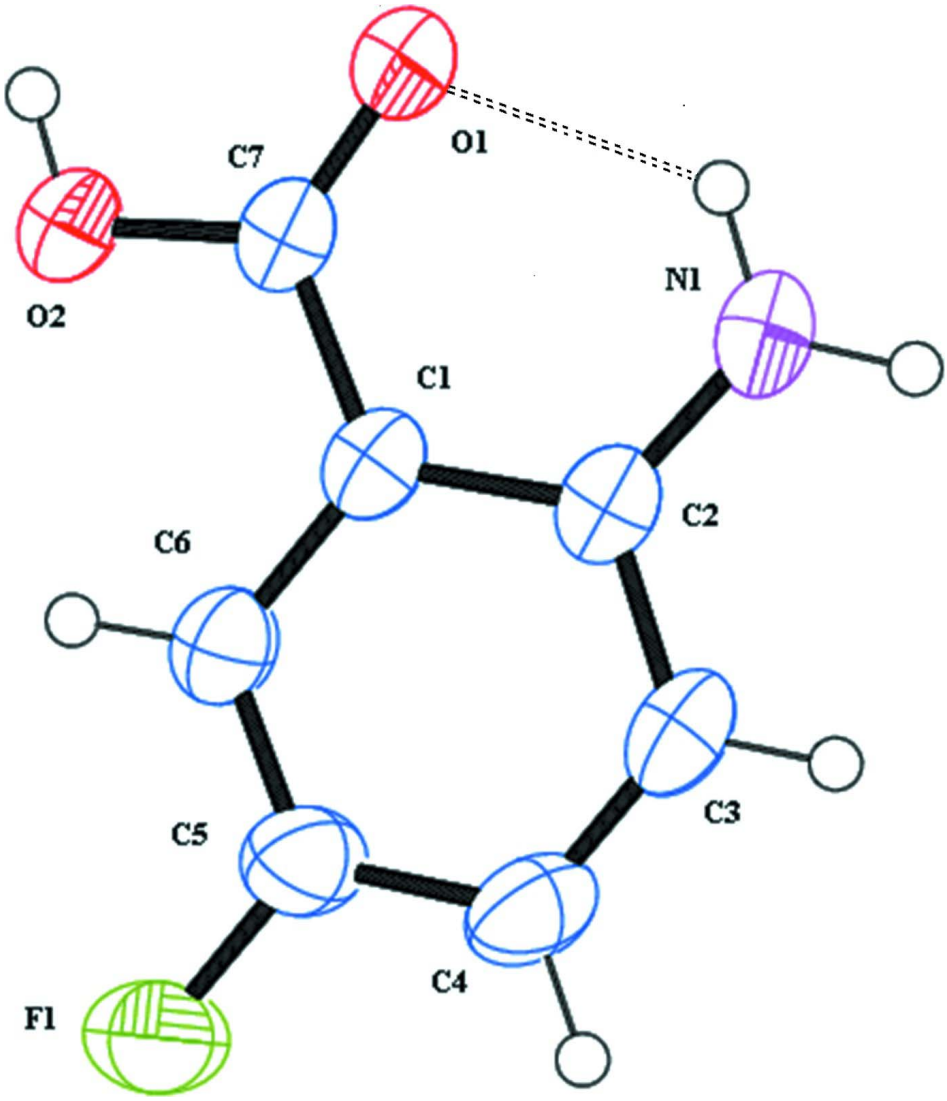

Figure 1

Molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

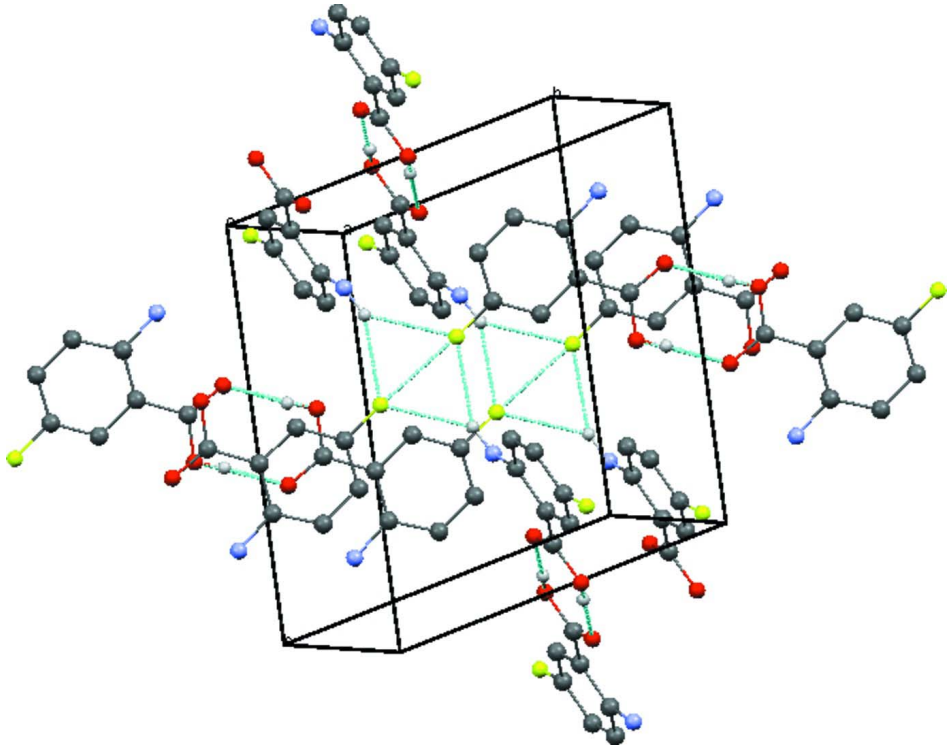

Figure 2

Molecular packing in the title compound. Hydrogen bonds are shown as dashed lines

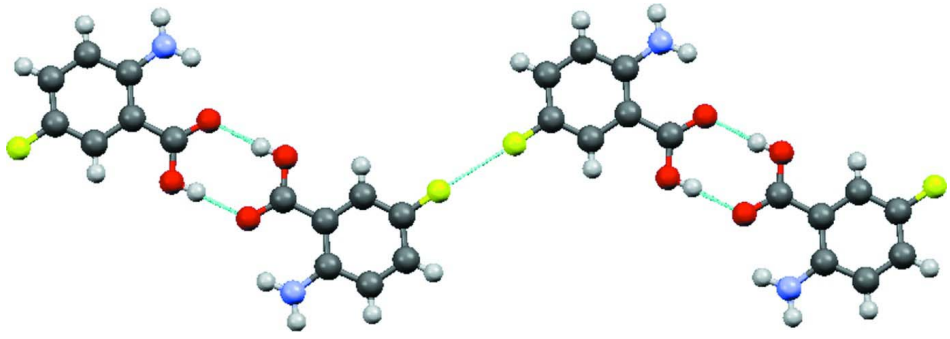

Figure 3

Display of F···F contacts and O–H···O Hydrogen bonds.

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Crystal data

$C_7H_6FNO_2$
$M_r = 155.13$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 4.9346\ (2)$ Å
$b = 11.7542\ (6)$ Å
$c = 11.9727\ (5)$ Å
$\beta = 96.782\ (3)°$
$V = 689.58\ (5)$ Å^3
$Z = 4$
$F(000) = 320$
Prism
$D_x = 1.494$ Mg m^{-3}
Melting point: 454 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 108 reflections
$\theta = 2.4–25.0°$
$\mu = 0.13$ mm^{-1}

T = 293 K
Prism, colourless

0.43 × 0.37 × 0.25 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.947, T_{max} = 0.969

5184 measured reflections
1207 independent reflections
1057 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 25.0°, θ_{min} = 2.4°
h = −5→5
k = −13→13
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.100
S = 1.09
1207 reflections
108 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2 + 0.0629P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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}
H1B	0.443 (4)	0.5012 (15)	0.2698 (16)	0.077 (5)*
H1A	0.681 (4)	0.4717 (14)	0.3630 (16)	0.078 (5)*
O1	0.20891 (18)	0.49475 (8)	0.11724 (8)	0.0572 (3)
C1	0.5279 (2)	0.34252 (10)	0.12427 (10)	0.0419 (3)
O2	0.20142 (19)	0.37877 (9)	−0.02978 (7)	0.0606 (3)
H2	0.0757	0.4209	−0.0541	0.091*
C2	0.6596 (2)	0.36817 (11)	0.23280 (10)	0.0458 (3)
C6	0.6146 (3)	0.24937 (12)	0.06514 (10)	0.0515 (3)
H6	0.5277	0.2315	−0.0059	0.062*
N1	0.5831 (3)	0.45571 (12)	0.29601 (11)	0.0688 (4)
C7	0.3008 (2)	0.41184 (10)	0.07158 (10)	0.0430 (3)
C4	0.9633 (3)	0.20846 (12)	0.21735 (11)	0.0561 (4)
H4	1.1092	0.1636	0.2474	0.067*
C3	0.8792 (3)	0.29852 (12)	0.27596 (11)	0.0529 (4)

H3	0.9699	0.3145	0.3468	0.063*
F1	0.9117 (2)	0.09467 (9)	0.05376 (8)	0.0924 (4)
C5	0.8272 (3)	0.18517 (12)	0.11232 (11)	0.0567 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0586 (6)	0.0593 (6)	0.0492 (6)	0.0139 (4)	−0.0129 (4)	−0.0088 (4)
C1	0.0393 (6)	0.0479 (7)	0.0374 (6)	−0.0016 (5)	0.0000 (5)	0.0045 (5)
O2	0.0619 (6)	0.0706 (6)	0.0439 (6)	0.0196 (5)	−0.0163 (4)	−0.0100 (4)
C2	0.0430 (6)	0.0513 (7)	0.0413 (7)	−0.0038 (5)	−0.0023 (5)	0.0027 (5)
C6	0.0566 (7)	0.0593 (7)	0.0370 (6)	0.0071 (6)	−0.0017 (5)	0.0009 (6)
N1	0.0719 (8)	0.0721 (8)	0.0549 (8)	0.0145 (7)	−0.0238 (6)	−0.0188 (6)
C7	0.0407 (6)	0.0477 (7)	0.0387 (6)	−0.0033 (5)	−0.0024 (5)	0.0009 (5)
C4	0.0538 (7)	0.0674 (9)	0.0461 (7)	0.0148 (6)	0.0018 (6)	0.0161 (6)
C3	0.0507 (7)	0.0664 (8)	0.0384 (6)	0.0003 (6)	−0.0077 (5)	0.0079 (6)
F1	0.1194 (8)	0.0939 (7)	0.0597 (6)	0.0593 (6)	−0.0071 (5)	−0.0108 (5)
C5	0.0665 (8)	0.0594 (8)	0.0442 (7)	0.0186 (6)	0.0061 (6)	0.0048 (6)

Geometric parameters (Å, º)

O1—C7	1.2299 (15)	C6—H6	0.9300
C1—C6	1.3982 (18)	N1—H1B	0.901 (19)
C1—C2	1.4150 (17)	N1—H1A	0.91 (2)
C1—C7	1.4667 (16)	C4—C3	1.361 (2)
O2—C7	1.3129 (14)	C4—C5	1.381 (2)
O2—H2	0.8200	C4—H4	0.9300
C2—N1	1.3571 (19)	C3—H3	0.9300
C2—C3	1.4069 (18)	F1—C5	1.3660 (16)
C6—C5	1.3599 (18)		
C6—C1—C2	119.80 (11)	O1—C7—O2	121.90 (10)
C6—C1—C7	118.77 (10)	O1—C7—C1	123.51 (10)
C2—C1—C7	121.43 (11)	O2—C7—C1	114.59 (11)
C7—O2—H2	109.5	C3—C4—C5	118.59 (11)
N1—C2—C3	119.29 (11)	C3—C4—H4	120.7
N1—C2—C1	123.08 (11)	C5—C4—H4	120.7
C3—C2—C1	117.63 (12)	C4—C3—C2	122.10 (11)
C5—C6—C1	119.44 (12)	C4—C3—H3	119.0
C5—C6—H6	120.3	C2—C3—H3	119.0
C1—C6—H6	120.3	C6—C5—F1	119.08 (12)
C2—N1—H1B	120.5 (12)	C6—C5—C4	122.44 (13)
C2—N1—H1A	119.8 (11)	F1—C5—C4	118.48 (12)
H1B—N1—H1A	119.5 (17)		
C6—C1—C2—N1	−178.62 (12)	C2—C1—C7—O2	179.10 (11)
C7—C1—C2—N1	1.46 (19)	C5—C4—C3—C2	−0.1 (2)
C6—C1—C2—C3	1.17 (18)	N1—C2—C3—C4	179.06 (13)

C7—C1—C2—C3	−178.75 (11)	C1—C2—C3—C4	−0.74 (19)
C2—C1—C6—C5	−0.75 (19)	C1—C6—C5—F1	−179.65 (12)
C7—C1—C6—C5	179.17 (11)	C1—C6—C5—C4	−0.1 (2)
C6—C1—C7—O1	179.42 (11)	C3—C4—C5—C6	0.6 (2)
C2—C1—C7—O1	−0.66 (18)	C3—C4—C5—F1	−179.91 (12)
C6—C1—C7—O2	−0.82 (16)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···O1	0.901 (19)	2.044 (19)	2.6959 (17)	128.2 (16)
N1—H1*A*···F1^{i}	0.91 (2)	2.55 (2)	3.3646 (17)	149.8 (14)
O2—H2···O1^{ii}	0.82	1.81	2.6279 (12)	175

Symmetry codes: (i) *x*, −*y*+1/2, *z*+1/2; (ii) −*x*, −*y*+1, −*z*.