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## Key indicators

Single-crystal X-ray study  
*T* = 298 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$   
*R* factor = 0.069  
*wR* factor = 0.142  
Data-to-parameter ratio = 9.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.2,2,2-Trifluoro-*N*-(2-hydroxy-5-nitrophenyl)acetamide

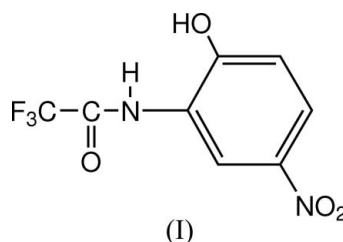
In the crystal structure of the title compound,  $\text{C}_8\text{H}_5\text{F}_3\text{N}_2\text{O}_4$ , all atoms apart from two F atoms are located on a crystallographic mirror plane. In the mirror plane, the molecules are linked by strong intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds, forming a chain along the *c* axis.

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## Comment

Substituted 2-aminophenol derivatives exhibit supramolecular assembly *via*  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds (Song *et al.*, 2002). In order to understand the hydrogen bonding pattern in *N*-substituted 2-aminophenol derivatives, the title compound, (I), was prepared by a typical synthetic route, *viz.* the condensation of an amine and acetic acid in the presence of a base (Li *et al.*, 1993).



All atoms of the title molecule are located on a crystallographic mirror plane except for two F atoms of the trifluoromethyl group (Fig. 1). An intramolecular  $\text{C}_6-\text{H}_6\cdots\text{O}_4$  hydrogen bond generates an *S*(6) ring motif (Bernstein *et al.*, 1995), and  $\text{N}_2-\text{H}_2\cdots\text{F}_2$  and  $\text{N}_2-\text{H}_2\cdots\text{O}_1$  (Table 1) interactions generate a pair of *S*(5) ring motifs. The molecules are linked by strong intermolecular  $\text{O}_1-\text{H}_1\cdots\text{O}_4(x, y, z - 1)$  hydrogen bonds into a chain along the *c* axis (Fig. 2).

## Experimental

Compound (I) was synthesized by a modification of the literature method of Li *et al.* (1993). Trifluoroacetic acid anhydride (1.55 ml, 10.00 mmol) in tetrahydrofuran (THF, 5 ml) was added dropwise to a solution of 2-amino-4-nitrophenol (1.5447 g, 10.00 mmol) in dried THF (35 ml) and pyridine (1.2 ml) at 273 K. The reaction mixture was slowly heated to room temperature and stirred under a nitrogen atmosphere for 24 h; water (5 ml) and brine (5 ml) were then successively added. The resultant organic layer was washed successively with 5% HCl (7.5 ml), saturated  $\text{NaHCO}_3$  (10 ml), and brine (10 ml). The aqueous layer was extracted with EtOAc ( $2 \times 10$  ml). The combined organic layer was then dried over anhydrous  $\text{Na}_2\text{SO}_4$  and the volatiles were removed using a rotary evaporator. The residue was purified by column chromatography ( $\text{SiO}_2$ ) using

EtOAc–hexane (1:1) and the compound was recrystallized from EtOAc–hexane (1:4 v/v) by slow evaporation (yield: 2.2411 g, 89.6%; m.p. 437–438 K).

Crystal data

$C_8H_5F_3N_2O_4$   
 $M_r = 250.14$   
 Orthorhombic, *Pnma*  
 $a = 19.7661(7) \text{ \AA}$   
 $b = 6.610(9) \text{ \AA}$   
 $c = 7.4321(8) \text{ \AA}$   
 $V = 971.0(13) \text{ \AA}^3$

$Z = 4$   
 $D_x = 1.711 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.17 \text{ mm}^{-1}$   
 $T = 298(2) \text{ K}$   
 Block, colourless  
 $0.39 \times 0.27 \times 0.24 \text{ mm}$

Data collection

Bruker APEX area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
 $T_{\min} = 0.936, T_{\max} = 0.960$

4879 measured reflections  
 954 independent reflections  
 848 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$   
 $\theta_{\text{max}} = 25.3^\circ$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.069$   
 $wR(F^2) = 0.142$   
 $S = 1.08$   
 954 reflections  
 100 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0736P)^2 + 1.1933P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.47 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.34 \text{ e \AA}^{-3}$

Table 1

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

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
O1–H1···O4 <sup>i</sup>	0.79	1.88	2.673 (4)	178
N2–H2···F2	0.86	2.22	2.628 (6)	109
N2–H2···O1	0.86	2.17	2.573 (6)	108
C6–H6···O4	0.93	2.25	2.839 (7)	121

Symmetry code: (i)  $x, y, z - 1$ .

All H atoms were found in difference density maps, but were then placed in calculated positions (O–H = 0.79 Å, N–H = 0.86 Å and C–H = 0.93 Å) and included in the refinement using a riding-model approximation, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N,O})$ . The displacement parameters of the F atoms suggest orientational disorder for the trifluoromethyl group, but attempts to use such a model did not improve the displacement parameters.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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, 1998); software used to prepare material for publication: *SHELXL97*.

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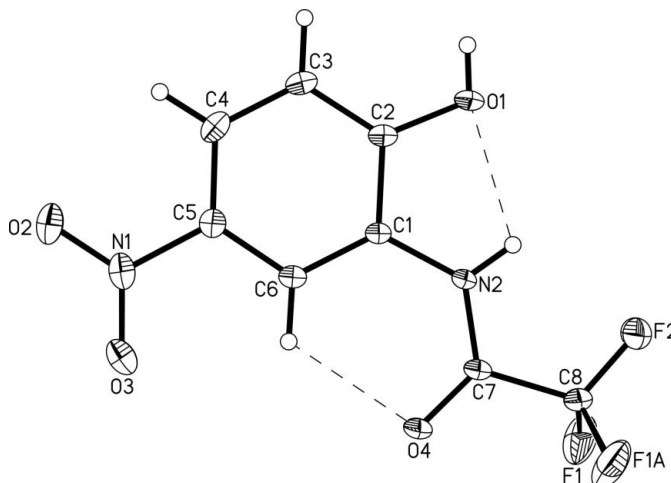


Figure 1

The molecular structure of (I), showing 50% probability displacement ellipsoids. Dashed lines indicate intramolecular hydrogen bonds. Atom F1A is generated by the symmetry operation  $(x, \frac{3}{2} - y, z)$

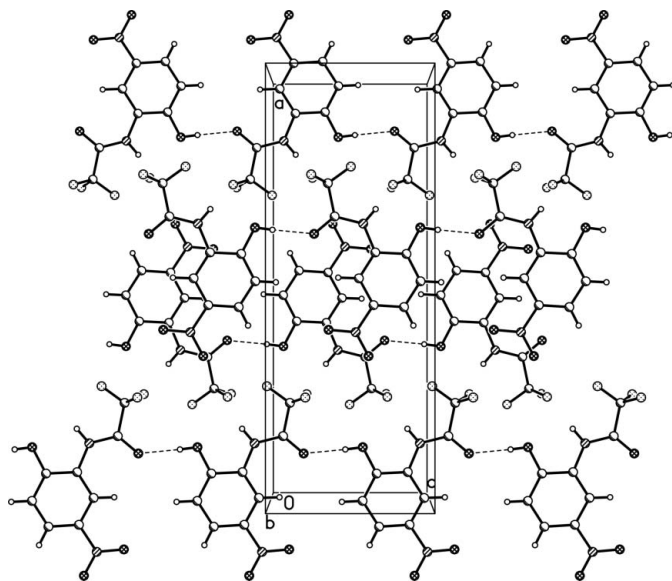


Figure 2

The crystal packing of (I), showing O–H···O hydrogen-bonded chains (dashed lines).

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