

2-Amino-4-(2,2,2-trifluoroethoxy)pyrimidine

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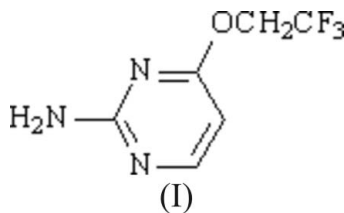
Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.052
 wR factor = 0.153
Data-to-parameter ratio = 12.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The crystal structure of the title compound, $\text{C}_6\text{H}_6\text{F}_3\text{N}_3\text{O}$, has two molecules in the asymmetric unit; these are linked by two intermolecular $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds to form a dimer. The planes of the rings of the two molecules are slightly inclined, with a dihedral angle of $27.1(3)^\circ$. The dimers are joined *via* a pair of $\text{N}-\text{H}\cdots\text{F}$ hydrogen bonds to form a tetramer.

Comment

Pyrimidine compounds have attracted much attention for their biological activities and molecular structures. The crystal structures of some 2-amino-substituted pyrimidine compounds, such as 2-amino-4-methoxy-6-methylpyrimidine (Glidewell *et al.*, 2003), 2-amino-4,6-dimethylpyrimidinium bromide (Panneerselvam *et al.*, 2004), 2-amino-4,6-dimethylpyrimidinium hydrogen sulfate (Hemamalini *et al.*, 2005), 2-amino-4,6-dimethylpyrimidine-cinnamic acid (Balasubramani *et al.*, 2005) and *catena*-2-aminopyrimidinecopper(II) (Bulut *et al.*, 2005), have previously been elucidated. Here, we report the crystal structure of the title compound, (I).



In the crystal structure of (I), the asymmetric unit is a hydrogen-bonded dimer (Fig. 1) containing two molecules of (I). All of the C, N and O atoms in one molecule, including the ethoxy substituent, are essentially coplanar, with a mean deviation of 0.0182 Å. In the other molecule, the pyrimidine ring and the N and O atoms directly attached to it are coplanar, with a mean deviation of 0.0079 Å, but the distal atom of the ethyl group is twisted out of this plane by about 10.5° , as shown by the torsion angle $\text{C8}-\text{O2}-\text{C11}-\text{C12} = 169.5(3)^\circ$. The dihedral angle between the planes of the two molecules is $27.1(3)^\circ$.

There is a pair of intermolecular hydrogen bonds, $\text{N1}-\text{H1A}\cdots\text{N6}$ and $\text{N4}-\text{H4B}\cdots\text{N3}$ (Table 1), between the two molecules in the dimeric asymmetric unit. Furthermore, another pair of hydrogen bonds, $\text{N4}-\text{H4A}\cdots\text{F4}^i$ and $\text{N4}^i-\text{H4A}^i\cdots\text{F4}$ [symmetry code: (i) $1-x, 2-y, -z$], join two dimers to form a tetramer (Fig. 2). The crystal structure is also stabilized by $\pi-\pi$ interactions between the pyrimidine rings of adjacent molecules (Fig. 3); the distance between the centroids

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of rings C1–C4/N2/N3 and C7–C10/N5/N6($\frac{1}{2} + x, \frac{3}{2} - x, \frac{1}{2} + z$) is 3.625 (3) Å.

Experimental

Na (0.8 g, 3.5 mmol) was dissolved in trifluoroethanol (20 ml); 2-amino-4-chloropyrimidine (2.0 g, 1.5 mmol) (Kuh & Clapper, 1947) was added, and the mixture was refluxed for 3 h. The solution was filtered and the excess trifluoroethanol was distilled off *in vacuo*. The residue was redissolved in 20% HCl (10 ml). After adjusting the pH to 8–9 with 20% NaOH, the precipitate which formed was filtered off and recrystallized from petroleum ether to give white crystals (m.p. 344–346 K; yield 59%). Elemental analysis, calculated for C₆H₆F₃N₃O: C 37.32, H 3.13, N 21.76%; found: C 37.18, H 3.13, N 21.60%. Colourless single crystals of (I) suitable for crystallographic analysis were obtained by the slow evaporation of an acetone solution at room temperature over 7 d.

Crystal data

C ₆ H ₆ F ₃ N ₃ O	Z = 8
$M_r = 193.14$	$D_x = 1.558 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 12.135 (6) \text{ \AA}$	$\mu = 0.16 \text{ mm}^{-1}$
$b = 10.537 (5) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 13.705 (7) \text{ \AA}$	Prism, colourless
$\beta = 109.989 (9)^\circ$	$0.24 \times 0.20 \times 0.12 \text{ mm}$
$V = 1646.8 (14) \text{ \AA}^3$	

Data collection

Bruker SMART CCD area-detector diffractometer	8219 measured reflections
φ and ω scans	2905 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1669 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.883, T_{\max} = 1.000$	$R_{\text{int}} = 0.044$
	$\theta_{\max} = 25.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0731P)^2 + 0.3351P]$
$R[F^2 > 2\sigma(F^2)] = 0.052$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.153$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.01$	$\Delta\rho_{\max} = 0.25 \text{ e \AA}^{-3}$
2905 reflections	$\Delta\rho_{\min} = -0.23 \text{ e \AA}^{-3}$
236 parameters	
H-atom parameters constrained	

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1–H1A \cdots N6	0.86	2.24	3.100 (7)	173
N4–H4B \cdots N3	0.86	2.21	2.999 (6)	153
N4–H4A \cdots F4 ⁱ	0.86	2.46	3.258 (7)	155

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

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C–H distances of 0.93 or 0.96 Å, N–H distances of 0.86 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent})$.

Data collection: SMART (Bruker, 1997); cell refinement: SMART; data reduction: SAINT (Bruker, 1997); 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.

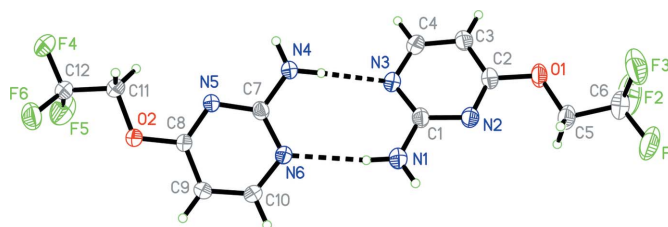


Figure 1

The asymmetric unit of (I), with displacement ellipsoids drawn at the 30% probability level. Intermolecular hydrogen bonds are indicated by dashed lines.

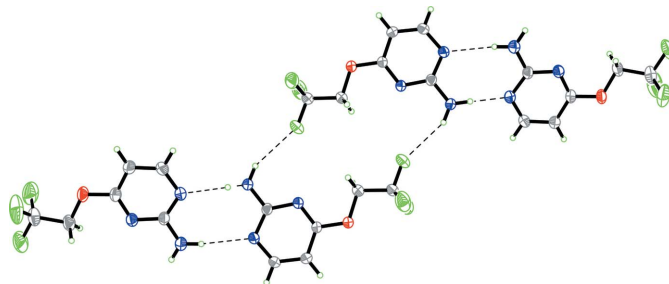


Figure 2

The tetramer structure of (I), with displacement ellipsoids drawn at the 30% probability level. Intermolecular hydrogen bonds are indicated by dashed lines.

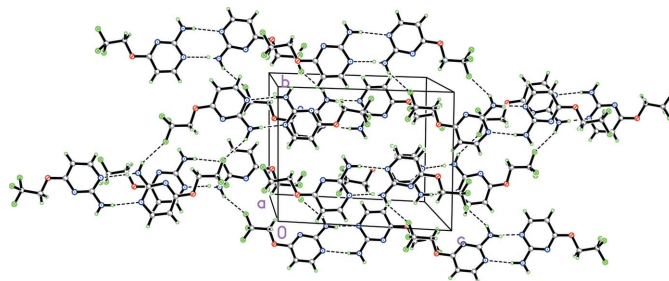


Figure 3

A molecular packing diagram, showing the π – π stacking interactions (superimposed pyrimidine rings). Hydrogen bonds are shown as dashed lines.

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