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#### Key indicators

Single-crystal X-ray study  
 $T = 150$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.058  
 $wR$  factor = 0.147  
Data-to-parameter ratio = 13.0

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

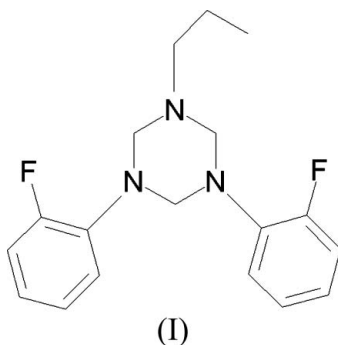
## 1,3-Bis(2-fluorophenyl)-5-propyl-1,3,5-triazacyclohexane

In the molecule of the title compound,  $\text{C}_{18}\text{H}_{21}\text{F}_2\text{N}_3$ , the 1,3,5-triazacyclohexane ring has a chair conformation. Intramolecular  $\text{C}-\text{H}\cdots\text{F}$  and  $\text{C}-\text{H}\cdots\text{N}$  hydrogen bonds may be effective in the stabilization of the structure.

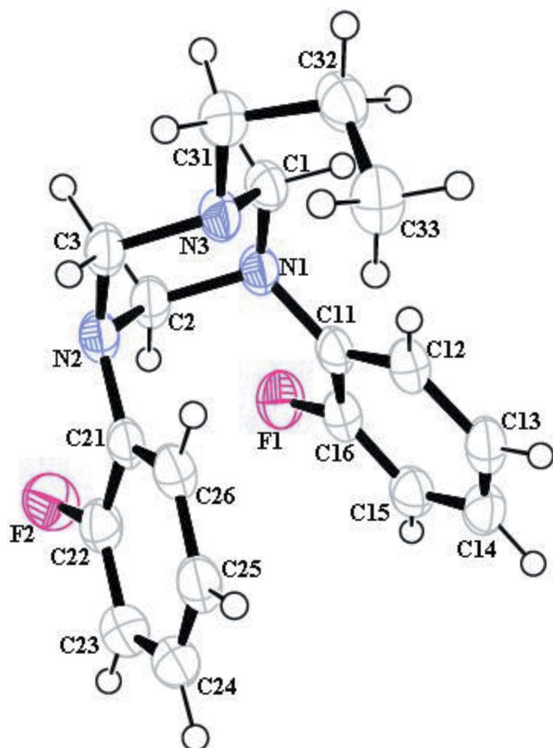
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#### Comment

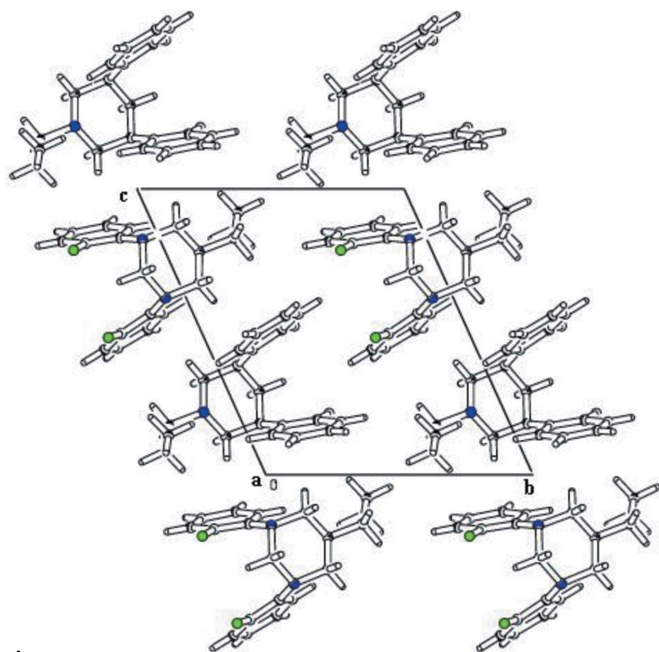
Conformational effects of non-bonding electrons are a feature of heterocyclic chemistry (Riddell, 1980). The heterocyclic nucleus in 1,3,5-triazacyclohexane is expected to adopt a chair conformation and four distinct types of substituent orientation can be postulated: eee, eea, eaa and aaa, where e is equatorial and a is axial. All four conformers have axial repulsions involving substituents and/or lone pairs of electrons on the N atoms. Several conformations of 1,3,5-trialkyl-1,3,5-triazacyclohexanes in solution have been investigated by dipole moment and NMR spectroscopy. The former approach suggests varying proportions of eee, eea and eaa conformers (Wellington & Tollens, 1885). X-ray studies of the 1,3,5-tricyclohexyl compound established that it adopts the eea conformation (Bouchemma *et al.*, 1988). Various 1,3,5-triaryl-1,3,5-triazacyclohexanes adopt the diaxial-equatorial orientation of substituents in the solid state, thus avoiding 1,3-diaxial lone-pair repulsions (Giumanini *et al.*, 1985; Gilardi *et al.*, 2003; Bouchemma *et al.*, 1990). The structure determination of the title compound, (I), was undertaken to compare the structural results obtained with those of 1,3,5-tris(*o*-fluorophenyl)-1,3,5-triazacyclohexane (Bouchemma *et al.*, 1989).



In the molecule of the title compound, (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). It was prepared from the condensation reaction of *o*-fluoroaniline and propylamine with formaldehyde. In this case, X-ray analysis proved that the product contains two aryl substituents and one alkyl group. The 1,3,5-triazacyclohexane ring has a total puckering amplitude  $Q_T$  of 1.925 (3) Å, and a



**Figure 1**  
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.



**Figure 2**  
A packing diagram of (I).

chair conformation [ $\varphi = 151.06(5)^\circ$  and  $\theta = 121.47(3)^\circ$ ] (Cremer & Pople, 1975), which is typical of these rings (Gilardi *et al.*, 2003). Rings *A* (C11–C16) and *B* (C21–C26) are, of course, planar, and the dihedral angle between them is  $33.85(4)^\circ$ .

There are 33 similar compounds in the Cambridge Structural Database (CSD, Version 5.24; Allen, 2002), all containing

the 1,3,5-triazacyclohexane ring with different substituents on the N atoms. 32 of these compounds have chair conformations, the exception being 1,3,5-tris(*p*-nitrophenyl)-1,3,5-triazacyclohexane (Adam *et al.*, 1993), which has a twist-boat conformation.

The title compound, (I), has the two *o*-fluorophenyl substituents in axial positions and the propyl group occupying an equatorial arrangement, leaving the N lone pairs in the thermodynamically stable equatorial position.

Intramolecular C–H···F and C–H···N hydrogen bonds (Table 1) may be effective in the stabilization of the structure of (I). In the crystal structure, the molecules are stacked in alternating layers along the *b* axis (Fig. 2).

## Experimental

The title compound was obtained from a mixture of propylamine and *o*-fluoroaniline with formalin (2:1:1) in ethanol (20 ml) at 293 K. The resulting solution was evaporated to dryness on a rotary evaporator and the white residue was crystallized from diethyl ether–petroleum ether (1:4).

### Crystal data

$C_{18}H_{21}F_2N_3$   
 $M_r = 317.38$   
Triclinic,  $P\bar{1}$   
 $a = 6.8130(6) \text{ \AA}$   
 $b = 10.4780(8) \text{ \AA}$   
 $c = 12.322(1) \text{ \AA}$   
 $\alpha = 114.089(4)^\circ$   
 $\beta = 94.033(4)^\circ$   
 $\gamma = 91.320(5)^\circ$

$V = 799.74(11) \text{ \AA}^3$   
 $Z = 2$   
 $D_x = 1.318 \text{ Mg m}^{-3}$   
Mo  $K\alpha$  radiation  
 $\mu = 0.10 \text{ mm}^{-1}$   
 $T = 150(2) \text{ K}$   
Prism, colourless  
 $0.35 \times 0.25 \times 0.18 \text{ mm}$

### Data collection

Nonius KappaCCD area-detector diffractometer  
 $\varphi$  scans, and  $\omega$  scans with  $\kappa$  offsets  
Absorption correction: none  
9398 measured reflections

2713 independent reflections  
2248 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.084$   
 $\theta_{\text{max}} = 25.0^\circ$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.058$   
 $wR(F^2) = 0.147$   
 $S = 1.09$   
2713 reflections  
208 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0293P)^2 + 1.3984P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.28 \text{ e \AA}^{-3}$   
Extinction correction: *SHELXL97* (Sheldrick, 1997)  
Extinction coefficient: none

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2–H2B···F1	0.99	2.25	2.904 (4)	123
C2–H2B···F2	0.99	2.28	2.920 (3)	121
C26–H26···N3	0.95	2.62	3.171 (3)	118

H atoms were positioned geometrically, with C–H = 0.95, 0.99 and 0.98  $\text{\AA}$  for aromatic, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$ , where  $x = 1.5$  for methyl H, and  $x = 1.2$  for all other H atoms.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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