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2-(1,3-Benzothiazol-2-yloxy)-*N*-(4-fluorophenyl)-*N*-isopropylacetamide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.061
wR factor = 0.150
Data-to-parameter ratio = 18.1

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

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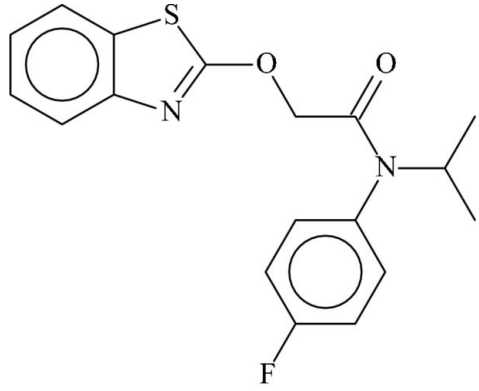
The asymmetric unit of the title compound, $C_{18}H_{17}FN_2O_2S$, contains two independent molecules related by a pseudo-inversion centre. The molecular packing is stabilized by C—H···O and C—H···π interactions.

Comment

We have reported the crystal structures of two nitrophenoxy-based herbicides produced by a commerical herbicide company in China (Gao & Ng, 2005*a*,*b*). We report here the crystal structure of the title compound, (I), a benzothiazolyl-oxy-bearing acetamide, which has bulky substituents on the amino N atom. The Cambridge Structural Database (Version 5.27; Allen, 2002) contains only one example of a benzothiazolyl ether compound, *viz.* ethyl 3-[4-(benzothiazol-2-yloxy)hydroxyphenyl]propionate (Mereiter & Mutuszczak, 2002).



(I)

Compound (I) crystallizes with two independent molecules in the asymmetric unit (Fig. 1), which are related by a pseudo inversion centre at (0.243, 0.876, 0.496). Bond lengths and angles observed in the two molecules are similar but the molecules have slightly different orientations for the isopropyl groups.

The crystal packing of (I) is stabilized by C—H···O hydrogen bonds and C—H···π interactions involving the aromatic C1–C6 and C19—C24 rings (Table 1).

Experimental

The title compound was purchased from Tianjian Bodi Chemical Reagent Company and recrystallized from ethanol.

Crystal data

$C_{18}H_{17}FN_2O_2S$
M_r = 344.40
Monoclinic, $P2_1/c$
a = 17.747 (2) Å
b = 15.266 (2) Å
c = 13.299 (1) Å
β = 108.243 (6)°
V = 3422.1 (7) Å^3
Z = 8
D_x = 1.337 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 293 (2) K
Block, colourless
0.4 × 0.3 × 0.2 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.909, T_{max} = 0.992
32053 measured reflections
7827 independent reflections
4363 reflections with $I > 2\sigma(I)$
R_{int} = 0.066
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.150
S = 1.01
7827 reflections
433 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0687P)^2 + 0.4362P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C19–C24 and C1–C6 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C23—H23···O2^{i}	0.93	2.52	3.289 (4)	140
C12—H12···*Cg*1^{ii}	0.93	2.70	3.573 (3)	156
C15—H15···*Cg*2^{iii}	0.93	2.70	3.509 (3)	146
C29—H29···*Cg*1^{iv}	0.93	2.78	3.617 (3)	151

Symmetry codes: (i) $x, y, z-1$; (ii) $-x+1, -y+2, -z+1$; (iii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (iv) $-x, -y+2, -z$.

H atoms were positioned geometrically [C—H = 0.93–0.98 Å] and were included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2 or 1.5 (methyl) times U_{eq}(C).

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

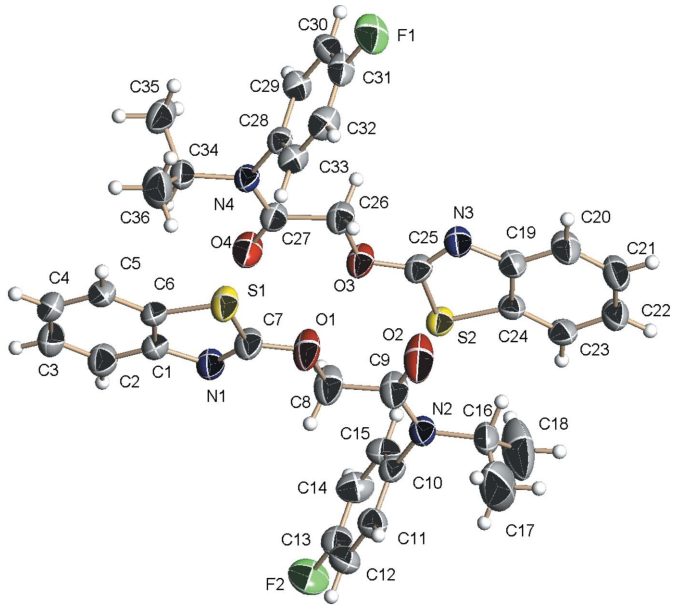


Figure 1
The asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii.

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