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2-Bromo-*N*′-[(*E*)-(4-fluorophenyl)-methylene]-5-methoxybenzohydrazide monohydrate

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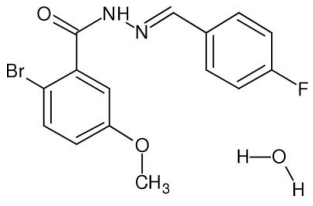
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.013 Å; R factor = 0.080; wR factor = 0.202; data-to-parameter ratio = 13.7.

The crystal packing of the title compound, $C_{15}H_{12}BrFN_2O_2\cdot H_2O$, is stabilized by N—H···O and O—H···O hydrogen bonds. There are two molecules in the asymmetric unit, differing in the dihedral angle between the two aromatic rings, which are 62.3 (2) and 49.9 (2)°.

Related literature

For related structures, see: Bruno *et al.* (1998); Harrison *et al.* (2005); Yathirajan, Sarojini *et al.* (2007); Yathirajan, Narayana, *et al.* (2007). For related literature, see: Varma *et al.* (1986); Misra *et al.* (1981); Agarwal *et al.* (1983); Singh *et al.* (1988); Hodnett *et al.* (1970).



Experimental

Crystal data

$C_{15}H_{12}BrFN_2O_2\cdot H_2O$
M_r = 369.19
Monoclinic, *Cc*
a = 30.1171 (18) Å
b = 8.0187 (7) Å
c = 13.4661 (8) Å
β = 111.902 (4)°
V = 3017.3 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.75 mm^{-1}
T = 173 (2) K
0.37 × 0.35 × 0.33 mm

Data collection

Stoe IPDS II two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.379, T_{max} = 0.394
16531 measured reflections
5477 independent reflections
4843 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.080
$wR(F^2)$ = 0.202
S = 1.02
5477 reflections
400 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}
Absolute structure: Flack (1983), 2642 Friedel pairs
Flack parameter: 0.018 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1*W*	0.88	2.03	2.901 (9)	172
N1*A*—H1*A*···O1*WA*	0.88	2.01	2.860 (9)	163
O1*W*—H1*W*1···O1^{i}	0.84	1.99	2.832 (8)	180
O1*W*—H1*W*2···O1*A*^{ii}	0.84	2.01	2.856 (8)	180
O1*WA*—H1*W*3···O1^{iii}	0.84	2.06	2.897 (8)	180
O1*WA*—H1*W*4···O1*A*^{iv}	0.84	1.96	2.802 (7)	180

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); 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: AT2297).

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