Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(4-Bromophenyl)-*N*-(3,4-difluorophenyl)acetamide

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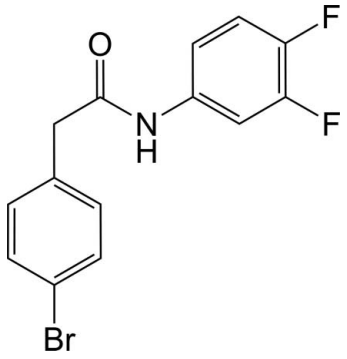
Received 6 May 2013; accepted 9 May 2013

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.009 Å; R factor = 0.041; wR factor = 0.106; data-to-parameter ratio = 13.9.

In the title compound, $C_{14}H_{10}BrF_2NO$, the dihedral angle between the mean planes of the 4-bromophenyl and 3,4-difluorophenyl rings is 66.4 (1)°. These two planes are twisted by 40.0 (5) and 86.3 (2)°, respectively, from that of the acetamide group. In the crystal, N—H···O hydrogen bonds and weak C—H···O and C—H···F interactions form infinite chains along [100].

Related literature

For the structural similarity of *N*-substituted 2-arylacetamides to the lateral chain of natural benzylpenicillin, see: Mijin & Marinkovic (2006); Mijin *et al.* (2008). For the coordination abilities of amides, see: Wu *et al.* (2008, 2010). For related structures, see: Praveen *et al.* (2011*a*,*b*,*c*, 2012). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{14}H_{10}BrF_2NO$
M_r = 326.14
Orthorhombic, $P2_12_12_1$
a = 4.9136 (3) Å
b = 6.0218 (4) Å
c = 42.514 (2) Å
V = 1257.96 (13) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 4.62 mm^{-1}
T = 173 K
0.48 × 0.32 × 0.16 mm

Data collection

Agilent Xcalibur (Eos, Gemini) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO* and *CrysAlis RED*; Agilent, 2012)
T_{min} = 0.257, T_{max} = 1.000
6592 measured reflections
2402 independent reflections
2388 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.106
S = 1.15
2402 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.87 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}
Absolute structure: Flack x determined using 915 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons & Flack, 2004)
Flack parameter: −0.01 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.88	1.97	2.851 (7)	175
C7—H7···O1^{ii}	0.95	2.63	3.309 (8)	129
C13—H13···F1^{iii}	0.95	2.50	3.426 (9)	164

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2012* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

ASP thanks the University of Mysore for research facilities. BN thanks the UGC for financial assistance through a BSR one-time grant for the purchase of chemicals. JPJ acknowledges the NSF–MRI program (grant No. CHE-1039027) for funds to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5313).

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supporting information

Acta Cryst. (2013). E**69**, o900–o901 [doi:10.1107/S1600536813012865]

2-(4-Bromophenyl)-*N*-(3,4-difluorophenyl)acetamide

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S1. Comment

N-Substituted 2-arylacetamides are very interesting compounds because of their structural similarity to the lateral chain of natural benzylpenicillin (Mijin *et al.*, 2006, 2008). Amides are also used as ligands due to their excellent coordination abilities (Wu *et al.*, 2008, 2010). Crystal structures of some acetamide derivatives viz., N-(3-chloro-4-fluoro-phenyl)-2-(naphthalen-1-yl)acetamide (Praveen *et al.*, 2011*a*), N-(4-chloro-1,3-benzothiazol-2-yl)-2- (3-methylphenyl)-acetamide monohydrate (Praveen *et al.*, 2011*b*), N-(3-chloro-4-fluorophenyl)-2,2-diphenylacetamide (Praveen *et al.*, 2011*c*) and N-(4,6-dimethoxypyrimidin-2-yl)-2-(3-methylphenyl)acetamide (Praveen *et al.*, 2012) have been reported. In view of the importance of amides, we report here in the crystal structure of the title compound, $C_{14}H_{10}BrF_2NO$, (I).

In (I) the dihedral angle between the mean planes of the 4-bromophenyl and 3,4-difluorophenyl rings is 66.4 (1)° (Fig. 1). These two planes are twisted by 40.0 (5)° and 86.3 (2)°, respectively, from that of the acetamide group. Bond lengths are in normal ranges (Allen *et al.*, 1987). In the crystal, N—H···O hydrogen bonds and weak C—H···O and C—H···F intermolecular interactions are observed forming a infinite chains along (100) and contribute to packing stability (Fig. 2).

S2. Experimental

4-bromophenylacetic acid (0.213 g, 1 mmol), 3,4-difluoro aniline (0.129 g, 1 mmol) and 1-ethyl-3-(3-dimethylamino-propyl)carbodiimide hydrochloride (1.0 g, 0.01 mol) were dissolved in dichloromethane (20 mL) (Fig. 3). The mixture was stirred in presence of triethylamine at 273 K for about 3 h. The contents were poured into 100 ml of ice-cold aqueous hydrochloric acid with stirring, which was extracted thrice with dichloromethane. The organic layer was washed with saturated $NaHCO_3$ solution and brine solution, dried and concentrated under reduced pressure to give the title compound (I). Single crystals were grown from methylene chloride by the slow evaporation method (m.p.: 423–425 K).

S3. Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with Atom—H lengths of 0.95Å (CH), 0.99Å (CH_2) or 0.88° (NH). Isotropic displacement parameters for these atoms were set to 1.2 (CH, CH_2, NH) times U_{eq} of the parent atom.

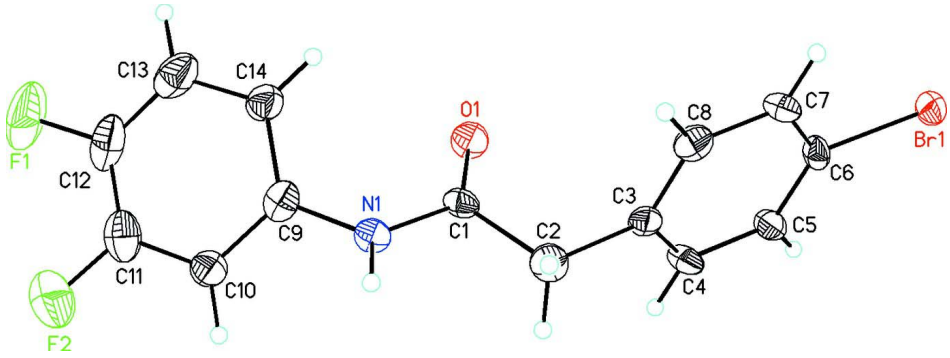

Figure 1

Molecular structure of the title compound showing the atom labeling scheme and 30% probability displacement ellipsoids.

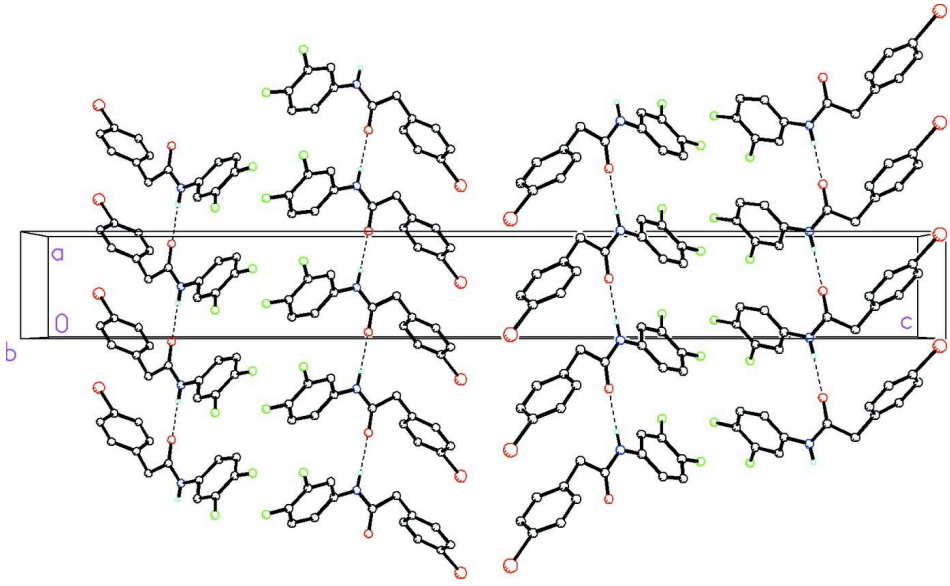

Figure 2

Packing diagram of the title compound viewed along the *b* axis. Dashed lines indicate N—H···O hydrogen bonds forming infinite chains along (100). H atoms not involved in hydrogen bonding have been deleted for clarity.

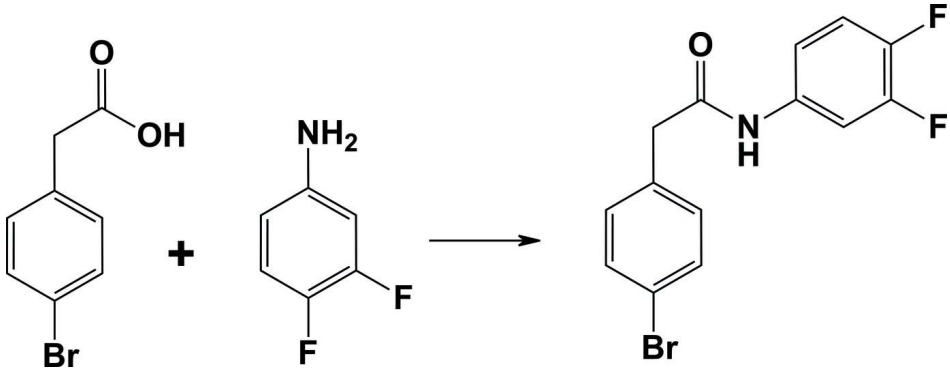

Figure 3

Synthesis of (I).

2-(4-Bromophenyl)-*N*-(3,4-difluorophenyl)acetamide

Crystal data

$C_{14}H_{10}BrF_2NO$
M_r = 326.14
Orthorhombic, $P2_12_12_1$
a = 4.9136 (3) Å
b = 6.0218 (4) Å
c = 42.514 (2) Å
V = 1257.96 (13) Å^3
Z = 4
$F(000)$ = 648
D_x = 1.722 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 3482 reflections
θ = 3.1–71.3°
μ = 4.62 mm^{-1}
T = 173 K
Block, colorless
0.48 × 0.32 × 0.16 mm

Data collection

Agilent Xcalibur (Eos, Gemini) diffractometer
Radiation source: Enhance (Cu) X-ray Source
Detector resolution: 16.1500 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO* and *CrysAlis RED*; Agilent, 2012)
T_{min} = 0.257, T_{max} = 1.000
6592 measured reflections
2402 independent reflections
2388 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 71.4°, θ_{min} = 4.2°
h = −5→4
k = −7→7
l = −51→52

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.106
S = 1.15
2402 reflections
173 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0518P)^2 + 2.6477P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.87 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}
Extinction correction: *SHELXL2012* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0034 (5)
Absolute structure: Flack x determined using 915 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons & Flack, 2004)
Absolute structure parameter: −0.01 (2)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Br1	0.05444 (13)	1.14849 (10)	0.52705 (2)	0.0255 (2)
F1	0.8291 (12)	−0.2536 (11)	0.73852 (13)	0.0682 (16)
F2	1.2315 (12)	−0.3056 (8)	0.69684 (13)	0.0577 (14)

O1	0.5535 (9)	0.4454 (8)	0.63179 (10)	0.0308 (9)
N1	0.9924 (9)	0.3661 (9)	0.64466 (11)	0.0243 (11)
H1	1.1630	0.3988	0.6404	0.029*
C1	0.7964 (12)	0.4695 (10)	0.62744 (13)	0.0203 (12)
C2	0.9134 (13)	0.6097 (10)	0.60058 (15)	0.0283 (13)
H2A	1.0489	0.7148	0.6093	0.034*
H2B	1.0088	0.5109	0.5856	0.034*
C3	0.6979 (12)	0.7387 (11)	0.58317 (14)	0.0222 (12)
C4	0.5905 (13)	0.6561 (11)	0.55519 (14)	0.0274 (12)
H4	0.6491	0.5161	0.5474	0.033*
C5	0.3960 (12)	0.7791 (10)	0.53850 (14)	0.0231 (13)
H5	0.3216	0.7238	0.5194	0.028*
C6	0.3155 (12)	0.9796 (10)	0.55018 (13)	0.0206 (11)
C7	0.4148 (13)	1.0645 (10)	0.57804 (14)	0.0235 (12)
H7	0.3531	1.2035	0.5858	0.028*
C8	0.6072 (12)	0.9412 (11)	0.59439 (13)	0.0255 (13)
H8	0.6779	0.9970	0.6136	0.031*
C9	0.9424 (13)	0.2099 (10)	0.66883 (13)	0.0247 (12)
C10	1.1086 (13)	0.0238 (12)	0.67050 (15)	0.0300 (14)
H10	1.2496	0.0018	0.6555	0.036*
C11	1.0656 (16)	−0.1289 (11)	0.69426 (16)	0.0365 (15)
C12	0.8674 (15)	−0.0986 (14)	0.71582 (17)	0.0427 (19)
C13	0.7024 (15)	0.0831 (15)	0.71475 (16)	0.0415 (19)
H13	0.5641	0.1022	0.7301	0.050*
C14	0.7366 (14)	0.2408 (13)	0.69109 (15)	0.0305 (14)
H14	0.6217	0.3675	0.6901	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0229 (3)	0.0270 (3)	0.0266 (3)	0.0051 (2)	0.0000 (2)	0.0054 (2)
F1	0.062 (3)	0.089 (4)	0.054 (3)	−0.020 (3)	−0.005 (3)	0.045 (3)
F2	0.063 (3)	0.045 (3)	0.065 (3)	0.010 (2)	−0.009 (3)	0.009 (2)
O1	0.015 (2)	0.045 (2)	0.032 (2)	0.003 (2)	0.0007 (18)	0.0076 (19)
N1	0.007 (2)	0.037 (3)	0.029 (2)	−0.001 (2)	0.0003 (16)	0.006 (2)
C1	0.011 (3)	0.025 (3)	0.025 (3)	0.001 (2)	0.000 (2)	−0.002 (2)
C2	0.016 (3)	0.031 (3)	0.038 (3)	−0.005 (3)	0.005 (2)	0.009 (2)
C3	0.012 (3)	0.030 (3)	0.024 (3)	0.002 (2)	0.004 (2)	0.006 (2)
C4	0.026 (3)	0.024 (3)	0.032 (3)	0.009 (3)	0.005 (2)	−0.002 (2)
C5	0.023 (3)	0.022 (3)	0.024 (3)	0.004 (2)	0.000 (2)	−0.002 (2)
C6	0.013 (3)	0.024 (3)	0.024 (3)	0.002 (2)	−0.003 (2)	0.007 (2)
C7	0.021 (3)	0.023 (3)	0.027 (3)	0.006 (3)	0.002 (2)	−0.005 (2)
C8	0.024 (3)	0.030 (3)	0.022 (3)	−0.003 (3)	0.001 (2)	−0.002 (2)
C9	0.017 (3)	0.033 (3)	0.024 (3)	−0.010 (3)	−0.006 (2)	0.003 (2)
C10	0.022 (3)	0.040 (4)	0.027 (3)	0.003 (3)	0.000 (2)	0.003 (3)
C11	0.038 (4)	0.031 (3)	0.041 (3)	−0.006 (4)	−0.013 (3)	0.006 (3)
C12	0.036 (4)	0.057 (5)	0.035 (3)	−0.016 (3)	−0.012 (3)	0.020 (3)
C13	0.025 (4)	0.069 (6)	0.029 (3)	−0.009 (4)	0.001 (3)	0.007 (3)

C14	0.024 (3)	0.042 (4)	0.025 (3)	0.002 (3)	0.001 (2)	0.003 (3)

Geometric parameters (Å, º)

Br1—C6	1.909 (6)	C5—C6	1.364 (9)
F1—C12	1.356 (8)	C5—H5	0.9500
F2—C11	1.345 (9)	C6—C7	1.379 (8)
O1—C1	1.217 (8)	C7—C8	1.389 (9)
N1—C1	1.360 (7)	C7—H7	0.9500
N1—C9	1.414 (8)	C8—H8	0.9500
N1—H1	0.8800	C9—C10	1.388 (10)
C1—C2	1.532 (8)	C9—C14	1.398 (9)
C2—C3	1.508 (8)	C10—C11	1.382 (9)
C2—H2A	0.9900	C10—H10	0.9500
C2—H2B	0.9900	C11—C12	1.350 (11)
C3—C8	1.383 (9)	C12—C13	1.362 (12)
C3—C4	1.393 (9)	C13—C14	1.394 (10)
C4—C5	1.402 (8)	C13—H13	0.9500
C4—H4	0.9500	C14—H14	0.9500
C1—N1—C9	124.9 (5)	C6—C7—C8	118.2 (5)
C1—N1—H1	117.5	C6—C7—H7	120.9
C9—N1—H1	117.5	C8—C7—H7	120.9
O1—C1—N1	123.9 (6)	C3—C8—C7	121.2 (6)
O1—C1—C2	123.2 (6)	C3—C8—H8	119.4
N1—C1—C2	112.8 (5)	C7—C8—H8	119.4
C3—C2—C1	112.7 (5)	C10—C9—C14	119.9 (6)
C3—C2—H2A	109.0	C10—C9—N1	118.2 (6)
C1—C2—H2A	109.0	C14—C9—N1	122.0 (6)
C3—C2—H2B	109.0	C11—C10—C9	119.0 (6)
C1—C2—H2B	109.0	C11—C10—H10	120.5
H2A—C2—H2B	107.8	C9—C10—H10	120.5
C8—C3—C4	119.2 (6)	F2—C11—C12	119.3 (6)
C8—C3—C2	120.7 (6)	F2—C11—C10	119.6 (7)
C4—C3—C2	120.1 (6)	C12—C11—C10	121.1 (7)
C3—C4—C5	120.1 (6)	C11—C12—F1	119.4 (8)
C3—C4—H4	119.9	C11—C12—C13	121.0 (7)
C5—C4—H4	119.9	F1—C12—C13	119.6 (8)
C6—C5—C4	118.8 (6)	C12—C13—C14	120.0 (7)
C6—C5—H5	120.6	C12—C13—H13	120.0
C4—C5—H5	120.6	C14—C13—H13	120.0
C5—C6—C7	122.5 (6)	C13—C14—C9	119.0 (7)
C5—C6—Br1	118.6 (4)	C13—C14—H14	120.5
C7—C6—Br1	118.9 (5)	C9—C14—H14	120.5
C9—N1—C1—O1	3.0 (10)	C1—N1—C9—C10	138.7 (6)
C9—N1—C1—C2	−173.6 (5)	C1—N1—C9—C14	−42.7 (9)
O1—C1—C2—C3	8.0 (9)	C14—C9—C10—C11	0.3 (9)

N1—C1—C2—C3	−175.4 (5)	N1—C9—C10—C11	179.0 (6)
C1—C2—C3—C8	83.5 (7)	C9—C10—C11—F2	−177.5 (6)
C1—C2—C3—C4	−97.5 (7)	C9—C10—C11—C12	−0.6 (10)
C8—C3—C4—C5	0.9 (9)	F2—C11—C12—F1	−3.9 (11)
C2—C3—C4—C5	−178.1 (5)	C10—C11—C12—F1	179.1 (6)
C3—C4—C5—C6	0.1 (9)	F2—C11—C12—C13	177.3 (7)
C4—C5—C6—C7	−1.1 (9)	C10—C11—C12—C13	0.3 (11)
C4—C5—C6—Br1	179.1 (5)	C11—C12—C13—C14	0.1 (11)
C5—C6—C7—C8	1.1 (9)	F1—C12—C13—C14	−178.6 (7)
Br1—C6—C7—C8	−179.1 (5)	C12—C13—C14—C9	−0.4 (11)
C4—C3—C8—C7	−1.0 (9)	C10—C9—C14—C13	0.1 (10)
C2—C3—C8—C7	178.0 (6)	N1—C9—C14—C13	−178.5 (6)
C6—C7—C8—C3	0.0 (9)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88	1.97	2.851 (7)	175
C7—H7···O1^{ii}	0.95	2.63	3.309 (8)	129
C13—H13···F1^{iii}	0.95	2.50	3.426 (9)	164

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*, *y*+1, *z*; (iii) −*x*+1, *y*+1/2, −*z*+3/2.