

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

4-(4-Fluoroanilino)-N-(4-fluorophenyl)-3-nitrobenzamide

Yong Wang,^{a*} Kaiqing Fan,^b Chenghong Li^a and Changhua Ge^a^aSchool of Pharmaceutical and Chemical Engineering, Taizhou University, Linhai 317000, People's Republic of China, and ^bAgronomy Department, Jiangsu Polytechnic College of Agriculture and Forestry, Jurong 212400 Jiangsu, People's Republic of China

Correspondence e-mail: yutaitang@hotmail.com

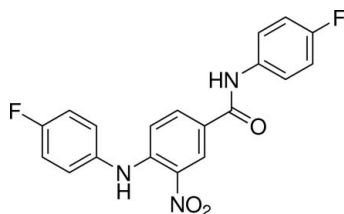
Received 16 September 2010; accepted 11 October 2010

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.058; wR factor = 0.155; data-to-parameter ratio = 12.1.

In the title compound, $\text{C}_{19}\text{H}_{13}\text{F}_2\text{N}_3\text{O}_3$, the anilino benzamide unit is essentially planar, with a maximum deviation of 0.036 (3) Å. The nitro group and the benzene ring form dihedral angles of 9.6 (5) and 62.20 (8)°, respectively, with the anilino benzamide unit. An intramolecular $\text{N}-\text{H}\cdots\text{O}$ interaction occurs. In the crystal, molecules are linked by weak intermolecular $\text{C}-\text{H}\cdots\text{O}$, $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{F}$ hydrogen bonds, which stabilize the structure.

Related literature

For comparison of bond lengths, see: Allen *et al.* (1987). For the synthetic procedure, see: Schelz & Inst (1978).



Experimental

Crystal data

$\text{C}_{19}\text{H}_{13}\text{F}_2\text{N}_3\text{O}_3$
 $M_r = 369.32$
 Triclinic, $P\bar{1}$
 $a = 7.8510$ (16) Å

$b = 8.2720$ (17) Å
 $c = 13.835$ (3) Å
 $\alpha = 74.75$ (3)°
 $\beta = 85.67$ (3)°

$\gamma = 70.76$ (3)°
 $V = 818.4$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation

$\mu = 0.12$ mm⁻¹
 $T = 293$ K
 $0.30 \times 0.20 \times 0.10$ mm

Data collection

Enraf-Nonius CAD-4 diffractometer
 Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\min} = 0.965$, $T_{\max} = 0.988$
 3198 measured reflections

2962 independent reflections
 1559 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$
 3 standard reflections every 200 reflections
 intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.058$
 $wR(F^2) = 0.155$
 $S = 1.00$
 2962 reflections

245 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.16$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.18$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O3}^i$	0.86	2.37	3.185 (4)	158
$\text{N2}-\text{H2A}\cdots\text{O2}$	0.86	1.98	2.636 (4)	132
$\text{C2}-\text{H2B}\cdots\text{O3}^i$	0.93	2.40	3.240 (5)	151
$\text{C10}-\text{H10A}\cdots\text{F1}^{ii}$	0.93	2.53	3.205 (4)	130
$\text{C15}-\text{H15A}\cdots\text{O1}^{iii}$	0.93	2.55	3.454 (4)	164
$\text{C16}-\text{H16A}\cdots\text{F2}^{iv}$	0.93	2.39	3.272 (5)	158

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+1, -y, -z$; (iii) $-x+1, -y, -z+1$; (iv) $-x+1, -y-1, -z+1$.

Data collection: *CAD-4 Software* (Enraf-Nonius, 1994); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

The authors thank Dr Shan Liu of Nanjing University of Technology for useful discussions and the Center of Testing and Analysis, Nanjing University, for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2329).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
 Enraf-Nonius (1994). *CAD-4 Software*. Enraf-Nonius, Delft, The Netherlands.
 Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
 North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.
 Schelz, D. & Inst, F. (1978). *Helv. Chim. Acta*, **61**, 2452–2462.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

supplementary materials

Acta Cryst. (2010). E66, o2909 [doi:10.1107/S1600536810040687]

4-(4-Fluoroanilino)-*N*-(4-fluorophenyl)-3-nitrobenzamide

Y. Wang, K. Fan, C. Li and C. Ge

Comment

The crystal structure of the title compound, (I), is presented in this article. In the title molecule (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The phenylaminobenzamide moiety (C1–C13/N1/O1) is essentially planar with maximum deviation of any atom being 0.036 (3) Å for C11 with F2 lying 0.109 (4) Å out of its plane, nitro group (N3/O2/O3) tilted at an angle 9.6 (5)° from its plane and the phenyl ring (C14–C19) inclined at 62.20 (8)° with its plane. In the crystal structure, weak intermolecular C—H···O, N—H···O and C—H···F hydrogen bonds (Table 1) link the molecules (Fig. 2), in which they may be effective in stabilizing the structure.

Experimental

4-Chloro-3-nitrobenzamide (4.0 g, 0.02 mol) was heated in 4-fluorobenzeneamine (10 ml) for 18 h at 403 K. On completion of the reaction (TLC control) was added ethanol (50 ml), at room temperature. The red precipitate thus formed was filtered, washed with cold ethanol (2 × 15 ml), dried over sodium sulfate to provide 5.8 g (79%) of (I) (Schelz & Inst, 1978). The compound (I) was purified by crystallizing from methanol. The crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a methanol solution.

Refinement

H atoms were positioned geometrically, with N—H = 0.86 and C—H = 0.93 Å, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C/N})$.

Figures

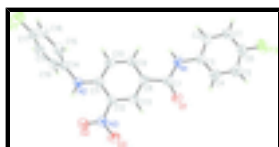


Fig. 1. The molecular structure of (I), showing the atom-numbering scheme and displacement ellipsoids at the 30% probability level.

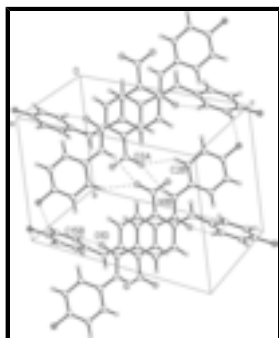


Fig. 2. A packing diagram of (I). The intermolecular hydrogen bonds are shown as dashed lines.

4-(4-Fluoroanilino)-N-(4-fluorophenyl)-3-nitrobenzamide

Crystal data

$C_{19}H_{13}F_2N_3O_3$	$Z = 2$
$M_r = 369.32$	$F(000) = 380$
Triclinic, PT	$D_x = 1.499 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 7.8510 (16) \text{ \AA}$	Cell parameters from 25 reflections
$b = 8.2720 (17) \text{ \AA}$	$\theta = 9\text{--}12^\circ$
$c = 13.835 (3) \text{ \AA}$	$\mu = 0.12 \text{ mm}^{-1}$
$\alpha = 74.75 (3)^\circ$	$T = 293 \text{ K}$
$\beta = 85.67 (3)^\circ$	Block, colourless
$\gamma = 70.76 (3)^\circ$	$0.30 \times 0.20 \times 0.10 \text{ mm}$
$V = 818.4 (3) \text{ \AA}^3$	

Data collection

Enraf-Nonius CAD-4 diffractometer	1559 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube graphite	$R_{\text{int}} = 0.026$
ω and 2θ scans	$\theta_{\text{max}} = 25.3^\circ$, $\theta_{\text{min}} = 1.5^\circ$
Absorption correction: ψ scan (North <i>et al.</i> , 1968)	$h = 0\text{--}9$
$T_{\text{min}} = 0.965$, $T_{\text{max}} = 0.988$	$k = -9\text{--}9$
3198 measured reflections	$l = -16\text{--}16$
2962 independent reflections	3 standard reflections every 200 reflections
	intensity decay: 1%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.058$	H-atom parameters constrained
$wR(F^2) = 0.155$	$w = 1/[\sigma^2(F_o^2) + (0.065P)^2]$
$S = 1.00$	where $P = (F_o^2 + 2F_c^2)/3$
2962 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
245 parameters	$\Delta\rho_{\text{max}} = 0.16 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.021 (4)

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	0.7511 (3)	0.0655 (3)	-0.12706 (14)	0.0823 (8)
N1	0.1978 (4)	-0.2157 (3)	0.58538 (17)	0.0468 (7)
H1A	0.2383	-0.2652	0.5372	0.056*
F2	-0.0468 (3)	-0.6359 (3)	0.90592 (15)	0.0839 (8)
C1	0.0848 (6)	-0.5958 (5)	0.7467 (3)	0.0687 (12)
H1C	0.0888	-0.7083	0.7443	0.082*
N2	0.4401 (4)	0.3033 (3)	0.20096 (18)	0.0511 (8)
H2A	0.4232	0.4141	0.1934	0.061*
O1	0.1462 (4)	0.0382 (3)	0.63333 (16)	0.0645 (8)
C2	0.1458 (5)	-0.4877 (4)	0.6679 (3)	0.0618 (11)
H2B	0.1932	-0.5290	0.6120	0.074*
O2	0.3708 (4)	0.5620 (3)	0.29073 (19)	0.0787 (9)
C3	0.1378 (4)	-0.3197 (4)	0.6703 (2)	0.0424 (8)
N3	0.3373 (4)	0.4670 (4)	0.3685 (2)	0.0579 (9)
C4	0.0683 (5)	-0.2610 (5)	0.7541 (2)	0.0515 (9)
H4A	0.0612	-0.1478	0.7569	0.062*
O3	0.3066 (5)	0.5176 (4)	0.4448 (2)	0.1081 (13)
C5	0.0093 (5)	-0.3689 (5)	0.8339 (2)	0.0573 (10)
H5A	-0.0360	-0.3301	0.8909	0.069*
C6	0.0189 (5)	-0.5329 (5)	0.8276 (3)	0.0577 (10)
C7	0.1996 (4)	-0.0465 (4)	0.5702 (2)	0.0413 (8)
C8	0.2697 (4)	0.0325 (4)	0.4724 (2)	0.0367 (7)
C9	0.3296 (4)	-0.0471 (4)	0.3930 (2)	0.0458 (9)
H9A	0.3288	-0.1616	0.3996	0.055*
C10	0.3893 (4)	0.0400 (4)	0.3058 (2)	0.0463 (9)
H10A	0.4292	-0.0178	0.2550	0.056*
C11	0.3924 (4)	0.2150 (4)	0.2904 (2)	0.0408 (8)
C12	0.3347 (4)	0.2909 (4)	0.3723 (2)	0.0411 (8)
C13	0.2751 (4)	0.2014 (4)	0.4597 (2)	0.0417 (8)
H13A	0.2376	0.2568	0.5116	0.050*
C14	0.5150 (5)	0.2322 (4)	0.1184 (2)	0.0422 (8)
C15	0.6711 (5)	0.0901 (5)	0.1283 (2)	0.0518 (9)
H15A	0.7234	0.0318	0.1914	0.062*

supplementary materials

C16	0.7504 (5)	0.0333 (5)	0.0459 (3)	0.0574 (10)
H16A	0.8563	-0.0623	0.0524	0.069*
C17	0.6702 (6)	0.1204 (5)	-0.0458 (3)	0.0554 (10)
C18	0.5142 (5)	0.2600 (5)	-0.0589 (2)	0.0566 (10)
H18A	0.4617	0.3155	-0.1221	0.068*
C19	0.4358 (5)	0.3171 (4)	0.0244 (2)	0.0495 (9)
H19A	0.3298	0.4126	0.0173	0.059*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.114 (2)	0.0861 (17)	0.0570 (13)	-0.0353 (15)	0.0258 (13)	-0.0374 (12)
N1	0.065 (2)	0.0442 (16)	0.0382 (15)	-0.0275 (15)	0.0133 (13)	-0.0135 (12)
F2	0.108 (2)	0.0535 (14)	0.0715 (14)	-0.0251 (13)	0.0345 (13)	0.0043 (11)
C1	0.094 (3)	0.038 (2)	0.068 (3)	-0.020 (2)	0.017 (2)	-0.0092 (19)
N2	0.078 (2)	0.0423 (16)	0.0389 (16)	-0.0291 (16)	0.0172 (15)	-0.0130 (13)
O1	0.104 (2)	0.0492 (15)	0.0487 (14)	-0.0345 (15)	0.0227 (14)	-0.0192 (12)
C2	0.090 (3)	0.044 (2)	0.050 (2)	-0.024 (2)	0.020 (2)	-0.0121 (17)
O2	0.136 (3)	0.0554 (16)	0.0587 (16)	-0.0535 (17)	0.0343 (16)	-0.0184 (13)
C3	0.052 (2)	0.042 (2)	0.0342 (18)	-0.0201 (17)	0.0066 (16)	-0.0069 (15)
N3	0.089 (3)	0.0494 (18)	0.0465 (18)	-0.0370 (18)	0.0176 (17)	-0.0165 (16)
C4	0.063 (3)	0.055 (2)	0.044 (2)	-0.031 (2)	0.0094 (18)	-0.0129 (17)
O3	0.225 (4)	0.072 (2)	0.0626 (18)	-0.087 (2)	0.050 (2)	-0.0403 (16)
C5	0.068 (3)	0.064 (3)	0.043 (2)	-0.028 (2)	0.0144 (18)	-0.0145 (18)
C6	0.062 (3)	0.046 (2)	0.049 (2)	-0.0125 (19)	0.0141 (18)	0.0043 (17)
C7	0.045 (2)	0.0400 (19)	0.0396 (18)	-0.0162 (17)	0.0017 (16)	-0.0091 (16)
C8	0.040 (2)	0.0355 (18)	0.0351 (17)	-0.0139 (15)	-0.0003 (14)	-0.0072 (14)
C9	0.061 (2)	0.043 (2)	0.0426 (19)	-0.0269 (18)	0.0063 (17)	-0.0134 (15)
C10	0.060 (2)	0.046 (2)	0.0427 (19)	-0.0260 (18)	0.0105 (17)	-0.0201 (16)
C11	0.044 (2)	0.0385 (19)	0.0412 (19)	-0.0149 (16)	0.0005 (15)	-0.0106 (15)
C12	0.053 (2)	0.0365 (18)	0.0384 (18)	-0.0195 (17)	0.0029 (16)	-0.0110 (15)
C13	0.053 (2)	0.0418 (19)	0.0339 (17)	-0.0186 (17)	0.0030 (15)	-0.0116 (14)
C14	0.060 (2)	0.0416 (19)	0.0353 (18)	-0.0296 (19)	0.0097 (16)	-0.0125 (15)
C15	0.062 (3)	0.050 (2)	0.043 (2)	-0.020 (2)	0.0041 (18)	-0.0094 (16)
C16	0.064 (3)	0.049 (2)	0.060 (2)	-0.0173 (19)	0.014 (2)	-0.0197 (19)
C17	0.082 (3)	0.060 (2)	0.041 (2)	-0.040 (2)	0.022 (2)	-0.0237 (18)
C18	0.073 (3)	0.065 (3)	0.039 (2)	-0.036 (2)	0.0023 (19)	-0.0083 (18)
C19	0.050 (2)	0.046 (2)	0.049 (2)	-0.0173 (18)	0.0048 (18)	-0.0066 (17)

Geometric parameters (\AA , $^\circ$)

F1—C17	1.358 (3)	C5—H5A	0.9300
N1—C7	1.365 (4)	C7—C8	1.490 (4)
N1—C3	1.413 (3)	C8—C13	1.376 (4)
N1—H1A	0.8600	C8—C9	1.400 (4)
F2—C6	1.373 (4)	C9—C10	1.369 (4)
C1—C6	1.354 (5)	C9—H9A	0.9300
C1—C2	1.382 (4)	C10—C11	1.415 (4)
C1—H1C	0.9300	C10—H10A	0.9300

N2—C11	1.357 (4)	C11—C12	1.412 (4)
N2—C14	1.421 (4)	C12—C13	1.378 (4)
N2—H2A	0.8600	C13—H13A	0.9300
O1—C7	1.225 (3)	C14—C15	1.376 (4)
C2—C3	1.379 (4)	C14—C19	1.388 (4)
C2—H2B	0.9300	C15—C16	1.375 (4)
O2—N3	1.222 (3)	C15—H15A	0.9300
C3—C4	1.380 (4)	C16—C17	1.366 (5)
N3—O3	1.214 (3)	C16—H16A	0.9300
N3—C12	1.451 (4)	C17—C18	1.363 (5)
C4—C5	1.381 (4)	C18—C19	1.384 (4)
C4—H4A	0.9300	C18—H18A	0.9300
C5—C6	1.360 (5)	C19—H19A	0.9300
C7—N1—C3	128.1 (3)	C10—C9—C8	121.5 (3)
C7—N1—H1A	115.9	C10—C9—H9A	119.3
C3—N1—H1A	115.9	C8—C9—H9A	119.3
C6—C1—C2	117.9 (4)	C9—C10—C11	122.1 (3)
C6—C1—H1C	121.0	C9—C10—H10A	118.9
C2—C1—H1C	121.0	C11—C10—H10A	118.9
C11—N2—C14	126.9 (3)	N2—C11—C12	123.5 (3)
C11—N2—H2A	116.6	N2—C11—C10	121.2 (3)
C14—N2—H2A	116.6	C12—C11—C10	115.2 (3)
C3—C2—C1	121.4 (3)	C13—C12—C11	121.9 (3)
C3—C2—H2B	119.3	C13—C12—N3	116.8 (3)
C1—C2—H2B	119.3	C11—C12—N3	121.2 (3)
C2—C3—C4	118.6 (3)	C8—C13—C12	121.9 (3)
C2—C3—N1	117.8 (3)	C8—C13—H13A	119.0
C4—C3—N1	123.6 (3)	C12—C13—H13A	119.0
O3—N3—O2	120.7 (3)	C15—C14—C19	119.5 (3)
O3—N3—C12	118.4 (3)	C15—C14—N2	121.5 (3)
O2—N3—C12	120.9 (3)	C19—C14—N2	118.8 (3)
C3—C4—C5	120.5 (3)	C16—C15—C14	120.6 (3)
C3—C4—H4A	119.7	C16—C15—H15A	119.7
C5—C4—H4A	119.7	C14—C15—H15A	119.7
C6—C5—C4	118.7 (3)	C17—C16—C15	118.5 (4)
C6—C5—H5A	120.7	C17—C16—H16A	120.7
C4—C5—H5A	120.7	C15—C16—H16A	120.7
C1—C6—C5	122.9 (3)	F1—C17—C18	119.1 (3)
C1—C6—F2	119.1 (3)	F1—C17—C16	118.1 (4)
C5—C6—F2	117.9 (3)	C18—C17—C16	122.8 (3)
O1—C7—N1	122.2 (3)	C17—C18—C19	118.3 (3)
O1—C7—C8	120.9 (3)	C17—C18—H18A	120.8
N1—C7—C8	116.9 (3)	C19—C18—H18A	120.8
C13—C8—C9	117.3 (3)	C18—C19—C14	120.2 (3)
C13—C8—C7	115.9 (3)	C18—C19—H19A	119.9
C9—C8—C7	126.8 (3)	C14—C19—H19A	119.9
C6—C1—C2—C3	-0.9 (6)	N2—C11—C12—C13	175.3 (3)
C1—C2—C3—C4	0.5 (6)	C10—C11—C12—C13	-1.7 (5)

supplementary materials

C1—C2—C3—N1	-178.1 (3)	N2—C11—C12—N3	-5.3 (5)
C7—N1—C3—C2	178.7 (3)	C10—C11—C12—N3	177.6 (3)
C7—N1—C3—C4	0.2 (5)	O3—N3—C12—C13	7.8 (5)
C2—C3—C4—C5	0.4 (5)	O2—N3—C12—C13	-172.6 (3)
N1—C3—C4—C5	178.9 (3)	O3—N3—C12—C11	-171.5 (4)
C3—C4—C5—C6	-0.9 (5)	O2—N3—C12—C11	8.1 (5)
C2—C1—C6—C5	0.5 (6)	C9—C8—C13—C12	0.8 (5)
C2—C1—C6—F2	178.4 (3)	C7—C8—C13—C12	-179.1 (3)
C4—C5—C6—C1	0.4 (6)	C11—C12—C13—C8	0.4 (5)
C4—C5—C6—F2	-177.5 (3)	N3—C12—C13—C8	-178.9 (3)
C3—N1—C7—O1	0.3 (5)	C11—N2—C14—C15	-56.2 (5)
C3—N1—C7—C8	-179.6 (3)	C11—N2—C14—C19	128.7 (3)
O1—C7—C8—C13	1.9 (5)	C19—C14—C15—C16	1.0 (5)
N1—C7—C8—C13	-178.2 (3)	N2—C14—C15—C16	-174.0 (3)
O1—C7—C8—C9	-178.0 (3)	C14—C15—C16—C17	-0.4 (5)
N1—C7—C8—C9	1.9 (5)	C15—C16—C17—F1	178.9 (3)
C13—C8—C9—C10	-0.7 (5)	C15—C16—C17—C18	-0.6 (5)
C7—C8—C9—C10	179.2 (3)	F1—C17—C18—C19	-178.4 (3)
C8—C9—C10—C11	-0.6 (5)	C16—C17—C18—C19	1.0 (5)
C14—N2—C11—C12	173.7 (3)	C17—C18—C19—C14	-0.4 (5)
C14—N2—C11—C10	-9.4 (5)	C15—C14—C19—C18	-0.5 (5)
C9—C10—C11—N2	-175.3 (3)	N2—C14—C19—C18	174.6 (3)
C9—C10—C11—C12	1.8 (5)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1A \cdots O3 ⁱ	0.86	2.37	3.185 (4)	158
N2—H2A \cdots O2	0.86	1.98	2.636 (4)	132
N2—H2A \cdots N3	0.86	2.58	2.917 (4)	105
C2—H2B \cdots O3 ⁱ	0.93	2.40	3.240 (5)	151
C4—H4A \cdots O1	0.93	2.20	2.821 (4)	123
C10—H10A \cdots F1 ⁱⁱ	0.93	2.53	3.205 (4)	130
C13—H13A \cdots O1	0.93	2.39	2.728 (4)	102
C13—H13A \cdots O3	0.93	2.33	2.661 (5)	100
C15—H15A \cdots O1 ⁱⁱⁱ	0.93	2.55	3.454 (4)	164
C16—H16A \cdots F2 ^{iv}	0.93	2.39	3.272 (5)	158

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+1, -y, -z$; (iii) $-x+1, -y, -z+1$; (iv) $-x+1, -y-1, -z+1$.

Fig. 1

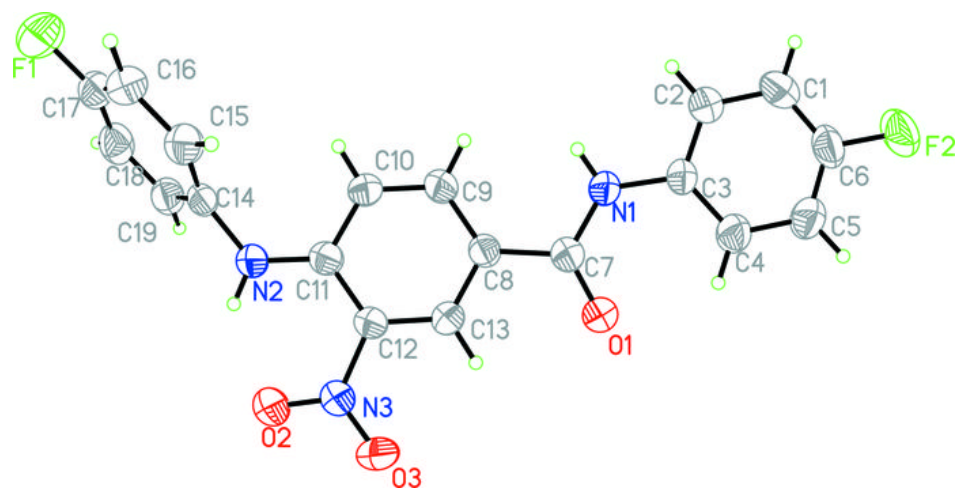


Fig. 2

