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3-(4-Fluorophenyl)-1,5-di-2-pyridylpentane-1,5-dione

Qing-Qing Shao,[a]* Dong-Qin Chen[b] and Feng Shi[a]

[a]School of Chemistry and Chemical Engineering, Xuzhou Normal University, Xuzhou 221116, People's Republic of China, and [b]Department of Chemistry, Xuzhou Medical College, Xuzhou 221004, People's Republic of China
Correspondence e-mail: laotu2001@263.net

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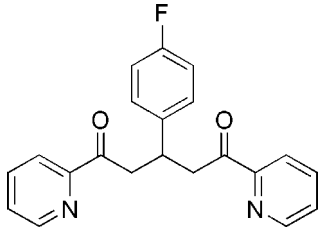
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.047; wR factor = 0.118; data-to-parameter ratio = 12.9.

The title compound, $C_{21}H_{17}FN_2O_2$, was prepared by the reaction of 4-fluorobenzaldehyde and 2-acetylpridine in *N*,*N*-dimethylformamide under microwave irradiation. In the molecular conformation, there are three planes: a benzene plane and two pyridine planes. The dihedral angles between the benzene plane and the pyridine planes are 88.38 (15) and 83.27 (13)°, and the dihedral angle between the two pyridine planes is 8.05 (10)°. There is an intramolecular C—H···N hydrogen bond. In the crystal structure, a supramolecular structure is constructed by the dimeration of two molecules *via* an intermolecular C—H···O hydrogen bond.

Related literature

For related literature, see: Chelucci & Thummel (2002); Clarke (2003); Islam *et al.* (2003); Jantunen & Scott (2006); Kröhnke (1976); Lehn (1995); Li *et al.* (2004); MacGillivray *et al.* (2000); Neve *et al.* (1997); Olenyuk *et al.* (1999); Raehm & Hamann (2000).



Experimental

Crystal data

$C_{21}H_{17}FN_2O_2$
M_r = 348.37
Triclinic, $P\overline{1}$
a = 8.6219 (15) Å
b = 10.4637 (18) Å
c = 10.7870 (19) Å
α = 94.045 (2)°
β = 112.017 (3)°
γ = 100.632 (2)°
V = 876.2 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.40 × 0.37 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.964, T_{max} = 0.989
4527 measured reflections
3037 independent reflections
1696 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.118
S = 1.01
3037 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···N1	0.97	2.50	2.838 (3)	100
C12—H12···O2^{i}	0.93	2.45	3.269 (3)	146

Symmetry code: (i) $-x+2, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2012).

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supplementary materials

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3-(4-Fluorophenyl)-1,5-di-2-pyridylpentane-1,5-dione

Q.-Q. Shao, D.-Q. Chen and F. Shi

Comment

Kröhnke type pyridines (Kröhnke, 1976) and other substituted pyridines (Neve *et al.*, 1997; MacGillivray *et al.*, 2000; Olenyuk *et al.*, 1999) were prominent building blocks in organic chemistry and substituted pyridines ligands have attracted widespread attention due to their ability to form complexes with transition metals, so substituted pyridines are applied extensively in coordinate chemistry (Li *et al.*, 2004; Jantunen *et al.* 2006; Raehm *et al.*, 2000). Also, the applications of pyridine derivatives have been found in various fields such as supramolecular chemistry (Lehn, 1995), asymmetric catalysis (Chelucci, 2002), photosensitization (Islam *et al.*, 2003) and antitumor compounds (Clarke *et al.*, 2003). In this paper we report the crystal structure of the title compound, (I).

In (I), there are three planes. They are benzene ring(C16—C21) and two pyridine planes. The dihedral angle between the C7/C8/C10/N1 plane and the C16—C21 benzene ring is 88.380 (146)°. The dihedral angle between the C12/C13/C15/N2 plane and the C16—C21 benzene ring is 83.267 (132)°. And the dihedral angle between the two pyridine planes is 8.049 (98)°. There is an intramolecular C(2)–H(2 A).·N(1) hydrogen bond. Besides, in the crystal structure, the supramolecular structure is constructed by the the dimeration of two molecules *via* a intermolecular C(12)–H(12).. O(2) hydrogen bond.

Experimental

The title compound, (I), was prepared by the reaction of 4-fluorobenzaldehyde(0.5 mmol,0.06 g) and 2-acetylpridine (1 mmol,0.12 g) in *N*,*N*-dimethylformamide(DMF)(1.5 ml) under microwave irradiation for 5 min. (microwave oven is EmrysTM Creator from Personal Chemistry, Uppsala, Sweden). Upon completion monitored by TLC, the reaction mixture was cooled to room temperature and then poured into cold water. The solid product was filtered, washed with water and EtOH (95%), and subsequently dried and recrystallized from EtOH (95%) to give the pure product(0.11 g). Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a 95% aqueous ethanol solution (yield 63%; m.p. 428–430 K). IR (cm^{-1}): 1698 (CO); ^{1}H NMR (DMSO-d_6): 8.70 (d, 2H, J = 4.4 Hz, ArH), 7.97 (t, 2H, ArH, J = 8.0 Hz), 7.86 (d, 2H, J = 7.2 Hz, ArH), 7.65 (t, 2H, ArH, J = 5.6 Hz), 7.38–7.34 (m, 2H, ArH), 7.04 (t, 2H, ArH, J = 8.8 Hz), 3.98–3.94 (m, 1H, CH), 3.78–3.71 (m, 2H, CH2), 3.58–3.50 (m, 2H, CH2)

Refinement

All H atoms were positioned geometrically and treated as riding, with C—H distances of 0.93–0.98 Å, and with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C,*N*) for others.

Figures

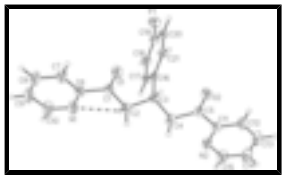

Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids.

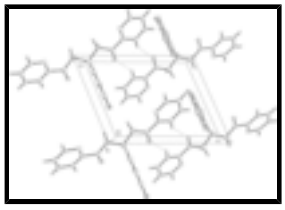

Fig. 2. A packing diagram of (I) projected along the *b* axis.

3-(4-Fluorophenyl)-1,5-di-2-pyridylpentane-1,5-dione

Crystal data

$C_{21}H_{17}FN_2O_2$	F_{000} = 364
M_r = 348.37	D_x = 1.320 Mg m^{-3}
Triclinic, $P\overline{1}$	Melting point: 428-430 K
a = 8.6219 (15) Å	Mo $K\alpha$ radiation λ = 0.71073 Å
b = 10.4637 (18) Å	Cell parameters from 1181 reflections
c = 10.7870 (19) Å	θ = 2.9–25.3º
α = 94.045 (2)º	μ = 0.09 mm^{-1}
β = 112.017 (3)º	T = 298 (2) K
γ = 100.632 (2)º	Prism, colourless
V = 876.2 (3) Å^3	0.40 × 0.37 × 0.12 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	3037 independent reflections
Radiation source: fine-focus sealed tube	1696 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.017
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −10→8
T_{min} = 0.964, T_{max} = 0.989	k = −10→12
4527 measured reflections	l = −11→12

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.118$	$w = 1/[\sigma^2(F_o^2) + (0.0395P)^2 + 0.2087P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
3037 reflections	$\Delta\rho_{max} = 0.15$ e Å^{-3}
235 parameters	$\Delta\rho_{min} = -0.15$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.4049 (2)	0.88118 (15)	0.11670 (16)	0.0739 (5)
N1	0.9292 (3)	0.8183 (2)	−0.2819 (2)	0.0730 (7)
N2	1.3438 (3)	0.8341 (2)	0.4885 (2)	0.0597 (6)
O1	0.7475 (2)	0.54540 (17)	−0.17159 (16)	0.0652 (6)
O2	0.9876 (2)	0.57115 (19)	0.31977 (17)	0.0739 (6)
C1	0.8471 (3)	0.6455 (2)	−0.1666 (2)	0.0442 (6)
C2	0.9899 (3)	0.7149 (2)	−0.0360 (2)	0.0478 (6)
H2A	1.0058	0.8091	−0.0358	0.057*
H2B	1.0956	0.6911	−0.0305	0.057*
C3	0.9560 (3)	0.6814 (2)	0.0888 (2)	0.0426 (6)
H3	0.9223	0.5854	0.0792	0.051*
C4	1.1168 (3)	0.7286 (2)	0.2194 (2)	0.0467 (6)
H4A	1.2145	0.7077	0.2051	0.056*
H4B	1.1389	0.8235	0.2412	0.056*
C5	1.1003 (3)	0.6672 (2)	0.3365 (2)	0.0483 (6)
C6	0.8302 (3)	0.7014 (2)	−0.2937 (2)	0.0450 (6)
C7	0.7154 (4)	0.6316 (3)	−0.4166 (2)	0.0640 (8)
H7	0.6484	0.5494	−0.4211	0.077*
C8	0.7003 (4)	0.6838 (3)	−0.5324 (3)	0.0811 (10)
H8	0.6235	0.6376	−0.6166	0.097*
C9	0.7988 (4)	0.8034 (3)	−0.5219 (3)	0.0909 (11)
H9	0.7911	0.8418	−0.5985	0.109*

C10	0.9099 (5)	0.8666 (3)	−0.3965 (3)	0.1043 (13)
H10	0.9770	0.9492	−0.3904	0.125*
C11	1.2313 (3)	0.7229 (2)	0.4757 (2)	0.0469 (6)
C12	1.2336 (4)	0.6589 (3)	0.5833 (3)	0.0662 (8)
H12	1.1515	0.5825	0.5712	0.079*
C13	1.3599 (4)	0.7104 (3)	0.7090 (3)	0.0773 (9)
H13	1.3657	0.6683	0.7832	0.093*
C14	1.4757 (4)	0.8230 (3)	0.7239 (3)	0.0723 (9)
H14	1.5620	0.8597	0.8081	0.087*
C15	1.4632 (4)	0.8816 (3)	0.6124 (3)	0.0747 (9)
H15	1.5426	0.9594	0.6236	0.090*
C16	0.8086 (3)	0.7357 (2)	0.0964 (2)	0.0387 (6)
C17	0.8156 (3)	0.8697 (2)	0.1086 (2)	0.0471 (6)
H17	0.9134	0.9275	0.1118	0.057*
C18	0.6816 (3)	0.9198 (2)	0.1161 (2)	0.0507 (7)
H18	0.6881	1.0099	0.1246	0.061*
C19	0.5394 (3)	0.8333 (3)	0.1107 (2)	0.0475 (6)
C20	0.5258 (3)	0.7011 (2)	0.1006 (2)	0.0475 (6)
H20	0.4277	0.6446	0.0985	0.057*
C21	0.6610 (3)	0.6531 (2)	0.0937 (2)	0.0436 (6)
H21	0.6534	0.5629	0.0869	0.052*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0651 (11)	0.0743 (11)	0.0899 (12)	0.0198 (9)	0.0376 (10)	0.0114 (9)
N1	0.0879 (18)	0.0666 (16)	0.0426 (13)	−0.0198 (13)	0.0190 (13)	0.0088 (11)
N2	0.0621 (15)	0.0574 (14)	0.0433 (13)	0.0006 (12)	0.0089 (12)	0.0077 (11)
O1	0.0736 (13)	0.0579 (12)	0.0498 (11)	−0.0143 (10)	0.0235 (10)	0.0022 (9)
O2	0.0670 (13)	0.0792 (14)	0.0534 (12)	−0.0155 (11)	0.0115 (10)	0.0255 (10)
C1	0.0440 (15)	0.0461 (15)	0.0401 (14)	0.0021 (12)	0.0189 (12)	0.0002 (11)
C2	0.0435 (15)	0.0565 (16)	0.0386 (14)	0.0005 (12)	0.0163 (12)	0.0047 (12)
C3	0.0432 (15)	0.0462 (14)	0.0335 (13)	0.0009 (12)	0.0142 (12)	0.0063 (11)
C4	0.0429 (15)	0.0559 (16)	0.0382 (14)	0.0045 (12)	0.0148 (12)	0.0126 (11)
C5	0.0436 (15)	0.0529 (16)	0.0456 (15)	0.0056 (13)	0.0158 (13)	0.0150 (12)
C6	0.0479 (15)	0.0471 (15)	0.0366 (14)	0.0032 (12)	0.0173 (12)	0.0018 (11)
C7	0.072 (2)	0.0620 (18)	0.0429 (16)	−0.0031 (15)	0.0161 (15)	0.0021 (13)
C8	0.094 (3)	0.092 (2)	0.0354 (17)	0.001 (2)	0.0127 (17)	0.0048 (16)
C9	0.114 (3)	0.100 (3)	0.0432 (18)	−0.003 (2)	0.0237 (19)	0.0252 (17)
C10	0.131 (3)	0.090 (2)	0.054 (2)	−0.037 (2)	0.022 (2)	0.0215 (18)
C11	0.0496 (16)	0.0526 (16)	0.0393 (14)	0.0111 (13)	0.0179 (13)	0.0116 (12)
C12	0.073 (2)	0.0723 (19)	0.0450 (17)	0.0033 (16)	0.0184 (16)	0.0177 (14)
C13	0.105 (3)	0.081 (2)	0.0402 (17)	0.024 (2)	0.0193 (18)	0.0189 (15)
C14	0.089 (2)	0.073 (2)	0.0371 (17)	0.0196 (18)	0.0057 (16)	−0.0004 (15)
C15	0.080 (2)	0.0667 (19)	0.0498 (18)	−0.0024 (16)	0.0058 (17)	0.0012 (15)
C16	0.0415 (14)	0.0411 (14)	0.0254 (12)	−0.0007 (11)	0.0088 (11)	0.0045 (10)
C17	0.0458 (16)	0.0465 (16)	0.0426 (15)	−0.0034 (12)	0.0162 (13)	0.0102 (11)
C18	0.0562 (17)	0.0425 (15)	0.0504 (16)	0.0055 (13)	0.0199 (14)	0.0105 (12)

C19	0.0432 (16)	0.0578 (18)	0.0421 (15)	0.0103 (13)	0.0184 (13)	0.0065 (12)
C20	0.0414 (16)	0.0505 (17)	0.0447 (15)	−0.0035 (12)	0.0177 (13)	0.0029 (12)
C21	0.0447 (15)	0.0390 (14)	0.0393 (14)	−0.0026 (12)	0.0145 (12)	0.0005 (11)

Geometric parameters (Å, °)

F1—C19	1.366 (3)	C8—H8	0.9300
N1—C6	1.323 (3)	C9—C10	1.361 (4)
N1—C10	1.333 (3)	C9—H9	0.9300
N2—C11	1.331 (3)	C10—H10	0.9300
N2—C15	1.334 (3)	C11—C12	1.376 (3)
O1—C1	1.209 (2)	C12—C13	1.374 (4)
O2—C5	1.212 (3)	C12—H12	0.9300
C1—C6	1.497 (3)	C13—C14	1.353 (4)
C1—C2	1.501 (3)	C13—H13	0.9300
C2—C3	1.531 (3)	C14—C15	1.365 (4)
C2—H2A	0.9700	C14—H14	0.9300
C2—H2B	0.9700	C15—H15	0.9300
C3—C16	1.510 (3)	C16—C17	1.388 (3)
C3—C4	1.528 (3)	C16—C21	1.388 (3)
C3—H3	0.9800	C17—C18	1.379 (3)
C4—C5	1.498 (3)	C17—H17	0.9300
C4—H4A	0.9700	C18—C19	1.362 (3)
C4—H4B	0.9700	C18—H18	0.9300
C5—C11	1.494 (3)	C19—C20	1.359 (3)
C6—C7	1.372 (3)	C20—C21	1.376 (3)
C7—C8	1.370 (3)	C20—H20	0.9300
C7—H7	0.9300	C21—H21	0.9300
C8—C9	1.347 (4)		
C6—N1—C10	116.3 (2)	C10—C9—H9	120.8
C11—N2—C15	116.6 (2)	N1—C10—C9	124.5 (3)
O1—C1—C6	119.6 (2)	N1—C10—H10	117.7
O1—C1—C2	121.7 (2)	C9—C10—H10	117.7
C6—C1—C2	118.68 (19)	N2—C11—C12	122.9 (2)
C1—C2—C3	113.06 (18)	N2—C11—C5	116.9 (2)
C1—C2—H2A	109.0	C12—C11—C5	120.2 (2)
C3—C2—H2A	109.0	C13—C12—C11	118.6 (3)
C1—C2—H2B	109.0	C13—C12—H12	120.7
C3—C2—H2B	109.0	C11—C12—H12	120.7
H2A—C2—H2B	107.8	C14—C13—C12	119.3 (3)
C16—C3—C4	111.00 (19)	C14—C13—H13	120.3
C16—C3—C2	111.1 (2)	C12—C13—H13	120.3
C4—C3—C2	112.02 (18)	C13—C14—C15	118.5 (3)
C16—C3—H3	107.5	C13—C14—H14	120.7
C4—C3—H3	107.5	C15—C14—H14	120.7
C2—C3—H3	107.5	N2—C15—C14	124.0 (3)
C5—C4—C3	112.65 (19)	N2—C15—H15	118.0
C5—C4—H4A	109.1	C14—C15—H15	118.0
C3—C4—H4A	109.1	C17—C16—C21	117.1 (2)

C5—C4—H4B	109.1	C17—C16—C3	121.7 (2)
C3—C4—H4B	109.1	C21—C16—C3	121.2 (2)
H4A—C4—H4B	107.8	C18—C17—C16	121.9 (2)
O2—C5—C11	119.9 (2)	C18—C17—H17	119.0
O2—C5—C4	121.4 (2)	C16—C17—H17	119.0
C11—C5—C4	118.6 (2)	C19—C18—C17	118.0 (2)
N1—C6—C7	122.6 (2)	C19—C18—H18	121.0
N1—C6—C1	117.5 (2)	C17—C18—H18	121.0
C7—C6—C1	119.9 (2)	C20—C19—C18	122.9 (3)
C8—C7—C6	119.5 (3)	C20—C19—F1	118.4 (2)
C8—C7—H7	120.2	C18—C19—F1	118.7 (2)
C6—C7—H7	120.2	C19—C20—C21	118.3 (2)
C9—C8—C7	118.6 (3)	C19—C20—H20	120.9
C9—C8—H8	120.7	C21—C20—H20	120.9
C7—C8—H8	120.7	C20—C21—C16	121.8 (2)
C8—C9—C10	118.5 (3)	C20—C21—H21	119.1
C8—C9—H9	120.8	C16—C21—H21	119.1
O1—C1—C2—C3	−22.3 (3)	C4—C5—C11—N2	7.6 (3)
C6—C1—C2—C3	158.6 (2)	O2—C5—C11—C12	5.8 (4)
C1—C2—C3—C16	−67.6 (3)	C4—C5—C11—C12	−171.5 (2)
C1—C2—C3—C4	167.7 (2)	N2—C11—C12—C13	−1.5 (4)
C16—C3—C4—C5	70.4 (3)	C5—C11—C12—C13	177.6 (3)
C2—C3—C4—C5	−164.8 (2)	C11—C12—C13—C14	1.2 (5)
C3—C4—C5—O2	14.9 (4)	C12—C13—C14—C15	−0.2 (5)
C3—C4—C5—C11	−167.9 (2)	C11—N2—C15—C14	0.3 (4)
C10—N1—C6—C7	1.0 (4)	C13—C14—C15—N2	−0.6 (5)
C10—N1—C6—C1	−179.1 (3)	C4—C3—C16—C17	63.5 (3)
O1—C1—C6—N1	172.6 (2)	C2—C3—C16—C17	−61.8 (3)
C2—C1—C6—N1	−8.2 (3)	C4—C3—C16—C21	−115.4 (2)
O1—C1—C6—C7	−7.5 (4)	C2—C3—C16—C21	119.3 (2)
C2—C1—C6—C7	171.7 (2)	C21—C16—C17—C18	−0.8 (3)
N1—C6—C7—C8	−0.4 (4)	C3—C16—C17—C18	−179.7 (2)
C1—C6—C7—C8	179.7 (3)	C16—C17—C18—C19	−0.2 (4)
C6—C7—C8—C9	−0.3 (5)	C17—C18—C19—C20	1.1 (4)
C7—C8—C9—C10	0.4 (5)	C17—C18—C19—F1	−179.4 (2)
C6—N1—C10—C9	−0.9 (6)	C18—C19—C20—C21	−0.9 (4)
C8—C9—C10—N1	0.2 (6)	F1—C19—C20—C21	179.5 (2)
C15—N2—C11—C12	0.7 (4)	C19—C20—C21—C16	−0.2 (3)
C15—N2—C11—C5	−178.3 (2)	C17—C16—C21—C20	1.0 (3)
O2—C5—C11—N2	−175.1 (2)	C3—C16—C21—C20	179.9 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2A···N1	0.97	2.50	2.838 (3)	100
C12—H12···O2^{i}	0.93	2.45	3.269 (3)	146

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1.

Fig. 1

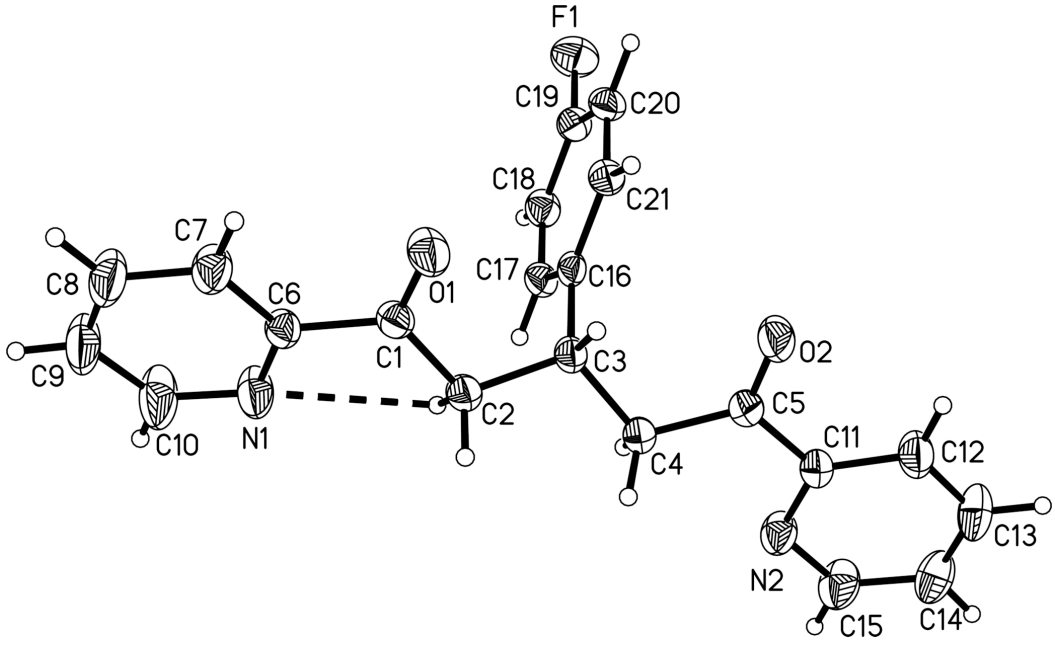
F1
C19
C20
C18
C21
C7
C8
C6
O1
C17
C16
C1
C3
O2
C9
C2
C5
C10
N1
C4
C11
C12
C13
N2
C15
C14

Fig. 2