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Molecular and crystal structure of 2,5-bis[(4-fluorophenyl)iminomethyl]furan

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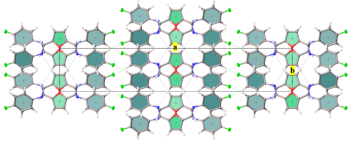
The title furan bis(imine) compound, 2,5-bis[(4-fluorophenyl)iminomethyl]-furan, $C_{18}H_{12}F_2N_2O$, was synthesized by condensation of 2,5-furandicarboxaldehyde with two equivalents of 4-fluoroaniline. The molecular structure consists of a central furan ring symmetrically bound to nearly coplanar iminomethyl groups with N-bonded 4-fluorophenyl rings that are significantly tipped out of the plane of the furan ring. In the crystal structure, the furan ring lies on a twofold rotation axis in space group *C*2/*c* with the furan ring and imine groups of adjacent molecules participating in C—H···N interactions to give furan-ring-centered hydrogen-bonded chains extending along [010]. Further cohesion of the crystal structure is achieved by participation of the peripheral 4-fluorophenyl rings in C—H···F hydrogen bonding and edge-to-face C—H···π interactions, resulting in a tri-periodic network. The resulting supramolecular chains formed by C—H···F hydrogen bonding extend in a direction parallel to [101].

1. Chemical context

The ongoing plastic pollution crisis and limited recycling strategies related to polyethylene terephthalate (PET) has led to significant research on the development of alternative materials possessing similar mechanical and gas barrier properties (Yoshida *et al.*, 2016; Thiounn & Smith, 2020; Lauer & Smith, 2020). Polyethylene furanoate (PEF) may function as a drop-in replacement for PET plastics due to the structural similarity of the furanic core of PEF relative to the phenyl core of PET (Fei *et al.*, 2020). Difluoro-terminated furanic monomers have already been developed and used to synthesize thermally robust (T_d-5% = 753–766 K) aryl ether ketones, but the synthesis of these monomers required the use of several deleterious reagents and yields were not published (Bao *et al.*, 2019). However, 2,5-furandicarboxaldehyde-derived imines can be synthesized in a single step in an environmentally friendly solvent with high yields, low energy requirements, facile isolation, and in excellent purity. This green chemistry approach was used to synthesize the title compound, 2,5-bis-[(4-fluorophenyl)iminomethyl]furan (Fig. 1), a possible



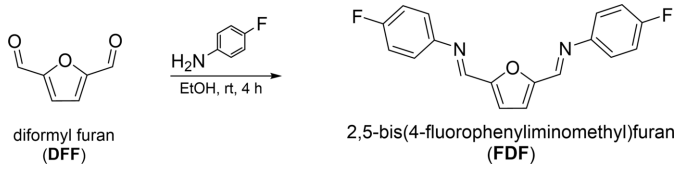
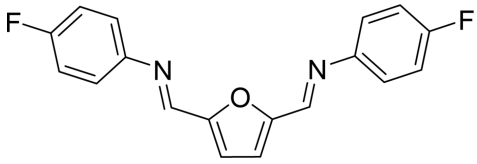


Figure 1
Single-step reaction of 2,5-bis[(4-fluorophenyl)iminomethyl]furan in the environmentally friendly solvent ethanol.

candidate for the development of next-generation bio-based polymeric materials.



2. Structural commentary

Molecules of 2,5-bis[(4-fluorophenyl)iminomethyl]furan crystallize in space group *C*2/*c* with one half molecule per asymmetric unit. Bond lengths alternate long [C1—C1^{i} = 1.411 (2) Å; symmetry code: (i) $-x+1, y, -z+\frac{1}{2}$] – short [C1—C2 = 1.3678 (15) Å] – long [C2—C3 = 1.4353 (15) Å], as expected for the central furan ring symmetrically bound to the C atoms of two methanimine groups (Fig. 2). The furan ring lies on a twofold rotation axis with nearly co-planar methanimine groups [small O1—C2—C3—N1 torsion angle of −3.35 (15)°] bound through their N atoms to 4-fluorophenyl groups as the *E* isomer in a *δ-cis* conformation (Fig. 2). In the crystal structure of the non-fluorinated 2,5-bis(phenyliminomethyl)furan molecule, a similar core structure was reported, with the peripheral benzene rings significantly tipped out of the plane of the central furan ring at a reported torsional angle of 38° (Mallet *et al.*, 2011). The title molecule displays a similar peripheral ring tip, with the planes of the 4-fluorophenyl groups tipped out of the plane of the central furan ring [34.38 (3)°] as well as the plane of the methanimine groups [39.03 (11)°].

3. Supramolecular features

The crystal structure of 2,5-bis[(4-fluorophenyl)iminomethyl] furan is consolidated by a tri-periodic network consisting of C—H···N and C—H···F hydrogen bonds as well as weaker edge-to-face C—H···π interactions. Molecules pack head

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···N1^{i}	0.970 (14)	2.576 (14)	3.5408 (14)	173.1 (10)
C8—H8···F1^{ii}	0.945 (14)	2.617 (14)	3.2815 (13)	127.8 (10)

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

(N1) to tail (C1*H*), held in place by four furan-ring-centered C1—H1···N1 intermolecular hydrogen bonds [2.576 (14) Å, Table 1] per molecule, forming chains that run along [010] (Fig. 3). Further, the two 4-fluorophenyl rings of each molecule interact with the 4-fluorophenyl rings of adjacent molecules, forming four additional C—H···F hydrogen bonds [2.617 (14) Å, Table 1] per molecule that repeat in a direction parallel to [101] (Fig. 3). Adjacent molecules pack along [001] in a head-to-head orientation, resulting in the O atoms of the co-parallel central furan rings facing opposite directions with an interplane spacing of 3.2026 (11) Å but with their centroids (*Cg*1) offset by 3.1666 (16) Å (Fig. 4). Although the planes of the 4-fluorophenyl rings (corresponding centroid is *Cg*2) are co-parallel along [010] (Fig. 3), they are mutually tilted at an angle of 58.35 (5)° along [001], giving edge-to-face 4-fluorophenyl group C—H···π contacts that involve H6···*Cg*2 [2.6004 (4) Å] and H9···*Cg*2 [2.6384 (4) Å interactions], see Fig. 4. Data for the non-fluorinated 2,5-bis(phenyliminomethyl)furan gave a furan ring-to-furan ring interplane spacing of 3.3 Å with a reported C—H···π contact distance of 2.63 Å (Mallet *et al.*, 2011). The C—H···F contact distance in the crystal structure for the title molecule [2.617 (14) Å, Table 1] is also consistent with the range of values reported for the perfluorophenyl compound, 2,5-bis(pentafluorophenyliminomethyl)furan [2.50 (4)–2.77 (5) Å; (Mallet *et al.*, 2011]. Although π–π stacking interactions were observed in the packing pattern of 2,5-bis(pentafluorophenyliminomethyl) furan (Mallet *et al.*, 2011), the incorporation of only one F atom on each peripheral ring in the title molecule produced a molecular and crystal structure that more closely resembles

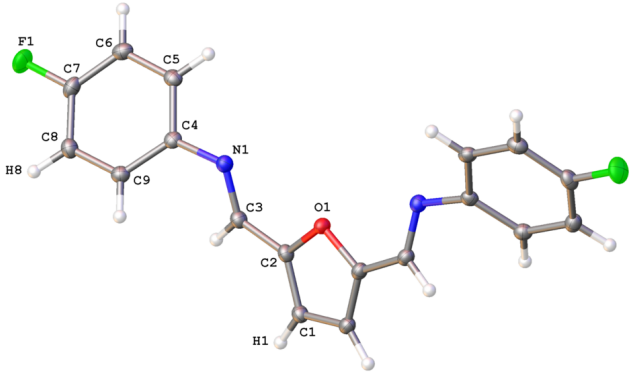


Figure 2
Molecular structure of 2,5-bis[(4-fluorophenyl)iminomethyl]furan. The central furan ring lies on a twofold rotation axis in space group *C*2/*c* with the planes of the 4-fluorophenyl rings tipped out of the central furan ring plane by 34.38 (3)°. Displacement ellipsoids are shown at the 50% probability level, with H atoms of arbitrary size; non-labeled atoms are generated by symmetry operation $-x+1, y, -z+\frac{1}{2}$.

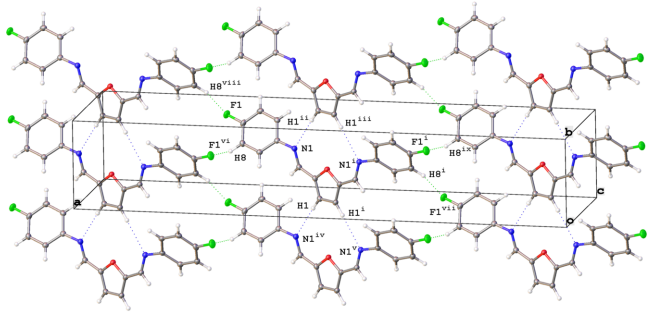


Figure 3
Hydrogen-bonding motif with unit cell overlay for 2,5-bis[(4-fluorophenyl)iminomethyl]furan. Each molecule forms eight hydrogen bonds using C—H···N [2.576 (14) Å] and C—-H···F [2.617 (14) Å] interactions. Displacement ellipsoids are shown at the 50% probability level, with H atoms of arbitrary size. [Symmetry codes: (i) $1-x, y, \frac{3}{2}-z$; (ii) $x, 1+y, z$; (iii) $1-x, 1+y, \frac{3}{2}-z$; (iv) $x, y-1, z$; (v) $1-x, y-1, \frac{3}{2}-z$; (vi) $\frac{1}{2}-x, y-\frac{1}{2}, \frac{1}{2}-z$; (vii) $\frac{1}{2}+x, y-\frac{1}{2}, 1+z$; (viii) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$; (ix) $\frac{1}{2}+x, \frac{1}{2}+y, 1+z$.]

that of the non-fluorinated 2,5-bis(phenyliminomethyl)furan, and that is consolidated by C—H···N and C—H···F hydrogen bonds as well as edge-to-face C—H···π interactions.

4. Database survey

The crystal structures of the related compounds, 2,5-bis-(phenyliminomethyl)furan [Cambridge Structural Database (CSD; Groom *et al.*, 2016) deposition identifier EBEVIS] and 2,5-bis(pentafluorophenyliminomethyl)furan (CSD deposition number EBEVUE) were previously reported (Mallet *et al.*, 2011). Compared to the title molecule, 2,5-bis(phenyliminomethylfuran) crystallizes in the same space group type (*C*2/*c*) with similar unit cell parameters (Mallet *et al.*, 2011), giving nearly identical molecular and crystal structures. However, 2,5-bis(pentafluorophenyliminomethyl)furan crystallizes in space group *P*1, having a molecular structure with one methanimine arm in the *δ-cis* conformation and the other arm in the *δ-trans* conformation in addition to a packing pattern featuring $\pi-\pi$ stacking interactions (Mallet *et al.*, 2011). The consolidating effect of C—H···N hydrogen bonding was not discussed for the reported crystal structures of 2,5-bis(phenyliminomethyl)furan and 2,5-bis(pentafluorophenyliminomethyl)furan, but C—H···F interactions were noted for the structure of 2,5-bis(pentafluorophenyliminomethyl)furan (Mallet *et al.*, 2011).

5. Synthesis and crystallization

To a well-stirred solution of 2,5-furandicarboxaldehyde (0.200 g, 1.6 mmol) in ethanol (20 ml) was added 4-fluoroaniline (0.394 g, 3.5 mmol), and the reaction mixture heated to 313 K. The reaction mixture was allowed to stir until all of the monosubstituted product had converted to the disubstituted product as determined by GC–MS. The reaction mixture was allowed to cool, diluted by half with water, filtered, and washed with water. After drying at 333 K under reduced pressure, a greenish-yellow-colored crystalline solid was obtained (0.402 g, 80%).

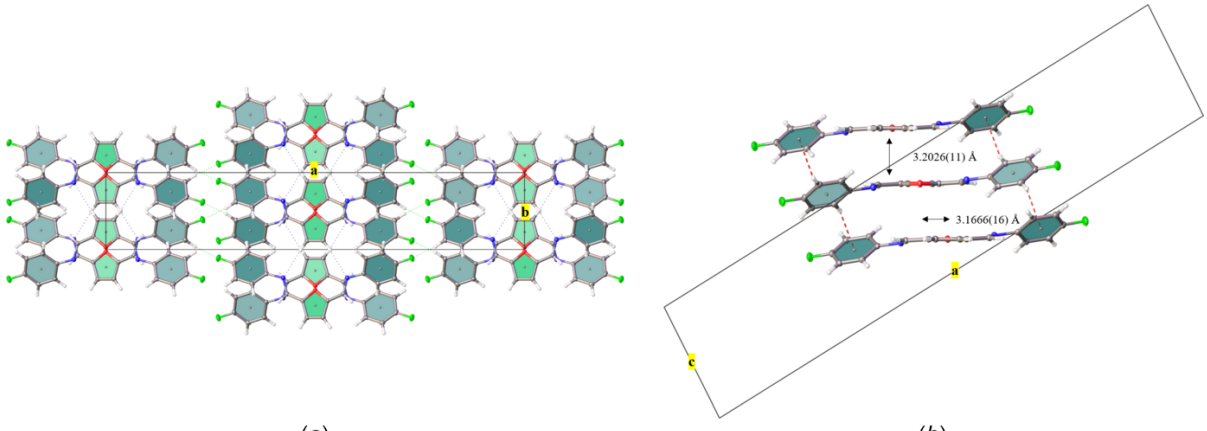
Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{12}F_2N_2O$
M_r	310.30
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	100
a, *b*, *c* (Å)	32.9033 (3), 6.02694 (5), 7.14998 (6)
β (°)	95.5021 (8)
V (Å^3)	1411.35 (2)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.93
Crystal size (mm)	0.21 × 0.11 × 0.07
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix3000
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2023)
T_{min}, T_{max}	0.671, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13137, 1312, 1252
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.605
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.029, 0.078, 1.05
No. of reflections	1312
No. of parameters	114
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.17

Computer programs: *CrysAlis PRO* (Rigaku OD, 2023), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All hydrogen atoms, except H1 and



(*a*) (*b*)

Figure 4
Details of the packing for 2,5-bis[(4-fluorophenyl)iminomethyl]furan. The view along [001] (*a*) shows the head-to-head arrangement of the central furan rings in addition to the edge-to-face interactions between peripheral 4-fluorophenyl groups. A portion of the view along [010] (*b*) depicts the offset furan ring-to-furan ring interplanar spacing as well as the C—H···π interactions [H6···*Cg*2 (2.6004 (4) Å] and H9···*Cg*2 [2.6384 (4) Å] that extend along [001]. Displacement ellipsoids are shown at the 50% probability level, with H atoms of arbitrary size.

H8, were placed using a riding model with their positions constrained relative to their parent C atom using the appropriate HFIX command in *SHELXL* (Sheldrick, 2015*b*). Hydrogen atoms H1 and H8 involved in C—H···N and C—H···F hydrogen bonding were placed from the electron-density map, and their C—H distances restrained (DFIX, C—H range 0.94–0.96 Å) at 0.95 Å with U_{iso}(H) = 1.2U_{eq}(C).

Acknowledgements

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Computing details

2,5-Bis[(4-fluorophenyl)iminomethyl]furan

Crystal data

$C_{18}H_{12}F_2N_2O$
$M_r = 310.30$
Monoclinic, $C2/c$
$a = 32.9033$ (3) Å
$b = 6.02694$ (5) Å
$c = 7.14998$ (6) Å
$\beta = 95.5021$ (8)°
$V = 1411.35$ (2) Å^3
$Z = 4$
$F(000) = 640$
$D_x = 1.460$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 10588 reflections
$\theta = 2.7$–$68.8°$
$\mu = 0.93$ mm^{-1}
$T = 100$ K
Rectangular prism, clear greenish yellow
0.21 × 0.11 × 0.07 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix3000 diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2023)
$T_{min} = 0.671$, $T_{max} = 1.000$
13137 measured reflections
1312 independent reflections
1252 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 68.9°$, $\theta_{min} = 2.7°$
$h = -31 \rightarrow 39$
$k = -7 \rightarrow 7$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.078$
$S = 1.05$
1312 reflections
114 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0395P)^2 + 1.169P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}
Extinction correction: SHELXL-2019/2 (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00100 (16)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.51924 (3)	0.11462 (17)	0.30286 (14)	0.0162 (3)
F1	0.73109 (2)	0.88737 (12)	0.71765 (9)	0.0280 (2)
N1	0.57648 (3)	0.62961 (15)	0.42481 (12)	0.0158 (2)
O1	0.500000	0.46983 (17)	0.250000	0.0150 (3)
C2	0.52992 (3)	0.33229 (18)	0.33073 (14)	0.0152 (2)
C3	0.56719 (3)	0.42300 (18)	0.41997 (14)	0.0160 (2)
H3	0.586445	0.322231	0.480032	0.019*
C4	0.61637 (3)	0.68551 (17)	0.50427 (14)	0.0149 (2)
C5	0.62174 (3)	0.88471 (17)	0.60383 (14)	0.0165 (3)
H5	0.598685	0.974298	0.621945	0.020*
C6	0.66028 (3)	0.95307 (19)	0.67642 (14)	0.0185 (3)
H6	0.663913	1.088192	0.744385	0.022*
C7	0.69331 (3)	0.81989 (19)	0.64753 (15)	0.0189 (3)
C8	0.68949 (3)	0.62270 (19)	0.54995 (15)	0.0180 (3)
C9	0.65075 (3)	0.55601 (18)	0.47783 (14)	0.0163 (3)
H9	0.647485	0.420854	0.409678	0.020*
H1	0.5356 (4)	−0.012 (2)	0.3467 (17)	0.019 (3)*
H8	0.7127 (4)	0.537 (2)	0.5300 (19)	0.027 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0153 (6)	0.0160 (5)	0.0175 (5)	0.0018 (4)	0.0024 (4)	0.0015 (4)
F1	0.0172 (4)	0.0342 (4)	0.0314 (4)	−0.0070 (3)	−0.0038 (3)	−0.0062 (3)
N1	0.0146 (5)	0.0164 (5)	0.0162 (4)	0.0003 (3)	0.0004 (3)	−0.0007 (3)
O1	0.0130 (5)	0.0137 (5)	0.0179 (5)	0.000	−0.0010 (4)	0.000
C2	0.0138 (5)	0.0168 (5)	0.0149 (5)	0.0023 (4)	0.0011 (4)	0.0014 (4)
C3	0.0153 (5)	0.0165 (5)	0.0160 (5)	0.0021 (4)	0.0011 (4)	0.0013 (4)
C4	0.0165 (5)	0.0146 (5)	0.0133 (5)	−0.0007 (4)	0.0004 (4)	0.0030 (4)
C5	0.0191 (6)	0.0143 (5)	0.0162 (5)	0.0016 (4)	0.0022 (4)	0.0025 (4)
C6	0.0240 (6)	0.0161 (5)	0.0155 (5)	−0.0030 (4)	0.0019 (4)	−0.0004 (4)
C7	0.0156 (5)	0.0236 (6)	0.0169 (5)	−0.0053 (4)	−0.0012 (4)	0.0022 (4)
C8	0.0161 (6)	0.0203 (6)	0.0177 (5)	0.0021 (4)	0.0021 (4)	0.0019 (4)
C9	0.0187 (5)	0.0152 (5)	0.0149 (5)	−0.0001 (4)	0.0009 (4)	0.0007 (4)

Geometric parameters (Å, º)

C1—C1^{i}	1.411 (2)	C4—C5	1.3983 (15)
C1—C2	1.3678 (15)	C4—C9	1.4020 (15)

C1—H1	0.970 (14)	C5—H5	0.9500
F1—C7	1.3573 (12)	C5—C6	1.3861 (15)
N1—C3	1.2819 (14)	C6—H6	0.9500
N1—C4	1.4198 (13)	C6—C7	1.3825 (16)
O1—C2^{i}	1.3712 (12)	C7—C8	1.3778 (16)
O1—C2	1.3712 (12)	C8—C9	1.3880 (15)
C2—C3	1.4353 (15)	C8—H8	0.945 (14)
C3—H3	0.9500	C9—H9	0.9500

C1^{i}—C1—H1	128.1 (8)	C6—C5—C4	120.82 (10)
C2—C1—C1^{i}	106.43 (6)	C6—C5—H5	119.6
C2—C1—H1	125.5 (8)	C5—C6—H6	120.8
C3—N1—C4	116.75 (9)	C7—C6—C5	118.40 (10)
C2^{i}—O1—C2	105.61 (12)	C7—C6—H6	120.8
C1—C2—O1	110.76 (10)	F1—C7—C6	118.43 (10)
C1—C2—C3	128.81 (10)	F1—C7—C8	118.77 (10)
O1—C2—C3	120.34 (10)	C8—C7—C6	122.79 (10)
N1—C3—C2	124.98 (10)	C7—C8—C9	118.29 (10)
N1—C3—H3	117.5	C7—C8—H8	120.8 (9)
C2—C3—H3	117.5	C9—C8—H8	120.9 (9)
C5—C4—N1	118.31 (9)	C4—C9—H9	119.6
C5—C4—C9	118.84 (10)	C8—C9—C4	120.86 (10)
C9—C4—N1	122.74 (10)	C8—C9—H9	119.6
C4—C5—H5	119.6		

C1^{i}—C1—C2—O1	0.69 (14)	C3—N1—C4—C9	37.67 (14)
C1^{i}—C1—C2—C3	−175.88 (10)	C4—N1—C3—C2	−174.20 (9)
C1—C2—C3—N1	172.93 (11)	C4—C5—C6—C7	0.19 (15)
F1—C7—C8—C9	−179.59 (9)	C5—C4—C9—C8	0.43 (15)
N1—C4—C5—C6	−176.78 (9)	C5—C6—C7—F1	179.63 (9)
N1—C4—C9—C8	176.64 (9)	C5—C6—C7—C8	−0.02 (17)
O1—C2—C3—N1	−3.35 (15)	C6—C7—C8—C9	0.05 (17)
C2^{i}—O1—C2—C1	−0.27 (6)	C7—C8—C9—C4	−0.26 (16)
C2^{i}—O1—C2—C3	176.63 (11)	C9—C4—C5—C6	−0.39 (15)
C3—N1—C4—C5	−146.10 (10)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···N1^{ii}	0.970 (14)	2.576 (14)	3.5408 (14)	173.1 (10)
C8—H8···F1^{iii}	0.945 (14)	2.617 (14)	3.2815 (13)	127.8 (10)

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