N-(4-Acetylphenyl)-N′-(4-fluorophenyl)urea

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In the title compound, $C_{15}H_{13}FN_2O_2$, the fluorophenyl and 4-acetylphenyl rings are twisted from each other by a dihedral angle of 11.6 (2)°. In the crystal, molecules are packed into layers parallel to (010). Each layer contains the molecules linked by a pair of strong N—H···O hydrogen bonds, with an $R_2^2(14)$ ring motif, while strong C—H···F hydrogen bonds forming $R_4^2(26)$ ring motifs connect molecules into a two-dimensional network. The intermolecular interactions have been investigated using Hirshfeld surface studies and two-dimensional fingerprint plots.

3D view
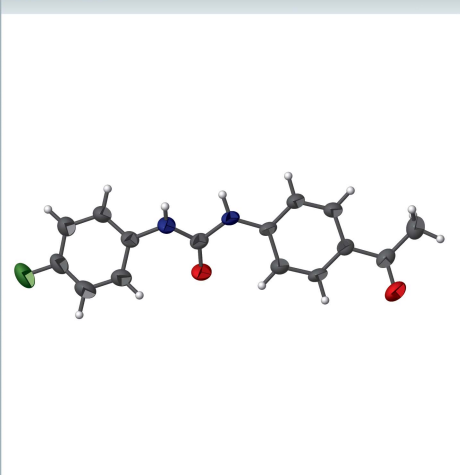
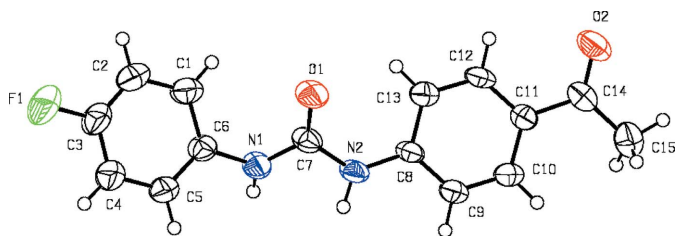

Chemical scheme
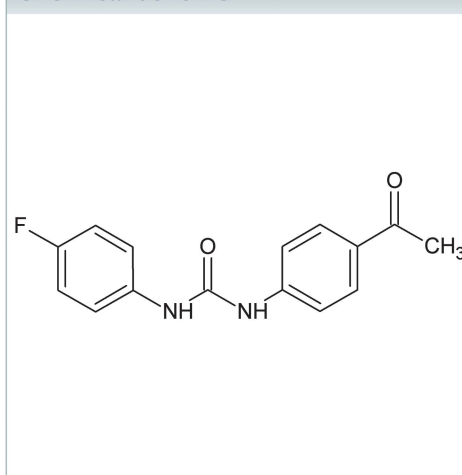
Structure description

Acetophenones having different substituents in synthetic organic chemistry are used as an important building block (Bing-Wei, 2010). In particular, they are frequently used in conjunction with aldehydes in the synthesis of chalcone derivatives (Kocyigit et al., 2018; Karaman et al., 2010; Ceylan et al., 2011), which are used as starting materials in the preparation of useful and multifunctional heterocyclic and bioactive compounds (Gürdere, Gümüş et al., 2017; Gürdere, Kamo et al., 2017; Gezegen et al., 2013). In this article we report the crystal structure of 4-fluorophenylurea-substituted acetophenone, namely N-(4-acetylphenyl)-N′-(4-fluorophenyl)urea.

In the title molecule (Fig. 1), the fluorophenyl ring (C1–C6) and the 4-acetylphenyl ring (C8–C13) are twisted from each other, making a dihedral angle of 11.6 (2)°. The mean plane of the four essentially planar atoms of the urea moiety (C7/N1/N2/O1; r.m.s deviation = 0.004 Å) forms dihedral angles of 35.9 (3) and 29.2 (2)°, respectively, with the mean planes of the fluorophenyl and 4-acetylphenyl rings. The molecular conformation is

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1[i]	0.79 (6)	2.17 (6)	2.927 (5)	160 (5)
N2—H2N···O2[ii]	0.88 (6)	2.30 (6)	3.070 (6)	147 (5)
C1—H1···O1	0.93	2.52	2.932 (6)	107
C10—H10···F1[iii]	0.93	2.49	3.386 (6)	162
C13—H13···O1	0.93	2.33	2.887 (7)	118

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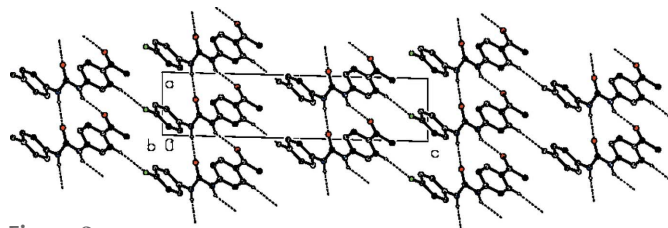

Figure 1
The molecular structure of the title compound, showing the displacement ellipsoids drawn at the 50% probability level.

stabilized by two weak intramolecular C—H···O interactions (Table 1). In the crystal (Figs. 2 and 3), N—H···O and C—H···F hydrogen bonds (Table 1) link the adjacent molecules into layers parallel to (010) forming $R_2^2(14)$ and $R_4^2(26)$ ring motifs. C—H···π and π–π interactions are not observed.
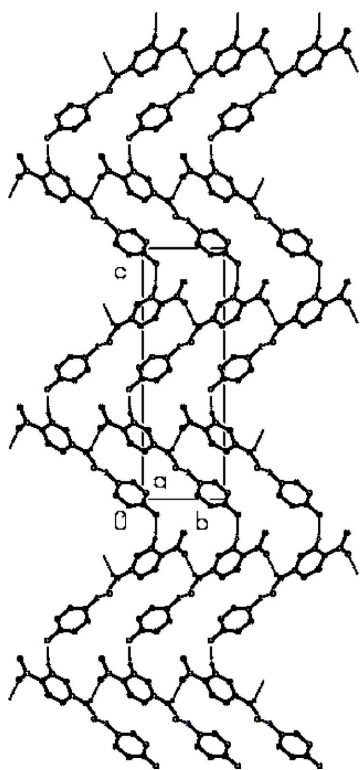
Figure 2
A view along the *a* axis of the crystal packing of the title compound. H atoms not involved in hydrogen bonding (dotted lines) are omitted for clarity.
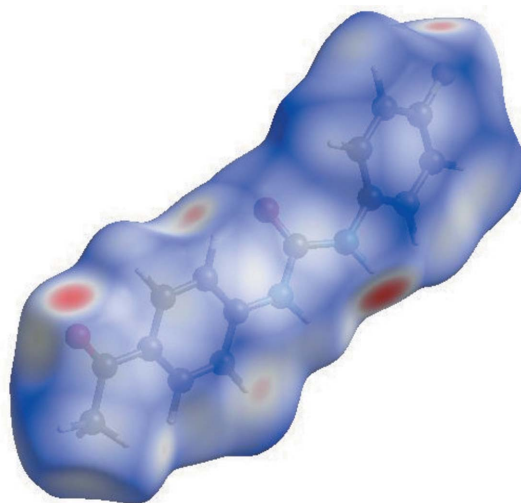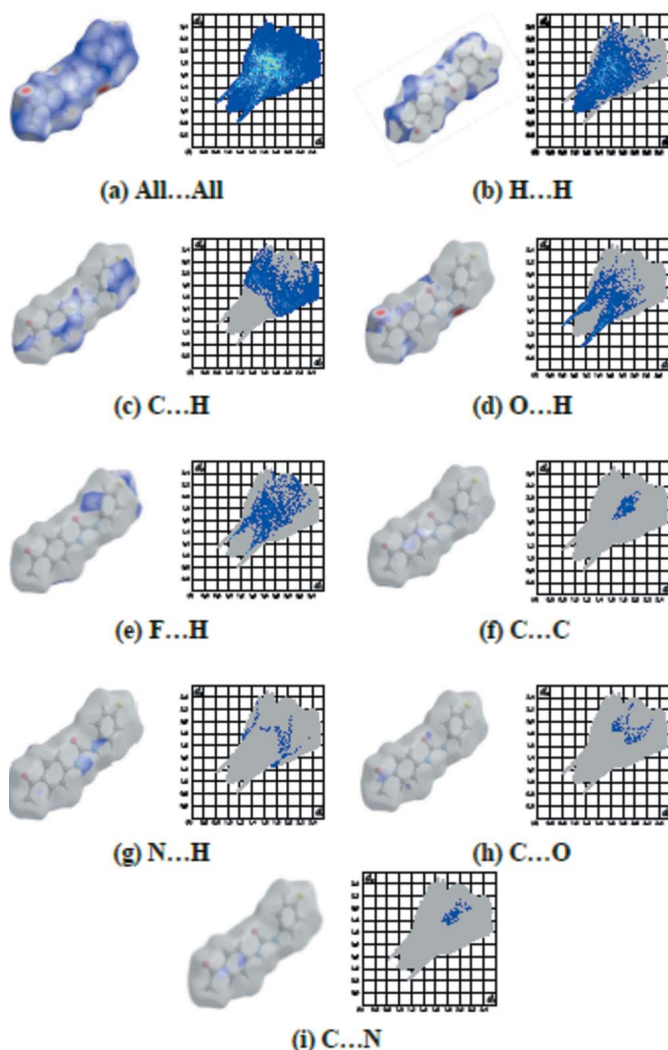

Figure 3
A view along the *b* axis of the crystal packing of the title compound. H atoms not involved in hydrogen bonding (dashed lines) are omitted for clarity.

The values of the geometric parameters of the title structure are comparable to those in the related structures N,N'-bis-(pentafluorophenyl)urea (Jai-nhuknan *et al.*, 1997), N,N'-bis(4-fluorophenyl)urea (Loh *et al.*, 2010) and polymorphs of 1,3-bis(3-fluorophenyl) urea (Capacci-Daniel *et al.*, 2016) and 1-(3-fluorophenyl)-3-(4-nitrophenyl)urea (Lin *et al.*, 2012).

The three-dimensional d_{norm} surface is a useful tool to analyse and visualize the inter-molecular interactions. d_{norm} takes negative or positive values depending on whether the intermolecular contact is shorter or longer than the van der Waals radii (Spackman & Jayatilaka, 2009). It is evident from the bright-red spots appearing near the oxygen atom on the Hirshfeld surface mapped over d_{norm} in Fig. 4 that these atoms play a significant role in the molecular packing. The donors and acceptors of N—H···O and C—H···F interactions are also represented with blue (positive potential) and red regions (negative potential), respectively, on the Hirshfeld surface mapped over the d_{norm} in Fig. 5. The red points, which represent closer contacts and negative d_{norm} values on the surface, correspond to the N—H···O, C—H···F and C—H···O interactions. The percentage contributions of various contacts to the total Hirshfeld surface are as follows: H···H (36.5%), F···H/H···F (13.3%), O···H/H···O (15.4%), C···H/H···C (24.7%), N···H/H···N (2.3%), C···C (3.1%), O···C/C···O (1.7%), C···N/N···C (1.5%) and F···C/C···F

Figure 4
View of the three-dimensional Hirshfeld surface of the title compound mapped with d_{norm}.

Figure 5
Two-dimensional fingerprint plots of the title compound, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) C···H, (*d*) O···H, (*e*) F···H, (*f*) C···C, (*g*) N···H, (*h*) C···O and (*i*) C···N interactions [d_e and d_i represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

(0.7%), as shown in the two-dimensional fingerprint plots in Fig. 5. The three-dimensional shape-index surface of the title compound is shown in Fig. 6.

Synthesis and crystallization

For the synthesis of 1-(4-acetylphenyl)-3-(4-fluorophenyl)urea, see Gezegen *et al.* (2017).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Seventeen reflections (3 1 23), ($\overline{1}$ 5 3), (0 8 0), (3 3 $\overline{10}$), (4 0 20), (1 5 $\overline{3}$), ($\overline{1}$ 4 $\overline{13}$), (1 4 13), ($\overline{4}$ 4 11), (2 5 $\overline{11}$), (0 6 7), (6 3 $\overline{1}$), ($\overline{3}$ 3 10), ($\overline{2}$ 6 $\overline{17}$), (0 6 $\overline{7}$), (5 1 $\overline{16}$) and

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{13}FN_2O_2$
M_r	272.27
Crystal system, space group	Monoclinic, *Pn*
Temperature (K)	296
a, b, c (Å)	4.8061 (15), 6.617 (2), 20.364 (7)
β (°)	91.417 (10)
V (Å^3)	647.4 (4)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	$0.15 \times 0.12 \times 0.11$
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 2003)
T_{min}, T_{max}	0.547, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15964, 2991, 2573
R_{int}	0.053
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.666
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.062, 0.134, 1.11
No. of reflections	2991
No. of parameters	191
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.18, −0.20

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

(0 1 14) were omitted from the refinement because of large differences between observed and calculated intensities.
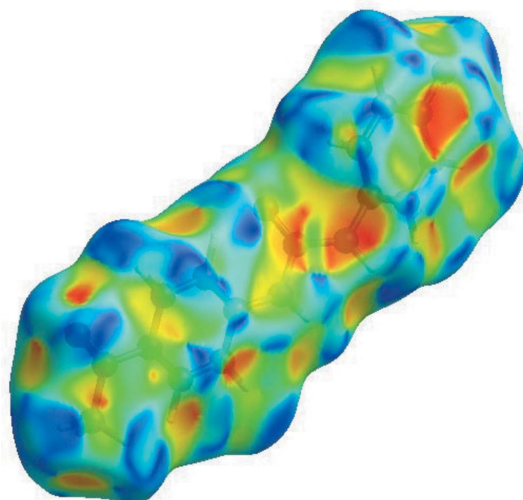
Figure 6
Hirshfeld surface of the title complex plotted over shape-index.

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full crystallographic data

N-(4-Acetylphenyl)-*N*′-(4-fluorophenyl)urea

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N-(4-Acetylphenyl)-N′-(4-fluorophenyl)urea

Crystal data

$C_{15}H_{13}FN_2O_2$	$F(000) = 284$
$M_r = 272.27$	$D_x = 1.397$ Mg m^{-3}
Monoclinic, Pn	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P -2yac	Cell parameters from 9977 reflections
$a = 4.8061$ (15) Å	$\theta = 3.0$–28.3°
$b = 6.617$ (2) Å	$\mu = 0.10$ mm^{-1}
$c = 20.364$ (7) Å	$T = 296$ K
$\beta = 91.417$ (10)°	Block, bronze
$V = 647.4$ (4) Å^3	$0.15 \times 0.12 \times 0.11$ mm
$Z = 2$	

Data collection

Bruker APEXII CCD diffractometer	2991 independent reflections
φ and ω scans	2573 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	$R_{int} = 0.053$
	$\theta_{max} = 28.3°$, $\theta_{min} = 3.1°$
$T_{min} = 0.547$, $T_{max} = 0.746$	$h = -6 \rightarrow 6$
15964 measured reflections	$k = -8 \rightarrow 8$
	$l = -27 \rightarrow 27$

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.062$	
$wR(F^2) = 0.134$	W = 1/[$\Sigma^2(FO^2) + 0.564P$] WHERE $P = (FO^2 + 2FC^2)/3$
$S = 1.11$	
2991 reflections	$(\Delta/\sigma)_{max} < 0.001$
191 parameters	$\Delta\rho_{max} = 0.18$ e Å^{-3}
2 restraints	$\Delta\rho_{min} = -0.20$ e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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.

H atoms of NH groups were located in difference Fourier maps [N1—H1N = 0.79 (6) and N2—H2N = 0.88 (6) Å] and refined freely. All H atoms attached to carbon were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances of 0.93 - 0.96 Å and $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$.

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.4143 (11)	0.6742 (8)	0.0165 (2)	0.0579 (13)
H1	0.5055	0.5510	0.0124	0.069*
C2	0.4738 (12)	0.8333 (10)	−0.0252 (3)	0.0686 (16)
H2	0.6100	0.8186	−0.0565	0.082*
C3	0.3346 (13)	1.0090 (8)	−0.0204 (3)	0.0620 (14)
C4	0.1366 (12)	1.0392 (9)	0.0249 (3)	0.0667 (15)
H4	0.0419	1.1615	0.0272	0.080*
C5	0.0800 (12)	0.8832 (8)	0.0676 (3)	0.0627 (14)
H5	−0.0538	0.9017	0.0992	0.075*
C6	0.2168 (8)	0.7011 (7)	0.0643 (2)	0.0430 (10)
C7	0.3297 (8)	0.4208 (7)	0.1394 (2)	0.0448 (10)
C8	0.3199 (8)	0.1346 (6)	0.2184 (2)	0.0390 (9)
C9	0.2016 (9)	0.0633 (7)	0.2753 (2)	0.0497 (11)
H9	0.0585	0.1364	0.2940	0.060*
C10	0.2898 (10)	−0.1112 (7)	0.3044 (2)	0.0519 (12)
H10	0.2057	−0.1544	0.3426	0.062*
C11	0.5022 (9)	−0.2266 (6)	0.2785 (2)	0.0395 (9)
C12	0.6243 (10)	−0.1525 (7)	0.2220 (2)	0.0512 (12)
H12	0.7700	−0.2244	0.2040	0.061*
C13	0.5364 (10)	0.0236 (8)	0.1921 (3)	0.0547 (12)
H13	0.6217	0.0684	0.1543	0.066*
C14	0.6020 (9)	−0.4180 (7)	0.3072 (2)	0.0483 (11)
C15	0.4600 (13)	−0.5012 (9)	0.3662 (3)	0.0676 (15)
H15A	0.4963	−0.4147	0.4032	0.101*
H15B	0.5298	−0.6343	0.3756	0.101*
H15C	0.2630	−0.5079	0.3574	0.101*
F1	0.3976 (9)	1.1663 (6)	−0.06090 (19)	0.1009 (14)
N1	0.1477 (8)	0.5458 (6)	0.1088 (2)	0.0486 (10)
N2	0.2112 (7)	0.3066 (6)	0.1886 (2)	0.0467 (9)
O1	0.5754 (6)	0.4085 (5)	0.12620 (19)	0.0573 (9)
O2	0.7956 (8)	−0.5106 (6)	0.2841 (2)	0.0702 (11)
H1N	−0.016 (12)	0.538 (8)	0.112 (3)	0.054 (15)*
H2N	0.057 (12)	0.366 (9)	0.200 (3)	0.074 (18)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.130 (3)	0.089 (3)	0.086 (3)	0.004 (3)	0.044 (2)	0.039 (2)
O1	0.0299 (14)	0.058 (2)	0.085 (2)	−0.0003 (15)	0.0178 (15)	0.0140 (18)
O2	0.065 (2)	0.052 (2)	0.094 (3)	0.0236 (18)	0.015 (2)	0.006 (2)
N1	0.0310 (18)	0.048 (2)	0.068 (3)	−0.0002 (17)	0.0132 (17)	0.0142 (19)
N2	0.0319 (18)	0.041 (2)	0.068 (2)	0.0071 (15)	0.0196 (17)	0.0078 (18)
C1	0.064 (3)	0.053 (3)	0.058 (3)	0.008 (2)	0.022 (2)	−0.002 (2)
C2	0.076 (4)	0.073 (4)	0.059 (3)	0.009 (3)	0.031 (3)	0.008 (3)
C3	0.075 (3)	0.056 (3)	0.057 (3)	−0.004 (3)	0.021 (3)	0.014 (3)
C4	0.084 (4)	0.053 (3)	0.063 (3)	0.014 (3)	0.025 (3)	0.013 (3)
C5	0.067 (3)	0.057 (3)	0.066 (3)	0.015 (3)	0.032 (3)	0.016 (3)
C6	0.036 (2)	0.043 (2)	0.050 (2)	−0.0046 (18)	0.0094 (18)	0.0023 (19)
C7	0.032 (2)	0.039 (2)	0.064 (3)	0.0008 (18)	0.0083 (19)	0.001 (2)
C8	0.0322 (18)	0.034 (2)	0.052 (2)	0.0072 (17)	0.0109 (16)	−0.0025 (18)
C9	0.048 (2)	0.044 (2)	0.058 (3)	0.014 (2)	0.018 (2)	0.004 (2)
C10	0.053 (3)	0.049 (3)	0.055 (3)	0.012 (2)	0.022 (2)	0.003 (2)
C11	0.0349 (19)	0.036 (2)	0.047 (2)	0.0022 (17)	0.0024 (17)	−0.0004 (17)
C12	0.044 (2)	0.047 (3)	0.063 (3)	0.019 (2)	0.020 (2)	0.000 (2)
C13	0.052 (3)	0.053 (3)	0.060 (3)	0.014 (2)	0.021 (2)	0.009 (2)
C14	0.044 (2)	0.040 (2)	0.060 (3)	0.007 (2)	−0.004 (2)	−0.004 (2)
C15	0.074 (4)	0.055 (3)	0.074 (4)	0.010 (3)	0.003 (3)	0.015 (3)

Geometric parameters (Å, º)

F1—C3	1.367 (7)	C9—C10	1.361 (6)
O1—C7	1.220 (5)	C10—C11	1.389 (6)
O2—C14	1.218 (6)	C11—C12	1.394 (6)
N1—C6	1.415 (6)	C11—C14	1.470 (6)
N1—C7	1.346 (6)	C12—C13	1.376 (7)
N2—C7	1.388 (6)	C14—C15	1.501 (7)
N2—C8	1.386 (6)	C1—H1	0.9300
C1—C2	1.387 (8)	C2—H2	0.9300
C1—C6	1.388 (6)	C4—H4	0.9300
N1—H1N	0.79 (6)	C5—H5	0.9300
C2—C3	1.346 (8)	C9—H9	0.9300
N2—H2N	0.88 (6)	C10—H10	0.9300
C3—C4	1.356 (9)	C12—H12	0.9300
C4—C5	1.381 (8)	C13—H13	0.9300
C5—C6	1.375 (7)	C15—H15A	0.9600
C8—C9	1.386 (6)	C15—H15B	0.9600
C8—C13	1.392 (6)	C15—H15C	0.9600
C6—N1—C7	125.7 (4)	C11—C12—C13	122.2 (4)
C7—N2—C8	127.3 (4)	C8—C13—C12	120.1 (5)
C2—C1—C6	119.2 (5)	O2—C14—C15	119.4 (4)
C6—N1—H1N	110 (4)	C11—C14—C15	118.9 (4)

C7—N1—H1N	124 (4)	O2—C14—C11	121.6 (4)
C7—N2—H2N	108 (4)	C2—C1—H1	120.00
C1—C2—C3	120.1 (5)	C6—C1—H1	120.00
C8—N2—H2N	124 (4)	C1—C2—H2	120.00
F1—C3—C2	119.7 (5)	C3—C2—H2	120.00
F1—C3—C4	117.9 (5)	C3—C4—H4	121.00
C2—C3—C4	122.3 (6)	C5—C4—H4	121.00
C3—C4—C5	118.1 (5)	C4—C5—H5	119.00
C4—C5—C6	121.5 (5)	C6—C5—H5	119.00
N1—C6—C5	119.0 (4)	C8—C9—H9	119.00
C1—C6—C5	118.9 (5)	C10—C9—H9	119.00
N1—C6—C1	122.1 (4)	C9—C10—H10	119.00
O1—C7—N1	124.1 (4)	C11—C10—H10	119.00
O1—C7—N2	122.6 (4)	C11—C12—H12	119.00
N1—C7—N2	113.3 (3)	C13—C12—H12	119.00
C9—C8—C13	117.9 (4)	C8—C13—H13	120.00
N2—C8—C9	119.2 (4)	C12—C13—H13	120.00
N2—C8—C13	122.8 (4)	C14—C15—H15A	109.00
C8—C9—C10	121.5 (4)	C14—C15—H15B	109.00
C9—C10—C11	121.7 (4)	C14—C15—H15C	109.00
C10—C11—C12	116.6 (4)	H15A—C15—H15B	110.00
C10—C11—C14	123.9 (4)	H15A—C15—H15C	109.00
C12—C11—C14	119.4 (4)	H15B—C15—H15C	109.00
C7—N1—C6—C1	42.0 (7)	C4—C5—C6—N1	−179.2 (5)
C7—N1—C6—C5	−139.4 (5)	C4—C5—C6—C1	−0.5 (8)
C6—N1—C7—O1	−9.9 (7)	N2—C8—C9—C10	176.2 (4)
C6—N1—C7—N2	169.5 (4)	C13—C8—C9—C10	−1.0 (7)
C7—N2—C8—C9	167.2 (4)	N2—C8—C13—C12	−176.2 (4)
C7—N2—C8—C13	−15.8 (7)	C9—C8—C13—C12	0.9 (7)
C8—N2—C7—N1	163.8 (4)	C8—C9—C10—C11	−0.1 (7)
C8—N2—C7—O1	−16.8 (7)	C9—C10—C11—C12	1.3 (7)
C6—C1—C2—C3	−2.1 (8)	C9—C10—C11—C14	−178.8 (4)
C2—C1—C6—N1	−179.5 (5)	C10—C11—C12—C13	−1.4 (7)
C2—C1—C6—C5	1.9 (7)	C14—C11—C12—C13	178.7 (4)
C1—C2—C3—C4	0.8 (9)	C10—C11—C14—O2	−177.4 (4)
C1—C2—C3—F1	178.9 (5)	C10—C11—C14—C15	3.0 (7)
F1—C3—C4—C5	−177.5 (5)	C12—C11—C14—O2	2.5 (7)
C2—C3—C4—C5	0.6 (9)	C12—C11—C14—C15	−177.2 (4)
C3—C4—C5—C6	−0.7 (9)	C11—C12—C13—C8	0.4 (8)

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O1[i]	0.79 (6)	2.17 (6)	2.927 (5)	160 (5)
N2—H2*N*···O2[ii]	0.88 (6)	2.30 (6)	3.070 (6)	147 (5)
C1—H1···O1	0.93	2.52	2.932 (6)	107

C10—H10···F1[iii]	0.93	2.49	3.386 (6)	162
C13—H13···O1	0.93	2.33	2.887 (7)	118

Symmetry codes: (i) $x-1, y, z$; (ii) $x-1, y+1, z$; (iii) $x-1/2, -y+1, z+1/2$.