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6-[(2-Chloropyridin-5-ylmethyl)(ethyl)-azanyl]-4-(2-fluorophenyl)-1-methyl-5-nitro-1,2,3,4-tetrahydropyridin-2-one

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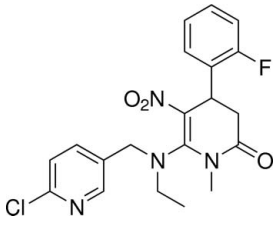
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.070; wR factor = 0.151; data-to-parameter ratio = 12.8.

In the title compound, $C_{20}H_{20}ClFN_4O_3$, the tetrahydropyridone ring adopts a skew boat conformation. The dihedral angle between the mean planes of the benzene and pyridine rings is 80.7 (3)°. In the crystal, weak C—H···O interactions are observed.

Related literature

For general background to neonicotinoid compounds and their application as insecticides, see: Jeschke & Nauen (2008); Kagabu & Matsuno (1997); Ohno *et al.* (2009); Shao *et al.* (2008); Tian *et al.* (2007); Tomizawa & Casida (2009). For the synthesis of the title compound, see: Zhang *et al.* (2010). For puckering parameters, see Cremer & Pople (1975).



Experimental

Crystal data

$C_{20}H_{20}ClFN_4O_3$
M_r = 418.85
Triclinic, $P\overline{1}$
a = 6.750 (2) Å
b = 8.262 (3) Å
c = 17.853 (6) Å
α = 94.981 (6)°
β = 91.302 (7)°
γ = 100.593 (7)°
V = 974.2 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 298 K
0.23 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.938, T_{max} = 0.954
5691 measured reflections
3391 independent reflections
1943 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.151
S = 0.96
3391 reflections
264 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8C···O1^{i}	0.96	2.46	3.383 (5)	161
C6—H6A···O3^{ii}	0.97	2.57	3.506 (5)	161
C3—H3···O1	0.93	2.53	3.320 (5)	143
C2—H2···O3^{iii}	0.93	2.46	3.344 (5)	159

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: JJ2119).

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supplementary materials

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6-[(2-Chloropyridin-5-ylmethyl)(ethyl)azanyl]-4-(2-fluorophenyl)-1-methyl-5-nitro-1,2,3,4-tetrahydropyridin-2-one

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Comment

In recent years, neonicotinoid insecticide compounds have rapidly grown and become a new chemical class of insecticides because of their novel structure and mode of action (Jeschke & Nauen,2008; Kagabu & Matsuno,1997; Ohno *et al.*, 2009; Shao *et al.*, 2008; Tian *et al.*, 2007; Tomizawa & Casida, 2009). We report here the synthesis and crystal structure of one of these compounds, $C_{20}H_{20}ClFN_4O_3$, the title compound, (I).

In (I) the tetrahydropyridone ring adopts a skew boat conformation with puckering paramers (Cremer & Pople, 1975) Q, θ and φ of 0.526 (4)Å, 113.2 (4)° and 22.0 (4)°) and a N2/C9/C10/N4 dihedral angle of -21.6 (6)° (Fig.1). In the tetrahydropyridone moiety, C11—C10, C12—C11 and C13—C12 bond lengths (1.499 (5) Å, 1.527 (5) Å and 1.503 (5) Å) are slightly shorter than normal. The C13—N3, C9—N3, and C10—N4 bond lengths (1.391 (4)Å, 1.417 (4)Å, and 1.422 (4)Å, respectively) are slightly shorter than normal while the C9═C10 bond length (1.360 (4)Å) is slightly longer than normal. The dihedral angle between the mean planes of the benzene and pryidine rings is 80.7 (3)°. In the crystal structure weak C2—H2···O3, C8—H8C···O1 and C6—H6A···O3 intermolecular interactions are observed which may influence crystal packing (Fig.2).

Experimental

In the preparation of the title compound, a solution of 2-fluorobenzaldehyde (15 mmol), Meldrum's acid (15 mmol) in ethanol (30 ml), with piperidine (0.1 mmol) used as catalyst, was added dropwise and the solution was stirred at room temperature for 2 h. Nitenpyram (2.75 g, 10 mmol) was added to the reaction mixture, heated to 65 °C for 6 h and then cooled to room temperature. The reaction mixture was concentrated under reduced pressure and treated with 20 ml of water whereby the solution was extracted three times with CH_2Cl_2, and the combined extracts were dried over $MgSO_4$. The organic phase was evaporated under reduced pressure and the crude product was subjected to flash chromatography on silica gel, eluting with ethyl acetate /petroleum ether to afford pure yellow crystals (yield 81%). Anal. calcd. for $C_{20}H_{20}ClFN_4O_3$ C 57.33, H 4.80, N 13.36% found, C 57.35, H 4.81, N 13.38%.

Refinement

All H atoms bonded to C were positioned geometrically [C—H = 0.93 Å (aromatic), 0.97 Å (methylene) and 0.96Å (methyl)] and refined in the riding mode with [U_{iso}(H) = 1.2U_{eq}(aromatic and methylene C) and 1.5U_{eq}(methyl C)].

Computing details

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART* (Bruker, 2001); data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication:

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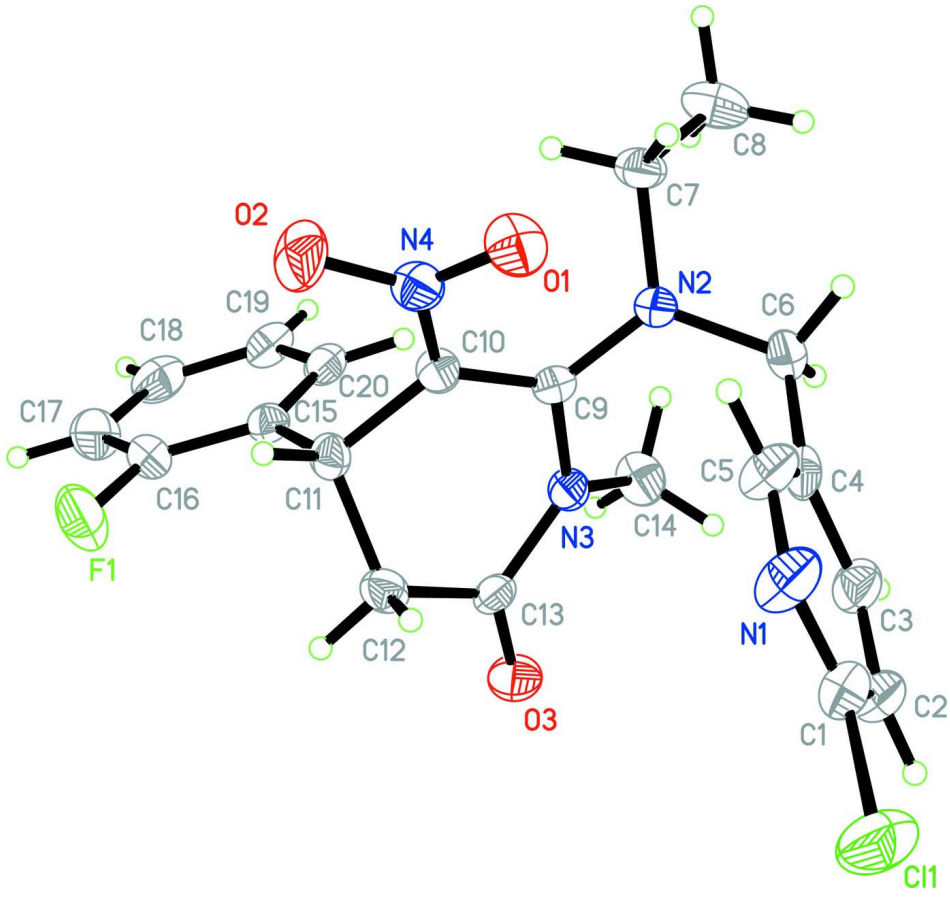

Figure 1

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

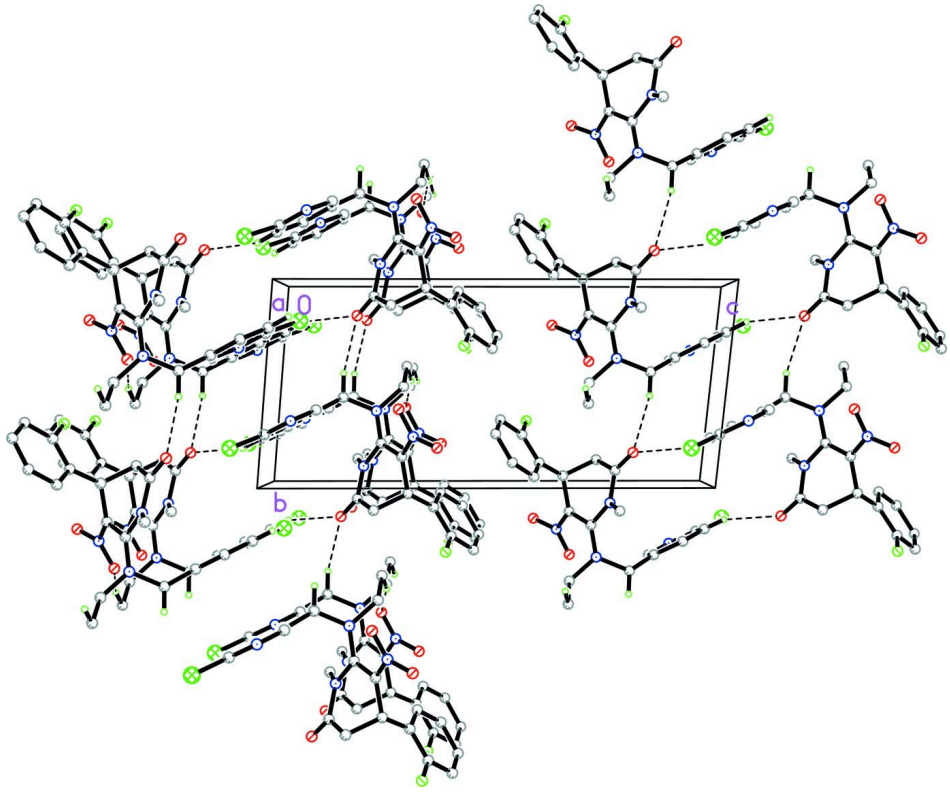

Figure 2

Packing of the title compound, (I), viewed along the *a* axis. Weak C2—H2···O3, C8—H8C···O1 and C6—H6A···O3 intermolecular interactions are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

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Crystal data

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Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.750$ (2) Å
$b = 8.262$ (3) Å
$c = 17.853$ (6) Å
$\alpha = 94.981$ (6)°
$\beta = 91.302$ (7)°
$\gamma = 100.593$ (7)°
$V = 974.2$ (6) Å^3
$Z = 2$
$F(000) = 436$
$D_x = 1.428$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 906 reflections
$\theta = 2.3$–19.9°
$\mu = 0.24$ mm^{-1}
$T = 298$ K
Block, yellow
0.23 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.938$, $T_{max} = 0.954$
5691 measured reflections
3391 independent reflections
1943 reflections with $I > 2\sigma(I)$

R_{int} = 0.073
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −7→8
k = −9→9
l = −21→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.151
S = 0.96
3391 reflections
264 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cl1	−0.0482 (2)	0.19595 (18)	1.06337 (7)	0.0963 (5)
F1	0.0556 (4)	−0.3141 (3)	0.57751 (14)	0.0768 (8)
O1	0.1183 (4)	0.3810 (3)	0.70839 (17)	0.0579 (8)
O2	0.0164 (4)	0.1954 (4)	0.61628 (17)	0.0745 (10)
O3	0.4797 (4)	−0.1603 (3)	0.82425 (15)	0.0613 (8)
N1	0.0698 (5)	0.3252 (5)	0.9407 (2)	0.0677 (11)
N2	0.5075 (4)	0.3694 (3)	0.76441 (15)	0.0358 (7)
N3	0.5073 (4)	0.0931 (3)	0.78309 (15)	0.0367 (7)
N4	0.1287 (5)	0.2474 (4)	0.67181 (19)	0.0457 (8)
C1	0.1333 (7)	0.2582 (5)	0.9985 (2)	0.0579 (12)
C2	0.3272 (8)	0.2367 (5)	1.0112 (2)	0.0620 (13)
H2	0.3632	0.1866	1.0528	0.074*
C3	0.2101 (7)	0.3769 (5)	0.8917 (2)	0.0595 (12)
H3	0.1690	0.4245	0.8501	0.071*
C4	0.4110 (6)	0.3647 (4)	0.8982 (2)	0.0431 (10)
C5	0.4664 (6)	0.2921 (5)	0.9599 (2)	0.0539 (11)
H5	0.5998	0.2804	0.9669	0.065*
C6	0.5569 (6)	0.4366 (4)	0.8427 (2)	0.0475 (11)
H6A	0.5631	0.5553	0.8461	0.057*
H6B	0.6899	0.4176	0.8567	0.057*
C7	0.5241 (6)	0.4907 (4)	0.7083 (2)	0.0468 (10)
H7A	0.4291	0.5638	0.7190	0.056*
H7B	0.4883	0.4331	0.6588	0.056*

C8	0.7339 (6)	0.5922 (5)	0.7079 (3)	0.0664 (13)
H8A	0.7682	0.6524	0.7563	0.100*
H8B	0.7388	0.6686	0.6701	0.100*
H8C	0.8283	0.5204	0.6970	0.100*
C9	0.4199 (5)	0.2097 (4)	0.74628 (18)	0.0333 (9)
C10	0.2653 (5)	0.1481 (4)	0.6955 (2)	0.0360 (9)
C11	0.2062 (5)	−0.0340 (4)	0.6735 (2)	0.0387 (9)
H11	0.0674	−0.0550	0.6527	0.046*
C12	0.2044 (5)	−0.1165 (4)	0.7469 (2)	0.0444 (10)
H12A	0.0999	−0.0843	0.7782	0.053*
H12B	0.1738	−0.2357	0.7359	0.053*
C13	0.4050 (6)	−0.0674 (5)	0.78885 (19)	0.0401 (9)
C14	0.7233 (5)	0.1245 (5)	0.8024 (2)	0.0539 (11)
H14A	0.7442	0.1457	0.8560	0.081*
H14B	0.7887	0.2190	0.7787	0.081*
H14C	0.7789	0.0297	0.7852	0.081*
C15	0.3356 (5)	−0.1057 (4)	0.6151 (2)	0.0371 (9)
C16	0.2525 (6)	−0.2468 (5)	0.5697 (2)	0.0491 (11)
C17	0.3578 (7)	−0.3229 (5)	0.5167 (2)	0.0621 (13)
H17	0.2958	−0.4175	0.4870	0.074*
C18	0.5569 (7)	−0.2557 (5)	0.5088 (2)	0.0590 (12)
H18	0.6323	−0.3060	0.4740	0.071*
C19	0.6450 (6)	−0.1144 (5)	0.5521 (2)	0.0500 (11)
H19	0.7796	−0.0685	0.5462	0.060*
C20	0.5345 (6)	−0.0401 (5)	0.6044 (2)	0.0418 (10)
H20	0.5957	0.0563	0.6330	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1069 (11)	0.1166 (12)	0.0622 (9)	0.0018 (9)	0.0239 (8)	0.0258 (8)
F1	0.0722 (17)	0.0626 (16)	0.0813 (18)	−0.0162 (13)	0.0080 (14)	−0.0141 (14)
O1	0.0526 (17)	0.0505 (18)	0.077 (2)	0.0280 (15)	−0.0045 (15)	0.0027 (16)
O2	0.074 (2)	0.072 (2)	0.077 (2)	0.0232 (17)	−0.0420 (18)	−0.0028 (17)
O3	0.087 (2)	0.0429 (17)	0.0585 (19)	0.0198 (16)	−0.0108 (16)	0.0156 (15)
N1	0.062 (2)	0.098 (3)	0.044 (2)	0.014 (2)	0.0000 (19)	0.013 (2)
N2	0.0406 (18)	0.0324 (17)	0.0344 (17)	0.0059 (14)	0.0014 (14)	0.0049 (14)
N3	0.0360 (17)	0.0358 (17)	0.0382 (18)	0.0071 (14)	−0.0067 (14)	0.0046 (14)
N4	0.0395 (19)	0.045 (2)	0.054 (2)	0.0081 (16)	−0.0040 (17)	0.0101 (17)
C1	0.073 (3)	0.059 (3)	0.038 (3)	0.006 (2)	0.003 (2)	−0.001 (2)
C2	0.089 (4)	0.059 (3)	0.038 (3)	0.010 (3)	−0.007 (2)	0.010 (2)
C3	0.067 (3)	0.077 (3)	0.037 (2)	0.015 (3)	−0.002 (2)	0.013 (2)
C4	0.050 (3)	0.040 (2)	0.036 (2)	0.008 (2)	−0.0077 (19)	−0.0111 (18)
C5	0.064 (3)	0.056 (3)	0.042 (3)	0.015 (2)	−0.012 (2)	0.004 (2)
C6	0.055 (3)	0.037 (2)	0.046 (2)	0.0004 (19)	−0.008 (2)	−0.0034 (18)
C7	0.056 (3)	0.037 (2)	0.050 (2)	0.0093 (19)	0.004 (2)	0.0132 (19)
C8	0.059 (3)	0.054 (3)	0.089 (4)	0.007 (2)	0.017 (3)	0.028 (3)
C9	0.036 (2)	0.035 (2)	0.031 (2)	0.0089 (17)	0.0030 (17)	0.0075 (16)
C10	0.033 (2)	0.035 (2)	0.041 (2)	0.0104 (17)	−0.0037 (17)	0.0038 (17)
C11	0.032 (2)	0.040 (2)	0.042 (2)	0.0021 (17)	−0.0060 (17)	0.0020 (18)

C12	0.046 (2)	0.040 (2)	0.045 (2)	0.0019 (18)	0.0107 (19)	0.0051 (18)
C13	0.056 (3)	0.039 (2)	0.026 (2)	0.012 (2)	0.0009 (18)	0.0049 (17)
C14	0.043 (2)	0.052 (3)	0.068 (3)	0.014 (2)	−0.010 (2)	0.003 (2)
C15	0.042 (2)	0.035 (2)	0.035 (2)	0.0100 (18)	−0.0018 (17)	0.0062 (17)
C16	0.054 (3)	0.041 (2)	0.048 (3)	−0.003 (2)	−0.001 (2)	0.006 (2)
C17	0.089 (4)	0.046 (3)	0.049 (3)	0.013 (3)	0.011 (3)	−0.006 (2)
C18	0.076 (3)	0.065 (3)	0.044 (3)	0.031 (3)	0.009 (2)	0.010 (2)
C19	0.054 (3)	0.064 (3)	0.037 (2)	0.022 (2)	0.001 (2)	0.009 (2)
C20	0.049 (2)	0.046 (2)	0.032 (2)	0.011 (2)	−0.0010 (18)	0.0057 (18)

Geometric parameters (Å, º)

Cl1—C1	1.744 (4)	C7—H7B	0.9700
F1—C16	1.358 (4)	C8—H8A	0.9600
O1—N4	1.247 (4)	C8—H8B	0.9600
O2—N4	1.231 (4)	C8—H8C	0.9600
O3—C13	1.206 (4)	C9—C10	1.360 (4)
N1—C1	1.312 (5)	C10—C11	1.499 (5)
N1—C3	1.342 (5)	C11—C15	1.526 (5)
N2—C9	1.352 (4)	C11—C12	1.527 (5)
N2—C6	1.467 (4)	C11—H11	0.9800
N2—C7	1.469 (4)	C12—C13	1.503 (5)
N3—C13	1.391 (4)	C12—H12A	0.9700
N3—C9	1.417 (4)	C12—H12B	0.9700
N3—C14	1.461 (4)	C14—H14A	0.9600
N4—C10	1.422 (4)	C14—H14B	0.9600
C1—C2	1.370 (6)	C14—H14C	0.9600
C2—C5	1.373 (5)	C15—C20	1.376 (5)
C2—H2	0.9300	C15—C16	1.381 (5)
C3—C4	1.381 (5)	C16—C17	1.373 (5)
C3—H3	0.9300	C17—C18	1.372 (5)
C4—C5	1.374 (5)	C17—H17	0.9300
C4—C6	1.495 (5)	C18—C19	1.371 (5)
C5—H5	0.9300	C18—H18	0.9300
C6—H6A	0.9700	C19—C20	1.381 (5)
C6—H6B	0.9700	C19—H19	0.9300
C7—C8	1.508 (5)	C20—H20	0.9300
C7—H7A	0.9700		

C1—N1—C3	115.8 (4)	N2—C9—N3	115.0 (3)
C9—N2—C6	121.8 (3)	C10—C9—N3	116.8 (3)
C9—N2—C7	121.2 (3)	C9—C10—N4	121.7 (3)
C6—N2—C7	116.1 (3)	C9—C10—C11	121.2 (3)
C13—N3—C9	122.3 (3)	N4—C10—C11	116.0 (3)
C13—N3—C14	115.9 (3)	C10—C11—C15	115.7 (3)
C9—N3—C14	120.6 (3)	C10—C11—C12	105.8 (3)
O2—N4—O1	121.0 (3)	C15—C11—C12	112.4 (3)
O2—N4—C10	118.5 (3)	C10—C11—H11	107.5
O1—N4—C10	120.4 (3)	C15—C11—H11	107.5
N1—C1—C2	125.1 (4)	C12—C11—H11	107.5

N1—C1—Cl1	115.6 (4)	C13—C12—C11	110.8 (3)
C2—C1—Cl1	119.3 (4)	C13—C12—H12A	109.5
C1—C2—C5	117.3 (4)	C11—C12—H12A	109.5
C1—C2—H2	121.4	C13—C12—H12B	109.5
C5—C2—H2	121.4	C11—C12—H12B	109.5
N1—C3—C4	125.0 (4)	H12A—C12—H12B	108.1
N1—C3—H3	117.5	O3—C13—N3	120.4 (3)
C4—C3—H3	117.5	O3—C13—C12	123.4 (3)
C5—C4—C3	116.0 (4)	N3—C13—C12	116.2 (3)
C5—C4—C6	123.5 (4)	N3—C14—H14A	109.5
C3—C4—C6	120.3 (4)	N3—C14—H14B	109.5
C2—C5—C4	120.8 (4)	H14A—C14—H14B	109.5
C2—C5—H5	119.6	N3—C14—H14C	109.5
C4—C5—H5	119.6	H14A—C14—H14C	109.5
N2—C6—C4	114.6 (3)	H14B—C14—H14C	109.5
N2—C6—H6A	108.6	C20—C15—C16	116.4 (4)
C4—C6—H6A	108.6	C20—C15—C11	124.4 (3)
N2—C6—H6B	108.6	C16—C15—C11	119.2 (3)
C4—C6—H6B	108.6	F1—C16—C17	118.1 (4)
H6A—C6—H6B	107.6	F1—C16—C15	118.4 (4)
N2—C7—C8	112.1 (3)	C17—C16—C15	123.6 (4)
N2—C7—H7A	109.2	C18—C17—C16	118.3 (4)
C8—C7—H7A	109.2	C18—C17—H17	120.9
N2—C7—H7B	109.2	C16—C17—H17	120.9
C8—C7—H7B	109.2	C19—C18—C17	120.1 (4)
H7A—C7—H7B	107.9	C19—C18—H18	119.9
C7—C8—H8A	109.5	C17—C18—H18	119.9
C7—C8—H8B	109.5	C18—C19—C20	120.2 (4)
H8A—C8—H8B	109.5	C18—C19—H19	119.9
C7—C8—H8C	109.5	C20—C19—H19	119.9
H8A—C8—H8C	109.5	C15—C20—C19	121.4 (4)
H8B—C8—H8C	109.5	C15—C20—H20	119.3
N2—C9—C10	128.1 (3)	C19—C20—H20	119.3

C3—N1—C1—C2	−0.7 (7)	O2—N4—C10—C11	−24.8 (5)
C3—N1—C1—Cl1	178.5 (3)	O1—N4—C10—C11	152.5 (3)
N1—C1—C2—C5	1.1 (7)	C9—C10—C11—C15	−80.5 (4)
Cl1—C1—C2—C5	−178.1 (3)	N4—C10—C11—C15	111.0 (3)
C1—N1—C3—C4	−0.2 (7)	C9—C10—C11—C12	44.6 (4)
N1—C3—C4—C5	0.7 (6)	N4—C10—C11—C12	−123.9 (3)
N1—C3—C4—C6	−175.9 (4)	C10—C11—C12—C13	−56.2 (4)
C1—C2—C5—C4	−0.5 (6)	C15—C11—C12—C13	70.9 (4)
C3—C4—C5—C2	−0.3 (6)	C9—N3—C13—O3	−175.8 (3)
C6—C4—C5—C2	176.2 (3)	C14—N3—C13—O3	17.0 (5)
C9—N2—C6—C4	−34.4 (5)	C9—N3—C13—C12	6.1 (5)
C7—N2—C6—C4	134.8 (3)	C14—N3—C13—C12	−161.1 (3)
C5—C4—C6—N2	124.5 (4)	C11—C12—C13—O3	−143.5 (4)
C3—C4—C6—N2	−59.1 (5)	C11—C12—C13—N3	34.5 (4)
C9—N2—C7—C8	−131.8 (4)	C10—C11—C15—C20	27.1 (5)

C6—N2—C7—C8	58.8 (4)	C12—C11—C15—C20	−94.5 (4)
C6—N2—C9—C10	136.3 (4)	C10—C11—C15—C16	−153.7 (3)
C7—N2—C9—C10	−32.4 (5)	C12—C11—C15—C16	84.6 (4)
C6—N2—C9—N3	−46.4 (4)	C20—C15—C16—F1	−179.0 (3)
C7—N2—C9—N3	144.8 (3)	C11—C15—C16—F1	1.8 (5)
C13—N3—C9—N2	160.7 (3)	C20—C15—C16—C17	0.9 (6)
C14—N3—C9—N2	−32.6 (4)	C11—C15—C16—C17	−178.4 (4)
C13—N3—C9—C10	−21.8 (5)	F1—C16—C17—C18	−179.8 (4)
C14—N3—C9—C10	144.9 (3)	C15—C16—C17—C18	0.4 (6)
N2—C9—C10—N4	−21.6 (6)	C16—C17—C18—C19	−1.2 (6)
N3—C9—C10—N4	161.2 (3)	C17—C18—C19—C20	0.7 (6)
N2—C9—C10—C11	170.6 (3)	C16—C15—C20—C19	−1.4 (5)
N3—C9—C10—C11	−6.6 (5)	C11—C15—C20—C19	177.8 (3)
O2—N4—C10—C9	166.7 (3)	C18—C19—C20—C15	0.7 (5)
O1—N4—C10—C9	−16.0 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*C*···O1^{i}	0.96	2.46	3.383 (5)	161
C6—H6*A*···O3^{ii}	0.97	2.57	3.506 (5)	161
C3—H3···O1	0.93	2.53	3.320 (5)	143
C2—H2···O3^{iii}	0.93	2.46	3.344 (5)	159

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