Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-[4-Chloro-2-methyl-6-(*N*-methylcarbamoyl)phenyl]-1-(3-chloro-2-pyridyl)-3-trifluoromethyl-1*H*-pyrazole-5-carboxamide

Huibin Yang, Haibo Yu and Bin Li*

Agrochemicals Division, Shenyang Research Institute of Chemical Industry, Shenyang 110021, People's Republic of China
Correspondence e-mail: libin1@sinochem.com

Received 8 August 2008; accepted 16 November 2008

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.034; wR factor = 0.082; data-to-parameter ratio = 11.5.

In the title compound, $C_{19}H_{14}Cl_2F_3N_5O_2$, which shows insecticidal activity, the dihedral angle between the pyrazole and pyridine rings is 68.15 (16)°. In the crystal structure, the molecules are linked by N—H···O and C—H···O hydrogen bonds and an intramolecular N—H···O interaction also occurs. The F atoms of the –CF_3 group are disordered over two sets of sites in a 0.800 (8):0.200 (8) ratio.

Related literature

For the synthesis and background to the insecticidal properties of the title compound, see: Lahm *et al.* (2003, 2005).

Experimental

Crystal data

$C_{19}H_{14}Cl_2F_3N_5O_2$
M_r = 472.25
Orthorhombic, *Fdd*2
a = 26.4612 (16) Å
b = 32.8657 (19) Å
c = 9.4679 (6) Å
V = 8233.9 (9) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 296 (2) K
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.917, T_{max} = 0.937
10439 measured reflections
3565 independent reflections
3284 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.082
S = 1.04
3565 reflections
310 parameters
49 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack (1983), 1621 Friedel pairs
Flack parameter: −0.01 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O2	0.86	2.37	2.673 (3)	101
N4—H4···O2^{i}	0.86	2.25	3.107 (3)	176
N5—H5···O1^{ii}	0.86	2.16	2.915 (3)	146
C8—H8···O2^{i}	0.93	2.50	3.168 (4)	129

Symmetry codes: (i) $-x+1, -y+2, z$; (ii) $x+\frac{1}{4}, -y+\frac{7}{4}, z-\frac{1}{4}$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2777).

References

Bruker (1999). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Lahm, G. P., Selby, T. P., Freudenberger, J. H., Stevenson, T. M., Myers, B. M., Seburyamo, G., Smith, B. K., Flexner, L., Clark, C. E. & Cordova, D. (2005). *Bioorg. Med. Chem. Lett.* **15**, 4898–4906.
Lahm, G. P., Selby, T. P. & Stevenson, T. M. (2003). International Patent Number WO 03/015 519.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, o2378 [doi:10.1107/S1600536808037604]

N-[4-Chloro-2-methyl-6-(*N*-methylcarbamoyl)phenyl]-1-(3-chloro-2-pyridyl)-3-trifluoromethyl-1*H*-pyrazole-5-carboxamide

Huibin Yang, Haibo Yu and Bin Li

S1. Comment

Anthranilamide compounds containing an N-pyridyl pyrazole grouping are a new class of inseticides showing potent activity against a broad spectrum of Lepidoptera and no-cross resistance to existing insecticides (Lahm *et al.*, 2003) and their mode of action has been been established (Lahm *et al.*, 2005). Anthranilamides show little effect on mammalian ryanodine receptors and as a result they show excellent insect *versus* mammalian selectivity. As part of our studies in this area, we now report the crystal structures of the title compound, (I), (Fig. 1) which possesses high insecticidal activity.

The pyrazole ring and pyridine rings are not coplanar, the dihedral angle formed by the least-squares planes of the rings being equal to 68.15 (16)°. The dihedral angle between the mean plane of the pyrazole ring and the plane of the C10/O1/N4 group is 23.4 (2)° and the dihedral angle between the mean plane of the phenyl ring and the plane of the C10/O1/N4 group is 59.9 (2)°.

An intramolecular N—H···O hydrogen bond (Table 1) is observed, which helps to establish the molecular conformation. Intermolecular N—H···O and C—H···O bonds result in a three-dimensional network.

S2. Experimental

The title compound was prepared by the literature method (Lahm *et al.*, 2003). The crude products were purified by silica-gel column chromatography and then grown from acetone to afford colourless blocks of (I).

Anal. Calcd for $C_{12}H_{14}N_4O_3$: C, 48.32; H, 2.99; N, 14.83. Found: C, 48.47; H, 3.04; N, 14.66. ^{1}H NMR($CDCl_3$): 2.19 (s, 3H, CH_3), 2.70 (d, J=4.5 Hz, 3H, CH_3), 7.30–7.31 (m, 2H, Ph), 7.57 (dd, 1H), 8.05 (d, J=8.1 Hz, 1H), 8.22 (br s, J=4.5 Hz, 1H, NH), 8.46 (d, J=4.8 Hz, 1H), 7.64 (s, 1H), 10.43 (s, 1H, NH).

S3. Refinement

Although all H atoms were visible in difference maps, they were placed in geometrically calculated positions, with C—H distances in the range 0.93–0.96Å and N—H distances of 0.86 Å, andincluded in the final refinement in the riding model approximation,with U_{iso}(H) = 1.2U_{eq}(C, N) or 1.5U_{eq}(methyl C). The F atoms of the -CF_3 are disordered over two sets of sites in a 0.800 (8):0.200 (8) ratio.

N-[4-Chloro-2-methyl-6-(N-methylcarbamoyl)phenyl]-1-(3-chloro-2- pyridyl)-3-trifluoromethyl-1*H*-pyrazole-5-carboxamide

Crystal data

$C_{19}H_{14}Cl_2F_3N_5O_2$	a = 26.4612 (16) Å
M_r = 472.25	b = 32.8657 (19) Å
Orthorhombic, *Fdd*2	c = 9.4679 (6) Å

V = 8233.9 (9) Å^3
Z = 16
F(000) = 3840
D_x = 1.524 Mg m^{-3}
Melting point: 492(1) K
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 3952 reflections
θ = 2.4–23.9°
μ = 0.37 mm^{-1}
T = 296 K
Block, colourless
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.917, T_{max} = 0.937

10439 measured reflections
3565 independent reflections
3284 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 25.0°, θ_{min} = 2.0°
h = −31→24
k = −34→38
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.082
S = 1.04
3565 reflections
310 parameters
49 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
$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2 + 8.8659P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack (1983), 1621 Friedel pairs
Absolute structure parameter: −0.01 (7)

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	0.28309 (3)	1.00598 (3)	0.40561 (10)	0.0647 (3)	
Cl2	0.46782 (4)	0.85540 (5)	−0.17854 (12)	0.1075 (5)	
F1	0.39895 (14)	1.06805 (12)	0.8595 (6)	0.1059 (17)	0.800 (8)
F2	0.4312 (2)	1.01859 (14)	0.9614 (4)	0.1148 (18)	0.800 (8)
F3	0.47071 (12)	1.04708 (16)	0.7981 (5)	0.0958 (15)	0.800 (8)
F1′	0.4028 (5)	1.0381 (5)	0.9535 (11)	0.074 (4)	0.200 (8)
F2′	0.4714 (4)	1.0263 (5)	0.8653 (18)	0.087 (5)	0.200 (8)
F3′	0.4283 (7)	1.0724 (3)	0.7878 (16)	0.106 (6)	0.200 (8)
O1	0.36097 (7)	0.91496 (6)	0.4022 (2)	0.0453 (5)	

O2	0.52136 (8)	0.96046 (6)	0.3535 (3)	0.0576 (6)
N1	0.35642 (9)	0.99358 (8)	0.7518 (3)	0.0445 (6)
N2	0.34753 (8)	0.97021 (6)	0.6376 (2)	0.0360 (5)
N3	0.28654 (9)	0.92344 (8)	0.7109 (3)	0.0479 (6)
N4	0.42127 (8)	0.95772 (6)	0.3170 (2)	0.0342 (5)
H4	0.4359	0.9808	0.3291	0.041*
N5	0.56488 (8)	0.90701 (7)	0.2779 (3)	0.0419 (6)
H5	0.5672	0.8873	0.2186	0.050*
C1	0.26575 (11)	0.96695 (9)	0.5174 (3)	0.0448 (7)
C2	0.21856 (11)	0.94974 (11)	0.5056 (4)	0.0566 (9)
H2	0.1958	0.9587	0.4375	0.068*
C3	0.20605 (12)	0.91908 (11)	0.5966 (4)	0.0602 (10)
H3	0.1747	0.9064	0.5899	0.072*
C4	0.23980 (14)	0.90720 (10)	0.6975 (4)	0.0592 (9)
H4A	0.2302	0.8869	0.7604	0.071*
C5	0.29811 (10)	0.95245 (8)	0.6209 (3)	0.0379 (6)
C6	0.40279 (10)	1.00776 (9)	0.7321 (3)	0.0434 (7)
C7	0.42585 (12)	1.03518 (11)	0.8368 (4)	0.0596 (9)
C8	0.42392 (10)	0.99401 (9)	0.6056 (3)	0.0429 (7)
H8	0.4558	1.0000	0.5695	0.052*
C9	0.38752 (10)	0.96987 (8)	0.5464 (3)	0.0346 (6)
C10	0.38824 (9)	0.94496 (7)	0.4152 (3)	0.0329 (6)
C11	0.43316 (10)	0.93476 (7)	0.1941 (3)	0.0323 (6)
C12	0.48281 (9)	0.92011 (7)	0.1738 (3)	0.0319 (6)
C13	0.49293 (10)	0.89622 (9)	0.0565 (3)	0.0415 (6)
H13	0.5254	0.8864	0.0410	0.050*
C14	0.45484 (12)	0.88718 (10)	−0.0367 (3)	0.0534 (8)
C15	0.40693 (11)	0.90324 (10)	−0.0207 (3)	0.0507 (8)
H15	0.3822	0.8976	−0.0875	0.061*
C16	0.39557 (10)	0.92751 (9)	0.0935 (3)	0.0401 (6)
C17	0.34412 (11)	0.94686 (11)	0.1030 (4)	0.0565 (8)
H17A	0.3290	0.9476	0.0108	0.085*
H17B	0.3474	0.9741	0.1385	0.085*
H17C	0.3232	0.9313	0.1656	0.085*
C18	0.52432 (10)	0.93058 (8)	0.2762 (3)	0.0334 (6)
C19	0.60538 (12)	0.91391 (11)	0.3778 (4)	0.0597 (9)
H19A	0.6216	0.9394	0.3571	0.090*
H19B	0.6296	0.8923	0.3708	0.090*
H19C	0.5918	0.9147	0.4718	0.090*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0572 (5)	0.0631 (5)	0.0737 (6)	0.0044 (4)	−0.0053 (4)	0.0203 (5)
Cl2	0.0781 (7)	0.1621 (12)	0.0821 (8)	0.0360 (7)	−0.0273 (6)	−0.0839 (8)
F1	0.090 (2)	0.090 (2)	0.137 (3)	0.0050 (19)	−0.020 (2)	−0.063 (2)
F2	0.168 (4)	0.117 (3)	0.059 (2)	−0.042 (3)	−0.040 (2)	−0.0052 (18)
F3	0.067 (2)	0.132 (3)	0.088 (3)	−0.0499 (19)	0.0139 (17)	−0.043 (2)

F1′	0.067 (6)	0.095 (6)	0.060 (6)	−0.014 (5)	0.009 (4)	−0.021 (5)
F2′	0.072 (6)	0.094 (6)	0.094 (7)	0.004 (5)	−0.017 (5)	−0.018 (5)
F3′	0.121 (8)	0.094 (7)	0.103 (7)	−0.008 (5)	−0.014 (5)	−0.004 (5)
O1	0.0485 (11)	0.0440 (11)	0.0433 (11)	−0.0146 (9)	0.0108 (10)	−0.0005 (9)
O2	0.0434 (12)	0.0537 (12)	0.0757 (17)	0.0105 (10)	−0.0185 (11)	−0.0324 (12)
N1	0.0407 (13)	0.0564 (15)	0.0365 (13)	−0.0054 (11)	0.0038 (10)	−0.0095 (11)
N2	0.0312 (11)	0.0441 (12)	0.0326 (12)	−0.0019 (9)	0.0043 (9)	−0.0051 (10)
N3	0.0511 (15)	0.0500 (14)	0.0426 (14)	−0.0052 (12)	0.0153 (11)	−0.0014 (12)
N4	0.0332 (11)	0.0331 (11)	0.0364 (13)	−0.0044 (9)	0.0052 (10)	−0.0030 (10)
N5	0.0347 (12)	0.0433 (13)	0.0478 (14)	0.0065 (10)	−0.0059 (10)	−0.0128 (11)
C1	0.0378 (16)	0.0472 (16)	0.0492 (18)	0.0027 (13)	0.0053 (13)	−0.0069 (14)
C2	0.0356 (17)	0.067 (2)	0.067 (2)	−0.0003 (15)	−0.0020 (16)	−0.0149 (18)
C3	0.0381 (17)	0.068 (2)	0.075 (2)	−0.0137 (16)	0.0124 (17)	−0.022 (2)
C4	0.065 (2)	0.0553 (19)	0.058 (2)	−0.0176 (17)	0.0271 (17)	−0.0078 (16)
C5	0.0335 (14)	0.0422 (15)	0.0380 (16)	−0.0023 (11)	0.0100 (12)	−0.0074 (12)
C6	0.0380 (16)	0.0545 (17)	0.0376 (16)	−0.0054 (13)	−0.0001 (12)	−0.0042 (13)
C7	0.0503 (19)	0.077 (2)	0.052 (2)	−0.0108 (18)	0.0062 (16)	−0.0155 (18)
C8	0.0326 (14)	0.0557 (17)	0.0405 (16)	−0.0058 (13)	0.0051 (12)	−0.0010 (13)
C9	0.0337 (14)	0.0392 (14)	0.0307 (13)	0.0022 (11)	0.0021 (11)	0.0020 (11)
C10	0.0288 (13)	0.0351 (13)	0.0347 (14)	0.0006 (11)	0.0028 (11)	0.0050 (11)
C11	0.0330 (13)	0.0329 (13)	0.0310 (14)	−0.0043 (11)	0.0016 (11)	0.0042 (10)
C12	0.0314 (13)	0.0310 (12)	0.0333 (14)	−0.0044 (10)	0.0008 (11)	0.0008 (11)
C13	0.0357 (14)	0.0499 (16)	0.0391 (15)	0.0027 (12)	0.0002 (12)	−0.0068 (13)
C14	0.0502 (18)	0.069 (2)	0.0405 (17)	0.0035 (16)	−0.0066 (13)	−0.0218 (16)
C15	0.0422 (17)	0.071 (2)	0.0392 (17)	−0.0054 (15)	−0.0108 (13)	−0.0092 (16)
C16	0.0319 (14)	0.0501 (16)	0.0383 (16)	−0.0040 (12)	0.0012 (11)	0.0034 (13)
C17	0.0365 (15)	0.085 (2)	0.0481 (19)	0.0068 (16)	−0.0051 (14)	0.0040 (16)
C18	0.0335 (14)	0.0308 (13)	0.0359 (15)	−0.0015 (11)	−0.0003 (11)	−0.0020 (11)
C19	0.0393 (17)	0.073 (2)	0.067 (2)	0.0107 (15)	−0.0141 (15)	−0.0186 (19)

Geometric parameters (Å, º)

Cl1—C1	1.725 (3)	C2—H2	0.9300
Cl2—C14	1.736 (3)	C3—C4	1.365 (5)
F1—C7	1.311 (4)	C3—H3	0.9300
F2—C7	1.307 (4)	C4—H4A	0.9300
F3—C7	1.303 (4)	C6—C8	1.397 (4)
F1′—C7	1.266 (8)	C6—C7	1.472 (4)
F2′—C7	1.269 (8)	C8—C9	1.368 (4)
F3′—C7	1.310 (8)	C8—H8	0.9300
O1—C10	1.228 (3)	C9—C10	1.488 (4)
O2—C18	1.227 (3)	C11—C16	1.397 (4)
N1—C6	1.326 (4)	C11—C12	1.412 (4)
N1—N2	1.347 (3)	C12—C13	1.387 (4)
N2—C9	1.366 (3)	C12—C18	1.505 (3)
N2—C5	1.441 (3)	C13—C14	1.372 (4)
N3—C5	1.315 (4)	C13—H13	0.9300
N3—C4	1.353 (4)	C14—C15	1.382 (4)

N4—C10	1.343 (3)	C15—C16	1.377 (4)
N4—C11	1.423 (3)	C15—H15	0.9300
N4—H4	0.8600	C16—C17	1.505 (4)
N5—C18	1.324 (3)	C17—H17A	0.9600
N5—C19	1.447 (4)	C17—H17B	0.9600
N5—H5	0.8600	C17—H17C	0.9600
C1—C2	1.375 (4)	C19—H19A	0.9600
C1—C5	1.386 (4)	C19—H19B	0.9600
C2—C3	1.367 (5)	C19—H19C	0.9600

C6—N1—N2	104.4 (2)	F3—C7—C6	111.8 (3)
N1—N2—C9	112.1 (2)	F2—C7—C6	113.4 (3)
N1—N2—C5	118.5 (2)	F3′—C7—C6	110.7 (7)
C9—N2—C5	129.1 (2)	F1—C7—C6	112.9 (3)
C5—N3—C4	116.0 (3)	C9—C8—C6	104.9 (2)
C10—N4—C11	123.0 (2)	C9—C8—H8	127.5
C10—N4—H4	118.5	C6—C8—H8	127.5
C11—N4—H4	118.5	N2—C9—C8	106.3 (2)
C18—N5—C19	121.1 (2)	N2—C9—C10	122.9 (2)
C18—N5—H5	119.5	C8—C9—C10	130.7 (2)
C19—N5—H5	119.5	O1—C10—N4	124.3 (2)
C2—C1—C5	118.5 (3)	O1—C10—C9	121.2 (2)
C2—C1—Cl1	119.8 (3)	N4—C10—C9	114.5 (2)
C5—C1—Cl1	121.7 (2)	C16—C11—C12	120.8 (2)
C3—C2—C1	118.1 (3)	C16—C11—N4	119.4 (2)
C3—C2—H2	120.9	C12—C11—N4	119.8 (2)
C1—C2—H2	120.9	C13—C12—C11	118.8 (2)
C4—C3—C2	119.6 (3)	C13—C12—C18	120.3 (2)
C4—C3—H3	120.2	C11—C12—C18	120.9 (2)
C2—C3—H3	120.2	C14—C13—C12	119.7 (3)
N3—C4—C3	123.4 (3)	C14—C13—H13	120.1
N3—C4—H4A	118.3	C12—C13—H13	120.1
C3—C4—H4A	118.3	C13—C14—C15	121.4 (3)
N3—C5—C1	124.3 (3)	C13—C14—Cl2	118.8 (2)
N3—C5—N2	115.7 (3)	C15—C14—Cl2	119.8 (2)
C1—C5—N2	119.9 (2)	C16—C15—C14	120.5 (3)
N1—C6—C8	112.2 (3)	C16—C15—H15	119.7
N1—C6—C7	120.2 (3)	C14—C15—H15	119.7
C8—C6—C7	127.6 (3)	C15—C16—C11	118.6 (3)
F1′—C7—F2′	106.9 (8)	C15—C16—C17	119.3 (3)
F1′—C7—F3	131.5 (6)	C11—C16—C17	122.1 (3)
F2′—C7—F3	42.6 (7)	C16—C17—H17A	109.5
F1′—C7—F2	45.3 (7)	C16—C17—H17B	109.5
F2′—C7—F2	67.0 (8)	H17A—C17—H17B	109.5
F3—C7—F2	106.3 (4)	C16—C17—H17C	109.5
F1′—C7—F3′	105.2 (8)	H17A—C17—H17C	109.5
F2′—C7—F3′	104.1 (8)	H17B—C17—H17C	109.5
F3—C7—F3′	64.8 (8)	O2—C18—N5	120.9 (2)

F2—C7—F3′	134.7 (7)	O2—C18—C12	121.4 (2)
F1′—C7—F1	62.1 (7)	N5—C18—C12	117.7 (2)
F2′—C7—F1	132.1 (7)	N5—C19—H19A	109.5
F3—C7—F1	107.1 (4)	N5—C19—H19B	109.5
F2—C7—F1	104.8 (4)	H19A—C19—H19B	109.5
F3′—C7—F1	46.8 (8)	N5—C19—H19C	109.5
F1′—C7—C6	115.8 (6)	H19A—C19—H19C	109.5
F2′—C7—C6	113.3 (7)	H19B—C19—H19C	109.5
C6—N1—N2—C9	−0.5 (3)	N1—N2—C9—C10	177.2 (2)
C6—N1—N2—C5	−175.3 (2)	C5—N2—C9—C10	−8.7 (4)
C5—C1—C2—C3	−0.1 (4)	C6—C8—C9—N2	−0.2 (3)
Cl1—C1—C2—C3	−179.5 (3)	C6—C8—C9—C10	−176.6 (3)
C1—C2—C3—C4	1.5 (5)	C11—N4—C10—O1	−8.6 (4)
C5—N3—C4—C3	1.0 (4)	C11—N4—C10—C9	170.3 (2)
C2—C3—C4—N3	−2.0 (5)	N2—C9—C10—O1	−22.0 (4)
C4—N3—C5—C1	0.5 (4)	C8—C9—C10—O1	154.0 (3)
C4—N3—C5—N2	178.7 (2)	N2—C9—C10—N4	159.1 (2)
C2—C1—C5—N3	−1.0 (4)	C8—C9—C10—N4	−24.9 (4)
Cl1—C1—C5—N3	178.5 (2)	C10—N4—C11—C16	64.7 (3)
C2—C1—C5—N2	−179.1 (3)	C10—N4—C11—C12	−116.2 (3)
Cl1—C1—C5—N2	0.4 (4)	C16—C11—C12—C13	−3.9 (4)
N1—N2—C5—N3	−69.8 (3)	N4—C11—C12—C13	177.1 (2)
C9—N2—C5—N3	116.4 (3)	C16—C11—C12—C18	175.2 (2)
N1—N2—C5—C1	108.4 (3)	N4—C11—C12—C18	−3.8 (3)
C9—N2—C5—C1	−65.4 (4)	C11—C12—C13—C14	−0.3 (4)
N2—N1—C6—C8	0.4 (3)	C18—C12—C13—C14	−179.4 (3)
N2—N1—C6—C7	179.6 (3)	C12—C13—C14—C15	3.7 (5)
N1—C6—C7—F1′	11.8 (10)	C12—C13—C14—Cl2	−177.2 (2)
C8—C6—C7—F1′	−169.1 (10)	C13—C14—C15—C16	−2.8 (5)
N1—C6—C7—F2′	135.8 (10)	Cl2—C14—C15—C16	178.0 (3)
C8—C6—C7—F2′	−45.1 (11)	C14—C15—C16—C11	−1.4 (4)
N1—C6—C7—F3	−177.9 (4)	C14—C15—C16—C17	175.9 (3)
C8—C6—C7—F3	1.1 (6)	C12—C11—C16—C15	4.7 (4)
N1—C6—C7—F2	61.9 (5)	N4—C11—C16—C15	−176.2 (2)
C8—C6—C7—F2	−119.0 (5)	C12—C11—C16—C17	−172.5 (3)
N1—C6—C7—F3′	−107.7 (10)	N4—C11—C16—C17	6.6 (4)
C8—C6—C7—F3′	71.4 (11)	C19—N5—C18—O2	4.6 (4)
N1—C6—C7—F1	−57.1 (5)	C19—N5—C18—C12	−177.1 (3)
C8—C6—C7—F1	122.0 (4)	C13—C12—C18—O2	157.4 (3)
N1—C6—C8—C9	−0.2 (3)	C11—C12—C18—O2	−21.8 (4)
C7—C6—C8—C9	−179.3 (3)	C13—C12—C18—N5	−21.0 (4)
N1—N2—C9—C8	0.4 (3)	C11—C12—C18—N5	159.9 (2)
C5—N2—C9—C8	174.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···O2	0.86	2.37	2.673 (3)	101
N4—H4···O2^{i}	0.86	2.25	3.107 (3)	176
N5—H5···O1^{ii}	0.86	2.16	2.915 (3)	146
C8—H8···O2^{i}	0.93	2.50	3.168 (4)	129

Symmetry codes: (i) −*x*+1, −*y*+2, *z*; (ii) *x*+1/4, −*y*+7/4, *z*−1/4.