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3-Bromo-1-(3-chloropyridin-2-yl)-*N*-(4-ethoxyphenyl)-1*H*-pyrazole-5-carboxamide

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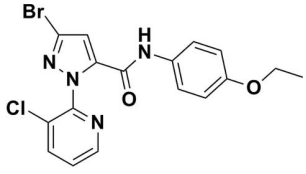
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.003 Å; R factor = 0.029; wR factor = 0.064; data-to-parameter ratio = 12.8.

In the title compound, $C_{17}H_{14}BrClN_4O_2$, the pyrazole ring is almost coplanar with the benzene ring [dihedral angle = 0.5 (2)°], whereas the pyrazole ring is close to perpendicular to the 3-chloropyridine ring [dihedral angle = 73.7 (2)°]. An intramolecular C—H···O hydrogen bond occurs. The dominant interaction in the crystal packing is an N—H···N hydrogen bond, which generates a chain along the c axis. Weak intermolecular C—H···O and C—H···N contacts are also observed

Related literature

For details of the synthesis, see: Dong *et al.* (2009). For the biological activity of related compounds, see: Gewehr *et al.* (2007); Dong *et al.* (2008*a*,*b*); Liu *et al.* (2007); Liu *et al.* (2009*a*,*b*,*c*).



Experimental

Crystal data

$C_{17}H_{14}BrClN_4O_2$
M_r = 421.68
Monoclinic, $P2_1/c$
a = 16.821 (3) Å
b = 10.195 (2) Å
c = 10.064 (2) Å
β = 101.09 (3)°
V = 1693.7 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.60 mm^{-1}
T = 113 K
0.16 × 0.12 × 0.08 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*CrystalClear*, Rigaku/MSC, 2002)
T_{min} = 0.681, T_{max} = 0.819
11217 measured reflections
2967 independent reflections
2459 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.064
S = 0.99
2967 reflections
231 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N4^{i}	0.88 (1)	2.21 (1)	3.059 (3)	165 (2)
C2—H2···O2	0.93	2.26	2.850 (3)	121
C6—H6···N4^{i}	0.93	2.60	3.358 (3)	140
C8—H8*A*···O2^{ii}	0.96	2.45	3.397 (3)	168
C11—H11···N4^{i}	0.93	2.55	3.390 (3)	151
C16—H16···O2^{iii}	0.93	2.33	3.244 (3)	167

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

Data collection: *CrystalClear* (Rigaku/MSC, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: KP2276).

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supporting information

Acta Cryst. (2010). E**66**, o2961 [https://doi.org/10.1107/S1600536810040158]

3-Bromo-1-(3-chloropyridin-2-yl)-*N*-(4-ethoxyphenyl)-1*H*-pyrazole-5-carboxamide

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S1. Comment

Due to the capability of insects to rapidly develop resistance, the discovery of agents that act on new biochemical targets is an important tool for effective pest management. Calcium channels, in particular, the ryanodine receptors (RyR) represent an attractive biological target for insect control and thus offer excellent promise in integrated pest management strategies.

Many pesticide contain amide structures (Liu *et al.* 2007; Dong *et al.* 2008*a*,*b*; Liu *et al.* 2009*a*,*b*,*c*). Recently, diamides have attracted considerable attention in the field of agrochemistry, owing to their prominent insecticidal activity (Gewehr *et al.* 2007), unique modes of action and good environmental profiles.

Thus, a series of novel amides containing *N*-pyridylpyrazole were synthesized and their insecticidal activities were tested. Here we present the crystal structure of the title compound,(I), which has been determined during a search for relationships between the structure and insecticidal activity of the above derivatives.

The molecular structure of title compound (Fig.1) reveals that the pyrazole ring is coplanar with the benzene ring [dihedral angle 179.5 (2)°] whereas the pyrazole ring is almost perpendicular to 3-chlorpyridine ring [dihedral angle 106.3 (2)°]. In the crystal packing dominating N—H···N interaction and weak C—H···O and C—H···N contacts were observed (Table 1, Fig. 2).

S2. Experimental

Compound (I) was prepared according to the reported procedure of Dong *et al.*(2009). Colourless single crystals suitable for X-ray diffraction analysis were obtained by recrystallization from ethanol.

S3. Refinement

H atom of N—H was located in a difference map and refined freely. All C—H atoms were generated by riding model with C—H distance fixed at 0.93(phenyl group), 0.97(methylene group).

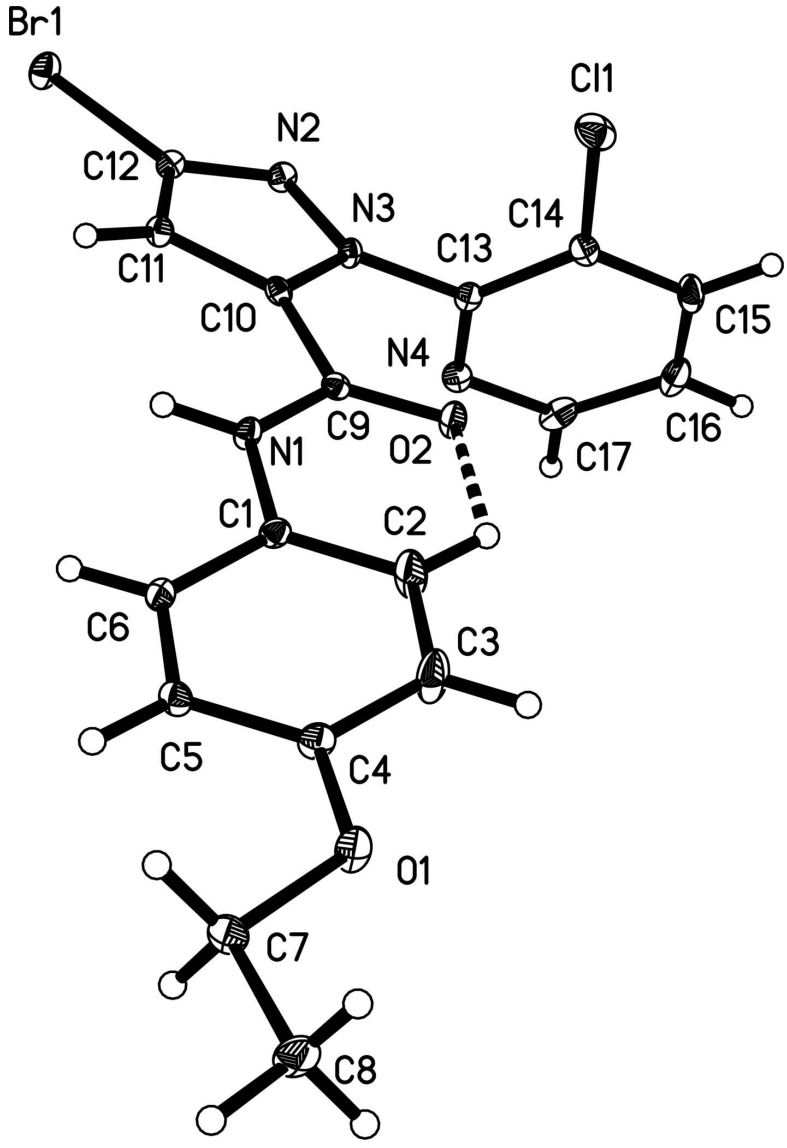

Figure 1

The molecular structure of (I) with intramolecular C—H···O interaction, showing displacement ellipsoids drawn at the 30% probability level.

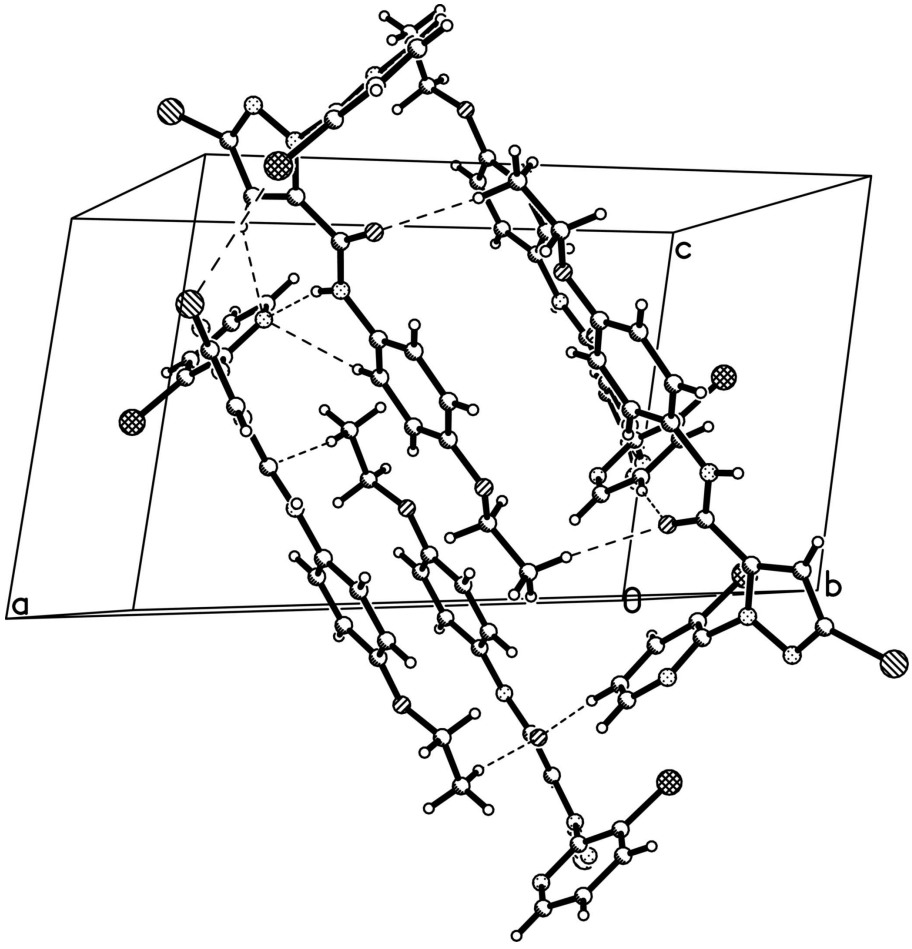

Figure 2

The crystal packing of I with hydrogen bonds shown (in dashed lines).

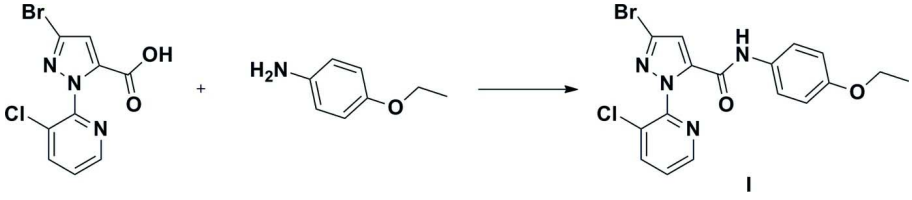

Figure 3

The formation of the title compound.

3-Bromo-1-(3-chloropyridin-2-yl)-*N*-(4-ethoxyphenyl)-1*H*-pyrazole- 5-carboxamide

Crystal data

$C_{17}H_{14}BrClN_4O_2$
$M_r = 421.68$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 16.821$ (3) Å
$b = 10.195$ (2) Å
$c = 10.064$ (2) Å
$\beta = 101.09$ (3)°
$V = 1693.7$ (6) Å^3
$Z = 4$
$F(000) = 848$
$D_x = 1.654$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4811 reflections
$\theta = 2.0$–27.1°
$\mu = 2.60$ mm^{-1}

T = 113 K
Ractangle, colourless

0.16 × 0.12 × 0.08 mm

Data collection

Rigaku Saturn diffractometer
Radiation source: rotating anode
Confocal monochromator
ω scans
Absorption correction: multi-scan (*CrystalClear*, Rigaku/MSC, 2002)
T_{min} = 0.681, T_{max} = 0.819

11217 measured reflections
2967 independent reflections
2459 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 25.0°, θ_{min} = 2.4°
h = −14→20
k = −11→12
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.064
S = 0.99
2967 reflections
231 parameters
1 restraint
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0325P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Br1	0.023579 (14)	0.06344 (2)	0.32526 (2)	0.02098 (9)
Cl1	0.07553 (4)	0.63129 (7)	0.54321 (6)	0.02706 (17)
O1	0.49241 (10)	0.39661 (16)	1.23908 (18)	0.0251 (4)
O2	0.25436 (9)	0.48804 (16)	0.66299 (16)	0.0182 (4)
N1	0.26429 (11)	0.29027 (19)	0.77115 (19)	0.0143 (5)
N2	0.09269 (10)	0.31241 (18)	0.35049 (19)	0.0148 (5)
N3	0.14508 (10)	0.38461 (18)	0.44293 (18)	0.0125 (4)
N4	0.21996 (11)	0.49665 (19)	0.3078 (2)	0.0171 (5)
C1	0.32339 (13)	0.3197 (2)	0.8882 (2)	0.0147 (5)
C2	0.34708 (16)	0.4465 (2)	0.9280 (3)	0.0292 (7)
H2	0.3250	0.5177	0.8759	0.035*
C3	0.40344 (16)	0.4662 (3)	1.0450 (3)	0.0318 (8)
H3	0.4189	0.5514	1.0712	0.038*

C4	0.43755 (13)	0.3629 (2)	1.1245 (2)	0.0181 (6)
C5	0.41491 (13)	0.2361 (2)	1.0851 (2)	0.0162 (6)
H5	0.4372	0.1650	1.1372	0.019*
C6	0.35841 (13)	0.2165 (2)	0.9668 (2)	0.0165 (6)
H6	0.3437	0.1313	0.9398	0.020*
C7	0.53387 (14)	0.2914 (2)	1.3173 (2)	0.0204 (6)
H7A	0.5647	0.2407	1.2631	0.024*
H7B	0.4954	0.2336	1.3481	0.024*
C8	0.58986 (14)	0.3521 (3)	1.4367 (3)	0.0257 (7)
H8A	0.6282	0.4079	1.4048	0.039*
H8B	0.6182	0.2841	1.4925	0.039*
H8C	0.5588	0.4031	1.4886	0.039*
C9	0.23427 (13)	0.3734 (2)	0.6695 (2)	0.0128 (5)
C10	0.17324 (13)	0.3141 (2)	0.5591 (2)	0.0133 (5)
C11	0.13590 (13)	0.1945 (2)	0.5421 (2)	0.0141 (5)
H11	0.1412	0.1253	0.6033	0.017*
C12	0.08813 (13)	0.1993 (2)	0.4129 (2)	0.0143 (5)
C13	0.17110 (13)	0.5071 (2)	0.3970 (2)	0.0144 (5)
C14	0.14284 (13)	0.6260 (2)	0.4354 (2)	0.0173 (6)
C15	0.16840 (15)	0.7398 (2)	0.3811 (3)	0.0247 (7)
H15	0.1510	0.8214	0.4056	0.030*
C16	0.21971 (15)	0.7303 (2)	0.2907 (3)	0.0257 (7)
H16	0.2381	0.8052	0.2532	0.031*
C17	0.24346 (14)	0.6071 (3)	0.2566 (2)	0.0226 (6)
H17	0.2777	0.6011	0.1945	0.027*
H1	0.2473 (12)	0.2088 (11)	0.765 (2)	0.013 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02471 (15)	0.01863 (15)	0.01646 (15)	−0.00563 (10)	−0.00392 (10)	−0.00200 (11)
Cl1	0.0241 (3)	0.0302 (4)	0.0266 (4)	0.0044 (3)	0.0042 (3)	−0.0100 (3)
O1	0.0317 (10)	0.0178 (10)	0.0183 (10)	−0.0035 (7)	−0.0142 (8)	0.0027 (8)
O2	0.0232 (9)	0.0126 (9)	0.0163 (9)	−0.0023 (7)	−0.0023 (7)	0.0005 (7)
N1	0.0168 (10)	0.0128 (11)	0.0113 (11)	−0.0031 (8)	−0.0022 (8)	−0.0001 (9)
N2	0.0165 (10)	0.0159 (11)	0.0107 (11)	−0.0010 (8)	−0.0011 (8)	−0.0029 (9)
N3	0.0162 (10)	0.0103 (10)	0.0101 (10)	−0.0011 (8)	0.0000 (8)	−0.0013 (8)
N4	0.0183 (11)	0.0175 (12)	0.0133 (11)	0.0002 (9)	−0.0025 (8)	−0.0013 (9)
C1	0.0139 (12)	0.0157 (13)	0.0136 (13)	−0.0017 (10)	0.0000 (10)	0.0007 (10)
C2	0.0378 (16)	0.0161 (15)	0.0250 (16)	0.0011 (11)	−0.0154 (12)	0.0036 (12)
C3	0.0452 (18)	0.0155 (14)	0.0260 (16)	−0.0053 (12)	−0.0145 (13)	−0.0015 (12)
C4	0.0191 (13)	0.0200 (14)	0.0127 (13)	−0.0019 (10)	−0.0034 (10)	−0.0002 (11)
C5	0.0185 (13)	0.0163 (13)	0.0124 (14)	0.0016 (10)	0.0000 (10)	0.0036 (10)
C6	0.0160 (12)	0.0133 (13)	0.0191 (15)	−0.0016 (9)	0.0006 (10)	−0.0003 (10)
C7	0.0213 (13)	0.0219 (14)	0.0153 (14)	0.0016 (10)	−0.0031 (11)	0.0036 (11)
C8	0.0240 (14)	0.0275 (16)	0.0209 (15)	−0.0052 (11)	−0.0078 (11)	0.0032 (12)
C9	0.0127 (12)	0.0136 (13)	0.0121 (13)	0.0016 (10)	0.0027 (9)	−0.0021 (10)
C10	0.0148 (12)	0.0129 (13)	0.0113 (13)	0.0029 (9)	0.0004 (10)	0.0025 (10)

C11	0.0173 (13)	0.0142 (13)	0.0109 (13)	0.0000 (10)	0.0025 (10)	0.0028 (10)
C12	0.0151 (12)	0.0155 (14)	0.0124 (13)	−0.0011 (10)	0.0029 (10)	−0.0013 (10)
C13	0.0153 (12)	0.0144 (13)	0.0104 (13)	−0.0012 (10)	−0.0050 (10)	0.0017 (10)
C14	0.0180 (13)	0.0170 (13)	0.0142 (13)	0.0026 (10)	−0.0035 (10)	−0.0030 (11)
C15	0.0277 (15)	0.0130 (13)	0.0275 (17)	0.0024 (11)	−0.0097 (12)	0.0010 (12)
C16	0.0294 (15)	0.0179 (15)	0.0241 (16)	−0.0075 (11)	−0.0090 (12)	0.0058 (12)
C17	0.0225 (14)	0.0299 (16)	0.0145 (14)	−0.0085 (11)	0.0008 (10)	0.0059 (12)

Geometric parameters (Å, º)

Br1—C12	1.873 (2)	C5—C6	1.387 (3)
Cl1—C14	1.713 (3)	C5—H5	0.9300
O1—C4	1.375 (3)	C6—H6	0.9300
O1—C7	1.430 (3)	C7—C8	1.510 (3)
O2—C9	1.222 (3)	C7—H7A	0.9700
N1—C9	1.350 (3)	C7—H7B	0.9700
N1—C1	1.419 (3)	C8—H8A	0.9600
N1—H1	0.877 (9)	C8—H8B	0.9600
N2—C12	1.322 (3)	C8—H8C	0.9600
N2—N3	1.367 (2)	C9—C10	1.488 (3)
N3—C10	1.376 (3)	C10—C11	1.367 (3)
N3—C13	1.429 (3)	C11—C12	1.391 (3)
N4—C17	1.330 (3)	C11—H11	0.9300
N4—C13	1.333 (3)	C13—C14	1.384 (3)
C1—C6	1.379 (3)	C14—C15	1.386 (4)
C1—C2	1.389 (3)	C15—C16	1.373 (4)
C2—C3	1.378 (3)	C15—H15	0.9300
C2—H2	0.9300	C16—C17	1.381 (4)
C3—C4	1.379 (3)	C16—H16	0.9300
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.384 (3)		
C4—O1—C7	116.83 (18)	C7—C8—H8A	109.5
C9—N1—C1	126.63 (19)	C7—C8—H8B	109.5
C9—N1—H1	117.9 (14)	H8A—C8—H8B	109.5
C1—N1—H1	115.4 (14)	C7—C8—H8C	109.5
C12—N2—N3	103.58 (17)	H8A—C8—H8C	109.5
N2—N3—C10	111.61 (18)	H8B—C8—H8C	109.5
N2—N3—C13	116.61 (17)	O2—C9—N1	125.03 (19)
C10—N3—C13	130.86 (17)	O2—C9—C10	120.47 (19)
C17—N4—C13	117.5 (2)	N1—C9—C10	114.5 (2)
C6—C1—C2	118.5 (2)	C11—C10—N3	106.54 (18)
C6—C1—N1	118.0 (2)	C11—C10—C9	133.6 (2)
C2—C1—N1	123.5 (2)	N3—C10—C9	119.8 (2)
C3—C2—C1	119.7 (2)	C10—C11—C12	104.7 (2)
C3—C2—H2	120.2	C10—C11—H11	127.6
C1—C2—H2	120.2	C12—C11—H11	127.6
C2—C3—C4	121.7 (2)	N2—C12—C11	113.5 (2)

C2—C3—H3	119.2	N2—C12—Br1	120.16 (16)
C4—C3—H3	119.2	C11—C12—Br1	126.31 (18)
O1—C4—C3	115.6 (2)	N4—C13—C14	123.2 (2)
O1—C4—C5	125.3 (2)	N4—C13—N3	114.5 (2)
C3—C4—C5	119.1 (2)	C14—C13—N3	122.1 (2)
C4—C5—C6	119.0 (2)	C13—C14—C15	118.3 (2)
C4—C5—H5	120.5	C13—C14—Cl1	120.6 (2)
C6—C5—H5	120.5	C15—C14—Cl1	121.1 (2)
C1—C6—C5	122.0 (2)	C16—C15—C14	119.0 (2)
C1—C6—H6	119.0	C16—C15—H15	120.5
C5—C6—H6	119.0	C14—C15—H15	120.5
O1—C7—C8	107.1 (2)	C15—C16—C17	118.5 (2)
O1—C7—H7A	110.3	C15—C16—H16	120.7
C8—C7—H7A	110.3	C17—C16—H16	120.7
O1—C7—H7B	110.3	N4—C17—C16	123.5 (3)
C8—C7—H7B	110.3	N4—C17—H17	118.2
H7A—C7—H7B	108.6	C16—C17—H17	118.2

C12—N2—N3—C10	1.4 (3)	N1—C9—C10—C11	5.7 (4)
C12—N2—N3—C13	171.6 (2)	O2—C9—C10—N3	6.4 (4)
C9—N1—C1—C6	−167.1 (2)	N1—C9—C10—N3	−172.7 (2)
C9—N1—C1—C2	13.5 (4)	N3—C10—C11—C12	1.4 (3)
C6—C1—C2—C3	−1.0 (4)	C9—C10—C11—C12	−177.1 (3)
N1—C1—C2—C3	178.3 (3)	N3—N2—C12—C11	−0.4 (3)
C1—C2—C3—C4	0.2 (5)	N3—N2—C12—Br1	−179.10 (15)
C7—O1—C4—C3	−174.8 (2)	C10—C11—C12—N2	−0.6 (3)
C7—O1—C4—C5	5.3 (4)	C10—C11—C12—Br1	177.93 (18)
C2—C3—C4—O1	−179.5 (3)	C17—N4—C13—C14	1.5 (3)
C2—C3—C4—C5	0.4 (5)	C17—N4—C13—N3	177.11 (17)
O1—C4—C5—C6	179.7 (2)	N2—N3—C13—N4	−69.3 (2)
C3—C4—C5—C6	−0.1 (4)	C10—N3—C13—N4	98.6 (3)
C2—C1—C6—C5	1.4 (4)	N2—N3—C13—C14	106.3 (2)
N1—C1—C6—C5	−178.0 (2)	C10—N3—C13—C14	−85.8 (3)
C4—C5—C6—C1	−0.8 (4)	N4—C13—C14—C15	−1.8 (3)
C4—O1—C7—C8	−179.8 (2)	N3—C13—C14—C15	−177.04 (19)
C1—N1—C9—O2	0.4 (4)	N4—C13—C14—Cl1	176.20 (16)
C1—N1—C9—C10	179.5 (2)	N3—C13—C14—Cl1	0.9 (3)
N2—N3—C10—C11	−1.8 (3)	C13—C14—C15—C16	0.7 (3)
C13—N3—C10—C11	−170.2 (2)	Cl1—C14—C15—C16	−177.25 (17)
N2—N3—C10—C9	176.95 (19)	C14—C15—C16—C17	0.5 (3)
C13—N3—C10—C9	8.6 (4)	C13—N4—C17—C16	−0.2 (3)
O2—C9—C10—C11	−175.3 (3)	C15—C16—C17—N4	−0.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N4^{i}	0.88 (1)	2.21 (1)	3.059 (3)	165 (2)
C2—H2···O2	0.93	2.26	2.850 (3)	121

C6—H6···N4^{i}	0.93	2.60	3.358 (3)	140
C8—H8*A*···O2^{ii}	0.96	2.45	3.397 (3)	168
C11—H11···N4^{i}	0.93	2.55	3.390 (3)	151
C16—H16···O2^{iii}	0.93	2.33	3.244 (3)	167

Symmetry codes: (i) x, $-y+1/2$, $z+1/2$; (ii) $-x+1$, $-y+1$, $-z+2$; (iii) x, $-y+3/2$, $z-1/2$.