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1-[(6-Chloropyridin-3-yl)methyl]-10-nitro-1,2,3,5,6,7,8,9-octahydro-5,9-methanoimidazo[1,2-a]azocin-5-ol

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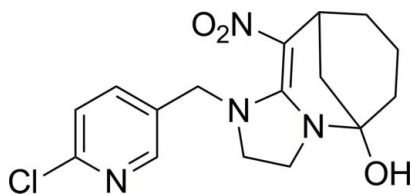
Received 10 April 2013; accepted 24 May 2013

 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.071; wR factor = 0.217; data-to-parameter ratio = 13.5.

In the title compound, $\text{C}_{16}\text{H}_{19}\text{ClN}_4\text{O}_3$, the cyclohexane ring displays a chair formation and the tetrahydropyridine ring displays an envelope conformation with the methylene C atom as the flap; the imidazolidine ring also displays an envelope conformation with a methylene C atom as the flap. In the crystal, $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds between hydroxy groups and pyridine rings link inversion-related molecules into dimers. Weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds further link the dimers into supramolecular chains running along the c axis.

Related literature

For background to the title compound, see: Jeschkel & Nauen (2008). For the synthesis, see: Tian *et al.* (2007).



Experimental

Crystal data

 $\text{C}_{16}\text{H}_{19}\text{ClN}_4\text{O}_3$
 $M_r = 350.80$

 Monoclinic, $P2_1/c$
 $a = 13.3975$ (14) Å
 $b = 18.7124$ (18) Å
 $c = 6.5721$ (8) Å
 $\beta = 97.897$ (10)°
 $V = 1632.0$ (3) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.26$ mm⁻¹
 $T = 296$ K
 $0.38 \times 0.24 \times 0.23$ mm

Data collection

 Bruker APEXII diffractometer
 Absorption correction: multi-scan
 (*SADABS*; Bruker, 2001)
 $T_{\min} = 0.93$, $T_{\max} = 0.94$

 7705 measured reflections
 2921 independent reflections
 1727 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.056$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.071$
 $wR(F^2) = 0.217$
 $S = 1.05$
 2921 reflections

 217 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.33$ e Å⁻³
 $\Delta\rho_{\min} = -0.34$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O3}-\text{H3}\cdots\text{N4}^i$	0.82	2.04	2.855 (4)	174
$\text{C11}-\text{H11A}\cdots\text{O1}^{ii}$	0.97	2.53	3.467 (5)	161
$\text{C13}-\text{H13}\cdots\text{O2}^{ii}$	0.93	2.48	3.265 (5)	142

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *S SAINT* (Bruker, 2007); data reduction: *S SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: XU5695).

References

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supporting information

Acta Cryst. (2013). E69, o1015 [https://doi.org/10.1107/S1600536813014402]

1-[(6-Chloropyridin-3-yl)methyl]-10-nitro-1,2,3,5,6,7,8,9-octahydro-5,9-methanoimidazo[1,2-a]azocin-5-ol

Shu-Xia Cui, Guang-You Zhang and Zhong-Zhen Tian

S1. Comment

The past decades have witnessed the great power and versatile ability of neonicotinoids as a novel class of insecticides (Jeschkel & Nauen, 2008). Several commercial neonicotinoid compounds were launched successively in the latest two decades, and they presented a broad spectrum performance in controlling various insects. Our interest was introducing bicyclic structure to fix the direction of the nitro group, and synthesized a class of novel *cis*-neonicotinoid compounds with carbon bicyclic, in which the title compound exhibited good insecticidal activities against pea aphids.

The structure of compound is shown in Fig. 1 with the atom-numbering scheme. In the title compound, the cyclohexane ring displays a chair formation while the hexahydroazocine ring displays an envelope conformation with the methylene C atom on the flap; the imidazolidine ring also displays an envelope conformation with a methylene C atom on the flap. In the crystal, intermolecular O—H···N hydrogen bonds between hydroxyl groups and pyridine rings link inversion-related molecules into dimer. Weak C—H···O hydrogen bonds further link the dimers into the supramolecular architecture.

S2. Experimental

The title compound was synthesized according to the literature (Tian *et al.*, 2007). Single crystals suitable for X-ray analysis were obtained by slow evaporation of the solution of dichloromethane and ether of the title compound.

S3. Refinement

Hydroxyl H atom was located in a difference map and refined with distance restraints of O—H = 0.82 Å, $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. Other H atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.98 Å, $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

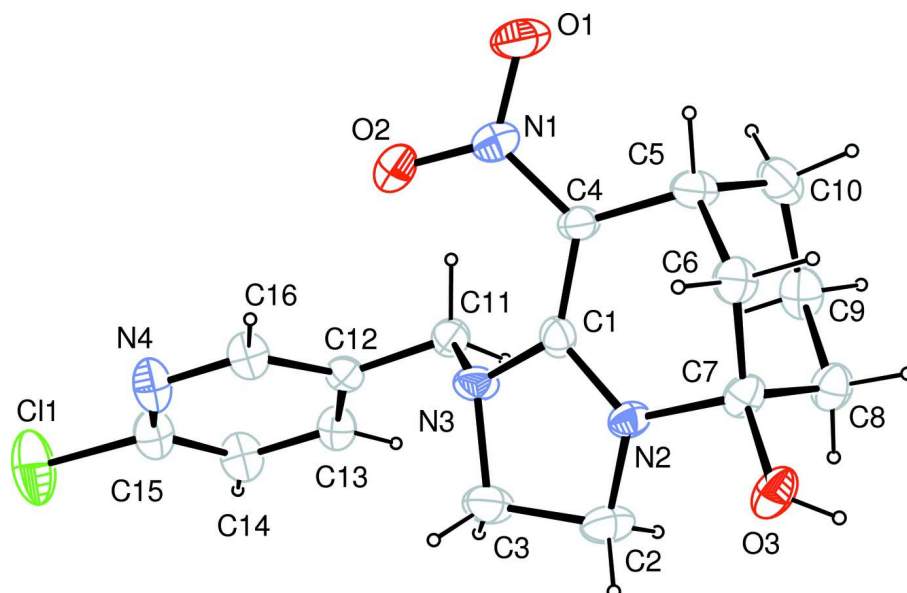


Figure 1

The molecular structure of the title compound with atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The H atoms are shown as circles of arbitrary size.

1-[(6-Chloropyridin-3-yl)methyl]-10-nitro-1,2,3,5,6,7,8,9-octahydro-5,9-methanoimidazo[1,2-a]azocin-5-ol

Crystal data

$C_{16}H_{19}ClN_4O_3$

$M_r = 350.80$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

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$b = 18.7124$ (18) Å

$c = 6.5721$ (8) Å

$\beta = 97.897$ (10)°

$V = 1632.0$ (3) Å³

$Z = 4$

$F(000) = 736$

$D_x = 1.428$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1166 reflections

$\theta = 2.6$ – 25.2 °

$\mu = 0.26$ mm⁻¹

$T = 296$ K

Prism, colourless

$0.38 \times 0.24 \times 0.23$ mm

Data collection

Bruker APEXII

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 16.03 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2001)

$T_{\min} = 0.93$, $T_{\max} = 0.94$

7705 measured reflections

2921 independent reflections

1727 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.056$

$\theta_{\max} = 25.2$ °, $\theta_{\min} = 2.7$ °

$h = -16 \rightarrow 16$

$k = -21 \rightarrow 22$

$l = -7 \rightarrow 6$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.071$

$wR(F^2) = 0.217$

$S = 1.05$

2921 reflections

217 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

$$w = 1/[\sigma^2(F_o^2) + (0.1042P)^2 + 0.1363P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.33 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.34 \text{ e } \text{\AA}^{-3}$

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.

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 $F^2 > 2\text{sigma}(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	-0.41200 (9)	0.65584 (9)	0.0781 (3)	0.0997 (6)
N1	0.1452 (3)	0.65779 (16)	0.7861 (5)	0.0462 (9)
N2	0.2189 (2)	0.53441 (15)	0.4048 (5)	0.0366 (8)
N3	0.0721 (2)	0.59219 (15)	0.3726 (5)	0.0437 (8)
N4	-0.2457 (2)	0.63479 (18)	0.3227 (6)	0.0571 (10)
O1	0.1870 (2)	0.69232 (16)	0.9378 (5)	0.0673 (9)
O2	0.0505 (2)	0.65481 (15)	0.7522 (5)	0.0588 (8)
O3	0.35157 (19)	0.45270 (13)	0.4224 (4)	0.0510 (8)
H3	0.3216	0.4252	0.4901	0.077*
C1	0.1637 (3)	0.58526 (18)	0.4877 (6)	0.0373 (9)
C2	0.1721 (3)	0.5161 (2)	0.1983 (6)	0.0533 (11)
H2A	0.1769	0.4653	0.1716	0.064*
H2B	0.2017	0.5427	0.0949	0.064*
C3	0.0639 (3)	0.5387 (2)	0.2069 (7)	0.0563 (12)
H3A	0.0341	0.5594	0.0774	0.068*
H3B	0.0233	0.4984	0.2386	0.068*
C4	0.2050 (3)	0.62191 (19)	0.6634 (6)	0.0388 (9)
C5	0.3162 (3)	0.61790 (18)	0.7288 (6)	0.0443 (10)
H5	0.3302	0.6297	0.8751	0.053*
C6	0.3494 (3)	0.54049 (19)	0.6983 (6)	0.0455 (10)
H6A	0.4208	0.5352	0.7467	0.055*
H6B	0.3123	0.5080	0.7752	0.055*
C7	0.3281 (3)	0.52359 (18)	0.4689 (6)	0.0388 (9)
C8	0.3893 (3)	0.57185 (19)	0.3484 (7)	0.0477 (10)
H8A	0.3741	0.5609	0.2032	0.057*
H8B	0.4605	0.5630	0.3904	0.057*
C9	0.3664 (3)	0.65028 (19)	0.3831 (7)	0.0515 (11)
H9A	0.4128	0.6797	0.3188	0.062*
H9B	0.2987	0.6609	0.3177	0.062*
C10	0.3751 (3)	0.6691 (2)	0.6090 (7)	0.0564 (12)

H10A	0.3502	0.7173	0.6229	0.068*
H10B	0.4455	0.6682	0.6680	0.068*
C11	0.0317 (3)	0.66343 (18)	0.3105 (6)	0.0400 (9)
H11A	0.0647	0.6811	0.1980	0.048*
H11B	0.0465	0.6963	0.4248	0.048*
C12	-0.0792 (3)	0.66095 (16)	0.2453 (6)	0.0347 (9)
C13	-0.1215 (3)	0.68244 (19)	0.0504 (6)	0.0450 (10)
H13	-0.0801	0.6977	-0.0435	0.054*
C14	-0.2246 (3)	0.6813 (2)	-0.0049 (7)	0.0539 (11)
H14	-0.2539	0.6961	-0.1346	0.065*
C15	-0.2822 (3)	0.6576 (2)	0.1372 (8)	0.0518 (11)
C16	-0.1457 (3)	0.6367 (2)	0.3742 (7)	0.0495 (11)
H16	-0.1190	0.6208	0.5044	0.059*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0386 (7)	0.1346 (13)	0.1228 (14)	0.0014 (7)	0.0000 (7)	0.0343 (10)
N1	0.055 (2)	0.042 (2)	0.042 (2)	0.0066 (15)	0.0090 (17)	-0.0048 (16)
N2	0.0401 (17)	0.0310 (17)	0.0390 (18)	0.0055 (12)	0.0071 (14)	-0.0050 (14)
N3	0.0452 (19)	0.0319 (17)	0.052 (2)	0.0061 (13)	-0.0022 (15)	-0.0140 (16)
N4	0.039 (2)	0.056 (2)	0.078 (3)	-0.0026 (15)	0.0113 (18)	0.014 (2)
O1	0.081 (2)	0.070 (2)	0.048 (2)	0.0147 (15)	0.0004 (16)	-0.0235 (16)
O2	0.0499 (19)	0.071 (2)	0.059 (2)	0.0059 (14)	0.0197 (14)	-0.0108 (15)
O3	0.0569 (18)	0.0363 (16)	0.064 (2)	0.0123 (12)	0.0222 (14)	0.0068 (13)
C1	0.034 (2)	0.032 (2)	0.047 (2)	-0.0027 (15)	0.0071 (16)	-0.0003 (18)
C2	0.067 (3)	0.042 (2)	0.049 (3)	0.0120 (19)	0.002 (2)	-0.012 (2)
C3	0.057 (3)	0.046 (2)	0.062 (3)	0.0052 (18)	-0.007 (2)	-0.017 (2)
C4	0.042 (2)	0.041 (2)	0.033 (2)	0.0023 (16)	0.0033 (16)	-0.0090 (17)
C5	0.050 (2)	0.041 (2)	0.040 (2)	0.0053 (17)	-0.0041 (18)	-0.0069 (18)
C6	0.044 (2)	0.045 (2)	0.046 (3)	0.0069 (17)	0.0016 (18)	0.0036 (19)
C7	0.045 (2)	0.026 (2)	0.047 (2)	0.0073 (15)	0.0114 (18)	0.0043 (17)
C8	0.044 (2)	0.046 (2)	0.055 (3)	0.0071 (17)	0.0116 (19)	0.005 (2)
C9	0.050 (2)	0.037 (2)	0.069 (3)	0.0002 (17)	0.012 (2)	0.014 (2)
C10	0.043 (2)	0.043 (2)	0.080 (3)	-0.0032 (17)	-0.003 (2)	-0.007 (2)
C11	0.043 (2)	0.033 (2)	0.046 (2)	-0.0023 (15)	0.0127 (17)	-0.0021 (17)
C12	0.041 (2)	0.0219 (18)	0.041 (2)	-0.0019 (14)	0.0067 (17)	0.0027 (16)
C13	0.045 (2)	0.040 (2)	0.050 (3)	0.0013 (16)	0.0093 (18)	0.0104 (19)
C14	0.050 (3)	0.057 (3)	0.053 (3)	0.002 (2)	0.001 (2)	0.018 (2)
C15	0.043 (2)	0.043 (2)	0.069 (3)	0.0056 (17)	0.007 (2)	0.013 (2)
C16	0.046 (2)	0.047 (2)	0.056 (3)	-0.0001 (17)	0.005 (2)	0.008 (2)

Geometric parameters (Å, °)

C11—C15	1.729 (4)	C5—H5	0.9800
N1—O1	1.254 (4)	C6—C7	1.529 (5)
N1—O2	1.258 (4)	C6—H6A	0.9700
N1—C4	1.386 (5)	C6—H6B	0.9700

N2—C1	1.363 (5)	C7—C8	1.515 (5)
N2—C2	1.456 (5)	C8—C9	1.523 (5)
N2—C7	1.480 (4)	C8—H8A	0.9700
N3—C1	1.357 (4)	C8—H8B	0.9700
N3—C3	1.472 (5)	C9—C10	1.515 (6)
N3—C11	1.475 (4)	C9—H9A	0.9700
N4—C15	1.320 (6)	C9—H9B	0.9700
N4—C16	1.337 (5)	C10—H10A	0.9700
O3—C7	1.407 (4)	C10—H10B	0.9700
O3—H3	0.8200	C11—C12	1.490 (5)
C1—C4	1.391 (5)	C11—H11A	0.9700
C2—C3	1.518 (5)	C11—H11B	0.9700
C2—H2A	0.9700	C12—C16	1.387 (5)
C2—H2B	0.9700	C12—C13	1.387 (5)
C3—H3A	0.9700	C13—C14	1.380 (5)
C3—H3B	0.9700	C13—H13	0.9300
C4—C5	1.495 (5)	C14—C15	1.364 (6)
C5—C10	1.527 (6)	C14—H14	0.9300
C5—C6	1.537 (5)	C16—H16	0.9300
O1—N1—O2	119.6 (3)	N2—C7—C8	110.8 (3)
O1—N1—C4	118.7 (3)	O3—C7—C6	113.1 (3)
O2—N1—C4	121.6 (3)	N2—C7—C6	107.2 (3)
C1—N2—C2	110.4 (3)	C8—C7—C6	110.5 (3)
C1—N2—C7	123.4 (3)	C7—C8—C9	111.2 (3)
C2—N2—C7	121.0 (3)	C7—C8—H8A	109.4
C1—N3—C3	108.5 (3)	C9—C8—H8A	109.4
C1—N3—C11	120.6 (3)	C7—C8—H8B	109.4
C3—N3—C11	115.0 (3)	C9—C8—H8B	109.4
C15—N4—C16	117.1 (4)	H8A—C8—H8B	108.0
C7—O3—H3	109.5	C10—C9—C8	112.4 (3)
N3—C1—N2	110.0 (3)	C10—C9—H9A	109.1
N3—C1—C4	129.9 (3)	C8—C9—H9A	109.1
N2—C1—C4	120.0 (3)	C10—C9—H9B	109.1
N2—C2—C3	101.0 (3)	C8—C9—H9B	109.1
N2—C2—H2A	111.6	H9A—C9—H9B	107.9
C3—C2—H2A	111.6	C9—C10—C5	112.6 (3)
N2—C2—H2B	111.6	C9—C10—H10A	109.1
C3—C2—H2B	111.6	C5—C10—H10A	109.1
H2A—C2—H2B	109.4	C9—C10—H10B	109.1
N3—C3—C2	104.0 (3)	C5—C10—H10B	109.1
N3—C3—H3A	110.9	H10A—C10—H10B	107.8
C2—C3—H3A	110.9	N3—C11—C12	111.4 (3)
N3—C3—H3B	110.9	N3—C11—H11A	109.4
C2—C3—H3B	110.9	C12—C11—H11A	109.4
H3A—C3—H3B	109.0	N3—C11—H11B	109.4
N1—C4—C1	121.8 (3)	C12—C11—H11B	109.4
N1—C4—C5	119.4 (3)	H11A—C11—H11B	108.0

C1—C4—C5	118.7 (3)	C16—C12—C13	116.4 (3)
C4—C5—C10	112.7 (3)	C16—C12—C11	122.2 (3)
C4—C5—C6	107.8 (3)	C13—C12—C11	121.4 (3)
C10—C5—C6	110.2 (4)	C14—C13—C12	120.4 (4)
C4—C5—H5	108.7	C14—C13—H13	119.8
C10—C5—H5	108.7	C12—C13—H13	119.8
C6—C5—H5	108.7	C15—C14—C13	117.7 (4)
C7—C6—C5	107.8 (3)	C15—C14—H14	121.2
C7—C6—H6A	110.2	C13—C14—H14	121.2
C5—C6—H6A	110.2	N4—C15—C14	124.4 (4)
C7—C6—H6B	110.2	N4—C15—C11	115.8 (3)
C5—C6—H6B	110.2	C14—C15—C11	119.8 (3)
H6A—C6—H6B	108.5	N4—C16—C12	124.0 (4)
O3—C7—N2	108.0 (3)	N4—C16—H16	118.0
O3—C7—C8	107.2 (3)	C12—C16—H16	118.0
C3—N3—C1—N2	3.5 (4)	C1—N2—C7—C8	-87.0 (4)
C11—N3—C1—N2	-132.3 (3)	C2—N2—C7—C8	65.2 (4)
C3—N3—C1—C4	-177.8 (4)	C1—N2—C7—C6	33.7 (4)
C11—N3—C1—C4	46.5 (6)	C2—N2—C7—C6	-174.1 (3)
C2—N2—C1—N3	13.0 (4)	C5—C6—C7—O3	-177.5 (3)
C7—N2—C1—N3	167.8 (3)	C5—C6—C7—N2	-58.5 (4)
C2—N2—C1—C4	-165.9 (3)	C5—C6—C7—C8	62.4 (4)
C7—N2—C1—C4	-11.1 (5)	O3—C7—C8—C9	178.1 (3)
C1—N2—C2—C3	-22.7 (4)	N2—C7—C8—C9	60.5 (4)
C7—N2—C2—C3	-178.2 (3)	C6—C7—C8—C9	-58.3 (4)
C1—N3—C3—C2	-17.4 (4)	C7—C8—C9—C10	51.5 (4)
C11—N3—C3—C2	121.1 (3)	C8—C9—C10—C5	-50.4 (5)
N2—C2—C3—N3	23.3 (4)	C4—C5—C10—C9	-65.2 (4)
O1—N1—C4—C1	-177.1 (3)	C6—C5—C10—C9	55.2 (4)
O2—N1—C4—C1	5.0 (5)	C1—N3—C11—C12	-162.0 (3)
O1—N1—C4—C5	7.4 (5)	C3—N3—C11—C12	64.9 (4)
O2—N1—C4—C5	-170.6 (3)	N3—C11—C12—C16	58.0 (4)
N3—C1—C4—N1	20.4 (6)	N3—C11—C12—C13	-121.5 (4)
N2—C1—C4—N1	-160.9 (3)	C16—C12—C13—C14	2.0 (5)
N3—C1—C4—C5	-164.0 (4)	C11—C12—C13—C14	-178.5 (3)
N2—C1—C4—C5	14.7 (5)	C12—C13—C14—C15	-0.8 (6)
N1—C4—C5—C10	-103.5 (4)	C16—N4—C15—C14	1.5 (6)
C1—C4—C5—C10	80.8 (4)	C16—N4—C15—C11	-178.9 (3)
N1—C4—C5—C6	134.7 (4)	C13—C14—C15—N4	-1.1 (7)
C1—C4—C5—C6	-41.0 (5)	C13—C14—C15—C11	179.3 (3)
C4—C5—C6—C7	63.1 (4)	C15—N4—C16—C12	0.0 (6)
C10—C5—C6—C7	-60.2 (4)	C13—C12—C16—N4	-1.7 (5)
C1—N2—C7—O3	155.9 (3)	C11—C12—C16—N4	178.8 (3)
C2—N2—C7—O3	-51.9 (4)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O3—H3 \cdots N4 ⁱ	0.82	2.04	2.855 (4)	174
C11—H11 <i>A</i> \cdots O1 ⁱⁱ	0.97	2.53	3.467 (5)	161
C13—H13 \cdots O2 ⁱⁱ	0.93	2.48	3.265 (5)	142

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