



# Crystal structure of 1-methyl-2-methylamino-3-nitro-1*H*-chromeno[2,3-*b*]-pyridin-5(10*aH*)-one

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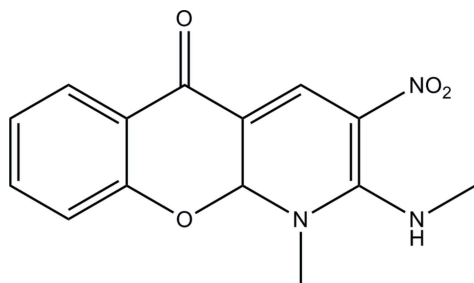
In the title compound, C<sub>14</sub>H<sub>13</sub>N<sub>3</sub>O<sub>4</sub>, the pyran ring adopts an envelope conformation with the methine C atom as the flap. The dihedral angle between the benzene and hydroypyridine rings is 29.33 (3)°. The methylamine C atom deviates from the plane of its attached ring by 0.380 (5) Å and an intramolecular N—H···O hydrogen bond closes an *S*(6) ring. In the crystal, weak C—H···O hydrogen bonds and aromatic  $\pi$ – $\pi$  stacking interactions [centroid–centroid distances vary from 3.6529 (10) to 3.6872 (10) Å] link the molecules, generating a three-dimensional network.

**Keywords:** crystal structure; chromene; hydrogen bonding;  $\pi$ – $\pi$  stacking.

**CCDC reference:** 1421106

## 1. Related literature

For the uses and biological importance of chromenes, see: Ercole *et al.* (2009); Geen *et al.* (1996); Khan *et al.* (2010); Raj *et al.* (2010).



## 2. Experimental

### 2.1. Crystal data

C <sub>14</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub>	<i>V</i> = 5102.6 (5) Å <sup>3</sup>
<i>M<sub>r</sub></i> = 287.27	<i>Z</i> = 16
Orthorhombic, <i>Fdd</i> 2	Mo <i>K</i> α radiation
<i>a</i> = 24.0182 (13) Å	$\mu$ = 0.11 mm <sup>-1</sup>
<i>b</i> = 26.8445 (14) Å	<i>T</i> = 293 K
<i>c</i> = 7.9140 (4) Å	0.35 × 0.30 × 0.25 mm

### 2.2. Data collection

Bruker SMART APEXII CCD diffractometer	12952 measured reflections
Absorption correction: multi-scan ( <i>SADABS</i> ; Bruker, 2008)	2261 independent reflections
<i>T<sub>min</sub></i> = 0.962, <i>T<sub>max</sub></i> = 0.972	2096 reflections with <i>I</i> > 2σ( <i>I</i> )
	<i>R<sub>int</sub></i> = 0.021

### 2.3. Refinement

<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )] = 0.030	H atoms treated by a mixture of independent and constrained refinement
<i>wR</i> ( <i>F</i> <sup>2</sup> ) = 0.076	$\Delta\rho_{\max}$ = 0.11 e Å <sup>-3</sup>
<i>S</i> = 1.04	$\Delta\rho_{\min}$ = -0.14 e Å <sup>-3</sup>
2261 reflections	
192 parameters	
1 restraint	

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

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N2—H2A···O1	0.86	1.83	2.543 (2)	139
C5—H5A···O2 <sup>i</sup>	0.96	2.46	3.376 (3)	159
C5—H5C···O3 <sup>ii</sup>	0.96	2.51	3.416 (3)	157
C6—H6A···O3 <sup>ii</sup>	0.96	2.55	3.429 (2)	152
C9—H9···O3 <sup>i</sup>	0.93	2.60	3.455 (2)	154

Symmetry codes: (i) *x*, *y*, *z* − 1; (ii) *x* +  $\frac{1}{4}$ , −*y* +  $\frac{1}{4}$ , *z* −  $\frac{3}{4}$ .

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7515).

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## supporting information

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## Crystal structure of 1-methyl-2-methylamino-3-nitro-1*H*-chromeno[2,3-*b*]pyridin-5(10*aH*)-one

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### S1. Comment

Chromene derivatives are very important heterocyclic compounds that have a variety of industrial, biological and chemical synthesis applications (Geen *et al.*, 1996; Ercole *et al.*, 2009). They exhibit a number of pharmacological activities such as anti-HIV, anti-inflammatory, anti-bacterial, anti-allergic, anti-cancer *etc.* (Khan *et al.*, 2010; Raj *et al.*, 2010). Against this background, X-ray analysis of the title compound has been carried out to study its structural aspects.

The molecular structure of the title molecule is shown in Fig. 1. The pyran ring (C1—C7—O4—C8—C13—C14) adopts an envelope conformation with the deviation of atoms O4 and C14 from the mean plane through atoms (C1—C7—C8—C13) being 0.475 and  $-0.095$  Å, respectively. The smallest displacement asymmetry parameters  $q_2$  and  $q_3$  are 0.421 (17) and  $-0.219$  (17) Å. The ring parameters  $Q$  and phase angle  $\theta$  are 0.475 (16) Å and  $117.5$  (2)°, respectively. The dihedral angle between the mean planes of the chromeno ring system (fusion of benzene and pyran rings) and the pyridine ring is  $29.37$  (7)°. The pyridine ring mean planes forms a dihedral angle of  $31.22$  (8)° with phenyl ring (C8—C13). The atoms O3 deviates by  $-0.295$  Å from the chromeno ring mean plane (O4/C1—C7).

An intramolecular N—H $\cdots$ O and N—H $\cdots$ N interaction occurs. In the crystal, molecules are linked by C—H $\cdots$ O hydrogen bonds, forming inversion dimers with an  $R_2^2(8)$  ring motif. The molecules are linked *via* C—H $\cdots$ O hydrogen bonds, forming ribbons along [110] direction. There are a number of  $\pi$ — $\pi$  interactions present linking the ribbons and forming a three dimensional structure [ $Cg2$ — $Cg3^i = 3.6529$  (10) Å,  $Cg2$ — $Cg3^{ii} = 3.6871$  (10) Å and  $Cg3$ — $Cg2^{iii} = 3.6528$  (10) Å; where  $Cg2$  and  $Cg3$  are the centroids of the N3/C4/C3/C2/C1/C7 and C8/C13 rings, respectively; symmetry codes: (i)  $-x, -y, -z$ ; (ii)  $1/4 + x, 1/4 - y, 1/4 + z$ ; (iii)  $-1/4 + x, 1/4 - y, -1/4 + z$ ].

### S2. Experimental

A mixture of 3-formylchromone (1 mmol), *N,N'*-dimethyl-2-nitroethene-1, 1-diamine (1 mmol) in ethanol (3 ml) and a catalytic amount (0.050 mmol) of In(OTf)<sub>3</sub> was added and refluxed for about 30 minutes. The product was purified by column chromatography (5/95% Ethylacetate/petether) to afford the pure product in 94% yield. The purified compound was recrystallized from DMSO-D<sub>6</sub> by using slow evaporation method to yield colourless blocks.

### S3. Refinement

N and C-bound H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and allowed to ride on their parent atoms, with  $U_{iso}(H) = 1.5U_{eq}(C)$  for methyl H atoms and  $1.2U_{eq}(C)$  for all other H atoms.

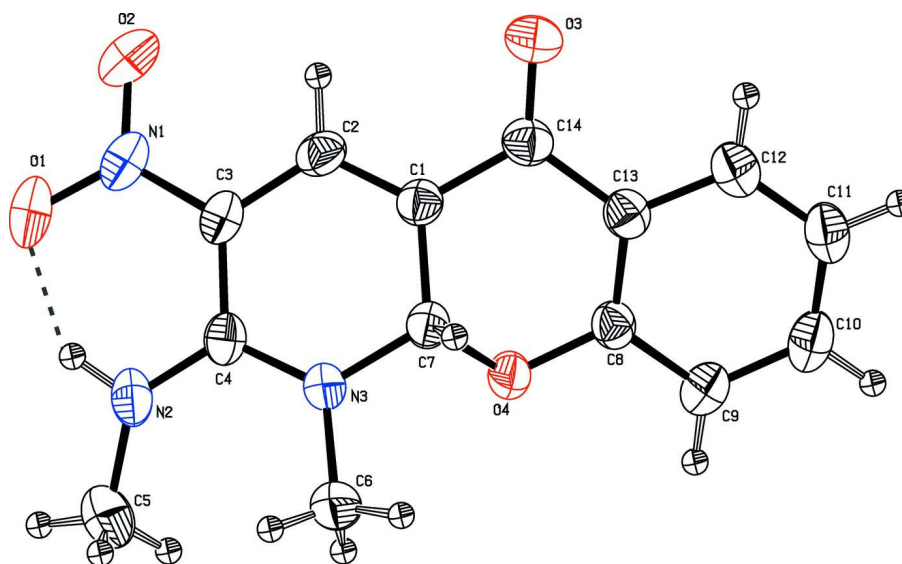


Figure 1

Molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

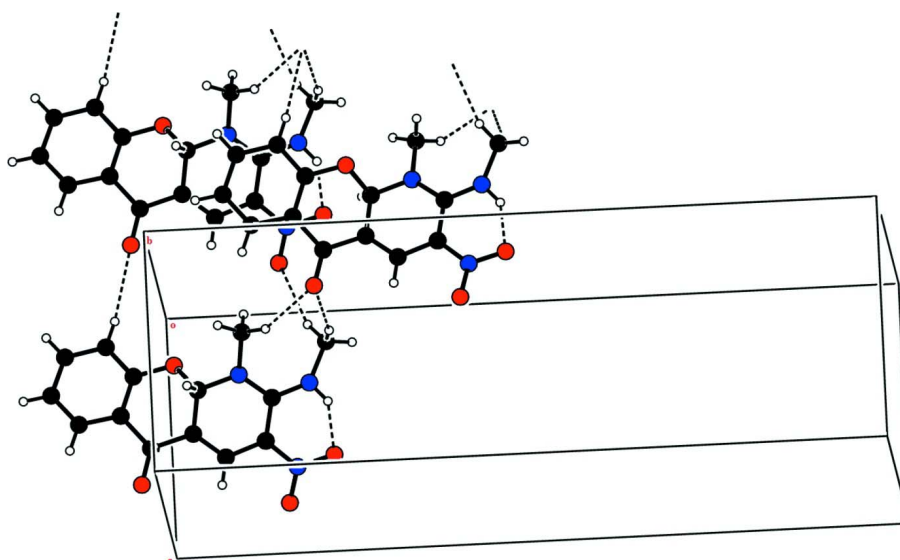


Figure 2

Viewed down the *c* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines (see Table 1 for details)

### 1-Methyl-2-methylamino-3-nitro-1*H*-chromeno[2,3-*b*]pyridin-5(10*aH*)-one

#### Crystal data

$C_{14}H_{13}N_3O_4$

$M_r = 287.27$

Orthorhombic, *Fdd2*

Hall symbol: *F* 2 -2*d*

$a = 24.0182$  (13) Å

$b = 26.8445$  (14) Å

$c = 7.9140$  (4) Å

$V = 5102.6$  (5) Å<sup>3</sup>

$Z = 16$

$F(000) = 2400$

$D_x = 1.496$  Mg m<sup>-3</sup>

Mo *K*α radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2096 reflections

$\theta = 2.3$ – $25.0^\circ$

$\mu = 0.11 \text{ mm}^{-1}$   
 $T = 293 \text{ K}$

Block, colourless  
 $0.35 \times 0.30 \times 0.25 \text{ mm}$

#### Data collection

Bruker SMART APEXII CCD  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\omega$  and  $\varphi$  scans  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2008)  
 $T_{\min} = 0.962$ ,  $T_{\max} = 0.972$

12952 measured reflections  
 2261 independent reflections  
 2096 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.021$   
 $\theta_{\max} = 25.0^\circ$ ,  $\theta_{\min} = 2.3^\circ$   
 $h = -27 \rightarrow 28$   
 $k = -31 \rightarrow 31$   
 $l = -9 \rightarrow 9$

#### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.030$   
 $wR(F^2) = 0.076$   
 $S = 1.04$   
 2261 reflections  
 192 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 1.3678P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.11 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.14 \text{ e } \text{\AA}^{-3}$

#### 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.03152 (7)	0.07119 (6)	0.5103 (2)	0.0316 (4)
C2	0.07422 (7)	0.05817 (6)	0.6093 (2)	0.0348 (4)
H2	0.0673	0.0483	0.7200	0.042*
C3	0.12950 (7)	0.05908 (6)	0.5492 (2)	0.0348 (4)
C4	0.14101 (7)	0.07284 (6)	0.3758 (2)	0.0323 (4)
C5	0.21801 (8)	0.07230 (9)	0.1521 (3)	0.0562 (6)
H5A	0.1937	0.0565	0.0723	0.084*
H5B	0.2531	0.0551	0.1543	0.084*
H5C	0.2239	0.1063	0.1193	0.084*
C6	0.10471 (8)	0.10996 (8)	0.1107 (2)	0.0514 (5)
H6A	0.1378	0.1300	0.1095	0.077*
H6B	0.0731	0.1305	0.0853	0.077*
H6C	0.1078	0.0841	0.0275	0.077*

C7	0.04068 (6)	0.08867 (6)	0.33547 (19)	0.0305 (4)
H7	0.0273	0.1231	0.3273	0.037*
C8	-0.04681 (7)	0.05675 (6)	0.2547 (2)	0.0315 (4)
C9	-0.08276 (7)	0.04527 (7)	0.1229 (2)	0.0400 (4)
H9	-0.0692	0.0389	0.0149	0.048*
C10	-0.13915 (8)	0.04360 (7)	0.1563 (3)	0.0439 (5)
H10	-0.1637	0.0361	0.0691	0.053*
C11	-0.16010 (8)	0.05281 (7)	0.3162 (3)	0.0428 (5)
H11	-0.1983	0.0528	0.3352	0.051*
C12	-0.12390 (8)	0.06192 (7)	0.4459 (3)	0.0403 (4)
H12	-0.1377	0.0669	0.5543	0.048*
C13	-0.06647 (7)	0.06394 (6)	0.4184 (2)	0.0333 (4)
C14	-0.02720 (8)	0.06748 (6)	0.5610 (2)	0.0353 (4)
O1	0.22180 (6)	0.04252 (6)	0.6136 (2)	0.0619 (4)
O2	0.15774 (6)	0.02632 (7)	0.79971 (18)	0.0710 (5)
O3	-0.04181 (6)	0.06418 (6)	0.70928 (16)	0.0523 (4)
O4	0.00911 (5)	0.05848 (4)	0.21703 (15)	0.0356 (3)
N1	0.17083 (7)	0.04246 (6)	0.6569 (2)	0.0458 (4)
N2	0.19283 (6)	0.07078 (5)	0.3198 (2)	0.0409 (4)
H2A	0.2169	0.0679	0.3996	0.049*
N3	0.09766 (5)	0.08753 (5)	0.27888 (17)	0.0339 (3)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0321 (9)	0.0326 (9)	0.0300 (9)	0.0013 (7)	-0.0007 (7)	-0.0038 (7)
C2	0.0399 (10)	0.0385 (9)	0.0262 (9)	-0.0023 (7)	-0.0043 (7)	-0.0041 (7)
C3	0.0317 (9)	0.0351 (9)	0.0376 (9)	0.0000 (7)	-0.0096 (8)	-0.0021 (7)
C4	0.0279 (9)	0.0299 (8)	0.0392 (9)	-0.0020 (7)	-0.0050 (8)	-0.0021 (8)
C5	0.0371 (11)	0.0692 (14)	0.0622 (13)	0.0076 (9)	0.0087 (10)	0.0000 (12)
C6	0.0379 (10)	0.0763 (14)	0.0399 (10)	0.0030 (9)	0.0018 (9)	0.0174 (10)
C7	0.0282 (9)	0.0317 (8)	0.0315 (8)	0.0012 (6)	-0.0022 (7)	-0.0017 (7)
C8	0.0280 (9)	0.0310 (9)	0.0356 (9)	0.0027 (6)	-0.0001 (7)	0.0029 (7)
C9	0.0395 (10)	0.0425 (10)	0.0378 (9)	-0.0006 (8)	-0.0079 (8)	-0.0006 (8)
C10	0.0364 (10)	0.0426 (10)	0.0527 (12)	-0.0032 (8)	-0.0143 (9)	0.0029 (9)
C11	0.0283 (10)	0.0424 (10)	0.0577 (12)	0.0009 (8)	-0.0010 (9)	0.0047 (9)
C12	0.0334 (9)	0.0393 (10)	0.0483 (11)	0.0010 (8)	0.0041 (9)	0.0015 (8)
C13	0.0318 (9)	0.0304 (8)	0.0376 (9)	0.0028 (7)	0.0014 (8)	0.0007 (7)
C14	0.0376 (10)	0.0344 (9)	0.0338 (10)	0.0029 (7)	0.0032 (8)	-0.0027 (8)
O1	0.0335 (8)	0.0824 (10)	0.0697 (11)	0.0039 (7)	-0.0197 (7)	0.0028 (9)
O2	0.0627 (10)	0.1090 (14)	0.0414 (8)	0.0052 (9)	-0.0172 (7)	0.0141 (9)
O3	0.0468 (8)	0.0771 (11)	0.0330 (7)	0.0008 (7)	0.0074 (6)	-0.0042 (7)
O4	0.0274 (7)	0.0480 (7)	0.0315 (6)	-0.0005 (5)	-0.0014 (5)	-0.0065 (5)
N1	0.0422 (10)	0.0525 (10)	0.0427 (10)	0.0006 (7)	-0.0168 (8)	-0.0015 (8)
N2	0.0252 (8)	0.0485 (9)	0.0492 (9)	-0.0011 (6)	-0.0038 (7)	-0.0018 (8)
N3	0.0263 (7)	0.0419 (8)	0.0334 (8)	0.0003 (6)	-0.0005 (6)	0.0026 (6)

*Geometric parameters (Å, °)*

C1—C2	1.337 (2)	C7—O4	1.4527 (19)
C1—C14	1.470 (2)	C7—H7	0.9800
C1—C7	1.478 (2)	C8—O4	1.3767 (19)
C2—C3	1.410 (2)	C8—C9	1.389 (2)
C2—H2	0.9300	C8—C13	1.392 (2)
C3—N1	1.383 (2)	C9—C10	1.381 (3)
C3—C4	1.448 (3)	C9—H9	0.9300
C4—N2	1.322 (2)	C10—C11	1.384 (3)
C4—N3	1.352 (2)	C10—H10	0.9300
C5—N2	1.459 (3)	C11—C12	1.367 (3)
C5—H5A	0.9600	C11—H11	0.9300
C5—H5B	0.9600	C12—C13	1.398 (2)
C5—H5C	0.9600	C12—H12	0.9300
C6—N3	1.471 (2)	C13—C14	1.474 (2)
C6—H6A	0.9600	C14—O3	1.228 (2)
C6—H6B	0.9600	O1—N1	1.271 (2)
C6—H6C	0.9600	O2—N1	1.250 (2)
C7—N3	1.440 (2)	N2—H2A	0.8600
C2—C1—C14	123.98 (15)	O4—C8—C13	121.86 (15)
C2—C1—C7	121.15 (15)	C9—C8—C13	121.26 (16)
C14—C1—C7	114.82 (14)	C10—C9—C8	118.23 (18)
C1—C2—C3	121.34 (16)	C10—C9—H9	120.9
C1—C2—H2	119.3	C8—C9—H9	120.9
C3—C2—H2	119.3	C9—C10—C11	121.74 (18)
N1—C3—C2	117.53 (16)	C9—C10—H10	119.1
N1—C3—C4	121.99 (16)	C11—C10—H10	119.1
C2—C3—C4	120.25 (15)	C12—C11—C10	119.15 (17)
N2—C4—N3	123.19 (16)	C12—C11—H11	120.4
N2—C4—C3	119.11 (15)	C10—C11—H11	120.4
N3—C4—C3	117.71 (15)	C11—C12—C13	121.18 (18)
N2—C5—H5A	109.5	C11—C12—H12	119.4
N2—C5—H5B	109.5	C13—C12—H12	119.4
H5A—C5—H5B	109.5	C8—C13—C12	118.32 (16)
N2—C5—H5C	109.5	C8—C13—C14	120.29 (15)
H5A—C5—H5C	109.5	C12—C13—C14	120.99 (16)
H5B—C5—H5C	109.5	O3—C14—C1	122.65 (16)
N3—C6—H6A	109.5	O3—C14—C13	122.98 (17)
N3—C6—H6B	109.5	C1—C14—C13	114.19 (15)
H6A—C6—H6B	109.5	C8—O4—C7	112.85 (13)
N3—C6—H6C	109.5	O2—N1—O1	119.09 (16)
H6A—C6—H6C	109.5	O2—N1—C3	119.25 (16)
H6B—C6—H6C	109.5	O1—N1—C3	121.65 (16)
N3—C7—O4	106.47 (12)	C4—N2—C5	133.91 (16)
N3—C7—C1	115.21 (13)	C4—N2—H2A	113.0
O4—C7—C1	110.46 (13)	C5—N2—H2A	113.0

N3—C7—H7	108.2	C4—N3—C7	124.17 (14)
O4—C7—H7	108.2	C4—N3—C6	122.96 (15)
C1—C7—H7	108.2	C7—N3—C6	112.47 (13)
O4—C8—C9	116.82 (15)		
C14—C1—C2—C3	175.22 (15)	C2—C1—C14—C13	-156.47 (16)
C7—C1—C2—C3	-2.0 (3)	C7—C1—C14—C13	20.9 (2)
C1—C2—C3—N1	-176.57 (17)	C8—C13—C14—O3	-165.56 (17)
C1—C2—C3—C4	-1.9 (2)	C12—C13—C14—O3	7.0 (3)
N1—C3—C4—N2	-1.9 (2)	C8—C13—C14—C1	9.7 (2)
C2—C3—C4—N2	-176.32 (15)	C12—C13—C14—C1	-177.78 (15)
N1—C3—C4—N3	178.45 (15)	C9—C8—O4—C7	157.13 (15)
C2—C3—C4—N3	4.0 (2)	C13—C8—O4—C7	-25.6 (2)
C2—C1—C7—N3	3.6 (2)	N3—C7—O4—C8	-179.19 (12)
C14—C1—C7—N3	-173.86 (14)	C1—C7—O4—C8	55.05 (17)
C2—C1—C7—O4	124.28 (17)	C2—C3—N1—O2	1.8 (3)
C14—C1—C7—O4	-53.19 (18)	C4—C3—N1—O2	-172.78 (17)
O4—C8—C9—C10	-179.54 (16)	C2—C3—N1—O1	-179.23 (17)
C13—C8—C9—C10	3.2 (2)	C4—C3—N1—O1	6.2 (3)
C8—C9—C10—C11	-0.2 (3)	N3—C4—N2—C5	-14.2 (3)
C9—C10—C11—C12	-2.6 (3)	C3—C4—N2—C5	166.2 (2)
C10—C11—C12—C13	2.5 (3)	N2—C4—N3—C7	178.08 (15)
O4—C8—C13—C12	179.59 (16)	C3—C4—N3—C7	-2.3 (2)
C9—C8—C13—C12	-3.3 (2)	N2—C4—N3—C6	-9.7 (2)
O4—C8—C13—C14	-7.7 (2)	C3—C4—N3—C6	169.90 (16)
C9—C8—C13—C14	169.44 (16)	O4—C7—N3—C4	-124.20 (15)
C11—C12—C13—C8	0.4 (3)	C1—C7—N3—C4	-1.4 (2)
C11—C12—C13—C14	-172.27 (16)	O4—C7—N3—C6	62.89 (17)
C2—C1—C14—O3	18.8 (3)	C1—C7—N3—C6	-174.29 (15)
C7—C1—C14—O3	-163.82 (17)		

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2A $\cdots$ O1	0.86	1.83	2.543 (2)	139
C5—H5A $\cdots$ O2 <sup>i</sup>	0.96	2.46	3.376 (3)	159
C5—H5C $\cdots$ O3 <sup>ii</sup>	0.96	2.51	3.416 (3)	157
C6—H6A $\cdots$ O3 <sup>ii</sup>	0.96	2.55	3.429 (2)	152
C9—H9 $\cdots$ O3 <sup>i</sup>	0.93	2.60	3.455 (2)	154

Symmetry codes: (i)  $x, y, z-1$ ; (ii)  $x+1/4, -y+1/4, z-3/4$ .