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## Structure Reports

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**(E)-Methyl N'-(2-furylmethylene)-hydrazinecarboxylate**Lu-Ping Lv,<sup>a</sup> Yong-Zhao Zhang,<sup>a</sup> Xiao-Min Ding,<sup>a</sup> Wen-Bo Yu<sup>b</sup> and Xian-Chao Hu<sup>c\*</sup>

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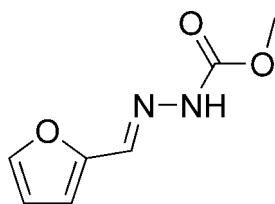
Received 15 October 2008; accepted 16 October 2008

Key indicators: single-crystal X-ray study;  $T = 193$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.031;  $wR$  factor = 0.085; data-to-parameter ratio = 7.3.

The title compound,  $\text{C}_7\text{H}_8\text{N}_2\text{O}_3$ , crystallizes with two independent but essentially identical molecules in the asymmetric unit. Each molecule adopts a *trans* configuration with respect to the  $\text{C}=\text{N}$  bond. The hydrazinecarboxylate group is twisted from the furan ring by  $7.78$  ( $13$ )° in one molecule and by  $7.01$  ( $17$ )° in the other. In the crystal structure, molecules are linked into chains running along  $[010]$  by bifurcated  $\text{N}-\text{H}\cdots(\text{N},\text{O})$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds. In addition, weak  $\text{C}-\text{H}\cdots\text{O}$  interactions and an  $\text{O}\cdots\text{C}$  short contact [ $2.896$  ( $3$ ) Å] are observed.

## Related literature

For general background, see: Parashar *et al.* (1988); Hadjoudis *et al.* (1987); Borg *et al.* (1999); Kahwa *et al.* (1986); Santos *et al.* (2001). For a related structure, see: Shang *et al.* (2007).



## Experimental

## Crystal data

$\text{C}_7\text{H}_8\text{N}_2\text{O}_3$   
 $M_r = 168.15$

Monoclinic,  $C2$   
 $a = 14.9185$  ( $17$ ) Å

$b = 7.8124$  ( $9$ ) Å  
 $c = 15.1299$  ( $19$ ) Å  
 $\beta = 105.251$  ( $7$ )°  
 $V = 1701.3$  ( $4$ ) Å<sup>3</sup>  
 $Z = 8$

Mo  $K\alpha$  radiation  
 $\mu = 0.10$  mm<sup>-1</sup>  
 $T = 193$  ( $2$ ) K  
 $0.19 \times 0.17 \times 0.16$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)  
 $T_{\min} = 0.978$ ,  $T_{\max} = 0.982$

4679 measured reflections  
1601 independent reflections  
1399 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.020$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.085$   
 $S = 1.07$   
1601 reflections  
218 parameters

1 restraint  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.10$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.09$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N2}-\text{H2A}\cdots\text{O5}$	0.86	2.36	3.138 (3)	151
$\text{N2}-\text{H2A}\cdots\text{N3}$	0.86	2.52	3.242 (3)	141
$\text{N4}-\text{H4}\cdots\text{O2}^i$	0.86	2.11	2.913 (3)	156
$\text{C2}-\text{H2}\cdots\text{O5}^{ii}$	0.93	2.60	3.521 (4)	172
$\text{C10}-\text{H10}\cdots\text{O5}^{iii}$	0.93	2.59	3.508 (4)	171

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2688).

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## supporting information

*Acta Cryst.* (2008). E64, o2146 [doi:10.1107/S1600536808033825]

**(E)-Methyl N'-(2-furylmethylene)hydrazinecarboxylate**

Lu-Ping Lv, Yong-Zhao Zhang, Xiao-Min Ding, Wen-Bo Yu and Xian-Chao Hu

**S1. Comment**

Benzaldehydhydrazone derivatives have attracted much attention due to their pharmacological activity (Parashar *et al.*, 1988) and their photochromic properties (Hadjoudis *et al.*, 1987). They are important intermediates of 1,3,4-oxadiazoles, which have been reported to be versatile compounds with many interesting properties (Borg *et al.*, 1999). Metal complexes based on Schiff bases have received considerable attention because they can be utilized as model compounds of active centres in various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*, 2001). We report here the crystal structure of the title compound (Fig. 1).

The title compound contains two independent, but essentially identical molecules in the asymmetric unit. Each independent molecule adopts a *trans* configuration with respect to the C=N bond. The N1/N2/O2/O3/C6/C7 and N3/N4/O5/O6/C13/C14 planes form dihedral angles of 7.78 (13) and 7.01 (17)°, respectively, with the O1/C1–C4 and O4/C8–C11 planes. The dihedral angle between the two independent furan rings is 85.17 (11)°. The bond lengths and angles are comparable to those observed for methyl N'-[(E)-4-methoxybenzylidene]hydrazinecarboxylate (Shang *et al.*, 2007).

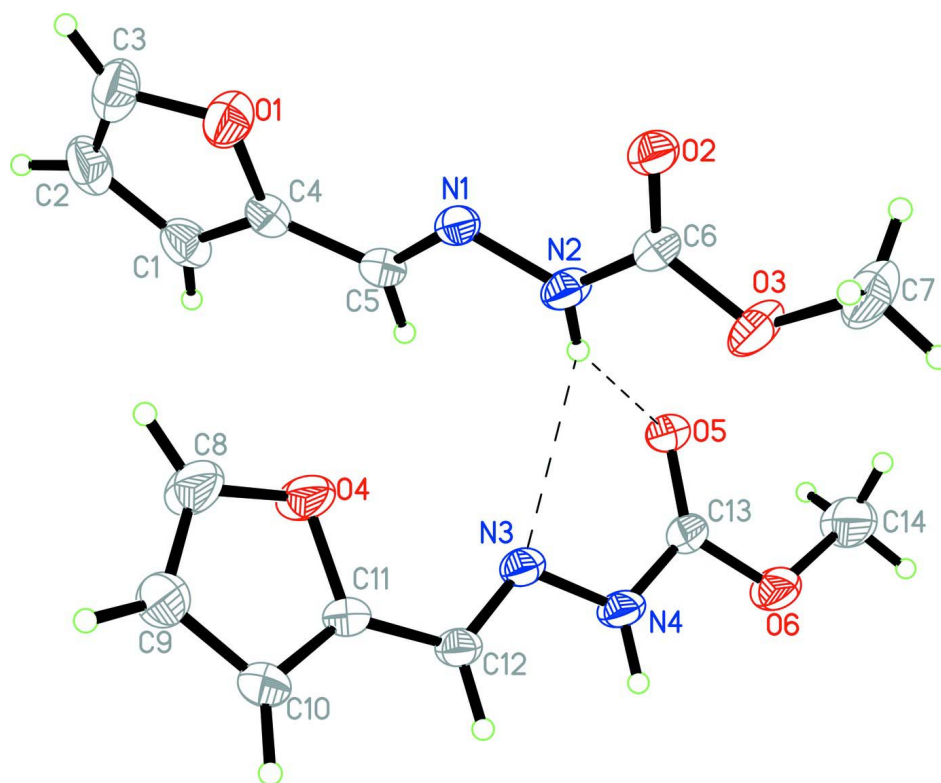
In the crystal structure, the molecules are linked into chains running along the [010] by N—H···O and N—H···N hydrogen bonds (Table 1 and Fig.2). In addition, weak C—H···O interactions and an O4···C5 short contact [2.896 (3) Å] are also observed.

**S2. Experimental**

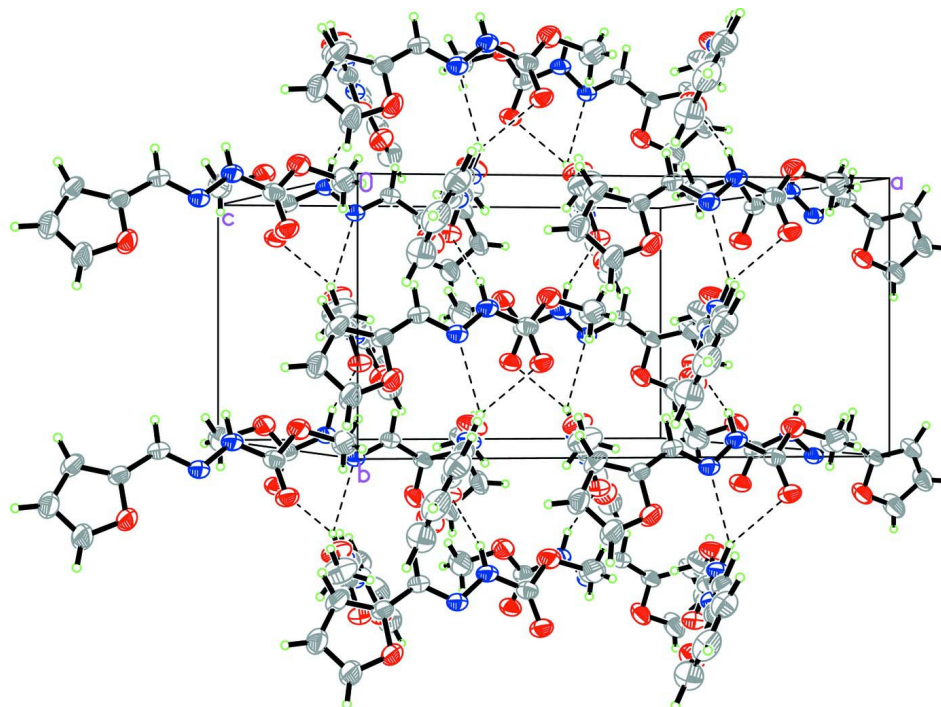
Furfuraldehyde (0.96 g, 0.01 mol) and methyl hydrazinecarboxylate (0.90 g, 0.01 mol) were dissolved in stirred methanol (20 ml) and left for 3 h at room temperature. The resulting solid was filtered off and recrystallized from ethanol to give the title compound in 85% yield. Single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution at room temperature (m.p. 408–413 K).

**S3. Refinement**

H atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93 or 0.96 Å) and refined using a riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$  and  $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$ . In the absence of significant anomalous scattering effects, Friedel pairs were averaged.

**Figure 1**

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Dashed lines indicate hydrogen bonds.

**Figure 2**

Crystal packing of the title compound. Hydrogen bonds are shown as dashed lines.

**(*E*)-Methyl *N*'-(2-furylmethylene)hydrazinecarboxylate**

*Crystal data*

$C_7H_8N_2O_3$

$M_r = 168.15$

Monoclinic,  $C2$

Hall symbol:  $C\ 2y$

$a = 14.9185\ (17)\ \text{\AA}$

$b = 7.8124\ (9)\ \text{\AA}$

$c = 15.1299\ (19)\ \text{\AA}$

$\beta = 105.251\ (7)^\circ$

$V = 1701.3\ (4)\ \text{\AA}^3$

$Z = 8$

$F(000) = 704$

$D_x = 1.313\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1601 reflections

$\theta = 1.4\text{--}25.0^\circ$

$\mu = 0.10\ \text{mm}^{-1}$

$T = 193\ \text{K}$

Block, colourless

$0.19 \times 0.17 \times 0.16\ \text{mm}$

*Data collection*

Bruker SMART CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2002)

$T_{\min} = 0.978$ ,  $T_{\max} = 0.982$

4679 measured reflections

1601 independent reflections

1399 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.020$

$\theta_{\max} = 25.0^\circ$ ,  $\theta_{\min} = 1.4^\circ$

$h = -17 \rightarrow 17$

$k = -9 \rightarrow 8$

$l = -17 \rightarrow 16$

*Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.031$  $wR(F^2) = 0.085$  $S = 1.07$ 

1601 reflections

218 parameters

1 restraint

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0464P)^2 + 0.2178P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} = 0.001$  $\Delta\rho_{\max} = 0.10 \text{ e } \text{\AA}^{-3}$  $\Delta\rho_{\min} = -0.09 \text{ e } \text{\AA}^{-3}$ Extinction correction: *SHELXL97* (Sheldrick,  
2008),  $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$ 

Extinction coefficient: 0.0051 (9)

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6802 (2)	0.5242 (5)	-0.0094 (2)	0.0834 (9)
H1	0.6985	0.4241	-0.0330	0.100*
C2	0.6239 (2)	0.6570 (6)	-0.0595 (2)	0.0971 (12)
H2	0.5969	0.6590	-0.1223	0.117*
C3	0.6170 (2)	0.7771 (6)	0.0000 (2)	0.1020 (12)
H3	0.5850	0.8797	-0.0152	0.122*
C4	0.70165 (17)	0.5730 (4)	0.07936 (17)	0.0617 (7)
C5	0.75360 (16)	0.4883 (3)	0.16066 (17)	0.0583 (6)
H5	0.7769	0.3792	0.1561	0.070*
C6	0.83278 (17)	0.5270 (4)	0.39638 (18)	0.0600 (6)
C7	0.8972 (3)	0.4683 (6)	0.5526 (2)	0.1191 (15)
H7A	0.9269	0.3773	0.5922	0.179*
H7B	0.8411	0.5010	0.5681	0.179*
H7C	0.9383	0.5648	0.5600	0.179*
C8	0.5302 (2)	0.2842 (6)	0.1389 (3)	0.1233 (17)
H8	0.5139	0.3884	0.1093	0.148*
C9	0.4711 (2)	0.1714 (5)	0.1540 (3)	0.0977 (11)
H9	0.4067	0.1801	0.1368	0.117*
C10	0.52379 (19)	0.0344 (5)	0.2012 (2)	0.0786 (8)
H10	0.5006	-0.0642	0.2216	0.094*
C11	0.61376 (17)	0.0724 (3)	0.21148 (18)	0.0615 (7)
C12	0.69799 (17)	-0.0134 (3)	0.25482 (16)	0.0586 (6)
H12	0.6952	-0.1248	0.2756	0.070*

C13	0.93793 (17)	0.0282 (4)	0.32608 (17)	0.0609 (6)
C14	1.0967 (2)	-0.0296 (6)	0.3959 (3)	0.1240 (16)
H14A	1.1351	-0.1178	0.4307	0.186*
H14B	1.1047	0.0743	0.4311	0.186*
H14C	1.1143	-0.0105	0.3400	0.186*
N1	0.76861 (13)	0.5587 (3)	0.23906 (14)	0.0552 (5)
N2	0.81642 (15)	0.4606 (3)	0.31122 (14)	0.0652 (6)
H2A	0.8355	0.3597	0.3025	0.078*
N3	0.77726 (14)	0.0577 (3)	0.26606 (14)	0.0596 (5)
N4	0.85235 (15)	-0.0392 (3)	0.31071 (16)	0.0692 (6)
H4	0.8447	-0.1414	0.3286	0.083*
O1	0.66343 (14)	0.7290 (3)	0.08659 (13)	0.0860 (7)
O2	0.81342 (12)	0.6698 (2)	0.41521 (12)	0.0673 (5)
O3	0.87484 (17)	0.4105 (3)	0.45826 (13)	0.0932 (7)
O4	0.61942 (13)	0.2275 (3)	0.17282 (18)	0.1027 (8)
O5	0.95630 (12)	0.1665 (2)	0.30007 (12)	0.0699 (5)
O6	0.99994 (13)	-0.0822 (3)	0.37459 (16)	0.0895 (7)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0933 (19)	0.090 (2)	0.0653 (18)	-0.024 (2)	0.0181 (15)	-0.0164 (18)
C2	0.090 (2)	0.131 (3)	0.0597 (19)	-0.034 (2)	0.0009 (16)	0.004 (2)
C3	0.097 (2)	0.118 (3)	0.080 (2)	0.012 (2)	0.0033 (18)	0.024 (2)
C4	0.0599 (13)	0.0630 (19)	0.0627 (17)	-0.0120 (13)	0.0170 (11)	-0.0070 (14)
C5	0.0606 (12)	0.0503 (16)	0.0669 (16)	-0.0080 (11)	0.0217 (11)	-0.0033 (13)
C6	0.0688 (14)	0.0525 (16)	0.0598 (16)	0.0034 (12)	0.0191 (11)	0.0131 (13)
C7	0.186 (4)	0.101 (3)	0.063 (2)	0.045 (3)	0.021 (2)	0.022 (2)
C8	0.0559 (16)	0.103 (3)	0.200 (4)	0.0057 (19)	0.014 (2)	0.072 (3)
C9	0.0562 (15)	0.102 (3)	0.129 (3)	-0.0063 (18)	0.0139 (16)	0.034 (3)
C10	0.0716 (16)	0.0723 (18)	0.088 (2)	-0.0234 (16)	0.0139 (14)	0.0125 (16)
C11	0.0673 (15)	0.0484 (16)	0.0684 (16)	-0.0082 (12)	0.0168 (12)	0.0072 (13)
C12	0.0711 (15)	0.0428 (14)	0.0618 (15)	-0.0042 (12)	0.0172 (11)	0.0016 (11)
C13	0.0668 (15)	0.0493 (15)	0.0629 (15)	0.0061 (13)	0.0108 (11)	0.0055 (13)
C14	0.0683 (19)	0.096 (3)	0.185 (4)	0.0045 (19)	-0.007 (2)	0.036 (3)
N1	0.0628 (11)	0.0452 (12)	0.0577 (13)	-0.0017 (9)	0.0159 (9)	0.0039 (10)
N2	0.0882 (15)	0.0433 (11)	0.0659 (14)	0.0111 (11)	0.0237 (11)	0.0071 (11)
N3	0.0637 (12)	0.0448 (12)	0.0693 (13)	0.0024 (10)	0.0158 (10)	0.0078 (10)
N4	0.0663 (12)	0.0437 (11)	0.0940 (16)	0.0038 (10)	0.0148 (11)	0.0182 (12)
O1	0.0971 (14)	0.0878 (16)	0.0700 (13)	0.0182 (12)	0.0162 (10)	0.0062 (11)
O2	0.0868 (12)	0.0485 (11)	0.0639 (11)	0.0061 (10)	0.0154 (9)	0.0031 (9)
O3	0.1460 (19)	0.0685 (15)	0.0641 (12)	0.0357 (14)	0.0256 (12)	0.0230 (11)
O4	0.0575 (10)	0.0748 (14)	0.171 (2)	-0.0016 (10)	0.0218 (12)	0.0520 (15)
O5	0.0733 (10)	0.0521 (11)	0.0783 (12)	-0.0049 (10)	0.0092 (9)	0.0131 (10)
O6	0.0698 (11)	0.0645 (14)	0.1240 (17)	0.0081 (10)	0.0075 (11)	0.0283 (13)

*Geometric parameters (Å, °)*

C1—C4	1.351 (4)	C8—H8	0.93
C1—C2	1.421 (6)	C9—C10	1.406 (5)
C1—H1	0.93	C9—H9	0.93
C2—C3	1.322 (6)	C10—C11	1.343 (4)
C2—H2	0.93	C10—H10	0.93
C3—O1	1.364 (4)	C11—O4	1.357 (3)
C3—H3	0.93	C11—C12	1.423 (3)
C4—O1	1.362 (4)	C12—N3	1.277 (3)
C4—C5	1.432 (4)	C12—H12	0.93
C5—N1	1.273 (3)	C13—O5	1.206 (3)
C5—H5	0.93	C13—O6	1.334 (3)
C6—O2	1.206 (4)	C13—N4	1.344 (3)
C6—O3	1.337 (3)	C14—O6	1.454 (4)
C6—N2	1.350 (3)	C14—H14A	0.96
C7—O3	1.450 (4)	C14—H14B	0.96
C7—H7A	0.96	C14—H14C	0.96
C7—H7B	0.96	N1—N2	1.370 (3)
C7—H7C	0.96	N2—H2A	0.86
C8—C9	1.309 (5)	N3—N4	1.373 (3)
C8—O4	1.368 (4)	N4—H4	0.86
C4—C1—C2	106.0 (3)	C11—C10—C9	107.4 (3)
C4—C1—H1	127.0	C11—C10—H10	126.3
C2—C1—H1	127.0	C9—C10—H10	126.3
C3—C2—C1	107.2 (3)	C10—C11—O4	108.7 (3)
C3—C2—H2	126.4	C10—C11—C12	133.1 (3)
C1—C2—H2	126.4	O4—C11—C12	118.1 (2)
C2—C3—O1	110.3 (4)	N3—C12—C11	122.1 (2)
C2—C3—H3	124.8	N3—C12—H12	119.0
O1—C3—H3	124.8	C11—C12—H12	119.0
C1—C4—O1	109.7 (3)	O5—C13—O6	125.1 (2)
C1—C4—C5	131.0 (3)	O5—C13—N4	125.6 (2)
O1—C4—C5	119.2 (2)	O6—C13—N4	109.4 (2)
N1—C5—C4	121.6 (2)	O6—C14—H14A	109.5
N1—C5—H5	119.2	O6—C14—H14B	109.5
C4—C5—H5	119.2	H14A—C14—H14B	109.5
O2—C6—O3	124.2 (3)	O6—C14—H14C	109.5
O2—C6—N2	125.9 (2)	H14A—C14—H14C	109.5
O3—C6—N2	109.9 (3)	H14B—C14—H14C	109.5
O3—C7—H7A	109.5	C5—N1—N2	115.3 (2)
O3—C7—H7B	109.5	C6—N2—N1	118.1 (2)
H7A—C7—H7B	109.5	C6—N2—H2A	120.9
O3—C7—H7C	109.5	N1—N2—H2A	120.9
H7A—C7—H7C	109.5	C12—N3—N4	115.6 (2)
H7B—C7—H7C	109.5	C13—N4—N3	118.9 (2)
C9—C8—O4	110.5 (3)	C13—N4—H4	120.5

C9—C8—H8	124.8	N3—N4—H4	120.5
O4—C8—H8	124.8	C4—O1—C3	106.7 (3)
C8—C9—C10	106.8 (3)	C6—O3—C7	114.9 (3)
C8—C9—H9	126.6	C11—O4—C8	106.6 (2)
C10—C9—H9	126.6	C13—O6—C14	116.3 (2)
C4—C1—C2—C3	1.7 (4)	C5—N1—N2—C6	-178.6 (2)
C1—C2—C3—O1	-1.6 (4)	C11—C12—N3—N4	178.7 (2)
C2—C1—C4—O1	-1.1 (3)	O5—C13—N4—N3	-3.8 (4)
C2—C1—C4—C5	177.6 (3)	O6—C13—N4—N3	176.4 (2)
C1—C4—C5—N1	178.0 (3)	C12—N3—N4—C13	-179.1 (2)
O1—C4—C5—N1	-3.3 (3)	C1—C4—O1—C3	0.2 (3)
O4—C8—C9—C10	0.8 (6)	C5—C4—O1—C3	-178.8 (2)
C8—C9—C10—C11	-0.6 (5)	C2—C3—O1—C4	0.9 (4)
C9—C10—C11—O4	0.1 (4)	O2—C6—O3—C7	-0.4 (4)
C9—C10—C11—C12	178.3 (3)	N2—C6—O3—C7	179.2 (3)
C10—C11—C12—N3	-171.0 (3)	C10—C11—O4—C8	0.3 (4)
O4—C11—C12—N3	7.0 (4)	C12—C11—O4—C8	-178.1 (3)
C4—C5—N1—N2	177.8 (2)	C9—C8—O4—C11	-0.7 (5)
O2—C6—N2—N1	-4.2 (4)	O5—C13—O6—C14	-0.8 (5)
O3—C6—N2—N1	176.2 (2)	N4—C13—O6—C14	179.0 (3)

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—H2 <i>A</i> ...O5	0.86	2.36	3.138 (3)	151
N2—H2 <i>A</i> ...N3	0.86	2.52	3.242 (3)	141
N4—H4...O2 <sup>i</sup>	0.86	2.11	2.913 (3)	156
C2—H2...O5 <sup>ii</sup>	0.93	2.60	3.521 (4)	172
C10—H10...O5 <sup>iii</sup>	0.93	2.59	3.508 (4)	171

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