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## Structure Reports

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 Methyl 1*H*-pyrrole-2-carboxylate

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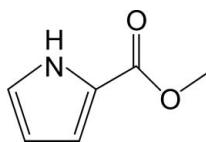
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 Key indicators: single-crystal X-ray study;  $T = 200$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.070;  $wR$  factor = 0.176; data-to-parameter ratio = 13.3.

The title compound,  $\text{C}_6\text{H}_7\text{NO}_2$ , is essentially planar with a dihedral angle of  $3.6(3)^\circ$  between the pyrrole ring and the methoxycarbonyl O/C/O/C plane. In the crystal structure, the N atom is a hydrogen-bond donor to the carboxylate C=O O atom of the neighboring molecule. These intermolecular hydrogen bonds lead to the formation of helical chains along the  $b$  axis.

## Related literature

For related structures, see: Kerscher, Klüfers, Kügel & Müller (2007); Kerscher, Klüfers & Kügel (2007). For graph-set analysis, see: Bernstein *et al.* (1995); Etter *et al.* (1990).



## Experimental

## Crystal data

$\text{C}_6\text{H}_7\text{NO}_2$   
 $M_r = 125.13$   
 Monoclinic,  $P2_1/c$   
 $a = 7.5346(19)$  Å  
 $b = 5.4598(14)$  Å  
 $c = 14.730(4)$  Å  
 $\beta = 100.55(2)^\circ$

$V = 595.7(3)$  Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.11$  mm<sup>-1</sup>  
 $T = 200$  K  
 $0.38 \times 0.16 \times 0.06$  mm

## Data collection

Oxford Xcalibur KappaCCD diffractometer  
 Absorption correction: none  
 2591 measured reflections

1103 independent reflections  
 528 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.112$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.070$   
 $wR(F^2) = 0.176$   
 $S = 0.95$   
 1103 reflections

83 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.27$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.26$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{O2}^{\text{i}}$	0.88	2.06	2.933 (4)	171
$\text{C4}-\text{H4}\cdots\text{Cg1}^{\text{ii}}$	0.95	2.63	3.401 (5)	139

Symmetry codes: (i)  $-x, y - \frac{1}{2}, -z + \frac{1}{2}$ ; (ii)  $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$ . Cg1 is the centroid of the pyrrole ring.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-III* (Burnett & Johnson, 1996), *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

TK is indebted to the Hanns-Seidel Stiftung for a PhD grant funded by the German Bundesministerium für Bildung und Forschung.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2445).

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## supporting information

*Acta Cryst.* (2009). E65, o2195 [doi:10.1107/S1600536809030906]

## Methyl 1*H*-pyrrole-2-carboxylate

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### S1. Comment

The title compound was prepared, in the attempt to create new complexing ligands, as a byproduct. The compound is quite similar to other compounds already published by our group (Kerscher, Klüfers, Kügel & Müller, 2007; Kerscher, Klüfers & Kügel, 2007).

In the molecule, a formic acid methyl ester is in the 2 position of the pyrrole ring (Fig. 1). With a torsion angle for C2–C1–C5–O1 of only about 2.9°, the molecule is, with the exception of the H atoms of the methyl group, nearly planar. Because of this small torsion angle, the molecule is not  $C_s$  symmetric.

The hydrogen bonds of the nitrogen to the carboxylate oxygen lead to a chain like hydrogen bonding system which can be described according to graph-set analysis (Etter *et al.*, 1990; Bernstein *et al.*, 1995) with a C(5) descriptor on the unitary level [the rpluto program (Cambridge Crystallographic Data Centre, England) was used for the graph set analyses; one of these strands is shown in Fig. 2].

Considering contacts whose range falls below the sum of van der Waals radii by only about 0.1 Å, a set of weak C–H $\cdots\pi$  interactions leads to the formation of a second system of strands along [0 1 0] which can be described by a C(2) descriptor (see Fig. 3).

The two strand systems alternate, which means two hydrogen bonding strands are interconnected by a strand of weak C–H $\cdots\pi$  contacts (this situation is illustrated in Fig. 4) and *vice versa*, two strands made of weak C–H $\cdots\pi$  contacts are interconnected by hydrogen bonding strands. This bonding pattern leads to sheet like structures normal to [0 0 1].

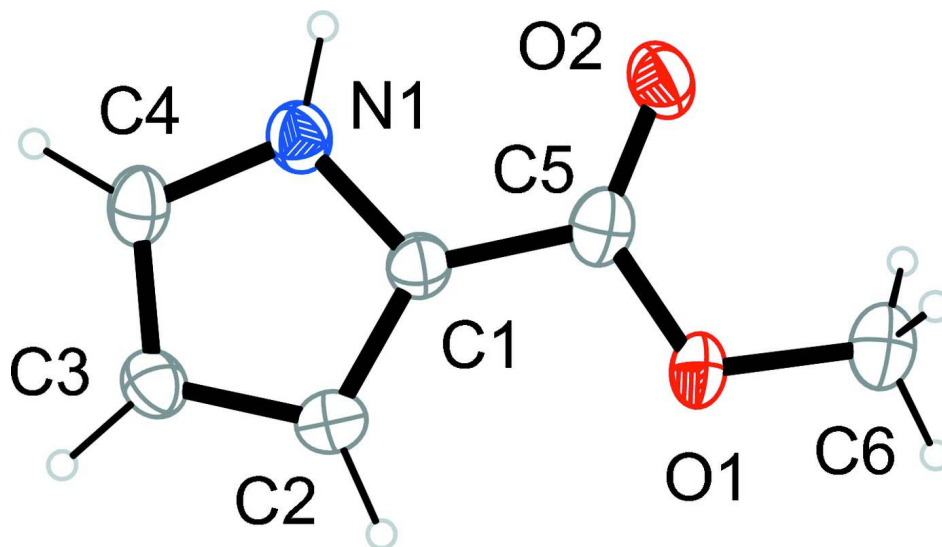
The molecular packing of the title compound is shown in Figure 5.

### S2. Experimental

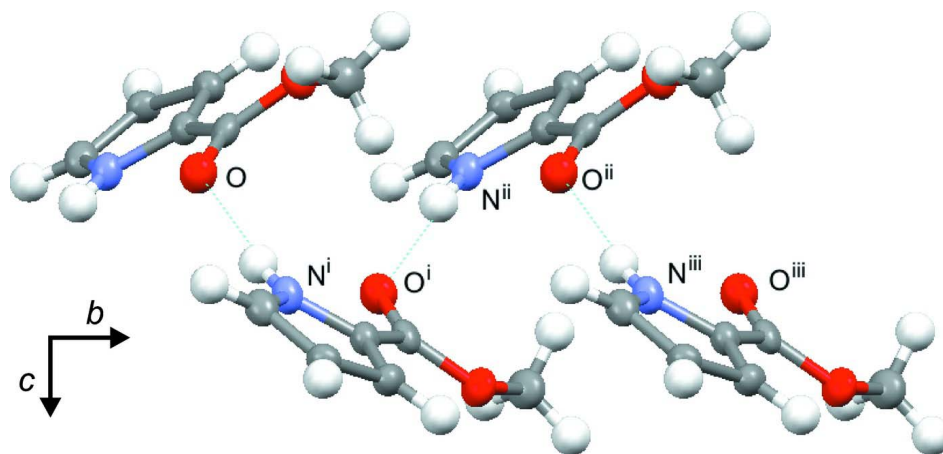
The title compound was obtained by reaction of 228 mg (3.40 mmol) of pyrrole with 280 mg (1.70 mmol) phosgene imminium chloride in 6 ml of dry acetonitrile. After removal of the solvent, the remaining green solid was purified by column chromatography on silica with chloroform as eluent. Sublimation of fraction five yielded the title compound as colorless crystals.

### S3. Refinement

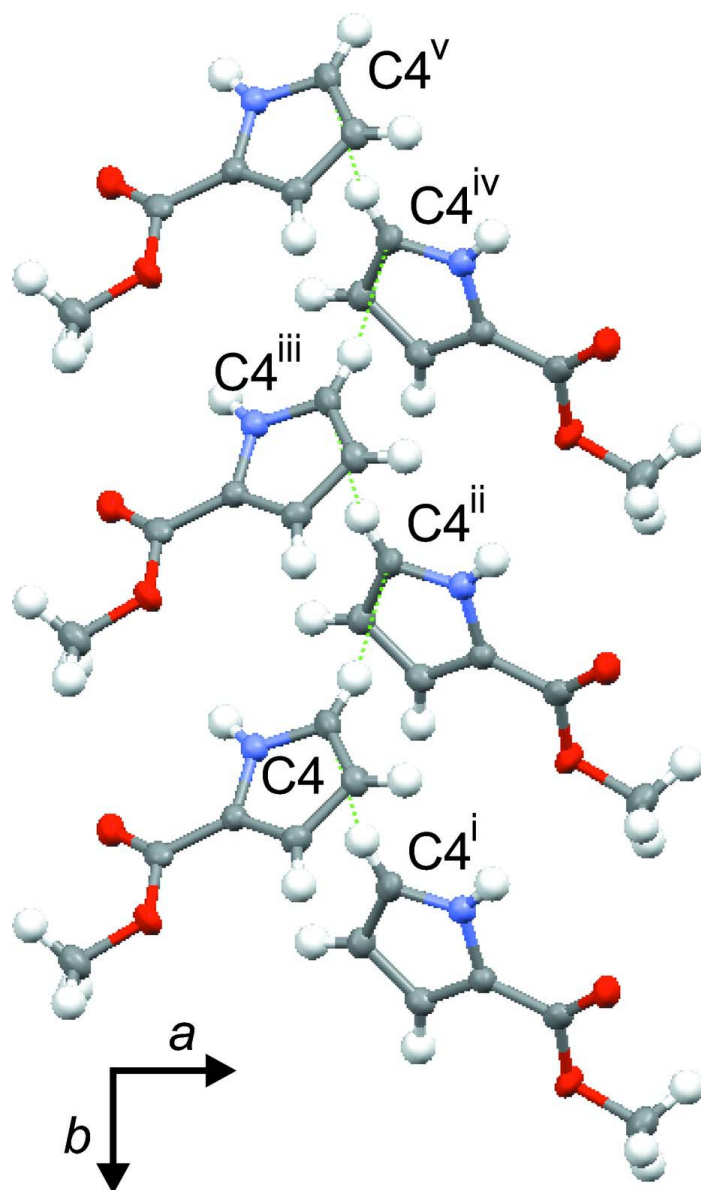
H atoms were calculated in ideal geometry, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C or N})$  for all aromatic C- and N-bound H atoms, and with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for the methylgroup H atoms.

**Figure 1**

The molecular structure of the title compound with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level) for non-H atoms.

**Figure 2**

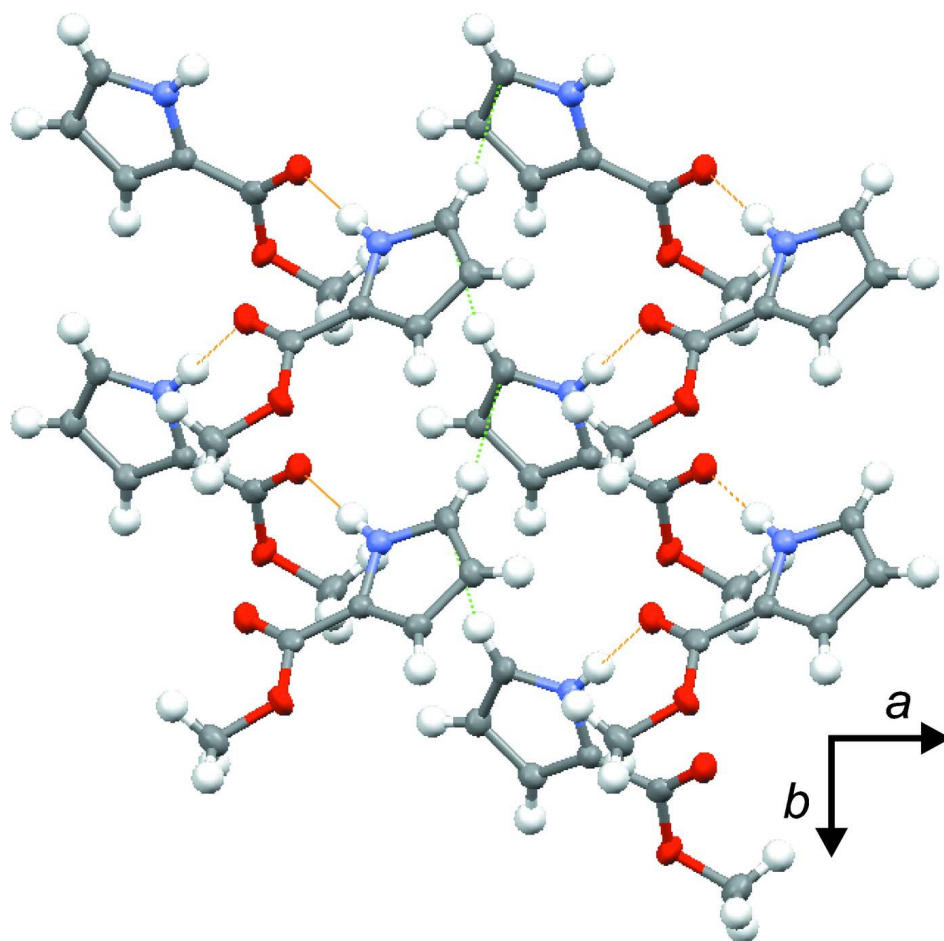
Strands formed by N–H...O hydrogen bonds along [0 1 0] in the crystal structure of the title compound, viewed along [1 0 0]. Symmetry codes: (i)  $-x, y + 1/2, 1/2 - z$ ; (ii)  $x, y + 1, z$ ; (iii)  $-x, y + 3/2, 1/2 - z$ .



**Figure 3**

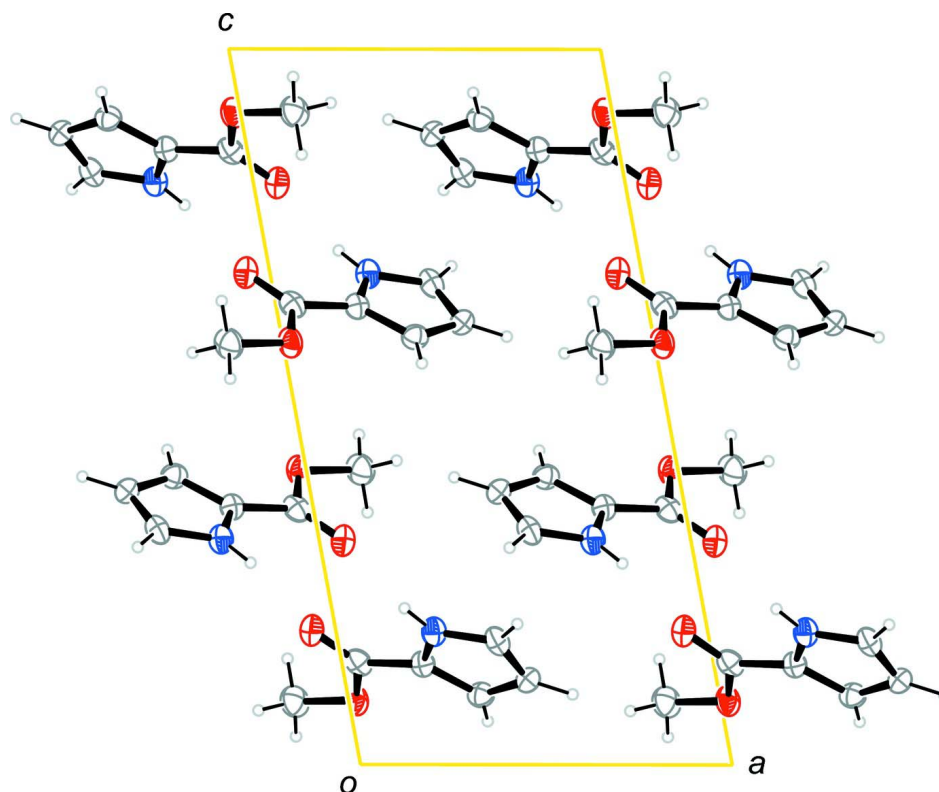
Strands formed by C-H... $\pi$  contacts along [0 1 0] in the crystal structure of the title compound, viewed along [0 0 1].

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



**Figure 4**

The strands formed by hydrogen bonding in the crystal structure are interconnected by the strands formed by C–H... $\pi$  contacts.

**Figure 5**

The packing of the title compound, viewed along [0 1 0].

### Methyl 1*H*-pyrrole-2-carboxylate

#### Crystal data

$C_6H_7NO_2$

$M_r = 125.13$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2ybc$

$a = 7.5346$  (19) Å

$b = 5.4598$  (14) Å

$c = 14.730$  (4) Å

$\beta = 100.55$  (2)°

$V = 595.7$  (3) Å<sup>3</sup>

$Z = 4$

$F(000) = 264$

$D_x = 1.395$  Mg m<sup>-3</sup>

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

Cell parameters from 1091 reflections

$\theta = 4.0$ – $27.5$ °

$\mu = 0.11$  mm<sup>-1</sup>

$T = 200$  K

Platelet, colourless

$0.38 \times 0.16 \times 0.06$  mm

#### Data collection

Oxford Xcalibur KappaCCD  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega$ -scans

2591 measured reflections

1103 independent reflections

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

$R_{int} = 0.112$

$\theta_{max} = 25.5$ °,  $\theta_{min} = 4.0$ °

$h = -9 \rightarrow 9$

$k = -6 \rightarrow 6$

$l = -17 \rightarrow 17$

Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.070$

$wR(F^2) = 0.176$

$S = 0.95$

1103 reflections

83 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

$w = 1/[\sigma^2(F_o^2) + (0.0745P)^2]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.27 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.0203 (3)	0.7534 (4)	0.08955 (19)	0.0312 (8)
O2	-0.0644 (3)	0.4755 (5)	0.18723 (19)	0.0331 (8)
N1	0.2637 (4)	0.2221 (6)	0.1856 (2)	0.0286 (9)
H1	0.1960	0.1417	0.2183	0.034*
C1	0.2176 (5)	0.4370 (7)	0.1405 (3)	0.0248 (10)
C5	0.0452 (5)	0.5519 (7)	0.1425 (3)	0.0276 (10)
C6	-0.1459 (5)	0.8847 (7)	0.0877 (3)	0.0378 (12)
H6A	-0.2475	0.7701	0.0753	0.057*
H6B	-0.1594	1.0093	0.0391	0.057*
H6C	-0.1439	0.9640	0.1476	0.057*
C3	0.4923 (5)	0.3236 (7)	0.1182 (3)	0.0275 (10)
H3	0.6054	0.3212	0.0984	0.033*
C4	0.4295 (5)	0.1506 (7)	0.1726 (3)	0.0300 (10)
H4	0.4914	0.0065	0.1967	0.036*
C2	0.3585 (5)	0.5042 (7)	0.0975 (3)	0.0276 (10)
H2	0.3638	0.6461	0.0608	0.033*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0235 (16)	0.0309 (17)	0.0388 (19)	0.0084 (12)	0.0042 (12)	0.0051 (13)
O2	0.0241 (16)	0.0352 (17)	0.041 (2)	0.0013 (13)	0.0090 (14)	-0.0012 (14)
N1	0.025 (2)	0.0251 (19)	0.036 (2)	-0.0002 (15)	0.0059 (15)	-0.0020 (16)
C1	0.024 (2)	0.022 (2)	0.028 (2)	-0.0012 (18)	0.0041 (18)	-0.0015 (17)
C5	0.028 (2)	0.022 (2)	0.030 (2)	0.0005 (18)	-0.0009 (19)	-0.0072 (18)
C6	0.034 (3)	0.037 (3)	0.041 (3)	0.009 (2)	0.004 (2)	0.001 (2)
C3	0.026 (2)	0.031 (2)	0.026 (2)	0.0016 (18)	0.0079 (17)	-0.0016 (19)
C4	0.023 (2)	0.029 (2)	0.035 (3)	0.0024 (19)	-0.0013 (18)	-0.0029 (19)
C2	0.030 (2)	0.026 (2)	0.026 (3)	-0.0026 (19)	0.0051 (19)	0.0019 (19)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

O1—C5	1.341 (4)	C6—H6A	0.9800
O1—C6	1.439 (4)	C6—H6B	0.9800

O2—C5	1.221 (5)	C6—H6C	0.9800
N1—C4	1.356 (5)	C3—C4	1.377 (5)
N1—C1	1.362 (5)	C3—C2	1.403 (5)
N1—H1	0.8800	C3—H3	0.9500
C1—C2	1.382 (5)	C4—H4	0.9500
C1—C5	1.447 (5)	C2—H2	0.9500
C5—O1—C6	116.6 (3)	O1—C6—H6C	109.5
C4—N1—C1	109.8 (3)	H6A—C6—H6C	109.5
C4—N1—H1	125.1	H6B—C6—H6C	109.5
C1—N1—H1	125.1	C4—C3—C2	107.4 (3)
N1—C1—C2	107.7 (3)	C4—C3—H3	126.3
N1—C1—C5	120.9 (3)	C2—C3—H3	126.3
C2—C1—C5	131.4 (4)	N1—C4—C3	108.0 (3)
O2—C5—O1	123.9 (4)	N1—C4—H4	126.0
O2—C5—C1	124.1 (4)	C3—C4—H4	126.0
O1—C5—C1	112.0 (4)	C1—C2—C3	107.2 (3)
O1—C6—H6A	109.5	C1—C2—H2	126.4
O1—C6—H6B	109.5	C3—C2—H2	126.4
H6A—C6—H6B	109.5		
C4—N1—C1—C2	0.0 (4)	C2—C1—C5—O1	2.9 (6)
C4—N1—C1—C5	179.3 (3)	C1—N1—C4—C3	0.3 (4)
C6—O1—C5—O2	0.7 (5)	C2—C3—C4—N1	-0.4 (4)
C6—O1—C5—C1	-179.0 (3)	N1—C1—C2—C3	-0.2 (4)
N1—C1—C5—O2	4.1 (6)	C5—C1—C2—C3	-179.4 (4)
C2—C1—C5—O2	-176.8 (4)	C4—C3—C2—C1	0.4 (4)
N1—C1—C5—O1	-176.2 (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>
N1—H1...O2 <sup>i</sup>	0.88	2.06	2.933 (4)	171
C4—H4...Cg1 <sup>ii</sup>	0.95	2.63	3.401 (5)	139

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