Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Methyl 2-(5-chloro-1-methyl-2-oxo-2,3-dihydro-1*H*-indol-3-ylidene)acetate

**Piskala Subburaman Kannan,[a] PanneerSelvam Yuvaraj,[b] Karthikeyan Manivannan,[b] Boreddy S. R. Reddy[b] and A. SubbiahPandi[c]***

[a]Department of Physics, S.M.K. Fomra Institute of Technology, Thaiyur, Chennai 603 103, India, [b]Industrial Chemistry Laboratory, Central Leather Research Institute, Adyar, Chennai 600 020, India, and [c]Department of Physics, Presidency College (Autonomous), Chennai 600 005, India
Correspondence e-mail: a_sp59@yahoo.in

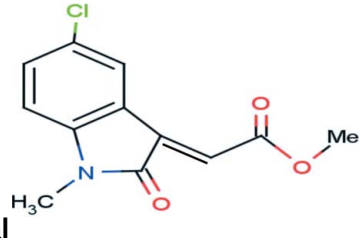
Received 10 April 2013; accepted 30 April 2013

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.038; $wR$ factor = 0.138; data-to-parameter ratio = 17.9.

The title compound, $C_{12}H_{10}ClNO_3$, the indoline ring system is essentially planar, with a maximum deviation of 0.009 Å for the N atom. The indoline ring and acetate group are essentially coplanar, with a maximum deviation of 0.086 Å for the O atom. The mean plane through the methoxycarbonylmethyl group forms a dihedral angle of 3.68 (5)° with the plane of the indoline ring system. The molecular structure is stabilized by an intramolecular C—H···O hydrogen-bond interaction. In the crystal, $\pi$–$\pi$ stacking interactions [centroid–centroid distance = 3.7677 (8) Å] occur between benzene rings, forming a chain running along the $c$-axis direction.

## Related literature

For the biological activity of indole derivatives, see: Chai *et al.* (2006); Nieto *et al.* (2005); Singh *et al.* (2000); Andreani *et al.* (2001); Quetin-Leclercq (1994); Mukhopadhyay *et al.* (1981); Taylor *et al.* (1999). For closely related structures, see: Hu *et al.* (2011); Han & Luo (2012); Deng (2011). For puckering parameters, see: Cremer & Pople (1975).




## Experimental

### Crystal data

$C_{12}H_{10}ClNO_3$
$M_r$ = 251.66
Monoclinic, $P2_1/c$
$a$ = 8.4709 (7) Å
$b$ = 17.1658 (13) Å
$c$ = 7.9481 (6) Å
$\beta$ = 107.228 (4)°
$V$ = 1103.88 (15) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.34 mm$^{-1}$
$T$ = 293 K
0.30 × 0.25 × 0.20 mm

### Data collection

Bruker SMART APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min}$ = 0.903, $T_{max}$ = 0.934
10447 measured reflections
2815 independent reflections
2410 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.138
$S$ = 1.13
2815 reflections
157 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C6—H6···O2 | 0.93 | 2.30 | 3.0181 (17) | 134 |

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).

The authors thank the TBI X-ray facility, CAS in Crystallography and BioPhysics, University of Madras, Chennai, India, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2438).

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# supplementary materials

*Acta Cryst.* (2013). E**69**, o856 [doi:10.1107/S1600536813011768]

## Methyl 2-(5-chloro-1-methyl-2-oxo-2,3-dihydro-1*H*-indol-3-ylidene)acetate

**Piskala Subburaman Kannan, PanneerSelvam Yuvaraj, Karthikeyan Manivannan, Boreddy S. R. Reddy and A. SubbiahPandi**

### Comment

Indole derivatives exhibit antihepatitis B virus (Chai *et al.*, 2006) and antibacterial (Nieto *et al.*, 2005) activities. Indole derivatives have been found to exhibit antibacterial, antifungal (Singh *et al.*, 2000) and antitumour activities (Andreani *et al.*, 2001). Some of the indole alkaloids extracted from plants possess interesting cytotoxic, antitumour or antiparasitic properties (Quetin-Leclercq, 1994; Mukhopadhyay *et al.*, 1981). Pyrido[1,2-a]indole derivatives have been identified as potent inhibitors of human immunodeficiency virus type 1 (Taylor *et al.*, 1999).

In the title compound, $C_{12}H_{10}Cl_1N_1O_3$,Figure 1 the indole ring system [C1-C8/N1] is essentially co-planar, with maxmium deviations of -0.009 Å for N1 atom. The indole ring and acetate group systems are essentially co-planar, with maxmium deviations of 0.086 Å for O2 atom. The mean plane through the methyl 4-oxobutanoate(acetate) group forms a dihedral angle of 3.68 (5)° with the plane of the indole ring system.

The geometric parameters of the title molecule (Fig. 1) agree well with the reported similar structures (Han *et al.*, 2012). The sum of the angles at N1 [359.98 (1)°] of the pyrrolidine rings are in accordance with $sp^2$ hybridizations.The crystal structure is stabilized by intramolecular C-H···O hydrogen bond interaction and $\pi$ -$\pi$ stacking interactions [centroid–centroid distance = 3.7677 (8) Å] between benzene rings [Cg1–Cg1$^{i}$ (Cg1:C1–C6) (i):symmetry code: -x,1-y,1-z]

### Experimental

To a mixture of 1eq of (*E*)-methyl 2-(5-chloro-1-methyl-2-oxoindolin- 3-ylidene) acetate, 1eq of isatin and 1.5eq of sarcosine were dissolved in acetonitrile. This reaction mixture refluxed at 80°C for 8hours. Completion of reaction monitor by Thin layar chromatography. The reaction mixture was extracted with ethyl acetate and water. The product was dried and purified by coloumn chromatography using ethyl acetate and hexane (1:9) as an elutent to afford pure Dispiro oxindole. Yield (90%). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a solution of the title compound in ethyl acetate at room temperature.

### Refinement

All H atoms were fixed geometrically and allowed to ride on their parent C atoms, with C—H distances fixed in the range 0.93–0.97 Å with $U_{iso}$(H) = 1.5$U_{eq}$(C) for methyl H 1.2$U_{eq}$(C) for other H atoms. The positions of methyl hydrogens were optimized rotationally.

### Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); 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* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

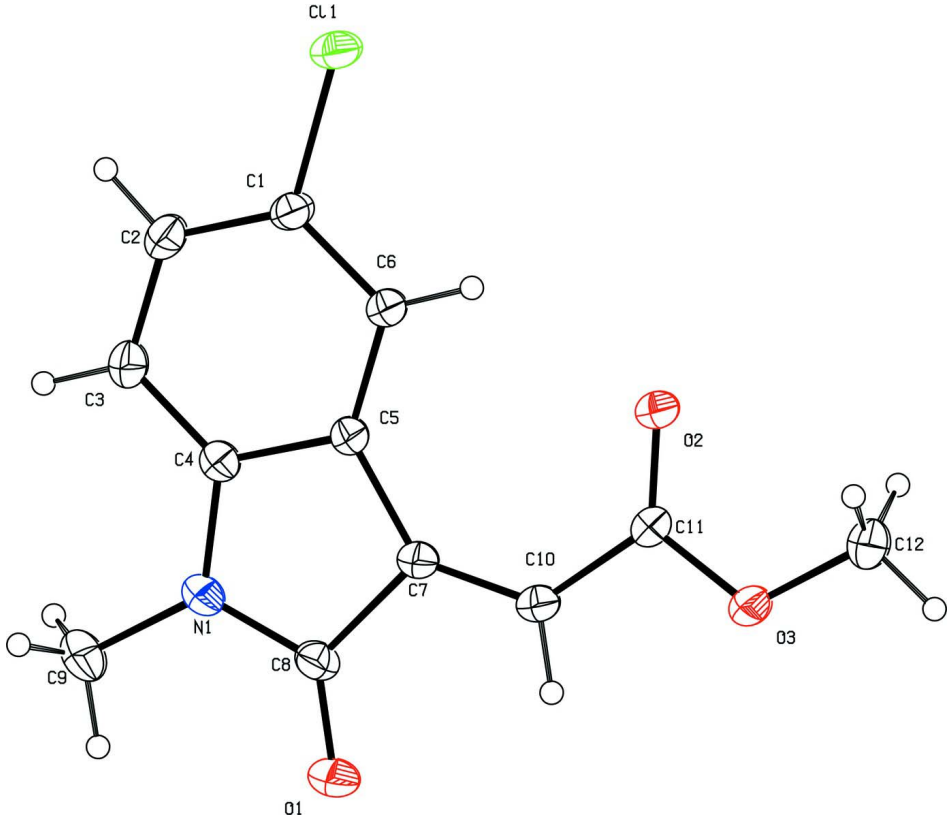


**Figure 1**

The structure of showing the atom-numbering scheme. The displacement ellipsoids are drawn at the 30% probability level.

### Methyl 2-(5-chloro-1-methyl-2-oxo-2,3-dihydro-1*H*-indol-3-ylidene)acetate

*Crystal data*

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$b = 17.1658\ (13)$ Å
$c = 7.9481\ (6)$ Å
$\beta = 107.228\ (4)°$
$V = 1103.88\ (15)$ Å$^3$
$Z = 4$
$F(000) = 520$
$D_x = 1.514$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2857 reflections
$\theta = 2.4$–$28.6°$
$\mu = 0.34$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.30 × 0.25 × 0.20 mm

*Data collection*

Bruker SMART APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.903$, $T_{max} = 0.934$
10447 measured reflections
2815 independent reflections
2410 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 28.6°$, $\theta_{min} = 2.4°$
$h = -11 \rightarrow 11$
$k = -23 \rightarrow 23$
$l = -10 \rightarrow 10$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.138$
$S = 1.13$
2815 reflections
157 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
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å$^{-3}$
$\Delta\rho_{min} = -0.21$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.008 (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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.18640 (15) | 0.52152 (8) | 0.41988 (16) | 0.0337 (3) |
| C2 | 0.22645 (18) | 0.44379 (9) | 0.44263 (18) | 0.0400 (3) |
| H2 | 0.3224 | 0.4283 | 0.5281 | 0.048* |
| C3 | 0.12324 (18) | 0.38846 (8) | 0.33765 (19) | 0.0396 (3) |
| H3 | 0.1487 | 0.3357 | 0.3514 | 0.047* |
| C4 | −0.01720 (16) | 0.41357 (7) | 0.21330 (17) | 0.0321 (3) |
| C5 | −0.05973 (15) | 0.49301 (7) | 0.18943 (15) | 0.0287 (3) |
| C6 | 0.04383 (15) | 0.54819 (7) | 0.29523 (15) | 0.0317 (3) |
| H6 | 0.0187 | 0.6010 | 0.2831 | 0.038* |
| C7 | −0.21570 (16) | 0.49743 (7) | 0.04971 (15) | 0.0306 (3) |
| C8 | −0.25984 (18) | 0.41402 (7) | −0.00755 (18) | 0.0344 (3) |
| C9 | −0.1339 (2) | 0.28462 (9) | 0.0829 (2) | 0.0509 (4) |
| H9A | −0.2332 | 0.2668 | −0.0022 | 0.076* |
| H9B | −0.1267 | 0.2625 | 0.1960 | 0.076* |
| H9C | −0.0398 | 0.2687 | 0.0476 | 0.076* |
| C10 | −0.31915 (15) | 0.55312 (8) | −0.03603 (16) | 0.0349 (3) |
| H10 | −0.4126 | 0.5363 | −0.1232 | 0.042* |
| C11 | −0.30207 (15) | 0.63753 (7) | −0.00835 (16) | 0.0341 (3) |
| C12 | −0.4227 (2) | 0.75770 (8) | −0.1167 (2) | 0.0499 (4) |
| H12A | −0.4311 | 0.7724 | −0.0031 | 0.075* |
| H12B | −0.5155 | 0.7782 | −0.2068 | 0.075* |
| H12C | −0.3222 | 0.7783 | −0.1314 | 0.075* |
| N1 | −0.13690 (14) | 0.36835 (6) | 0.09414 (14) | 0.0370 (3) |
| O1 | −0.38178 (14) | 0.39168 (7) | −0.12194 (15) | 0.0484 (3) |

| | | | | |
|---|---|---|---|---|
| O2 | −0.19597 (13) | 0.67151 (6) | 0.10265 (16) | 0.0503 (3) |
| O3 | −0.42172 (12) | 0.67452 (6) | −0.12966 (13) | 0.0426 (3) |
| Cl1 | 0.31706 (4) | 0.58922 (2) | 0.55565 (4) | 0.04557 (17) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0283 (6) | 0.0363 (7) | 0.0319 (6) | −0.0017 (5) | 0.0015 (5) | 0.0008 (4) |
| C2 | 0.0347 (7) | 0.0386 (7) | 0.0406 (6) | 0.0058 (6) | 0.0016 (5) | 0.0059 (5) |
| C3 | 0.0409 (7) | 0.0302 (6) | 0.0437 (7) | 0.0054 (5) | 0.0065 (6) | 0.0047 (5) |
| C4 | 0.0331 (7) | 0.0284 (6) | 0.0340 (6) | −0.0013 (4) | 0.0084 (5) | −0.0007 (4) |
| C5 | 0.0277 (6) | 0.0265 (6) | 0.0306 (5) | 0.0001 (4) | 0.0065 (4) | −0.0003 (4) |
| C6 | 0.0285 (6) | 0.0303 (6) | 0.0324 (6) | −0.0003 (5) | 0.0031 (4) | −0.0001 (4) |
| C7 | 0.0289 (6) | 0.0299 (6) | 0.0307 (6) | −0.0030 (4) | 0.0052 (4) | −0.0027 (4) |
| C8 | 0.0372 (7) | 0.0298 (6) | 0.0346 (6) | −0.0055 (5) | 0.0084 (5) | −0.0045 (4) |
| C9 | 0.0618 (10) | 0.0273 (7) | 0.0595 (9) | −0.0019 (6) | 0.0116 (7) | −0.0034 (6) |
| C10 | 0.0298 (6) | 0.0344 (7) | 0.0346 (6) | −0.0026 (5) | 0.0003 (5) | −0.0025 (5) |
| C11 | 0.0298 (6) | 0.0345 (7) | 0.0332 (6) | 0.0040 (5) | 0.0021 (4) | 0.0012 (5) |
| C12 | 0.0546 (9) | 0.0351 (8) | 0.0501 (8) | 0.0081 (6) | 0.0003 (7) | 0.0075 (6) |
| N1 | 0.0406 (6) | 0.0272 (6) | 0.0399 (6) | −0.0034 (4) | 0.0068 (5) | −0.0045 (4) |
| O1 | 0.0443 (6) | 0.0404 (5) | 0.0503 (6) | −0.0094 (4) | −0.0018 (5) | −0.0099 (4) |
| O2 | 0.0423 (6) | 0.0347 (5) | 0.0547 (6) | 0.0022 (4) | −0.0151 (4) | −0.0065 (4) |
| O3 | 0.0408 (6) | 0.0336 (5) | 0.0406 (5) | 0.0029 (4) | −0.0074 (4) | 0.0021 (4) |
| Cl1 | 0.0370 (2) | 0.0450 (3) | 0.0434 (2) | −0.00716 (13) | −0.00546 (16) | −0.00314 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.3753 (19) | C8—O1 | 1.2183 (18) |
| C1—C6 | 1.3932 (16) | C8—N1 | 1.3615 (18) |
| C1—Cl1 | 1.7415 (13) | C9—N1 | 1.4408 (18) |
| C2—C3 | 1.389 (2) | C9—H9A | 0.9600 |
| C2—H2 | 0.9300 | C9—H9B | 0.9600 |
| C3—C4 | 1.3717 (18) | C9—H9C | 0.9600 |
| C3—H3 | 0.9300 | C10—C11 | 1.4661 (19) |
| C4—N1 | 1.3995 (16) | C10—H10 | 0.9300 |
| C4—C5 | 1.4089 (17) | C11—O2 | 1.2070 (16) |
| C5—C6 | 1.3917 (16) | C11—O3 | 1.3346 (15) |
| C5—C7 | 1.4545 (17) | C12—O3 | 1.4320 (16) |
| C6—H6 | 0.9300 | C12—H12A | 0.9600 |
| C7—C10 | 1.3389 (19) | C12—H12B | 0.9600 |
| C7—C8 | 1.5153 (17) | C12—H12C | 0.9600 |
| | | | |
| C2—C1—C6 | 122.71 (12) | N1—C8—C7 | 106.77 (11) |
| C2—C1—Cl1 | 118.64 (10) | N1—C9—H9A | 109.5 |
| C6—C1—Cl1 | 118.64 (10) | N1—C9—H9B | 109.5 |
| C1—C2—C3 | 119.83 (13) | H9A—C9—H9B | 109.5 |
| C1—C2—H2 | 120.1 | N1—C9—H9C | 109.5 |
| C3—C2—H2 | 120.1 | H9A—C9—H9C | 109.5 |
| C4—C3—C2 | 118.36 (12) | H9B—C9—H9C | 109.5 |
| C4—C3—H3 | 120.8 | C7—C10—C11 | 127.50 (11) |

| | | | |
|---|---|---|---|
| C2—C3—H3 | 120.8 | C7—C10—H10 | 116.3 |
| C3—C4—N1 | 127.82 (11) | C11—C10—H10 | 116.3 |
| C3—C4—C5 | 122.27 (12) | O2—C11—O3 | 122.67 (12) |
| N1—C4—C5 | 109.92 (11) | O2—C11—C10 | 127.33 (11) |
| C6—C5—C4 | 119.15 (11) | O3—C11—C10 | 109.98 (11) |
| C6—C5—C7 | 133.90 (11) | O3—C12—H12A | 109.5 |
| C4—C5—C7 | 106.94 (11) | O3—C12—H12B | 109.5 |
| C5—C6—C1 | 117.68 (11) | H12A—C12—H12B | 109.5 |
| C5—C6—H6 | 121.2 | O3—C12—H12C | 109.5 |
| C1—C6—H6 | 121.2 | H12A—C12—H12C | 109.5 |
| C10—C7—C5 | 137.34 (12) | H12B—C12—H12C | 109.5 |
| C10—C7—C8 | 117.12 (12) | C8—N1—C4 | 110.84 (10) |
| C5—C7—C8 | 105.52 (11) | C8—N1—C9 | 124.20 (12) |
| O1—C8—N1 | 126.31 (12) | C4—N1—C9 | 124.94 (12) |
| O1—C8—C7 | 126.92 (13) | C11—O3—C12 | 116.21 (11) |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | 0.6 (2) | C5—C7—C8—O1 | 179.90 (14) |
| Cl1—C1—C2—C3 | 179.16 (10) | C10—C7—C8—N1 | 178.76 (11) |
| C1—C2—C3—C4 | −0.1 (2) | C5—C7—C8—N1 | 0.12 (13) |
| C2—C3—C4—N1 | 179.68 (12) | C5—C7—C10—C11 | −0.4 (2) |
| C2—C3—C4—C5 | −0.2 (2) | C8—C7—C10—C11 | −178.48 (12) |
| C3—C4—C5—C6 | 0.01 (19) | C7—C10—C11—O2 | −4.1 (2) |
| N1—C4—C5—C6 | −179.87 (10) | C7—C10—C11—O3 | 174.29 (13) |
| C3—C4—C5—C7 | −179.19 (12) | O1—C8—N1—C4 | −179.33 (13) |
| N1—C4—C5—C7 | 0.93 (13) | C7—C8—N1—C4 | 0.45 (14) |
| C4—C5—C6—C1 | 0.42 (17) | O1—C8—N1—C9 | −0.9 (2) |
| C7—C5—C6—C1 | 179.36 (11) | C7—C8—N1—C9 | 178.84 (12) |
| C2—C1—C6—C5 | −0.71 (19) | C3—C4—N1—C8 | 179.24 (13) |
| Cl1—C1—C6—C5 | −179.32 (9) | C5—C4—N1—C8 | −0.88 (14) |
| C6—C5—C7—C10 | 2.1 (2) | C3—C4—N1—C9 | 0.9 (2) |
| C4—C5—C7—C10 | −178.84 (15) | C5—C4—N1—C9 | −179.26 (13) |
| C6—C5—C7—C8 | −179.66 (13) | O2—C11—O3—C12 | −2.8 (2) |
| C4—C5—C7—C8 | −0.63 (12) | C10—C11—O3—C12 | 178.73 (12) |
| C10—C7—C8—O1 | −1.5 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C6—H6···O2 | 0.93 | 2.30 | 3.0181 (17) | 134 |