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# Dipentyl 2,6-diaminobenzo[1,2-*b*:4,5-*b*′]-difuran-3,7-dicarboxylate

**Giuseppina Roviello,[a] Fabio Borbone,[b] Antonio Carella,[b] Giovanni N. Roviello[c]* and Angela Tuzi[b]***

[a]Dipartimento di Ingegneria, Università di Napoli 'Parthenope', Centro Direzionale di Napoli, Isola C4, 80143 Napoli, Italy, [b]Dipartimento di Scienze Chimiche, Università degli Studi di Napoli 'Federico II', Complesso di Monte S. Angelo, Via Cinthia, 80126 Napoli, Italy, and [c]Istituto di Biostrutture e Bioimmagini, CNR, Via Mezzocannone 16, 80134 Naples, Italy
Correspondence e-mail: giuseppina.roviello@uniparthenope.it, angela.tuzi@unina.it

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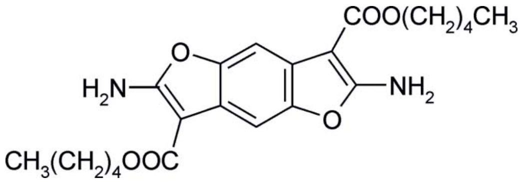
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.055; $wR$ factor = 0.134; data-to-parameter ratio = 18.5.

The title compound, $C_{22}H_{28}N_2O_6$, crystallizes with one half-molecule in the independent unit, the molecule being located on an inversion centre. The penthyl groups are in the all-*trans* conformation and an almost planar conformation of the whole molecule is observed [maximum deviation from the least-squares plane through all non-H atoms is 0.0229 (17) Å for an N atom]. The amino groups are involved in intra- and intermolecular hydrogen bonds. Intramolecular hydrogen bonding involving the amino group and ester carbonyl helps to lock the *syn* conformation of the ester with respect to the amino group. In the crystal, N—H$\cdots$O hydrogen bonding involving the amino group and the furan and ester carbonyl O atoms self-assembles the molecules into a two-dimensional hydrogen-bonded network parallel to (010) that displays interdigital packing sustained by alkyl–alkyl interactions.

## Related literature

For the synthesis and properties of aminobenzodifurane derivatives, see: Caruso *et al.* (2009). For O- and N-rich aromatic heterocycles, see: Roviello *et al.* (2007, 2012). For molecules with optical and opto-electronical properties, see: Carella *et al.* (2012); Centore *et al.* (2007); Roviello *et al.* (2009); Ricciotti *et al.* (2013); Vitaliano *et al.* (2009). For hydrogen bonding in heterocycles, see: Centore *et al.* (2013*a*,*b*).



## Experimental

### Crystal data

$C_{22}H_{28}N_2O_6$
$M_r$ = 416.46
Monoclinic, $P2_1/c$
$a$ = 8.267 (1) Å
$b$ = 7.994 (1) Å
$c$ = 17.582 (3) Å
$\beta$ = 98.98 (2)°
$V$ = 1147.7 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 173 K
0.50 × 0.04 × 0.01 mm

### Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.957, $T_{max}$ = 0.999
11093 measured reflections
2626 independent reflections
1258 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.096

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.134
$S$ = 0.93
2626 reflections
142 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.20 e Å$^{-3}$

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

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| N1—H1$A\cdots$O2$^{i}$ | 0.83 (2) | 2.11 (2) | 2.935 (3) | 171 (2) |
| N1—H1$B\cdots$O1$^{ii}$ | 0.84 (2) | 2.34 (2) | 3.066 (2) | 144 (2) |
| N1—H1$B\cdots$O2 | 0.84 (2) | 2.41 (2) | 2.942 (3) | 122.2 (18) |

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

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg *et al.*, 2000); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DS2234).

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# supporting information

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## Dipentyl 2,6-diaminobenzo[1,2-*b*:4,5-*b′*]difuran-3,7-dicarboxylate

**Giuseppina Roviello, Fabio Borbone, Antonio Carella, Giovanni N. Roviello and Angela Tuzi**

### S1. Comment

In the field of our studies on the synthesis and properties of aminobenzodifurane derivatives (Caruso *et al.* 2009) we prepared the title compound, $C_{22}H_{28}N_2O_6$. The presence of an aromatic heterocyclic core in the molecule makes this kind of compound interesting in organic electronics (Carella *et al.* 2012; Centore *et al.* 2007). 2,6-diamino-benzo[1,2 - b;4,5 - b′]difuran-3,7-dicarboxylic acid (Fig. 1) crystallizes in $P2_1/c$ space group with one half molecule in the independent unit. The molecule is located on a crystallographic inversion center and exhibits an all planar shape (maximum deviation from least square plane of the molecule is -0.0229 (17) for N1). The planarity of the molecule is a consequence of the all-*trans* conformation of penthyl groups and of the torsion angle at C6–O3 bond (C4—C6—O3—C7 = 179.7 (2)°). The planar conformation is also stabilized by intramolecular N—H···O=C hydrogen bonds (Table 1). In fact, the intramolecular hydrogen bonding involving the amino group and ester carbonyl helps to lock the *syn* conformation of ester with respect to amino group. The amino $NH_2$ group is also involved in intermolecular hydrogen bonds, acting as donor towards benzodifurane oxigen (O1) and ester carbonyl oxygen (O2) acceptors (see Table 1). In the crystal packing (Fig. 2), molecules self-assemble into a two-dimensional hydrogen bonded network that display interdigital packing sustained by alkyl-alkyl interactions.

### S2. Experimental

2,6-diamino-benzo[1,2 - b;4,5 - b′]difuran-3,7-dicarboxylic acid was prepared according to the procedure described in the literature (Caruso *et al.* 2009). Crystals suitable for X-ray analysis were obtained by slow evaporation of dioxane/water solution.

### S3. Refinement

All NH hydrogen atoms were located in difference Fourier maps and refined with $U_{iso}=1.2U_{eq}(N)$ of the carrier atom. All the other H atoms were generated stereochemically and refined by the riding model with $U_{iso}=1.2\times U_{eq}$ of the carrier atom (1.5 for H atoms of the methyl groups).

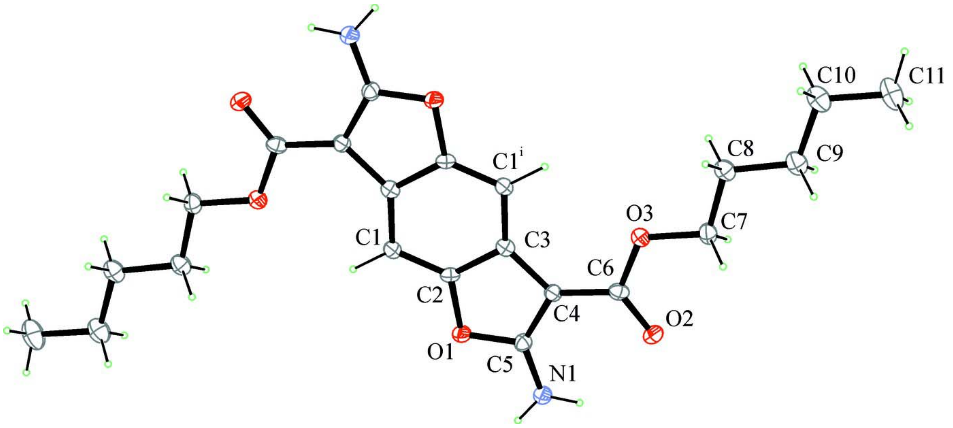

**Figure 1**

*ORTEP* view of the title compound. Thermal ellipsoids are drawn at 30% probability level.

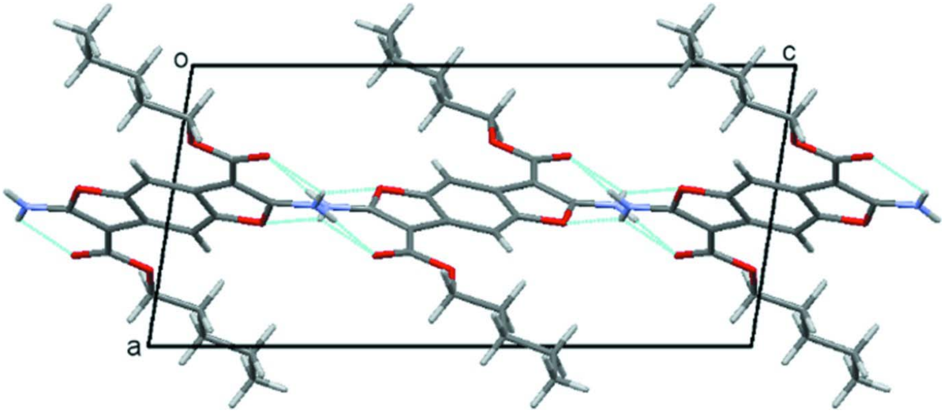

**Figure 2**

Crystal packing viewed along **b** axis. Hydrogen bonds are drawn as dashed lines.

## Dipentyl 2,6-diaminobenzo[1,2-*b*:4,5-*b*′]difuran-3,7-dicarboxylate

### *Crystal data*

$C_{22}H_{28}N_2O_6$
$M_r = 416.46$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.267$ (1) Å
$b = 7.994$ (1) Å
$c = 17.582$ (3) Å
$\beta = 98.98$ (2)°
$V = 1147.7$ (3) Å$^3$
$Z = 2$
$F(000) = 444$
$D_x = 1.205$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 75 reflections
$\theta = 3.1$–16.9°
$\mu = 0.09$ mm$^{-1}$
$T = 173$ K
Block, grey
0.50 × 0.04 × 0.01 mm

### *Data collection*

Bruker–Nonius KappaCCD diffractometer
Radiation source: normal-focus sealed tube
Graphite monochromator
Detector resolution: 9 pixels mm$^{-1}$
CCD rotation images, thick slices scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.957$, $T_{max} = 0.999$
11093 measured reflections

2626 independent reflections
1258 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.096$
$\theta_{\text{max}} = 27.5°$, $\theta_{\text{min}} = 3.2°$

$h = -10 \rightarrow 10$
$k = -10 \rightarrow 9$
$l = -22 \rightarrow 22$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.134$
$S = 0.93$
2626 reflections
142 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.061P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\text{max}} < 0.001$
$\Delta\rho_{\text{max}} = 0.19$ e Å$^{-3}$
$\Delta\rho_{\text{min}} = -0.20$ e Å$^{-3}$

*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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{\text{iso}}$*/$U_{\text{eq}}$ |
|---|---|---|---|---|
| C1 | 0.5923 (2) | 0.1341 (3) | 0.04464 (11) | 0.0257 (5) |
| H1 | 0.6556 | 0.2314 | 0.0731 | 0.026* |
| C2 | 0.5354 (2) | −0.0094 (3) | 0.07682 (11) | 0.0246 (5) |
| C3 | 0.4461 (2) | −0.1426 (3) | 0.03695 (11) | 0.0255 (5) |
| C4 | 0.4171 (2) | −0.2648 (3) | 0.09645 (11) | 0.0254 (5) |
| C5 | 0.4884 (3) | −0.1957 (3) | 0.16650 (12) | 0.0282 (5) |
| C6 | 0.3356 (2) | −0.4269 (3) | 0.09113 (12) | 0.0288 (6) |
| C7 | 0.1878 (3) | −0.6355 (3) | 0.00858 (11) | 0.0326 (6) |
| H7A | 0.0935 | −0.6356 | 0.0370 | 0.033* |
| H7B | 0.2644 | −0.7250 | 0.0301 | 0.033* |
| C8 | 0.1290 (3) | −0.6679 (3) | −0.07634 (12) | 0.0340 (6) |
| H8A | 0.2242 | −0.6700 | −0.1043 | 0.034* |
| H8B | 0.0556 | −0.5760 | −0.0979 | 0.034* |
| C9 | 0.0363 (3) | −0.8366 (3) | −0.08811 (12) | 0.0382 (6) |
| H9A | 0.1101 | −0.9271 | −0.0654 | 0.038* |
| H9B | −0.0583 | −0.8331 | −0.0598 | 0.038* |
| C10 | −0.0261 (3) | −0.8793 (3) | −0.17302 (13) | 0.0472 (7) |
| H10A | 0.0678 | −0.8822 | −0.2017 | 0.047* |
| H10B | −0.1019 | −0.7904 | −0.1958 | 0.047* |
| C11 | −0.1155 (4) | −1.0494 (3) | −0.18205 (16) | 0.0632 (8) |

| | | | | |
|---|---|---|---|---|
| H11A | −0.1539 | −1.0711 | −0.2367 | 0.063* |
| H11B | −0.2094 | −1.0467 | −0.1542 | 0.063* |
| H11C | −0.0400 | −1.1383 | −0.1609 | 0.063* |
| N1 | 0.4973 (3) | −0.2479 (3) | 0.23935 (11) | 0.0383 (6) |
| H1A | 0.550 (3) | −0.192 (3) | 0.2748 (12) | 0.038* |
| H1B | 0.454 (3) | −0.340 (3) | 0.2485 (12) | 0.038* |
| O1 | 0.56177 (16) | −0.04310 (18) | 0.15705 (7) | 0.0292 (4) |
| O2 | 0.32315 (19) | −0.51874 (18) | 0.14725 (8) | 0.0377 (4) |
| O3 | 0.27143 (17) | −0.47150 (17) | 0.01739 (8) | 0.0324 (4) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0243 (13) | 0.0246 (14) | 0.0275 (12) | 0.0019 (10) | 0.0017 (10) | −0.0028 (10) |
| C2 | 0.0267 (12) | 0.0283 (14) | 0.0184 (11) | 0.0051 (11) | 0.0018 (9) | 0.0001 (10) |
| C3 | 0.0225 (12) | 0.0268 (14) | 0.0271 (12) | 0.0040 (10) | 0.0039 (10) | −0.0032 (10) |
| C4 | 0.0263 (12) | 0.0216 (13) | 0.0271 (12) | 0.0021 (10) | 0.0009 (10) | −0.0009 (10) |
| C5 | 0.0289 (13) | 0.0252 (15) | 0.0303 (13) | 0.0008 (11) | 0.0039 (10) | 0.0012 (11) |
| C6 | 0.0260 (13) | 0.0305 (15) | 0.0286 (13) | 0.0076 (11) | −0.0001 (10) | −0.0006 (11) |
| C7 | 0.0304 (13) | 0.0269 (14) | 0.0400 (14) | −0.0019 (11) | 0.0041 (11) | −0.0014 (11) |
| C8 | 0.0282 (13) | 0.0345 (16) | 0.0385 (13) | 0.0024 (11) | 0.0029 (11) | −0.0043 (11) |
| C9 | 0.0292 (13) | 0.0355 (16) | 0.0487 (15) | 0.0032 (11) | 0.0025 (12) | −0.0065 (12) |
| C10 | 0.0432 (16) | 0.0499 (18) | 0.0483 (15) | −0.0056 (14) | 0.0068 (13) | −0.0135 (13) |
| C11 | 0.0620 (19) | 0.054 (2) | 0.073 (2) | −0.0181 (16) | 0.0085 (16) | −0.0242 (15) |
| N1 | 0.0530 (14) | 0.0320 (14) | 0.0268 (12) | −0.0109 (11) | −0.0033 (10) | 0.0022 (10) |
| O1 | 0.0350 (9) | 0.0296 (10) | 0.0224 (8) | −0.0013 (7) | 0.0025 (7) | 0.0006 (7) |
| O2 | 0.0489 (10) | 0.0313 (10) | 0.0307 (9) | −0.0033 (8) | −0.0003 (7) | 0.0075 (7) |
| O3 | 0.0373 (9) | 0.0293 (10) | 0.0289 (9) | −0.0043 (7) | 0.0001 (7) | −0.0010 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.393 (3) | C7—H7B | 0.9900 |
| C1—C3$^{i}$ | 1.422 (3) | C8—C9 | 1.549 (3) |
| C1—H1 | 1.0231 | C8—H8A | 0.9900 |
| C2—C3 | 1.418 (3) | C8—H8B | 0.9900 |
| C2—O1 | 1.419 (2) | C9—C10 | 1.540 (3) |
| C3—C1$^{i}$ | 1.422 (3) | C9—H9A | 0.9900 |
| C3—C4 | 1.477 (3) | C9—H9B | 0.9900 |
| C4—C5 | 1.394 (3) | C10—C11 | 1.543 (3) |
| C4—C6 | 1.457 (3) | C10—H10A | 0.9900 |
| C5—N1 | 1.338 (3) | C10—H10B | 0.9900 |
| C5—O1 | 1.384 (2) | C11—H11A | 0.9800 |
| C6—O2 | 1.247 (2) | C11—H11B | 0.9800 |
| C6—O3 | 1.369 (2) | C11—H11C | 0.9800 |
| C7—O3 | 1.479 (2) | N1—H1A | 0.83 (2) |
| C7—C8 | 1.518 (3) | N1—H1B | 0.84 (2) |
| C7—H7A | 0.9900 | | |

| | | | |
|---|---|---|---|
| C2—C1—C3$^{i}$ | 114.40 (18) | C7—C8—H8B | 109.5 |
| C2—C1—H1 | 127.3 | C9—C8—H8B | 109.5 |
| C3$^{i}$—C1—H1 | 118.3 | H8A—C8—H8B | 108.1 |
| C1—C2—C3 | 126.93 (18) | C10—C9—C8 | 114.01 (19) |
| C1—C2—O1 | 123.44 (18) | C10—C9—H9A | 108.8 |
| C3—C2—O1 | 109.63 (17) | C8—C9—H9A | 108.8 |
| C2—C3—C1$^{i}$ | 118.67 (18) | C10—C9—H9B | 108.8 |
| C2—C3—C4 | 106.02 (17) | C8—C9—H9B | 108.8 |
| C1$^{i}$—C3—C4 | 135.31 (19) | H9A—C9—H9B | 107.6 |
| C5—C4—C6 | 122.45 (19) | C9—C10—C11 | 112.2 (2) |
| C5—C4—C3 | 105.72 (18) | C9—C10—H10A | 109.2 |
| C6—C4—C3 | 131.82 (18) | C11—C10—H10A | 109.2 |
| N1—C5—O1 | 115.50 (19) | C9—C10—H10B | 109.2 |
| N1—C5—C4 | 132.4 (2) | C11—C10—H10B | 109.2 |
| O1—C5—C4 | 112.08 (18) | H10A—C10—H10B | 107.9 |
| O2—C6—O3 | 121.9 (2) | C10—C11—H11A | 109.5 |
| O2—C6—C4 | 124.58 (19) | C10—C11—H11B | 109.5 |
| O3—C6—C4 | 113.54 (18) | H11A—C11—H11B | 109.5 |
| O3—C7—C8 | 109.05 (16) | C10—C11—H11C | 109.5 |
| O3—C7—H7A | 109.9 | H11A—C11—H11C | 109.5 |
| C8—C7—H7A | 109.9 | H11B—C11—H11C | 109.5 |
| O3—C7—H7B | 109.9 | C5—N1—H1A | 119.4 (15) |
| C8—C7—H7B | 109.9 | C5—N1—H1B | 119.5 (15) |
| H7A—C7—H7B | 108.3 | H1A—N1—H1B | 121 (2) |
| C7—C8—C9 | 110.81 (18) | C5—O1—C2 | 106.54 (16) |
| C7—C8—H8A | 109.5 | C6—O3—C7 | 115.84 (15) |
| C9—C8—H8A | 109.5 | | |

| | | | |
|---|---|---|---|
| C3$^{i}$—C1—C2—C3 | 0.1 (3) | C5—C4—C6—O2 | −0.8 (3) |
| C3$^{i}$—C1—C2—O1 | 179.41 (17) | C3—C4—C6—O2 | 178.5 (2) |
| C1—C2—C3—C1$^{i}$ | −0.1 (3) | C5—C4—C6—O3 | 179.06 (18) |
| O1—C2—C3—C1$^{i}$ | −179.49 (16) | C3—C4—C6—O3 | −1.6 (3) |
| C1—C2—C3—C4 | 179.22 (19) | O3—C7—C8—C9 | −178.43 (16) |
| O1—C2—C3—C4 | −0.2 (2) | C7—C8—C9—C10 | −179.49 (19) |
| C2—C3—C4—C5 | 0.7 (2) | C8—C9—C10—C11 | 179.2 (2) |
| C1$^{i}$—C3—C4—C5 | 179.8 (2) | N1—C5—O1—C2 | −178.64 (17) |
| C2—C3—C4—C6 | −178.7 (2) | C4—C5—O1—C2 | 0.8 (2) |
| C1$^{i}$—C3—C4—C6 | 0.4 (4) | C1—C2—O1—C5 | −179.79 (18) |
| C6—C4—C5—N1 | −2.1 (4) | C3—C2—O1—C5 | −0.3 (2) |
| C3—C4—C5—N1 | 178.4 (2) | O2—C6—O3—C7 | −0.4 (3) |
| C6—C4—C5—O1 | 178.55 (17) | C4—C6—O3—C7 | 179.72 (16) |
| C3—C4—C5—O1 | −0.9 (2) | C8—C7—O3—C6 | −178.24 (17) |

Symmetry code: (i) $-x+1, -y, -z$.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*A*···O2$^{ii}$ | 0.83 (2) | 2.11 (2) | 2.935 (3) | 171 (2) |

| | | | | |
|---|---|---|---|---|
| N1—H1*B*···O1$^{iii}$ | 0.84 (2) | 2.34 (2) | 3.066 (2) | 144 (2) |
| N1—H1*B*···O2 | 0.84 (2) | 2.41 (2) | 2.942 (3) | 122.2 (18) |

Symmetry codes: (ii) −*x*+1, *y*+1/2, −*z*+1/2; (iii) −*x*+1, *y*−1/2, −*z*+1/2.