Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(1*H*-Benzotriazol-1-yl)-1-(furan-2-yl)-ethanol

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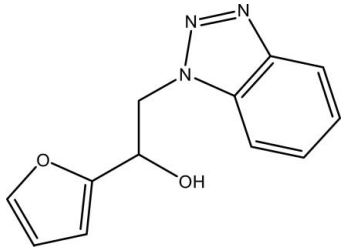
Received 30 November 2011; accepted 1 December 2011

Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.054; wR factor = 0.139; data-to-parameter ratio = 16.3.

In the title compound, $C_{12}H_{11}N_3O_2$, the benzotriazole ring system is approximately planar [maximum deviation = 0.008 (1) Å] and its mean plane is oriented at a dihedral angle of 24.05 (4)° with respect to the furan ring. In the crystal, O—H···N hydrogen bonds link the molecules into chains along the *ac* diagonal. π–π stacking between the furan rings, between the triazole and benzene rings, and between the benzene rings [centroid–centroid distances = 3.724 (1), 3.786 (1) and 3.8623 (9) Å] are also observed.

Related literature

For general background to the biological activity of benzotriazole derivatives, see: Hirokawa *et al.* (1998); Yu *et al.* (2003); Kopanska *et al.* (2004). For related structures, see: Caira *et al.* (2004); Katritzky *et al.* (2001); Özel Güven *et al.* (2008, 2010, 2011); Nanjunda Swamy *et al.* (2006).



Experimental

Crystal data

$C_{12}H_{11}N_3O_2$
M_r = 229.24
Monoclinic, $P2_1/c$
a = 11.3606 (4) Å
b = 11.1034 (4) Å
c = 8.7860 (2) Å
β = 96.938 (2)°
V = 1100.16 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 120 K
0.50 × 0.50 × 0.20 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.953, T_{max} = 0.981
12372 measured reflections
2531 independent reflections
2166 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.139
S = 1.11
2531 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N3^{i}	0.82	2.26	2.7968 (18)	123

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; 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, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

The authors acknowledge the Zonguldak Karaelmas University Research Fund (project No. 2010-13-02-05).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5402).

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supporting information

Acta Cryst. (2012). E**68**, o72 [doi:10.1107/S1600536811051798]

2-(1*H*-Benzotriazol-1-yl)-1-(furan-2-yl)ethanol

Özden Özel Güven, Meral Bayraktar, Simon J. Coles and Tuncer Hökelek

S1. Comment

Azole compounds have important biological activities. Benzotriazol derivatives also exhibit a good degree of analgesic, anti-inflammatory, diuretic, antiviral and antihypertensive activities (Kopanska *et al.*, 2004; Yu *et al.*, 2003; Hirokawa *et al.*, 1998). Crystal structures of similar compounds like 1-phenyl-2-(1*H*-1,2,4-triazol-1-yl)ethanol (Özel Güven *et al.*, 2008), 2-(1*H*-benzotriazol-1-yl)-1-phenylethanol (Özel Güven *et al.*, 2010), 2-(1*H*-benzotriazol-1-yl)-3-(2,6-dichlorophenyl)-1-phenylpropan-1-ol (Özel Güven *et al.*, 2011), fluconazole (Caira *et al.*, 2004), and other benzotriazole ring possesing compounds (Katritzky *et al.*, 2001; Nanjunda Swamy *et al.*, 2006) have been reported before. Now, we report herein the crystal structure of the title alcohol, (I).

In the molecule of the title compound (Fig. 1), the bond lengths and angles are generally within normal ranges. The planar benzotriazole ring [B (N1-N3/C7-C12)] is oriented with respect to the furan [A (O2/C2-C5)] ring at a dihedral angle of A/B = 24.05 (4)°. Atom C6 is 0.043 (2) Å away from the plane of the benzotriazole ring and atoms C1 and O1 are 0.010 (2) and 0.043 (1) Å away from the plane of the furan ring, respectively.

In the crystal, O—H···N hydrogen bonds (table 1) link the molecules into chains (Fig. 2). There also exist $\pi\cdots\pi$ contacts between the furan rings, between the triazole and benzene rings and between the benzene rings, Cg1—Cg1^{i}, Cg2—Cg3^{ii} and Cg3—Cg3^{ii}, may further stabilize the structure [centroid-centroid distances = 3.724 (1), 3.786 (1) and 3.8623 (9) Å; symmetry codes: (i) 1 - x, 1 - y, 1 - z; (ii) -x, 1 - y, 1 - z; Cg1, Cg2 and Cg3 are the centroids of the rings A (O2/C2-C5), C (N1-N3/C7/C12) and D (C7-C12), respectively].

S2. Experimental

The title compound, (I), was synthesized by reduction of 2-(1*H*-benzotriazol-1-yl)-1-(furan-2-yl)ethanone with sodiumborohydrate. A mixture of 2-(1*H*-benzotriazol-1-yl)-1-(furan-2-yl)ethanone (1010 mg, 4.44 mmol) and sodium borohydrate (561 mg, 8.89 mmol) in ethanol (50 ml) was refluxed for 4 h. After evaporation of the solvent, the mixture was neutralized with dilute HCl, and then refluxed for 30 min. After the mixture was cooled, the solution was alkalinized with dilute NaOH and the resulting precipitate was filtered. The filtrate was extracted with chloroform, then the organic phase was dried and evaporated. The residue was crystallized from 2-propanol to obtain colorless crystals suitable for X-ray analysis (yield; 634 mg, 62%).

S3. Refinement

H atoms were positioned geometrically with O—H = 0.82 Å (for OH group), C—H = 0.98, 0.93 and 0.97 Å for methine, aromatic and methylene H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = k × U_{eq}(C,O), where k = 1.5 for OH H-atom and k = 1.2 for all other H-atoms.

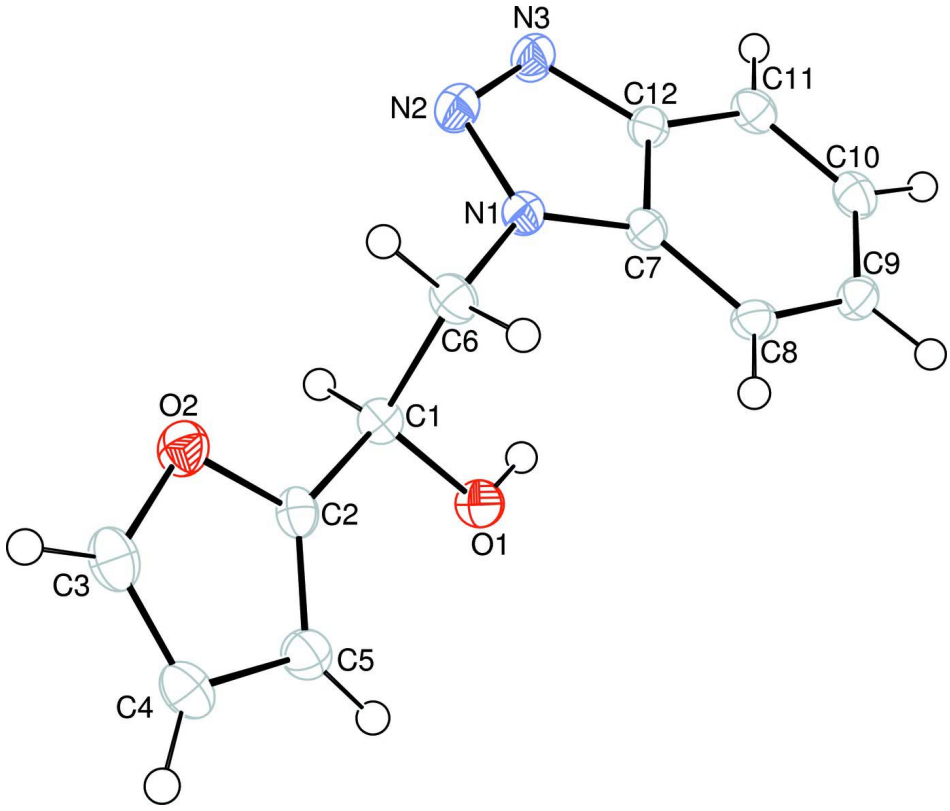

Figure 1

The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

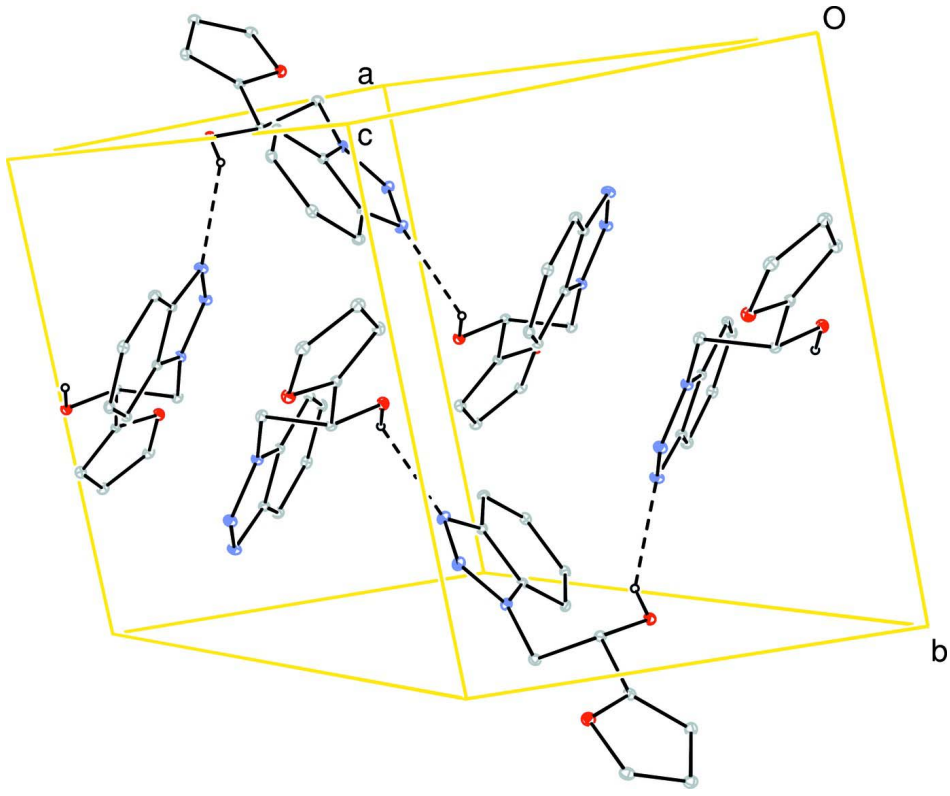

Figure 2

A partial packing diagram. Hydrogen bonds are shown as dashed lines. Hydrogen atoms not involved in hydrogen bonding have been omitted for clarity.

2-(1*H*-Benzotriazol-1-yl)-1-(furan-2-yl)ethanol

Crystal data

$C_{12}H_{11}N_3O_2$
$M_r = 229.24$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.3606$ (4) Å
$b = 11.1034$ (4) Å
$c = 8.7860$ (2) Å
$\beta = 96.938$ (2)°
$V = 1100.16$ (6) Å^3
$Z = 4$

$F(000) = 480$
$D_x = 1.384$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6399 reflections
$\theta = 2.9$–27.5°
$\mu = 0.10$ mm^{-1}
$T = 120$ K
Block, colorless
0.50 × 0.50 × 0.20 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
$T_{min} = 0.953$, $T_{max} = 0.981$

12372 measured reflections
2531 independent reflections
2166 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -14 \rightarrow 14$
$k = -14 \rightarrow 14$
$l = -10 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.139$
$S = 1.11$
2531 reflections
155 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
$w = 1/[\sigma^2(F_o^2) + (0.0748P)^2 + 0.4779P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.58$ e Å^{-3}
$\Delta\rho_{min} = -0.55$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.144 (12)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.20677 (10)	0.98199 (10)	0.08354 (12)	0.0223 (3)
H1	0.1559	0.9346	0.1048	0.033*
O2	0.50236 (10)	1.06715 (11)	0.24705 (13)	0.0247 (3)
N1	0.18510 (11)	0.91870 (12)	0.39959 (14)	0.0196 (3)
N2	0.22565 (12)	0.82297 (13)	0.48488 (16)	0.0249 (3)
N3	0.13604 (12)	0.75376 (13)	0.50674 (16)	0.0248 (3)
C1	0.30653 (14)	0.97510 (14)	0.19621 (17)	0.0193 (3)
H1A	0.3392	0.8933	0.1989	0.023*
C2	0.39723 (13)	1.06237 (14)	0.15318 (17)	0.0194 (3)
C3	0.57056 (15)	1.15175 (15)	0.18424 (19)	0.0257 (4)
H3	0.6471	1.1732	0.2247	0.031*
C4	0.51146 (15)	1.19920 (15)	0.05628 (19)	0.0252 (4)
H4	0.5385	1.2581	−0.0062	0.030*
C5	0.39773 (14)	1.14020 (15)	0.03582 (18)	0.0238 (4)
H5	0.3367	1.1533	−0.0429	0.029*
C6	0.26911 (14)	1.00691 (14)	0.35398 (17)	0.0214 (3)
H6A	0.3386	1.0091	0.4298	0.026*
H6B	0.2330	1.0862	0.3496	0.026*
C7	0.06500 (13)	0.91156 (13)	0.36343 (16)	0.0178 (3)
C8	−0.01985 (14)	0.98551 (14)	0.27982 (17)	0.0202 (3)
H8	0.0010	1.0560	0.2326	0.024*
C9	−0.13571 (14)	0.94734 (15)	0.27193 (17)	0.0226 (4)
H9	−0.1949	0.9939	0.2182	0.027*

C10	−0.16792 (14)	0.83958 (15)	0.34283 (17)	0.0232 (4)
H10	−0.2474	0.8174	0.3339	0.028*
C11	−0.08469 (14)	0.76679 (14)	0.42472 (18)	0.0222 (4)
H11	−0.1059	0.6962	0.4713	0.027*
C12	0.03398 (13)	0.80499 (13)	0.43403 (17)	0.0191 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0207 (6)	0.0231 (6)	0.0226 (6)	−0.0047 (4)	0.0004 (4)	−0.0002 (4)
O2	0.0204 (6)	0.0259 (6)	0.0271 (6)	−0.0032 (4)	−0.0001 (4)	0.0002 (4)
N1	0.0181 (6)	0.0205 (6)	0.0205 (6)	0.0001 (5)	0.0030 (5)	0.0020 (5)
N2	0.0224 (7)	0.0249 (7)	0.0272 (7)	0.0045 (5)	0.0023 (5)	0.0044 (5)
N3	0.0231 (7)	0.0221 (7)	0.0293 (7)	0.0043 (5)	0.0038 (5)	0.0059 (6)
C1	0.0204 (7)	0.0172 (7)	0.0203 (7)	−0.0007 (6)	0.0028 (6)	−0.0012 (5)
C2	0.0168 (7)	0.0204 (7)	0.0213 (7)	0.0006 (6)	0.0031 (6)	−0.0038 (6)
C3	0.0203 (8)	0.0251 (8)	0.0322 (8)	−0.0052 (6)	0.0054 (6)	−0.0052 (6)
C4	0.0246 (8)	0.0237 (8)	0.0285 (8)	−0.0047 (6)	0.0087 (6)	−0.0016 (6)
C5	0.0223 (8)	0.0264 (8)	0.0228 (7)	−0.0012 (6)	0.0029 (6)	0.0007 (6)
C6	0.0201 (7)	0.0221 (8)	0.0223 (7)	−0.0039 (6)	0.0041 (6)	−0.0025 (6)
C7	0.0185 (7)	0.0178 (7)	0.0173 (7)	−0.0002 (6)	0.0034 (5)	−0.0017 (5)
C8	0.0248 (8)	0.0178 (7)	0.0184 (7)	0.0020 (6)	0.0040 (6)	0.0030 (5)
C9	0.0213 (8)	0.0274 (8)	0.0185 (7)	0.0056 (6)	0.0002 (6)	−0.0009 (6)
C10	0.0190 (7)	0.0286 (8)	0.0224 (7)	−0.0031 (6)	0.0043 (6)	−0.0042 (6)
C11	0.0243 (8)	0.0191 (8)	0.0244 (8)	−0.0022 (6)	0.0074 (6)	−0.0004 (6)
C12	0.0212 (8)	0.0169 (7)	0.0195 (7)	0.0022 (6)	0.0041 (6)	0.0004 (5)

Geometric parameters (Å, º)

O1—C1	1.4139 (18)	C4—H4	0.9300
O1—H1	0.8200	C5—C4	1.440 (2)
O2—C2	1.3681 (19)	C5—H5	0.9300
O2—C3	1.375 (2)	C6—H6A	0.9700
N1—N2	1.3492 (18)	C6—H6B	0.9700
N1—C6	1.4571 (19)	C7—C12	1.401 (2)
N1—C7	1.365 (2)	C8—C7	1.404 (2)
N3—N2	1.308 (2)	C8—C9	1.376 (2)
N3—C12	1.377 (2)	C8—H8	0.9300
C1—C6	1.539 (2)	C9—H9	0.9300
C1—H1A	0.9800	C10—C9	1.417 (2)
C2—C1	1.496 (2)	C10—H10	0.9300
C2—C5	1.346 (2)	C11—C10	1.379 (2)
C3—C4	1.345 (2)	C11—C12	1.406 (2)
C3—H3	0.9300	C11—H11	0.9300
C1—O1—H1	109.5	N1—C6—C1	110.77 (12)
C2—O2—C3	106.13 (12)	N1—C6—H6A	109.5
N2—N1—C7	110.36 (12)	N1—C6—H6B	109.5

N2—N1—C6	119.43 (12)	C1—C6—H6A	109.5
C7—N1—C6	130.13 (13)	C1—C6—H6B	109.5
N3—N2—N1	108.96 (13)	H6A—C6—H6B	108.1
N2—N3—C12	108.40 (13)	N1—C7—C8	133.73 (14)
O1—C1—C2	107.84 (12)	N1—C7—C12	104.11 (13)
O1—C1—C6	109.45 (12)	C12—C7—C8	122.15 (14)
O1—C1—H1A	109.6	C7—C8—H8	122.0
C2—C1—C6	110.64 (12)	C9—C8—C7	115.98 (14)
C2—C1—H1A	109.6	C9—C8—H8	122.0
C6—C1—H1A	109.6	C8—C9—C10	122.27 (15)
O2—C2—C1	116.78 (13)	C8—C9—H9	118.9
C5—C2—O2	110.66 (14)	C10—C9—H9	118.9
C5—C2—C1	132.56 (14)	C9—C10—H10	119.1
O2—C3—H3	124.6	C11—C10—C9	121.81 (15)
C4—C3—O2	110.75 (14)	C11—C10—H10	119.1
C4—C3—H3	124.6	C10—C11—C12	116.47 (14)
C3—C4—C5	106.01 (14)	C10—C11—H11	121.8
C3—C4—H4	127.0	C12—C11—H11	121.8
C5—C4—H4	127.0	N3—C12—C7	108.16 (13)
C2—C5—C4	106.45 (14)	N3—C12—C11	130.53 (15)
C2—C5—H5	126.8	C7—C12—C11	121.31 (14)
C4—C5—H5	126.8		

C6—N1—N2—N3	−177.41 (13)	C5—C2—C1—O1	0.9 (2)
C7—N1—N2—N3	−0.44 (17)	C5—C2—C1—C6	−118.73 (19)
N2—N1—C6—C1	92.27 (16)	O2—C2—C5—C4	−0.09 (18)
C7—N1—C6—C1	−84.02 (19)	C1—C2—C5—C4	−179.58 (15)
N2—N1—C7—C8	179.68 (16)	O2—C3—C4—C5	−0.27 (18)
N2—N1—C7—C12	0.62 (16)	C2—C5—C4—C3	0.21 (18)
C6—N1—C7—C8	−3.8 (3)	N1—C7—C12—N3	−0.58 (16)
C6—N1—C7—C12	177.17 (14)	N1—C7—C12—C11	179.06 (14)
C12—N3—N2—N1	0.05 (17)	C8—C7—C12—N3	−179.77 (13)
N2—N3—C12—C7	0.34 (17)	C8—C7—C12—C11	−0.1 (2)
N2—N3—C12—C11	−179.25 (15)	C9—C8—C7—N1	−178.60 (15)
C3—O2—C2—C1	179.51 (13)	C9—C8—C7—C12	0.3 (2)
C3—O2—C2—C5	−0.07 (17)	C7—C8—C9—C10	−0.4 (2)
C2—O2—C3—C4	0.22 (18)	C11—C10—C9—C8	0.3 (2)
O1—C1—C6—N1	64.08 (16)	C10—C11—C12—N3	179.57 (15)
C2—C1—C6—N1	−177.23 (12)	C10—C11—C12—C7	0.0 (2)
O2—C2—C1—O1	−178.53 (12)	C12—C11—C10—C9	−0.1 (2)
O2—C2—C1—C6	61.80 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N3^{i}	0.82	2.26	2.7968 (18)	123

Symmetry code: (i) x, $-y+3/2$, $z-1/2$.