

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

1-[2-(2,6-Dichlorobenzoyloxy)-2-(2-furyl)-ethyl]-1*H*-1,2,4-triazole

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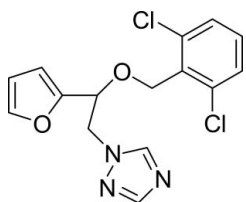
Received 4 December 2009; accepted 7 December 2009

 Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.067; wR factor = 0.180; data-to-parameter ratio = 17.2.

In the molecule of the title compound, $\text{C}_{15}\text{H}_{13}\text{Cl}_2\text{N}_3\text{O}_2$, the triazole ring is oriented at dihedral angles of 2.54 (13) and 44.43 (12)°, respectively with respect to the furan and dichlorobenzene rings. The dihedral angle between the dichlorobenzene and furan rings is 46.75 (12)°. In the crystal structure, intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules into centrosymmetric dimers and $\pi-\pi$ contacts between dichlorobenzene rings [centroid-centroid distance = 3.583 (2) Å] may further stabilize the structure. Intermolecular $\text{C}-\text{H}\cdots\pi$ contacts between the triazole and furan rings also occur.

Related literature

For general background to antifungal agents, see: Caira *et al.* (2004); Godefroi *et al.* (1969); Özel Güven *et al.* (2007a,b); Paulvannan *et al.* (2001); Peeters *et al.* (1996); Wahbi *et al.* (1995). For related structures, see: Freer *et al.* (1986); Özel Güven *et al.* (2008a,b,c,d,e,f); Özel Güven *et al.* (2009); Peeters *et al.* (1979).



Experimental

Crystal data

 $\text{C}_{15}\text{H}_{13}\text{Cl}_2\text{N}_3\text{O}_2$
 $M_r = 338.18$
 Monoclinic, $P2_1/n$
 $a = 10.5853$ (3) Å

 $b = 12.4960$ (2) Å
 $c = 12.5850$ (3) Å
 $\beta = 114.455$ (1)°
 $V = 1515.32$ (6) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.44$ mm⁻¹
 $T = 120$ K
 $0.40 \times 0.40 \times 0.10$ mm

Data collection

 Bruker–Nonius KappaCCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2007)
 $T_{\min} = 0.837$, $T_{\max} = 0.955$

 33067 measured reflections
 3438 independent reflections
 2775 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.058$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.067$
 $wR(F^2) = 0.180$
 $S = 1.04$
 3438 reflections

 200 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.20$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.76$ e Å⁻³

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

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}2-\text{H}2\cdots\text{O}1^{\text{i}}$	0.93	2.44	3.363 (3)	173
$\text{C}9-\text{H}9\text{B}\cdots\text{Cl}2$	0.97	2.62	3.109 (3)	112
$\text{C}1-\text{H}1\cdots\text{C}g2^{\text{ii}}$	0.93	2.79	3.488 (4)	133
$\text{C}7-\text{H}7\cdots\text{C}g1^{\text{iii}}$	0.93	2.93	3.570 (4)	127

Symmetry codes: (i) $-x, -y + 1, -z + 2$; (ii) $x - \frac{3}{2}, -y - \frac{1}{2}, z - \frac{3}{2}$; (iii) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$. $\text{C}g1$ and $\text{C}g2$ are the centroids of the $\text{N}1-\text{N}3/\text{C}1/\text{C}2$ and $\text{O}2/\text{C}5-\text{C}8$ rings, respectively.

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) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors acknowledge Zonguldak Karaelmas University Research Fund (project No. 2008–13–02–06) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2704).

References

- Caira, M. R., Alkhamis, K. A. & Obaidat, R. M. (2004). *J. Pharm. Sci.* **93**, 601–611.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
 Freer, A. A., Pearson, A. & Salole, E. G. (1986). *Acta Cryst.* **C42**, 1350–1352.
 Godefroi, E. F., Heeres, J., Van Cutsem, J. & Janssen, P. A. J. (1969). *J. Med. Chem.* **12**, 784–791.
 Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
 Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
 Özel Güven, Ö., Erdoğan, T., Coles, S. J. & Hökelek, T. (2008a). *Acta Cryst.* **E64**, o1437.
 Özel Güven, Ö., Erdoğan, T., Coles, S. J. & Hökelek, T. (2008b). *Acta Cryst.* **E64**, o1496–o1497.
 Özel Güven, Ö., Erdoğan, T., Coles, S. J. & Hökelek, T. (2008c). *Acta Cryst.* **E64**, o1588–o1589.
 Özel Güven, Ö., Erdoğan, T., Coles, S. J. & Hökelek, T. (2008d). *Acta Cryst.* **E64**, o1655–o1656.

- Özel Güven, Ö., Erdoğan, T., Göker, H. & Yıldız, S. (2007a). *Bioorg. Med. Chem. Lett.* **17**, 2233–2236.
- Özel Güven, Ö., Erdoğan, T., Göker, H. & Yıldız, S. (2007b). *J. Heterocycl. Chem.* **44**, 731–734.
- Özel Güven, Ö., Tahtacı, H., Coles, S. J. & Hökelek, T. (2008e). *Acta Cryst. E64*, o1914–o1915.
- Özel Güven, Ö., Tahtacı, H., Coles, S. J. & Hökelek, T. (2009). *Acta Cryst. E65*, o2868–o2869.
- Özel Güven, Ö., Tahtacı, H., Tahir, M. N. & Hökelek, T. (2008f). *Acta Cryst. E64*, o2465.
- Paulvannan, K., Hale, R., Sedehi, D. & Chen, T. (2001). *Tetrahedron*, **57**, 9677–9682.
- Peeters, O. M., Blaton, N. M. & De Ranter, C. J. (1979). *Acta Cryst. B35*, 2461–2464.
- Peeters, O. M., Blaton, N. M. & De Ranter, C. J. (1996). *Acta Cryst. C52*, 2225–2229.
- Sheldrick, G. M. (2007). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (2008). *Acta Cryst. A64*, 112–122.
- Spek, A. L. (2009). *Acta Cryst. D65*, 148–155.
- Wahbi, Y., Caujolle, R., Tournaire, C., Payard, M., Linas, M. D. & Seguela, J. P. (1995). *Eur. J. Med. Chem.* **30**, 955–962.

supporting information

Acta Cryst. (2010). E66, o107–o108 [doi:10.1107/S1600536809052568]

1-[2-(2,6-Dichlorobenzyloxy)-2-(2-furyl)ethyl]-1*H*-1,2,4-triazole**Özden Özel Güven, Hakan Tahtacı, Simon J. Coles and Tuncer Hökelek****S1. Comment**

In recent years, among antifungal agents, azole derivatives still have an important place in the class of systemic antifungal drugs. Some ether structures containing 1*H*-imidazole ring like miconazole, econazole and sulconazole have been synthesized and developed for clinical uses as antifungal agents (Godefroi *et al.*, 1969). The crystal structures of these ether derivatives like miconazole (Peeters *et al.*, 1979), econazole (Freer *et al.*, 1986) have been reported previously. Also, antifungal activity of aromatic ethers possessing 1*H*-1,2,4-triazole ring have been reported (Wahbi *et al.*, 1995). Itraconazole (Peeters *et al.*, 1996) and fluconazole (Caira *et al.*, 2004) are 1*H*-1,2,4-triazole ring containing azole derivatives. 1,2,4-Triazoles are biologically interesting molecules and their chemistry is receiving considerable attention due to antihypertensive, antifungal and antibacterial properties (Paulvannan *et al.*, 2001). Ether structures possessing 1*H*-benzimidazole ring have been reported to show antibacterial activity more than antifungal activity (Özel Güven *et al.*, 2007*a,b*). The crystal structures of 1*H*-benzimidazole ring containing ether derivatives (Özel Güven *et al.*, 2008*a,b,c,d*) and also, 1*H*-1,2,4-triazole ring containing ether derivatives have been reported recently (Özel Güven *et al.*, 2008*e,f*; Özel Güven *et al.*, 2009). Now, we report herein the crystal structure of 2,6-dichloro- derivative of 1*H*-1,2,4-triazole and furyl rings containing ether structure.

In the molecule of the title compound (Fig. 1) the bond lengths and angles are generally within normal ranges. The planar triazole ring is oriented with respect to the furan and dichlorobenzene rings at dihedral angles of 2.54 (13)° and 44.43 (12)°, respectively. Atoms C3, C4 and C9 are -0.064 (3), 0.039 (3) and -0.073 (3) Å away from the planes of the triazole, furan and dichlorobenzene, respectively. So, they are nearly coplanar with the adjacent rings. The dichlorobenzene ring is oriented with respect to the furan ring at a dihedral angle of 46.75 (12)°. An intramolecular C—H···Cl hydrogen bond (Table 1) results in the formation of a five-membered ring (C12/H9B/C9/C10/C15) adopting envelope conformation with H9B atom displaced by 0.210 (1) Å from the plane of the other ring atoms.

In the crystal structure, intermolecular C—H···O hydrogen bonds (Table 1) link the molecules into centrosymmetric dimers (Fig. 2), in which they may be effective in the stabilization of the structure. The π - π contact between the dichlorobenzene rings, Cg3—Cg3ⁱ [symmetry code: (i) -x, -y, 1 - z, where Cg3 is centroid of the ring (C10-C15)] may further stabilize the structure, with centroid-centroid distance of 3.583 (2) Å. Intermolecular C—H··· π interactions (Table 1) are also observed between the triazole and furan rings.

S2. Experimental

The title compound was synthesized by the reaction of 1-(furan-2-yl)-2-(1*H*-1,2,4-triazol-1-yl)ethanol (unpublished results) with NaH and appropriate benzyl halide. To a solution of alcohol (500 mg, 2.791 mmol) in DMF (4 ml) was added NaH (112 mg, 2.791 mmol) in small fractions. The appropriate benzyl halide (669 mg, 2.791 mmol) was added dropwise. The mixture was stirred at room temperature for 3 h, and excess hydride was decomposed with methyl alcohol (5 ml). After evaporation to dryness under reduced pressure, the crude residue was suspended with water and extracted

with methylene chloride. The organic layer was dried over anhydrous sodium sulfate and then evaporated to dryness. The crude residue was purified by chromatography on a silica-gel column using chloroform as eluent. Crystals suitable for X-ray analysis were obtained by the recrystallization of the ether from isopropanol solution (yield; 500 mg, 53%).

S3. Refinement

H atoms were positioned geometrically, with C–H = 0.93, 0.98 and 0.97 Å for aromatic, methine and methylene H, respectively, and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

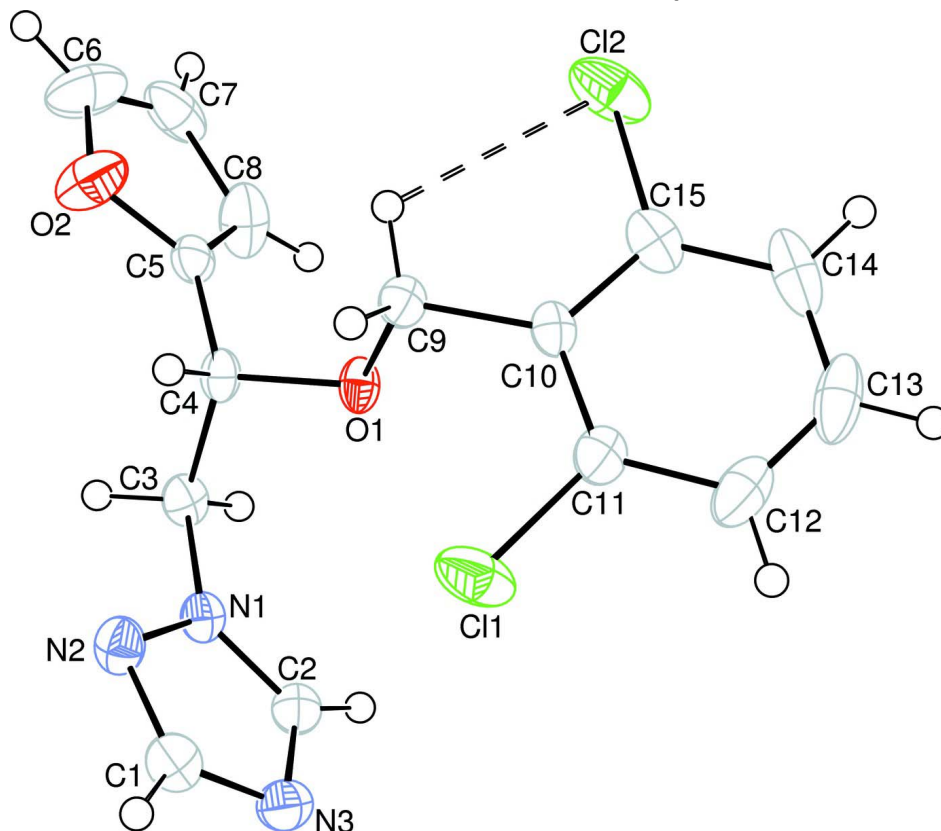
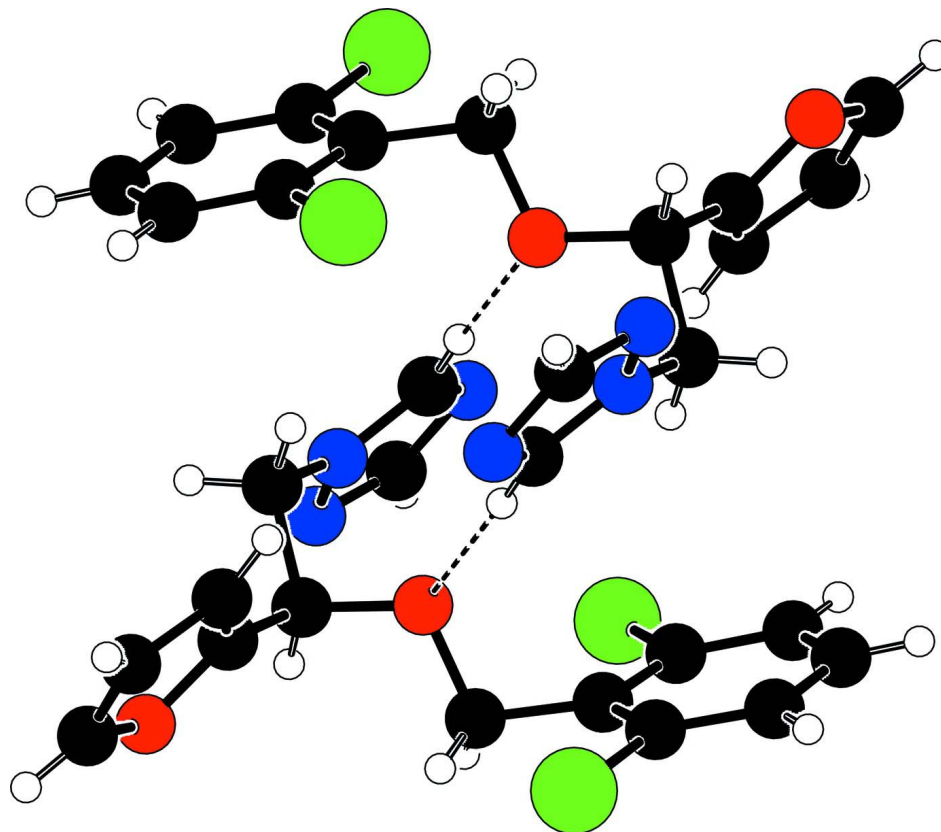


Figure 1

The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The dashed line indicates a hydrogen bond.

**Figure 2**

A partial packing diagram.

1-[2-(2,6-Dichlorobenzoyloxy)-2-(2-furyl)ethyl]-1H-1,2,4-triazole

Crystal data

$C_{15}H_{13}Cl_2N_3O_2$

$M_r = 338.18$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1n$

$a = 10.5853\ (3)\ \text{\AA}$

$b = 12.4960\ (2)\ \text{\AA}$

$c = 12.5850\ (3)\ \text{\AA}$

$\beta = 114.455\ (1)^\circ$

$V = 1515.32\ (6)\ \text{\AA}^3$

$Z = 4$

$F(000) = 696$

$D_x = 1.482\ \text{Mg m}^{-3}$

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

Cell parameters from 23020 reflections

$\theta = 2.9\text{--}27.5^\circ$

$\mu = 0.44\ \text{mm}^{-1}$

$T = 120\ \text{K}$

Plate, colorless

$0.40 \times 0.40 \times 0.10\ \text{mm}$

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)

$T_{\min} = 0.837$, $T_{\max} = 0.955$

33067 measured reflections

3438 independent reflections

2775 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.058$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.3^\circ$

$h = -13 \rightarrow 13$

$k = -14 \rightarrow 15$

$l = -16 \rightarrow 16$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.067$ $wR(F^2) = 0.180$ $S = 1.04$

3438 reflections

200 parameters

0 restraints

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

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0984P)^2 + 1.9705P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 1.20 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.76 \text{ e } \text{\AA}^{-3}$ Extinction correction: *SHELXL97* (Sheldrick,
2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.051 (5)

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.32066 (8)	0.66344 (7)	1.08482 (8)	0.0470 (3)
Cl2	0.29005 (8)	0.31220 (7)	0.82358 (9)	0.0497 (3)
O1	0.07950 (17)	0.54757 (14)	0.86960 (15)	0.0231 (4)
O2	-0.1088 (3)	0.5914 (2)	0.5685 (2)	0.0483 (6)
N1	-0.0576 (2)	0.71549 (17)	0.93071 (19)	0.0226 (5)
N2	-0.0121 (2)	0.81516 (18)	0.9183 (2)	0.0284 (5)
N3	0.0458 (2)	0.7770 (2)	1.1089 (2)	0.0298 (5)
C1	0.0483 (3)	0.8475 (2)	1.0282 (3)	0.0300 (6)
H1	0.0898	0.9144	1.0487	0.036*
C2	-0.0207 (3)	0.6947 (2)	1.0435 (2)	0.0255 (5)
H2	-0.0393	0.6309	1.0724	0.031*
C3	-0.1260 (3)	0.6463 (2)	0.8301 (2)	0.0248 (5)
H3A	-0.2023	0.6846	0.7706	0.030*
H3B	-0.1638	0.5842	0.8530	0.030*
C4	-0.0241 (2)	0.6098 (2)	0.7800 (2)	0.0228 (5)
H4	0.0197	0.6727	0.7628	0.027*
C5	-0.0952 (3)	0.5454 (2)	0.6705 (2)	0.0250 (5)
C6	-0.1805 (4)	0.5198 (4)	0.4817 (3)	0.0582 (11)
H6	-0.2048	0.5311	0.4026	0.070*
C7	-0.2101 (3)	0.4328 (3)	0.5259 (3)	0.0457 (9)
H7	-0.2564	0.3726	0.4847	0.055*
C8	-0.1574 (3)	0.4484 (3)	0.6500 (3)	0.0429 (8)
H8	-0.1646	0.4016	0.7047	0.051*

C9	0.2081 (3)	0.5444 (2)	0.8579 (2)	0.0244 (5)
H9A	0.2416	0.6164	0.8565	0.029*
H9B	0.1961	0.5086	0.7859	0.029*
C10	0.3091 (2)	0.4839 (2)	0.9611 (2)	0.0224 (5)
C11	0.3640 (3)	0.5315 (2)	1.0718 (2)	0.0283 (6)
C12	0.4517 (3)	0.4781 (3)	1.1713 (3)	0.0424 (8)
H12	0.4849	0.5122	1.2435	0.051*
C13	0.4890 (3)	0.3753 (3)	1.1629 (3)	0.0459 (9)
H13	0.5469	0.3388	1.2297	0.055*
C14	0.4416 (3)	0.3250 (2)	1.0558 (4)	0.0427 (9)
H14	0.4695	0.2555	1.0500	0.051*
C15	0.3507 (3)	0.3794 (2)	0.9559 (3)	0.0304 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0272 (4)	0.0521 (5)	0.0535 (5)	0.0023 (3)	0.0085 (3)	-0.0273 (4)
C12	0.0340 (4)	0.0412 (5)	0.0711 (6)	-0.0067 (3)	0.0191 (4)	-0.0283 (4)
O1	0.0144 (8)	0.0260 (9)	0.0257 (9)	0.0012 (6)	0.0052 (7)	0.0068 (7)
O2	0.0633 (16)	0.0525 (15)	0.0306 (12)	-0.0134 (12)	0.0208 (11)	-0.0054 (10)
N1	0.0183 (10)	0.0227 (11)	0.0247 (11)	-0.0008 (8)	0.0069 (8)	0.0013 (8)
N2	0.0284 (12)	0.0243 (12)	0.0289 (12)	-0.0032 (9)	0.0082 (9)	0.0016 (9)
N3	0.0262 (11)	0.0356 (13)	0.0269 (12)	0.0010 (10)	0.0105 (9)	-0.0031 (9)
C1	0.0244 (13)	0.0283 (14)	0.0341 (15)	-0.0025 (10)	0.0089 (11)	-0.0028 (11)
C2	0.0228 (12)	0.0282 (13)	0.0282 (13)	0.0003 (10)	0.0131 (11)	0.0020 (10)
C3	0.0172 (11)	0.0250 (13)	0.0271 (13)	-0.0020 (9)	0.0041 (10)	-0.0012 (10)
C4	0.0168 (11)	0.0230 (12)	0.0233 (12)	0.0005 (9)	0.0032 (9)	0.0040 (9)
C5	0.0201 (12)	0.0264 (13)	0.0247 (13)	0.0046 (9)	0.0057 (10)	0.0000 (10)
C6	0.065 (3)	0.077 (3)	0.0307 (17)	-0.009 (2)	0.0176 (17)	-0.0201 (17)
C7	0.0299 (15)	0.0392 (18)	0.051 (2)	0.0080 (13)	-0.0004 (14)	-0.0203 (15)
C8	0.0333 (16)	0.0322 (16)	0.0470 (19)	-0.0052 (12)	0.0004 (14)	0.0062 (13)
C9	0.0177 (11)	0.0308 (13)	0.0254 (13)	0.0016 (9)	0.0096 (10)	0.0038 (10)
C10	0.0152 (11)	0.0240 (12)	0.0286 (13)	0.0001 (9)	0.0095 (10)	0.0050 (10)
C11	0.0165 (11)	0.0400 (15)	0.0289 (14)	0.0013 (10)	0.0098 (10)	0.0039 (11)
C12	0.0208 (13)	0.080 (3)	0.0261 (15)	0.0038 (14)	0.0098 (12)	0.0119 (15)
C13	0.0222 (14)	0.068 (2)	0.0461 (19)	0.0056 (14)	0.0131 (13)	0.0354 (17)
C14	0.0233 (14)	0.0281 (15)	0.080 (3)	0.0056 (11)	0.0243 (16)	0.0228 (15)
C15	0.0190 (12)	0.0248 (13)	0.0472 (17)	-0.0040 (10)	0.0134 (12)	-0.0008 (11)

Geometric parameters (Å, °)

N1—N2	1.367 (3)	C7—C8	1.438 (5)
C1—N2	1.324 (4)	C7—H7	0.9300
C1—N3	1.352 (4)	C8—H8	0.9300
C1—H1	0.9300	C9—O1	1.429 (3)
C2—N3	1.323 (4)	C9—H9A	0.9700
C2—N1	1.333 (3)	C9—H9B	0.9700
C2—H2	0.9300	C10—C9	1.501 (3)

C3—N1	1.455 (3)	C10—C11	1.401 (4)
C3—H3A	0.9700	C10—C15	1.389 (4)
C3—H3B	0.9700	C11—C11	1.737 (3)
C4—O1	1.434 (3)	C11—C12	1.383 (4)
C4—C3	1.527 (4)	C12—C13	1.361 (6)
C4—C5	1.501 (4)	C12—H12	0.9300
C4—H4	0.9800	C13—C14	1.380 (6)
C5—O2	1.359 (4)	C13—H13	0.9300
C5—C8	1.352 (4)	C14—C15	1.403 (4)
C6—O2	1.373 (4)	C14—H14	0.9300
C6—C7	1.317 (6)	C15—C12	1.733 (3)
C6—H6	0.9300		
C9—O1—C4	112.62 (18)	C6—C7—C8	107.1 (3)
C5—O2—C6	106.5 (3)	C6—C7—H7	126.5
N2—N1—C3	120.9 (2)	C8—C7—H7	126.5
C2—N1—N2	109.7 (2)	C5—C8—C7	105.6 (3)
C2—N1—C3	129.2 (2)	C5—C8—H8	127.2
C1—N2—N1	101.5 (2)	C7—C8—H8	127.2
C2—N3—C1	102.1 (2)	O1—C9—C10	107.01 (19)
N2—C1—N3	115.7 (2)	O1—C9—H9A	110.3
N2—C1—H1	122.1	O1—C9—H9B	110.3
N3—C1—H1	122.1	C10—C9—H9A	110.3
N1—C2—H2	124.5	C10—C9—H9B	110.3
N3—C2—N1	110.9 (2)	H9A—C9—H9B	108.6
N3—C2—H2	124.5	C11—C10—C9	120.1 (2)
N1—C3—C4	110.8 (2)	C15—C10—C9	124.0 (2)
N1—C3—H3A	109.5	C15—C10—C11	115.9 (2)
N1—C3—H3B	109.5	C10—C11—C11	118.7 (2)
C4—C3—H3A	109.5	C12—C11—C10	122.9 (3)
C4—C3—H3B	109.5	C12—C11—C11	118.5 (3)
H3A—C3—H3B	108.1	C11—C12—H12	120.3
O1—C4—C3	106.1 (2)	C13—C12—C11	119.5 (3)
O1—C4—C5	111.1 (2)	C13—C12—H12	120.3
O1—C4—H4	109.3	C12—C13—C14	120.5 (3)
C3—C4—H4	109.3	C12—C13—H13	119.8
C5—C4—C3	111.5 (2)	C14—C13—H13	119.8
C5—C4—H4	109.3	C13—C14—C15	119.5 (3)
O2—C5—C4	117.2 (2)	C13—C14—H14	120.3
C8—C5—O2	110.3 (3)	C15—C14—H14	120.3
C8—C5—C4	132.5 (3)	C10—C15—C12	120.2 (2)
O2—C6—H6	124.7	C10—C15—C14	121.8 (3)
C7—C6—O2	110.6 (3)	C14—C15—C12	118.1 (2)
C7—C6—H6	124.7		
C2—N1—N2—C1	-1.0 (3)	C7—C6—O2—C5	-0.4 (4)
C3—N1—N2—C1	-176.9 (2)	O2—C6—C7—C8	1.3 (4)
N3—C1—N2—N1	0.4 (3)	C6—C7—C8—C5	-1.7 (4)

N2—C1—N3—C2	0.3 (3)	C10—C9—O1—C4	176.0 (2)
N3—C2—N1—N2	1.3 (3)	C11—C10—C9—O1	-73.1 (3)
N3—C2—N1—C3	176.7 (2)	C15—C10—C9—O1	104.8 (3)
N1—C2—N3—C1	-1.0 (3)	C9—C10—C11—C11	-3.8 (3)
C4—C3—N1—C2	-107.0 (3)	C9—C10—C11—C12	176.5 (2)
C4—C3—N1—N2	68.0 (3)	C15—C10—C11—C11	178.21 (19)
C3—C4—O1—C9	-156.0 (2)	C15—C10—C11—C12	-1.5 (4)
C5—C4—O1—C9	82.6 (3)	C9—C10—C15—C12	2.2 (3)
O1—C4—C3—N1	63.3 (3)	C9—C10—C15—C14	-177.5 (2)
C5—C4—C3—N1	-175.5 (2)	C11—C10—C15—C12	-179.85 (19)
O1—C4—C5—O2	-132.0 (2)	C11—C10—C15—C14	0.4 (4)
O1—C4—C5—C8	51.7 (4)	C10—C11—C12—C13	0.9 (4)
C3—C4—C5—O2	109.7 (3)	C11—C11—C12—C13	-178.8 (2)
C3—C4—C5—C8	-66.6 (4)	C11—C12—C13—C14	0.9 (4)
C4—C5—O2—C6	-177.9 (3)	C12—C13—C14—C15	-2.0 (4)
C8—C5—O2—C6	-0.8 (4)	C13—C14—C15—C12	-178.4 (2)
O2—C5—C8—C7	1.5 (4)	C13—C14—C15—C10	1.3 (4)
C4—C5—C8—C7	178.0 (3)		

Hydrogen-bond geometry (\AA , $^\circ$)

Cg1 and Cg2 are the centroids of the N1–N3/C1/C2 and O2/C5–C8 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 \cdots O1 ⁱ	0.93	2.44	3.363 (3)	173
C9—H9B \cdots C12	0.97	2.62	3.109 (3)	112
C1—H1 \cdots Cg2 ⁱⁱ	0.93	2.79	3.488 (4)	133
C7—H7 \cdots Cg1 ⁱⁱⁱ	0.93	2.93	3.570 (4)	127

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