

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

1-[2-(2,5-Dichlorobenzyloxy)-2-phenylethyl]-1H-benzotriazole

 Özden Özel Güven,^a Meral Bayraktar,^a Simon J. Coles^b and Tuncer Hökelek^{c*}
^aDepartment of Chemistry, Zonguldak Karaelmas University, 67100 Zonguldak, Turkey, ^bDepartment of Chemistry, Southampton University, Southampton SO17 1BJ, England, and ^cDepartment of Physics, Hacettepe University, 06800 Beytepe, Ankara, Turkey

Correspondence e-mail: merzifon@hacettepe.edu.tr

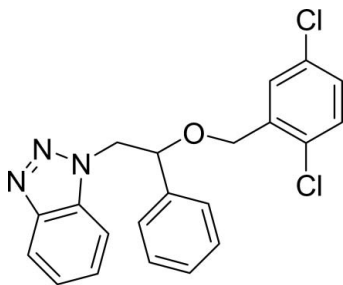
Received 21 October 2011; accepted 26 October 2011

 Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.043; wR factor = 0.120; data-to-parameter ratio = 17.5.

In the title molecule, $\text{C}_{21}\text{H}_{17}\text{Cl}_2\text{N}_3\text{O}$, the benzotriazole ring is oriented at dihedral angles of $48.72(6)$ and $62.94(5)^\circ$, respectively, to the phenyl and benzene rings and the dihedral angle between the phenyl and benzene rings is $88.95(6)^\circ$. In the crystal, weak $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds link the molecules into chains. $\pi-\pi$ contacts between the triazole and benzene rings [centroid-centroid distance = $3.678(1)$ Å] and a weak $\text{C}-\text{H}\cdots\pi$ interaction 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: Katritzky *et al.* (2001); Özel Güven *et al.* (2007*a,b*, 2010*a,b*, 2011); Swamy *et al.* (2006).



Experimental

Crystal data

 $\text{C}_{21}\text{H}_{17}\text{Cl}_2\text{N}_3\text{O}$
 $M_r = 398.28$
 Triclinic, $P\bar{1}$
 $a = 8.6970(3)$ Å
 $b = 8.8385(3)$ Å

 $c = 13.3918(4)$ Å
 $\alpha = 105.840(3)^\circ$
 $\beta = 104.453(3)^\circ$
 $\gamma = 99.713(2)^\circ$
 $V = 927.47(6)$ Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.37$ mm⁻¹
 $T = 120$ K
 $0.20 \times 0.13 \times 0.08$ mm

Data collection

 Bruker–Nonius KappaCCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2007)
 $T_{\min} = 0.930$, $T_{\max} = 0.971$

 21356 measured reflections
 4271 independent reflections
 3391 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.055$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.120$
 $S = 1.12$
 4271 reflections

 244 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.47$ e Å⁻³
 $\Delta\rho_{\min} = -0.50$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C2–C7 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C19–H19 \cdots N3 ⁱ	0.93	2.62	3.549 (2)	174
C18–H18 \cdots Cg1 ⁱⁱ	0.93	2.69	3.605 (2)	168

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

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: SU2333).

References

- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
 Hirokawa, Y., Yamazaki, H., Yoshida, N. & Kato, S. (1998). *Bioorg. Med. Chem. Lett.* **8**, 1973–1978.
 Katritzky, A. R., Zhang, S. M., Kurz, T., Wang, M. Y. & Steel, P. J. (2001). *Org. Lett.* **3**, 2807–2809.
 Kopanska, K., Najda, A., Zebrowska, J., Chomicz, L., Piekarczyk, J., Myjak, P. & Bretner, M. (2004). *Bioorg. Med. Chem.* **12**, 2617–2624.
 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., Bayraktar, M., Coles, S. J. & Hökelek, T. (2010*a*). *Acta Cryst. E* **66**, o959.
 Özel Güven, Ö., Bayraktar, M., Coles, S. J. & Hökelek, T. (2010*b*). *Acta Cryst. E* **66**, o1246–o1247.
 Özel Güven, Ö., Çapanlar, S., Coles, S. J. & Hökelek, T. (2011). *Acta Cryst. E* **67**, o2510.
 Özel Güven, Ö., Erdoğan, T., Göker, H. & Yıldız, S. (2007*a*). *Bioorg. Med. Chem. Lett.* **17**, 2233–2236.
 Özel Güven, Ö., Erdoğan, T., Göker, H. & Yıldız, S. (2007*b*). *J. Heterocycl. Chem.* **44**, 731–734.
 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.

Swamy, S. N., Basappa, Sarala G., Priya, B. S., Gaonkar, S. L., Prasad, J. S. &

Rangappa, K. S. (2006). *Bioorg. Med. Chem. Lett.* **16**, 999–1004.

Yu, K. L., Zhang, Y., Civiello, R. L., Kadow, K. F., Cianci, C., Krystal, M. & Meanwell, N. A. (2003). *Bioorg. Med. Chem. Lett.* **13**, 2141–2144.

supporting information

Acta Cryst. (2011). E67, o3177–o3178 [https://doi.org/10.1107/S1600536811044783]

1-[2-(2,5-Dichlorobenzoyloxy)-2-phenylethyl]-1*H*-benzotriazole**Özden Özel Güven, Meral Bayraktar, Simon J. Coles and Tuncer Hökelek****S1. Comment**

Clotrimazole, miconazole, econazole, ketoconazole, itraconazole and fluconazole have been developed for clinical uses as antifungal agents. Lately, similar structures containing benzimidazole ring have been reported as antibacterial agents (Özel Güven *et al.*, 2007*a,b*). Benzotriazole derivatives also exhibit a good degree of analgesic, anti-inflammatory, diuretic, antiviral and antihypertensive activities (Hirokawa *et al.*, 1998; Yu *et al.*, 2003; Kopanska *et al.*, 2004). Crystal structures of benzotriazole ring possessing compounds have been reported before (Katritzky *et al.*, 2001; Swamy *et al.*, 2006; Özel Güven *et al.*, 2010*a,b*; Özel Güven *et al.*, 2011). Now, we report herein the crystal structure of the title benzotriazole derivative, (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/C9–C14)] is oriented with respect to the phenyl [A (C2–C7)] and benzene [C (C16–C21)] rings at dihedral angles of A/B = 48.72 (6) and B/C = 62.94 (5)°. The dihedral angle between phenyl and benzene rings is A/C = 88.95 (6)°. Atom C8 is -0.017 (2) Å away from the plane of the benzotriazole ring and atom C1 is 0.069 (2) Å away from the plane of the phenyl ring, while atoms O1 and C15 are -0.052 (1) and 0.010 (2) Å away from the plane of the benzene ring.

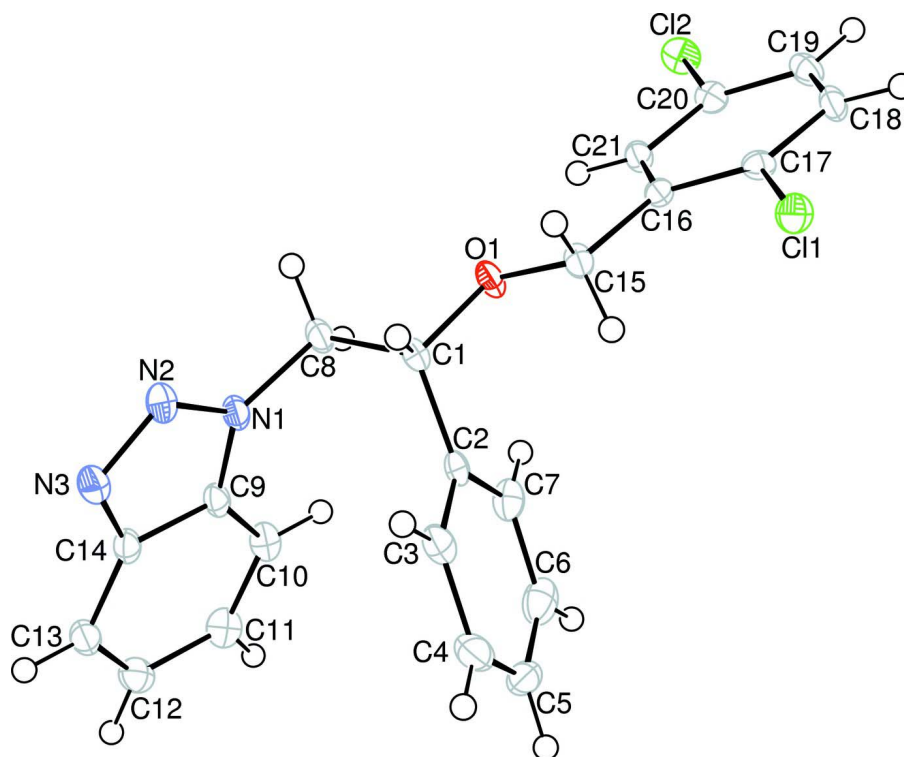
In the crystal, weak C—H···N hydrogen bonds (table 1) link the molecules into chains (Fig. 2). There also exists a π – π contact between the triazole and benzene rings, Cg4—Cg5ⁱ, may further stabilize the structure [centroid-centroid distance = 3.678 (1) Å; symmetry code: (i) 2 - x, 1 - y, 1 - z; Cg4 and Cg5 are the centroids of the rings D (N1—N3/C9/C14) and E (C9—C14)]. A weak C—H··· π interaction (Table 1) may stabilize the structure.

S2. Experimental

The title compound was synthesized by the reaction of 2-(1*H*-benzotriazol-1-yl)-1-phenylethanol (Özel Güven *et al.*, 2010*a*) with aryl halide using NaH. 2-(1*H*-benzotriazol-1-yl)-1-phenylethanol (200 mg, 0.84 mmol) was dissolved in DMF (3–4 ml). NaH (33 mg, 0.84 mmol) was added to the solution portionwise. After stirring the mixture a few minutes, 2,5-dichlorobenzyl bromide (200 mg, 0.84 mmol) was added dropwise. Then, the reaction mixture was stirred additional 3 h at room temperature. Adding methanol (5 ml) reaction was stopped. After evaporation of the solvent, dichloromethane was added to the reaction mixture and extracted with water. Then, the organic phase was separated, dried, filtered and evaporated. The precipitate formed was purified by column chromatography using chloroform and crystallized from *iso*-propanol to obtain colorless crystals suitable for X-ray analysis (yield; 231 mg, 69%).

S3. Refinement

H atoms were positioned geometrically with 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 $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

**Figure 1**

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

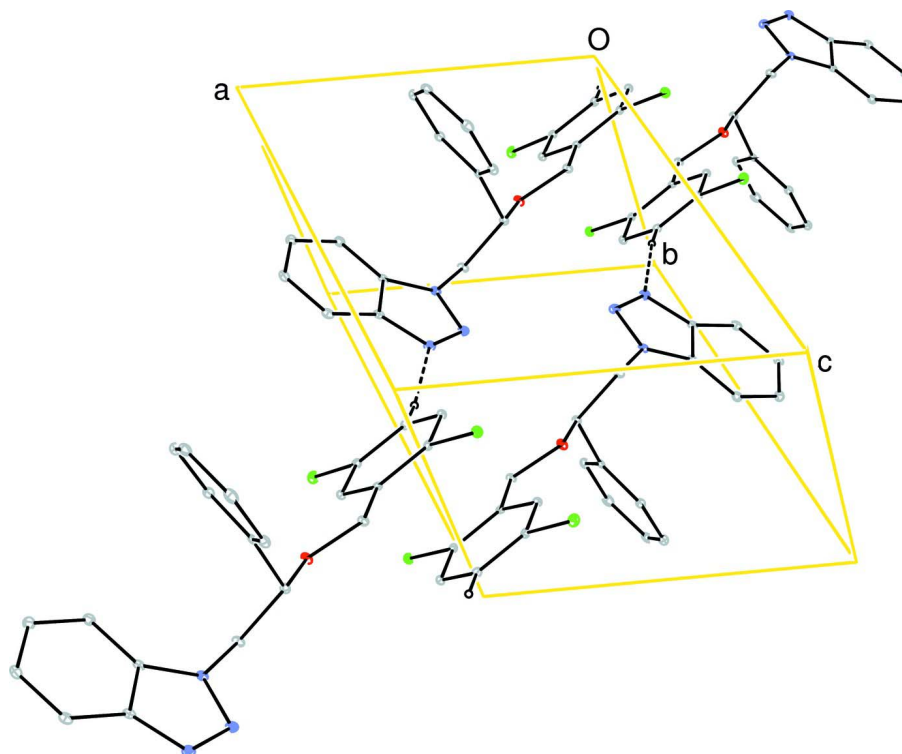


Figure 2

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

1-[2-(2,5-Dichlorobenzyloxy)-2-phenylethyl]-1*H*-benzotriazole

Crystal data

$C_{21}H_{17}Cl_2N_3O$

$M_r = 398.28$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.6970$ (3) Å

$b = 8.8385$ (3) Å

$c = 13.3918$ (4) Å

$\alpha = 105.840$ (3)°

$\beta = 104.453$ (3)°

$\gamma = 99.713$ (2)°

$V = 927.47$ (6) Å³

$Z = 2$

$F(000) = 412$

$D_x = 1.426$ Mg m⁻³

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

Cell parameters from 14295 reflections

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

$\mu = 0.37$ mm⁻¹

$T = 120$ K

Block, colorless

$0.20 \times 0.13 \times 0.08$ 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)

$T_{\min} = 0.930$, $T_{\max} = 0.971$

21356 measured reflections

4271 independent reflections

3391 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.055$

$\theta_{\max} = 27.6^\circ$, $\theta_{\min} = 3.0^\circ$

$h = -11 \rightarrow 11$

$k = -11 \rightarrow 11$

$l = -17 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.120$

$S = 1.12$

4271 reflections

244 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

$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 0.2097P]$

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

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

$\Delta\rho_{\max} = 0.47 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.50 \text{ e } \text{\AA}^{-3}$

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 $F^2 > 2\sigma(F^2)$ 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	1.14499 (5)	0.89780 (6)	0.93114 (4)	0.02094 (14)
Cl2	0.71261 (6)	0.46919 (6)	1.10951 (4)	0.02373 (14)
O1	0.61227 (15)	0.66913 (16)	0.77690 (10)	0.0196 (3)
N1	0.25973 (19)	0.61345 (19)	0.54291 (12)	0.0178 (3)
N2	0.2767 (2)	0.5667 (2)	0.44128 (12)	0.0224 (4)
N3	0.1660 (2)	0.6091 (2)	0.37527 (12)	0.0229 (4)
C1	0.5343 (2)	0.7104 (2)	0.68405 (14)	0.0164 (4)
H1	0.5981	0.6965	0.6329	0.020*
C2	0.5167 (2)	0.8836 (2)	0.71551 (14)	0.0171 (4)
C3	0.5459 (2)	0.9801 (2)	0.65228 (15)	0.0224 (4)
H3	0.5803	0.9394	0.5922	0.027*
C4	0.5241 (3)	1.1372 (3)	0.67827 (18)	0.0297 (5)
H4	0.5451	1.2016	0.6362	0.036*
C5	0.4709 (2)	1.1970 (3)	0.76725 (18)	0.0307 (5)
H5	0.4540	1.3009	0.7841	0.037*
C6	0.4431 (2)	1.1023 (3)	0.83084 (17)	0.0304 (5)
H6	0.4084	1.1432	0.8908	0.036*
C7	0.4665 (2)	0.9469 (2)	0.80589 (15)	0.0230 (4)
H7	0.4486	0.8844	0.8496	0.028*
C8	0.3692 (2)	0.5830 (2)	0.63280 (14)	0.0200 (4)
H8A	0.3884	0.4765	0.6063	0.024*
H8B	0.3164	0.5821	0.6885	0.024*
C9	0.1356 (2)	0.6899 (2)	0.54283 (14)	0.0172 (4)
C10	0.0700 (2)	0.7613 (2)	0.62427 (15)	0.0214 (4)
H10	0.1098	0.7626	0.6958	0.026*

C11	-0.0566 (2)	0.8293 (3)	0.59197 (16)	0.0244 (4)
H11	-0.1025	0.8795	0.6436	0.029*
C12	-0.1196 (2)	0.8254 (2)	0.48260 (16)	0.0238 (4)
H12	-0.2064	0.8717	0.4643	0.029*
C13	-0.0554 (2)	0.7549 (2)	0.40323 (15)	0.0220 (4)
H13	-0.0968	0.7527	0.3316	0.026*
C14	0.0754 (2)	0.6861 (2)	0.43453 (14)	0.0179 (4)
C15	0.7840 (2)	0.7424 (2)	0.81794 (14)	0.0184 (4)
H15A	0.8037	0.8585	0.8309	0.022*
H15B	0.8360	0.6971	0.7646	0.022*
C16	0.8562 (2)	0.7120 (2)	0.92259 (14)	0.0157 (4)
C17	1.0225 (2)	0.7779 (2)	0.98111 (14)	0.0159 (4)
C18	1.0947 (2)	0.7531 (2)	1.07830 (14)	0.0190 (4)
H18	1.2057	0.7998	1.1157	0.023*
C19	1.0001 (2)	0.6582 (2)	1.11903 (14)	0.0197 (4)
H19	1.0464	0.6388	1.1834	0.024*
C20	0.8346 (2)	0.5930 (2)	1.06155 (14)	0.0176 (4)
C21	0.7616 (2)	0.6186 (2)	0.96475 (14)	0.0173 (4)
H21	0.6501	0.5735	0.9284	0.021*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0188 (2)	0.0214 (3)	0.0219 (2)	0.00319 (19)	0.00663 (19)	0.00705 (19)
C12	0.0264 (3)	0.0283 (3)	0.0226 (2)	0.0087 (2)	0.0116 (2)	0.0132 (2)
O1	0.0155 (7)	0.0245 (7)	0.0166 (6)	0.0027 (5)	-0.0012 (5)	0.0103 (5)
N1	0.0169 (8)	0.0191 (8)	0.0136 (7)	0.0020 (6)	0.0000 (6)	0.0053 (6)
N2	0.0253 (9)	0.0251 (9)	0.0137 (7)	0.0057 (7)	0.0029 (7)	0.0050 (7)
N3	0.0253 (9)	0.0257 (9)	0.0157 (7)	0.0075 (7)	0.0026 (7)	0.0066 (7)
C1	0.0153 (9)	0.0209 (9)	0.0124 (8)	0.0048 (7)	0.0015 (7)	0.0070 (7)
C2	0.0088 (8)	0.0200 (9)	0.0168 (8)	0.0013 (7)	-0.0019 (7)	0.0042 (7)
C3	0.0172 (10)	0.0272 (11)	0.0205 (9)	0.0043 (8)	0.0015 (8)	0.0094 (8)
C4	0.0226 (11)	0.0273 (11)	0.0355 (12)	0.0043 (9)	-0.0021 (9)	0.0160 (9)
C5	0.0179 (10)	0.0170 (10)	0.0434 (12)	0.0060 (8)	-0.0049 (9)	0.0007 (9)
C6	0.0184 (10)	0.0312 (12)	0.0318 (11)	0.0041 (9)	0.0057 (9)	-0.0014 (9)
C7	0.0178 (10)	0.0261 (11)	0.0200 (9)	0.0016 (8)	0.0044 (8)	0.0033 (8)
C8	0.0198 (10)	0.0202 (10)	0.0157 (8)	0.0025 (8)	-0.0020 (7)	0.0074 (7)
C9	0.0144 (9)	0.0175 (9)	0.0155 (8)	-0.0013 (7)	-0.0001 (7)	0.0065 (7)
C10	0.0186 (10)	0.0256 (10)	0.0177 (9)	0.0013 (8)	0.0046 (8)	0.0074 (8)
C11	0.0214 (10)	0.0270 (11)	0.0240 (10)	0.0037 (8)	0.0086 (8)	0.0072 (8)
C12	0.0165 (10)	0.0230 (10)	0.0291 (10)	0.0025 (8)	0.0026 (8)	0.0101 (8)
C13	0.0218 (10)	0.0204 (10)	0.0194 (9)	0.0005 (8)	0.0000 (8)	0.0086 (8)
C14	0.0180 (9)	0.0166 (9)	0.0143 (8)	-0.0011 (7)	0.0005 (7)	0.0049 (7)
C15	0.0169 (9)	0.0193 (10)	0.0159 (8)	0.0033 (8)	0.0010 (7)	0.0055 (7)
C16	0.0169 (9)	0.0148 (9)	0.0132 (8)	0.0068 (7)	0.0029 (7)	0.0013 (7)
C17	0.0157 (9)	0.0156 (9)	0.0184 (8)	0.0064 (7)	0.0070 (7)	0.0056 (7)
C18	0.0132 (9)	0.0241 (10)	0.0155 (8)	0.0065 (8)	0.0003 (7)	0.0024 (7)
C19	0.0210 (10)	0.0270 (10)	0.0135 (8)	0.0124 (8)	0.0050 (7)	0.0072 (8)

C20	0.0188 (9)	0.0200 (9)	0.0162 (8)	0.0069 (8)	0.0079 (7)	0.0060 (7)
C21	0.0142 (9)	0.0188 (9)	0.0158 (8)	0.0052 (7)	0.0018 (7)	0.0032 (7)

Geometric parameters (Å, °)

C11—C17	1.7518 (19)	C8—H8B	0.9700
C12—C20	1.7514 (19)	C9—C10	1.404 (3)
O1—C1	1.432 (2)	C10—C11	1.374 (3)
O1—C15	1.422 (2)	C10—H10	0.9300
N1—N2	1.363 (2)	C11—H11	0.9300
N1—C8	1.456 (2)	C12—C11	1.418 (3)
N1—C9	1.366 (2)	C12—H12	0.9300
N3—N2	1.314 (2)	C13—C12	1.372 (3)
N3—C14	1.383 (2)	C13—C14	1.405 (3)
C1—C8	1.530 (3)	C13—H13	0.9300
C1—H1	0.9800	C14—C9	1.403 (2)
C2—C1	1.517 (3)	C15—H15A	0.9700
C2—C3	1.392 (3)	C15—H15B	0.9700
C2—C7	1.395 (3)	C16—C15	1.501 (2)
C3—C4	1.395 (3)	C16—C17	1.395 (3)
C3—H3	0.9300	C18—C17	1.390 (3)
C4—H4	0.9300	C18—H18	0.9300
C5—C4	1.388 (3)	C19—C18	1.385 (3)
C5—H5	0.9300	C19—C20	1.386 (3)
C6—C5	1.381 (3)	C19—H19	0.9300
C6—H6	0.9300	C21—C16	1.391 (3)
C7—C6	1.385 (3)	C21—C20	1.390 (2)
C7—H7	0.9300	C21—H21	0.9300
C8—H8A	0.9700		
C15—O1—C1	111.82 (13)	C9—C10—H10	122.0
N2—N1—C8	120.18 (15)	C11—C10—C9	115.98 (17)
N2—N1—C9	110.27 (14)	C11—C10—H10	122.0
C9—N1—C8	129.53 (15)	C10—C11—C12	122.25 (19)
N3—N2—N1	108.69 (15)	C10—C11—H11	118.9
N2—N3—C14	108.37 (15)	C12—C11—H11	118.9
O1—C1—C2	112.30 (14)	C11—C12—H12	119.2
O1—C1—C8	103.20 (14)	C13—C12—C11	121.54 (19)
O1—C1—H1	109.3	C13—C12—H12	119.2
C2—C1—C8	113.11 (15)	C12—C13—C14	117.29 (17)
C2—C1—H1	109.3	C12—C13—H13	121.4
C8—C1—H1	109.3	C14—C13—H13	121.4
C3—C2—C1	120.21 (16)	N3—C14—C9	108.34 (16)
C3—C2—C7	119.01 (18)	N3—C14—C13	131.14 (17)
C7—C2—C1	120.75 (16)	C9—C14—C13	120.51 (17)
C2—C3—C4	120.57 (19)	O1—C15—C16	109.65 (14)
C2—C3—H3	119.7	O1—C15—H15A	109.7
C4—C3—H3	119.7	O1—C15—H15B	109.7

C3—C4—H4	120.2	C16—C15—H15A	109.7
C5—C4—C3	119.61 (19)	C16—C15—H15B	109.7
C5—C4—H4	120.2	H15A—C15—H15B	108.2
C4—C5—H5	120.0	C17—C16—C15	120.42 (16)
C6—C5—C4	120.05 (19)	C21—C16—C15	121.89 (16)
C6—C5—H5	120.0	C21—C16—C17	117.70 (16)
C5—C6—C7	120.41 (19)	C16—C17—C11	118.97 (14)
C5—C6—H6	119.8	C18—C17—C11	118.58 (14)
C7—C6—H6	119.8	C18—C17—C16	122.45 (17)
C2—C7—H7	119.8	C17—C18—H18	120.3
C6—C7—C2	120.33 (19)	C19—C18—C17	119.48 (17)
C6—C7—H7	119.8	C19—C18—H18	120.3
N1—C8—C1	112.73 (15)	C18—C19—C20	118.36 (16)
N1—C8—H8A	109.0	C18—C19—H19	120.8
N1—C8—H8B	109.0	C20—C19—H19	120.8
C1—C8—H8A	109.0	C19—C20—C12	119.43 (14)
C1—C8—H8B	109.0	C19—C20—C21	122.33 (17)
H8A—C8—H8B	107.8	C21—C20—C12	118.22 (14)
N1—C9—C10	133.25 (16)	C16—C21—H21	120.2
N1—C9—C14	104.33 (16)	C20—C21—C16	119.67 (17)
C14—C9—C10	122.42 (18)	C20—C21—H21	120.2
C15—O1—C1—C2	-74.67 (18)	C2—C7—C6—C5	-0.7 (3)
C15—O1—C1—C8	163.19 (14)	N1—C9—C10—C11	179.31 (19)
C1—O1—C15—C16	173.24 (14)	C14—C9—C10—C11	-0.6 (3)
C8—N1—N2—N3	-179.18 (16)	C9—C10—C11—C12	1.1 (3)
C9—N1—N2—N3	-0.7 (2)	C13—C12—C11—C10	-0.9 (3)
N2—N1—C8—C1	81.4 (2)	C14—C13—C12—C11	0.1 (3)
C9—N1—C8—C1	-96.7 (2)	C12—C13—C14—N3	-179.28 (19)
N2—N1—C9—C10	-179.3 (2)	C12—C13—C14—C9	0.4 (3)
N2—N1—C9—C14	0.61 (19)	N3—C14—C9—N1	-0.3 (2)
C8—N1—C9—C10	-1.0 (3)	N3—C14—C9—C10	179.59 (17)
C8—N1—C9—C14	178.92 (17)	C13—C14—C9—N1	179.96 (17)
C14—N3—N2—N1	0.5 (2)	C13—C14—C9—C10	-0.1 (3)
N2—N3—C14—C9	-0.1 (2)	C17—C16—C15—O1	-177.33 (15)
N2—N3—C14—C13	179.59 (19)	C21—C16—C15—O1	2.6 (2)
O1—C1—C8—N1	173.19 (14)	C15—C16—C17—C11	0.5 (2)
C2—C1—C8—N1	51.6 (2)	C15—C16—C17—C18	179.99 (17)
C3—C2—C1—O1	139.00 (17)	C21—C16—C17—C11	-179.40 (13)
C3—C2—C1—C8	-104.68 (19)	C21—C16—C17—C18	0.1 (3)
C7—C2—C1—O1	-43.0 (2)	C19—C18—C17—C11	-179.81 (14)
C7—C2—C1—C8	73.4 (2)	C19—C18—C17—C16	0.7 (3)
C1—C2—C3—C4	177.58 (17)	C20—C19—C18—C17	-1.0 (3)
C7—C2—C3—C4	-0.5 (3)	C18—C19—C20—C12	178.73 (14)
C1—C2—C7—C6	-176.83 (17)	C18—C19—C20—C21	0.5 (3)
C3—C2—C7—C6	1.2 (3)	C20—C21—C16—C15	179.49 (16)
C2—C3—C4—C5	-0.8 (3)	C20—C21—C16—C17	-0.6 (3)
C6—C5—C4—C3	1.3 (3)	C16—C21—C20—C12	-177.96 (13)

C7—C6—C5—C4	-0.6 (3)	C16—C21—C20—C19	0.3 (3)
-------------	----------	-----------------	---------

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the C2–C7 ring.

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C19—H19 \cdots N3 ⁱ	0.93	2.62	3.549 (2)	174
C18—H18 \cdots Cg1 ⁱⁱ	0.93	2.69	3.605 (2)	168

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