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2-(1*H*-Benzotriazol-1-yl)-1-phenylethanol

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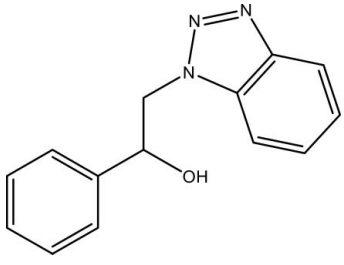
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.045; wR factor = 0.105; data-to-parameter ratio = 12.9.

In the title compound, $C_{14}H_{13}N_3O$, the benzotriazole ring is oriented at a dihedral angle of 13.43 (4)° with respect to the phenyl ring. In the crystal structure, intermolecular O—H···N hydrogen bonds link the molecules into chains along the b axis. Aromatic π–π contacts between benzene rings and between triazole and benzene rings [centroid–centroid distances = 3.8133 (8) and 3.7810 (8) Å, respectively], as well as a weak C—H···π interaction involving the phenyl ring, are also observed.

Related literature

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



Experimental

Crystal data

$C_{14}H_{13}N_3O$
M_r = 239.27
Orthorhombic, *Pbca*
a = 11.0731 (3) Å
b = 8.6571 (2) Å
c = 25.3436 (7) Å
V = 2429.5 (1) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 120 K
0.40 × 0.30 × 0.20 mm

Data collection

Nonius Kappa CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.968, T_{max} = 0.981
11997 measured reflections
2772 independent reflections
2447 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.105
S = 1.06
2772 reflections
215 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.85 (2)	1.92 (2)	2.766 (2)	170 (2)
C11—H11···$Cg3^{i}$	1.01 (2)	2.94 (2)	3.850 (2)	151 (1)

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2186).

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.
Hirokawa, Y., Yamazaki, H., Yoshida, N. & Kato, S. (1998). *Bioorg. Med. Chem. Lett.* **8**, 1973–1978.
Katritzky, A. R., Zhang, S., Kurz, T., Wang, M. & Steel, P. J. (2001). *Org. Lett.* **3**, 2807–2809.
Kopańska, K., Najda, A., Żebrowska, J., Chomicz, L., Piekarczyk, J., Myjak, P. & Bretner, M. (2004). *Bioorg. Med. Chem.* **12**, 2317–2624.
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., Tahtacı, H., Coles, S. J. & Hökelek, T. (2008). *Acta Cryst.* E**64**, o1254.
Sheldrick, G. M. (2007). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 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.

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2-(1*H*-Benzotriazol-1-yl)-1-phenylethanol

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S1. Comment

Azole compounds have important antifungal and antibacterial activities. Benzotriazole derivatives also exhibit a good degree of analgesic, anti-inflammatory, diuretic, antiviral and antihypertensive activities (Kopańska *et al.*, 2004; Yu *et al.*, 2003; Hirokawa *et al.*, 1998). Crystal structures of similar compounds such as 1-phenyl-2-(1*H*-1,2,4-triazol-1-yl)ethanol (Özel Güven *et al.*, 2008), fluconazole (Caira *et al.*, 2004) and benzotriazole ring possessing compounds (Katritzky *et al.*, 2001; Swamy *et al.*, 2006) have been reported. Now, we report herein the crystal structure of the title benzotriazole derivative, (I).

In the molecule of the title compound (Fig. 1), bond lengths and angles are generally within normal ranges. The planar benzotriazole ring system is oriented with respect to the phenyl ring at a dihedral angle of 13.43 (4)°. Exocyclic carbon atoms C7 and C8 are 0.062 (1) and -0.028 (1) Å away from the planes of the benzotriazole and phenyl rings, respectively. So, they are almost coplanar with the adjacent rings.

In the crystal structure, intermolecular O-H···N hydrogen bonds (Table 1) link the molecules into chains along the *b*-axis (Fig. 2), in which they may be effective in the stabilization of the structure. The π–π contacts between the benzene rings and between the triazole and the benzene rings , Cg2—Cg2^{i} and Cg1—Cg2^{i} [symmetry code: (i) 1 - x, 1 - y, -z, where Cg1 and Cg2 are centroids of the rings (C1/C6/N1-N3) and (C1-C6), respectively] with centroid-centroid distances of 3.8133 (8) and 3.7810 (8) Å are also observed in the crystal structure. respectively. A weak C—H···π interaction (Table 1) involving the phenyl ring also occurs.

S2. Experimental

The title compound was synthesized by the reduction of 2-(-benzotriazol-1-yl)-1-phenylethanone with sodiumborohydride. A mixture of 2-(-benzotriazol-1-yl)-1-phenylethanone (500 mg, 2.10 mmol) and sodiumborohydride (159.5 mg, 4.21 mmol) in ethanol (25 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 ethyl acetate to obtain colorless crystals suitable for X-ray analysis (yield; 216 mg, 43%).

S3. Refinement

H atoms were located in a difference Fourier map and refined isotropically.

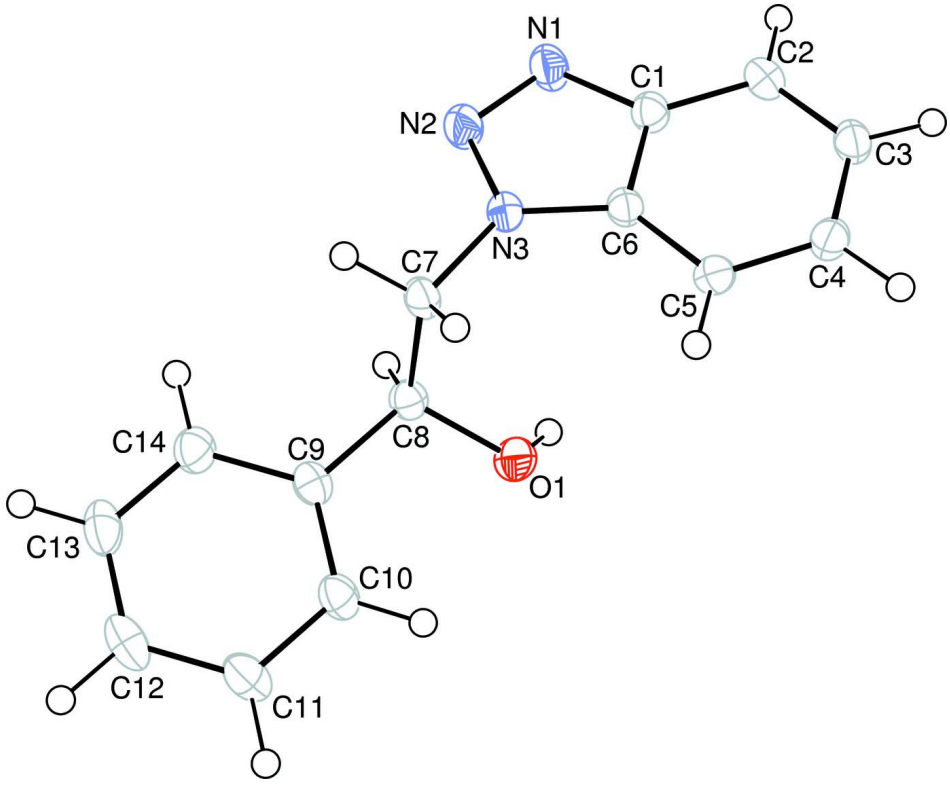

Figure 1

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

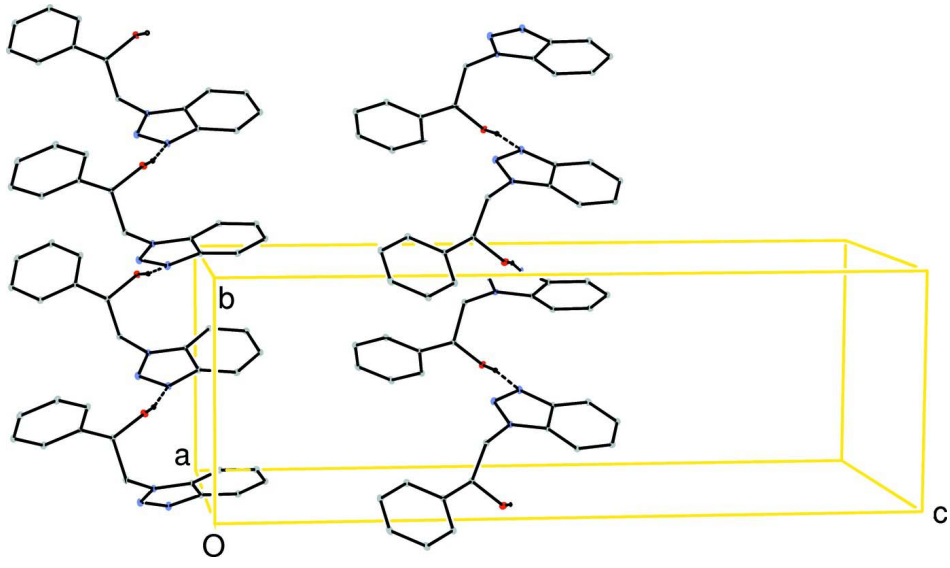

Figure 2

A partial packing diagram. Hydrogen bonds are shown as dashed lines.

2-(1*H*-Benzotriazol-1-yl)-1-phenylethanol

Crystal data

$C_{14}H_{13}N_3O$
$M_r = 239.27$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 11.0731$ (3) Å
$b = 8.6571$ (2) Å
$c = 25.3436$ (7) Å
$V = 2429.5$ (1) Å^3
$Z = 8$
$F(000) = 1008$
$D_x = 1.308$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 13033 reflections
$\theta = 2.9$–$27.5°$
$\mu = 0.09$ mm^{-1}
$T = 120$ K
Block, colorless
0.40 × 0.30 × 0.20 mm

Data collection

Nonius Kappa CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
$T_{min} = 0.968$, $T_{max} = 0.981$
11997 measured reflections
2772 independent reflections
2447 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -14 \rightarrow 14$
$k = -10 \rightarrow 11$
$l = -32 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.105$
$S = 1.06$
2772 reflections
215 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0259P)^2 + 1.6489P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.02061 (10)	0.04949 (12)	0.40376 (4)	0.0279 (2)
H1	0.090 (2)	0.038 (2)	0.4178 (9)	0.054 (6)*
N1	0.25101 (12)	0.48299 (16)	0.44171 (5)	0.0300 (3)
N2	0.18457 (11)	0.44939 (15)	0.40068 (5)	0.0295 (3)
N3	0.08582 (11)	0.37136 (13)	0.41711 (4)	0.0222 (3)

C1	0.19546 (12)	0.42532 (16)	0.48602 (5)	0.0224 (3)
C2	0.22997 (13)	0.43162 (17)	0.53950 (5)	0.0240 (3)
H2	0.3052 (16)	0.479 (2)	0.5494 (7)	0.029 (4)*
C3	0.15335 (14)	0.36306 (17)	0.57508 (5)	0.0253 (3)
H3	0.1736 (15)	0.3631 (19)	0.6119 (7)	0.030 (4)*
C4	0.04479 (14)	0.29030 (16)	0.55904 (6)	0.0255 (3)
H4	−0.0089 (16)	0.240 (2)	0.5866 (8)	0.036 (5)*
C5	0.01041 (13)	0.28261 (16)	0.50680 (6)	0.0228 (3)
H5	−0.0631 (15)	0.232 (2)	0.4957 (7)	0.028 (4)*
C6	0.08867 (12)	0.35214 (15)	0.47059 (5)	0.0199 (3)
C7	0.00031 (13)	0.31427 (16)	0.37785 (5)	0.0229 (3)
H71	−0.0807 (15)	0.3138 (18)	0.3945 (6)	0.022 (4)*
H72	0.0019 (15)	0.388 (2)	0.3473 (7)	0.028 (4)*
C8	0.03379 (12)	0.15050 (16)	0.36022 (5)	0.0216 (3)
H8	0.1203 (14)	0.1535 (17)	0.3473 (6)	0.021 (4)*
C9	−0.04730 (12)	0.09913 (16)	0.31533 (5)	0.0214 (3)
C10	−0.13758 (13)	−0.00987 (17)	0.32359 (5)	0.0248 (3)
H10	−0.1479 (15)	−0.0567 (19)	0.3588 (7)	0.032 (4)*
C11	−0.21348 (14)	−0.05425 (19)	0.28253 (6)	0.0303 (3)
H11	−0.2784 (17)	−0.134 (2)	0.2882 (7)	0.039 (5)*
C12	−0.19924 (15)	0.00902 (19)	0.23260 (6)	0.0317 (3)
H12	−0.2518 (18)	−0.023 (2)	0.2038 (8)	0.043 (5)*
C13	−0.10914 (15)	0.11692 (19)	0.22396 (6)	0.0318 (3)
H13	−0.0995 (17)	0.162 (2)	0.1892 (8)	0.041 (5)*
C14	−0.03327 (14)	0.16238 (17)	0.26496 (6)	0.0270 (3)
H14	0.0301 (16)	0.238 (2)	0.2584 (7)	0.032 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0291 (6)	0.0264 (5)	0.0282 (5)	−0.0010 (4)	−0.0097 (4)	0.0070 (4)
N1	0.0289 (6)	0.0409 (7)	0.0201 (6)	−0.0107 (5)	0.0015 (5)	−0.0021 (5)
N2	0.0311 (6)	0.0367 (7)	0.0206 (6)	−0.0111 (6)	0.0016 (5)	0.0001 (5)
N3	0.0250 (6)	0.0238 (6)	0.0176 (5)	−0.0032 (5)	−0.0009 (4)	0.0004 (4)
C1	0.0222 (6)	0.0248 (7)	0.0202 (6)	−0.0007 (5)	0.0013 (5)	−0.0008 (5)
C2	0.0235 (7)	0.0265 (7)	0.0221 (7)	0.0007 (6)	−0.0024 (5)	−0.0037 (5)
C3	0.0339 (8)	0.0237 (7)	0.0184 (6)	0.0030 (6)	−0.0022 (6)	−0.0002 (5)
C4	0.0332 (8)	0.0219 (7)	0.0213 (7)	−0.0005 (6)	0.0047 (6)	0.0012 (5)
C5	0.0245 (7)	0.0213 (7)	0.0227 (7)	−0.0025 (5)	0.0015 (5)	−0.0003 (5)
C6	0.0227 (6)	0.0191 (6)	0.0178 (6)	0.0017 (5)	−0.0009 (5)	−0.0002 (5)
C7	0.0269 (7)	0.0240 (7)	0.0178 (6)	0.0001 (5)	−0.0051 (5)	−0.0004 (5)
C8	0.0205 (6)	0.0232 (7)	0.0212 (6)	0.0001 (5)	−0.0013 (5)	−0.0002 (5)
C9	0.0212 (6)	0.0233 (7)	0.0197 (6)	0.0048 (5)	0.0004 (5)	−0.0042 (5)
C10	0.0239 (7)	0.0307 (7)	0.0197 (6)	0.0000 (6)	0.0014 (5)	−0.0046 (6)
C11	0.0269 (7)	0.0376 (8)	0.0263 (7)	−0.0032 (6)	−0.0011 (6)	−0.0098 (6)
C12	0.0322 (8)	0.0401 (9)	0.0227 (7)	0.0071 (7)	−0.0065 (6)	−0.0109 (6)
C13	0.0439 (9)	0.0340 (8)	0.0176 (7)	0.0078 (7)	−0.0013 (6)	−0.0024 (6)
C14	0.0317 (8)	0.0274 (7)	0.0218 (7)	0.0015 (6)	0.0033 (6)	−0.0016 (6)

Geometric parameters (Å, º)

O1—C8	1.4154 (17)	C7—H71	0.992 (17)
O1—H1	0.86 (2)	C7—H72	1.003 (17)
N1—C1	1.3743 (18)	C8—C7	1.5320 (19)
N2—N1	1.3067 (17)	C8—C9	1.5161 (18)
N3—N2	1.3511 (16)	C8—H8	1.012 (16)
N3—C6	1.3659 (16)	C9—C10	1.390 (2)
N3—C7	1.4597 (17)	C9—C14	1.3978 (19)
C1—C2	1.4091 (18)	C10—C11	1.392 (2)
C2—H2	0.962 (18)	C10—H10	0.986 (18)
C3—C2	1.373 (2)	C11—H11	1.005 (19)
C3—H3	0.960 (17)	C12—C13	1.384 (2)
C4—C3	1.417 (2)	C12—C11	1.388 (2)
C4—C5	1.3793 (19)	C12—H12	0.98 (2)
C4—H4	1.014 (19)	C13—H13	0.97 (2)
C5—H5	0.965 (17)	C14—C13	1.393 (2)
C6—C1	1.3974 (19)	C14—H14	0.972 (18)
C6—C5	1.3983 (19)		
C8—O1—H1	107.8 (15)	C8—C7—H71	109.9 (9)
N2—N1—C1	108.51 (12)	C8—C7—H72	111.1 (10)
N1—N2—N3	108.76 (11)	H71—C7—H72	110.3 (13)
N2—N3—C6	110.37 (11)	O1—C8—C7	108.63 (11)
N2—N3—C7	118.95 (11)	O1—C8—C9	110.04 (11)
C6—N3—C7	130.55 (12)	O1—C8—H8	111.5 (9)
N1—C1—C2	130.58 (13)	C9—C8—C7	110.30 (11)
N1—C1—C6	108.35 (12)	C9—C8—H8	108.9 (9)
C6—C1—C2	121.07 (13)	C7—C8—H8	107.4 (9)
C1—C2—H2	120.1 (10)	C10—C9—C8	120.79 (12)
C3—C2—C1	116.58 (13)	C10—C9—C14	118.89 (13)
C3—C2—H2	123.2 (10)	C14—C9—C8	120.31 (13)
C2—C3—C4	121.87 (13)	C9—C10—C11	120.60 (14)
C2—C3—H3	119.6 (10)	C9—C10—H10	119.9 (10)
C4—C3—H3	118.5 (10)	C11—C10—H10	119.5 (10)
C3—C4—H4	119.4 (11)	C10—C11—H11	120.9 (11)
C5—C4—C3	122.08 (13)	C12—C11—C10	120.28 (15)
C5—C4—H4	118.5 (11)	C12—C11—H11	118.8 (10)
C4—C5—C6	115.99 (13)	C11—C12—H12	120.1 (12)
C4—C5—H5	122.4 (10)	C13—C12—C11	119.50 (14)
C6—C5—H5	121.6 (10)	C13—C12—H12	120.4 (12)
N3—C6—C1	104.01 (12)	C12—C13—C14	120.49 (14)
N3—C6—C5	133.57 (13)	C12—C13—H13	119.5 (11)
C1—C6—C5	122.41 (12)	C14—C13—H13	120.0 (12)
N3—C7—C8	110.81 (11)	C9—C14—H14	120.0 (11)
N3—C7—H71	107.3 (9)	C13—C14—C9	120.24 (14)
N3—C7—H72	107.4 (10)	C13—C14—H14	119.8 (11)

N2—N1—C1—C2	−179.62 (15)	C5—C6—C1—N1	−179.32 (13)
N2—N1—C1—C6	0.05 (17)	C5—C6—C1—C2	0.4 (2)
N3—N2—N1—C1	0.35 (17)	N3—C6—C5—C4	−178.54 (14)
C6—N3—N2—N1	−0.64 (16)	C1—C6—C5—C4	0.0 (2)
C7—N3—N2—N1	−177.00 (12)	O1—C8—C7—N3	65.40 (14)
N2—N3—C6—C1	0.64 (15)	C9—C8—C7—N3	−173.92 (11)
N2—N3—C6—C5	179.36 (15)	O1—C8—C9—C10	13.06 (17)
N2—N3—C7—C8	90.35 (15)	O1—C8—C9—C14	−167.73 (12)
C6—N3—C7—C8	−85.16 (17)	C7—C8—C9—C10	−106.78 (15)
C7—N3—C6—C1	176.45 (13)	C7—C8—C9—C14	72.44 (16)
C7—N3—C6—C5	−4.8 (3)	C8—C9—C10—C11	178.62 (13)
N1—C1—C2—C3	179.42 (15)	C14—C9—C10—C11	−0.6 (2)
C6—C1—C2—C3	−0.2 (2)	C8—C9—C14—C13	−178.95 (13)
C4—C3—C2—C1	−0.3 (2)	C10—C9—C14—C13	0.3 (2)
C5—C4—C3—C2	0.7 (2)	C9—C10—C11—C12	0.5 (2)
C3—C4—C5—C6	−0.5 (2)	C13—C12—C11—C10	−0.2 (2)
N3—C6—C1—N1	−0.42 (15)	C11—C12—C13—C14	−0.2 (2)
N3—C6—C1—C2	179.29 (13)	C9—C14—C13—C12	0.1 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.85 (2)	1.92 (2)	2.766 (2)	170 (2)
C11—H11···*Cg*3^{i}	1.01 (2)	2.94 (2)	3.850 (2)	151 (1)

Symmetry code: (i) *x*, −*y*−3/2, *z*−1/2.