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2-[(1*H*-Benzimidazol-1-yl)methyl]phenol benzene hemisolvateAugusto Rivera,^{a*} Leonardo Jiménez-Cruz^a and Michael Bolte^b

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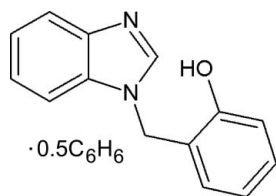
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.040; wR factor = 0.108; data-to-parameter ratio = 14.0.

In the title solvate, $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O} \cdot 0.5\text{C}_6\text{H}_6$, the complete benzene molecule is generated by a crystallographic inversion centre. The dihedral angle between the planes of the benzimidazole moiety and the phenol substituent is $75.28(3)^\circ$. In the crystal, $\text{O}-\text{H} \cdots \text{N}$ hydrogen bonds link the molecules into parallel chains propagating along [100]. The molecules are further connected by $\text{C}-\text{H} \cdots \pi$ interactions.

Related literature

For related structures, see: Cai *et al.* (2006); Rivera *et al.* (2012); Shi *et al.* (2011). For another synthesis procedure, see: Milata *et al.* (2001); Rivera *et al.* (2008). For the pharmacological use of benzimidazoles, see: Alamgir *et al.* (2007). For $\text{C}-\text{H} \cdots \pi$ interactions, see: Malathy Sony & Ponnuswamy (2005).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{12}\text{N}_2\text{O} \cdot 0.5\text{C}_6\text{H}_6$
 $M_r = 263.31$
Triclinic, $P\bar{1}$
 $a = 8.9351(11)$ Å
 $b = 9.3268(10)$ Å

$c = 9.9579(11)$ Å
 $\alpha = 73.098(8)^\circ$
 $\beta = 69.124(8)^\circ$
 $\gamma = 62.148(8)^\circ$
 $V = 677.75(15)$ Å³

$Z = 2$
Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹

$T = 173$ K
 $0.42 \times 0.12 \times 0.12$ mm

Data collection

Stoe IPDS II two-circle diffractometer
Absorption correction: multi-scan (*X-AREA*; Stoe & Cie, 2001)
 $T_{\text{min}} = 0.967$, $T_{\text{max}} = 0.990$

8981 measured reflections
2591 independent reflections
2314 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.043$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.108$
 $S = 1.12$
2591 reflections
185 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.20$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.17$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C2–C7 ring.

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{O1}-\text{H1} \cdots \text{N2}^i$	0.98 (2)	1.74 (2)	2.7200 (16)	174 (2)
$\text{C22}-\text{H22} \cdots \text{Cg1}$	0.95	3.25	3.868	124

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SJ5381).

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supporting information

Acta Cryst. (2014). E70, o177 [doi:10.1107/S1600536814000841]

2-[(1*H*-Benzimidazol-1-yl)methyl]phenol benzene hemisolvate

Augusto Rivera, Leonardo Jiménez-Cruz and Michael Bolte

S1. Introduction

Appropriately substituted benzimidazole derivatives have found diverse therapeutic applications as antiulcer, anti-hypertensive, antiviral, antifungal, anticancer, and antihistaminic agents [Alamgir *et al.* 2007]. Although the synthesis of the title compound has been reported in the literature (Milata *et al.*, 2001; Rivera *et al.*, 2008), we have developed an alternative route to prepare this compound starting from *N*¹,*N*²-bis((1*H*-benzotriazol-1-yl)methyl)benzene-1,2-diamine.

The asymmetric unit contains one molecule of 2-((1*H*-benzimidazol-1-yl)methyl)phenol and half a molecule of benzene (Fig. 1). The solvent molecule subtends a dihedral angle of 78.90 (6)° with respect to the phenol substituent and 70.99 (6)° with respect to the benzimidazole moiety, which suggest an edge-to-face (T-shaped) C—H⋯ π interaction according to the literature (Malathy Sony *et al.* 2005). The dihedral angle between the phenol substituent and the benzimidazole ring [75.28 (3)°] is similar to the one in a related structure (Cai *et al.*, 2006). In the benzimidazole moiety, the bond distances and angles are in good agreement with those found in bis(1*H*-benzimidazol-1-yl)methane monohydrate (Shi *et al.*, 2011), 1-(6-chloropyridin-3-ylmethyl)-1*H*-benzimidazole (Cai *et al.*, 2006) and (1*H*-benzimidazol-1-yl)methanol (Rivera *et al.*, 2012).

An intermolecular hydrogen bond was observed in the crystal packing (Fig. 2) between the hydroxyl group of one molecule and a nitrogen atom of another one (Table 1). The O—H distance is longer than in (1*H*-benzimidazol-1-yl)methanol [0.894 (19)Å] (Rivera *et al.*, 2012). However, the O⋯N distance [2.7200 (16)Å and 2.7355 (16)Å] and the O—H⋯N angle [174 (2)°, 173.8 (17)°] are similar in both structures. The O—H⋯N hydrogen bond connects the molecules forming chains running along the *a*-axis. The benzene molecule is linked to molecules of 2-((1*H*-benzimidazol-1-yl)methyl)phenol via C—H⋯ π interactions (Fig. 3) acting as both a donor and an acceptor, Table 1. The benzimidazole moiety also forms two C—H⋯ π interactions to the phenol rings of neighbouring molecules. These values are similar to the values reported for other C—H⋯ π interactions (Malathy Sony *et al.* 2005).

S2. Experimental

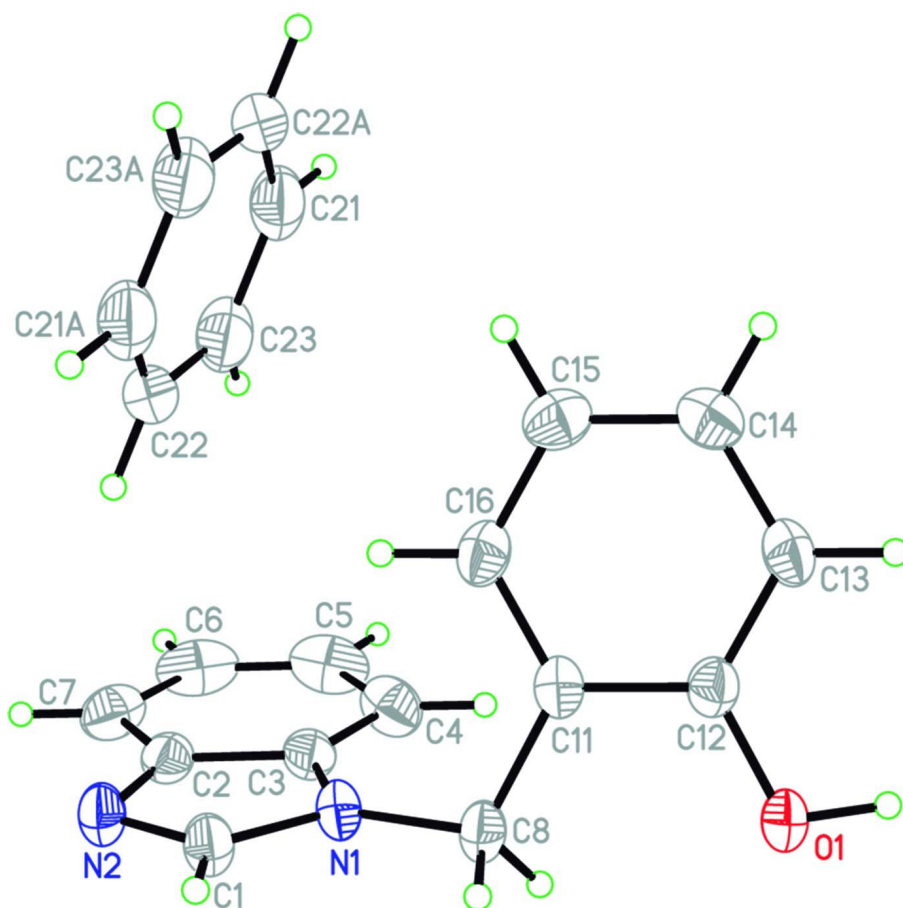
S2.1. Synthesis and crystallization

A mixture of phenol (0.282 g, 3.00 mmol) and *N*¹,*N*²-bis((1*H*-benzotriazol-1-yl)methyl)benzene-1,2-diamine (0.370 g, 1.00 mmol) was heated to 160 °C, after 5 minutes the mixture was cooled at room temperature until a sticky residue appeared. The product was purified by column chromatography using a mixture of benzene: ethyl acetate (80:20) as the mobile phase (yield 25 %, m.p.= 489-490 K). Single crystals were grown from a benzene:ethyl acetate solution by slow evaporation of the solvent at room temperature over a period of about one week.

S2.2. Refinement

All H atoms were located in a difference map. The hydroxyl H atom was freely refined. H atoms bonded to C atoms were refined using a riding model, with secondary C—H = 0.99 Å and aromatic C—H = 0.95 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

S3. Results and discussion

**Figure 1**

A view of the crystal structure of the title compound with the numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

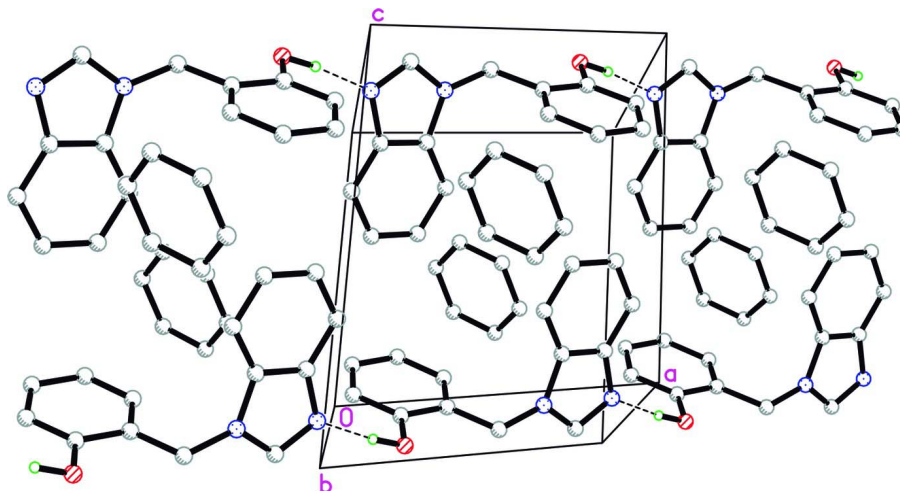


Figure 2

Packing of the molecules of the title compound viewed along the *b* axis. H atoms bonded to C atoms are omitted for clarity. O—H···N hydrogen bonds are drawn as dashed lines.

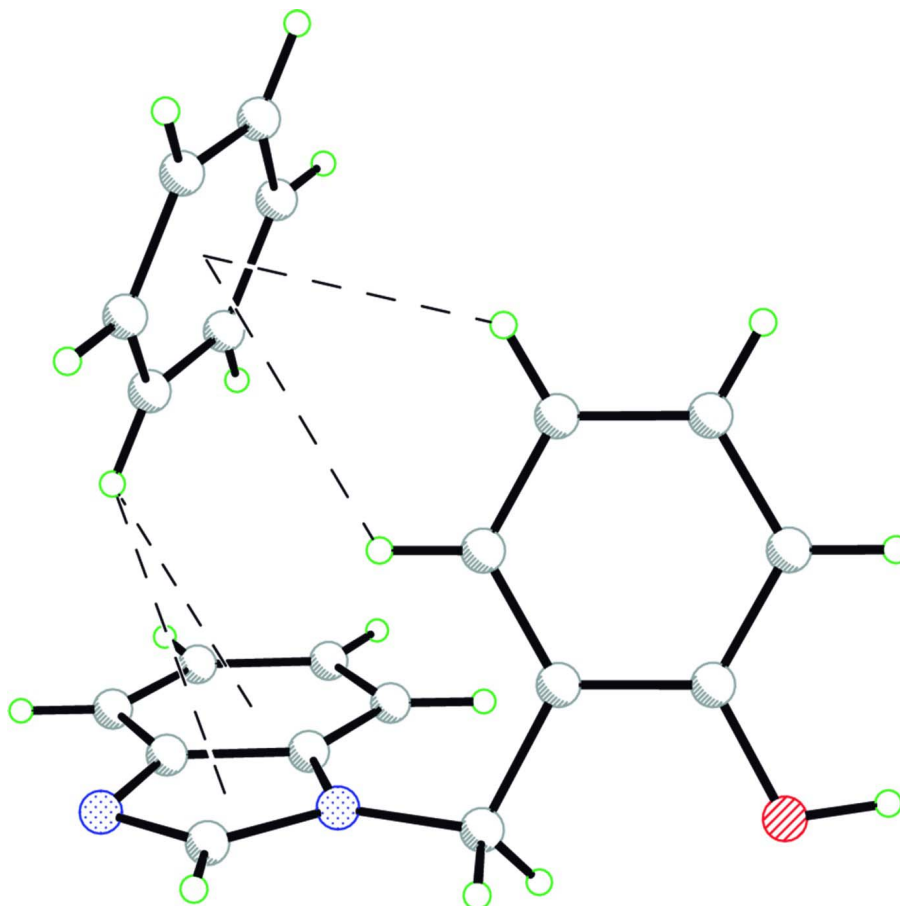


Figure 3

C—H··· π interactions between 2-((1*H*-benzimidazol-1-yl)methyl)phenol and the benzene molecule.

2-[(1*H*-Benzimidazol-1-yl)methyl]phenol benzene hemisolvate*Crystal data*C₁₄H₁₂N₂O·0.5C₆H₆ $M_r = 263.31$ Triclinic, $P\bar{1}$ $a = 8.9351$ (11) Å $b = 9.3268$ (10) Å $c = 9.9579$ (11) Å $\alpha = 73.098$ (8)° $\beta = 69.124$ (8)° $\gamma = 62.148$ (8)° $V = 677.75$ (15) Å³ $Z = 2$ $F(000) = 278$ $D_x = 1.290$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 14234 reflections

 $\theta = 3.6$ – 26.3 ° $\mu = 0.08$ mm⁻¹ $T = 173$ K

Needle, light brown

 $0.42 \times 0.12 \times 0.12$ mm*Data collection*Stoe IPDS II two-circle
diffractometerRadiation source: Genix 3D I μ S microfocus X-
ray source ω scansAbsorption correction: multi-scan
(*X-AREA*; Stoe & Cie, 2001) $T_{\min} = 0.967$, $T_{\max} = 0.990$

8981 measured reflections

2591 independent reflections

2314 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.043$ $\theta_{\max} = 25.9$ °, $\theta_{\min} = 3.9$ ° $h = -10 \rightarrow 10$ $k = -11 \rightarrow 11$ $l = -12 \rightarrow 12$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.040$ $wR(F^2) = 0.108$ $S = 1.12$

2591 reflections

185 parameters

0 restraints

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 0.238P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.20$ e Å⁻³ $\Delta\rho_{\min} = -0.17$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.26163 (13)	0.72436 (14)	0.00166 (12)	0.0358 (3)
H1	0.155 (3)	0.706 (3)	0.023 (2)	0.064 (6)*
N1	0.72313 (15)	0.66159 (14)	0.07264 (13)	0.0272 (3)
N2	0.96889 (15)	0.66557 (15)	0.07838 (14)	0.0323 (3)
C1	0.84911 (18)	0.71998 (18)	0.00788 (16)	0.0298 (3)
H1A	0.8506	0.7939	-0.0809	0.036*
C2	0.91796 (18)	0.56313 (17)	0.20031 (15)	0.0286 (3)
C3	0.76391 (18)	0.55998 (16)	0.19817 (15)	0.0274 (3)
C4	0.6810 (2)	0.46847 (19)	0.30695 (17)	0.0383 (4)
H4	0.5766	0.4670	0.3040	0.046*

C5	0.7585 (3)	0.3802 (2)	0.41906 (19)	0.0478 (4)
H5	0.7057	0.3167	0.4963	0.057*
C6	0.9130 (3)	0.3812 (2)	0.42267 (18)	0.0487 (5)
H6	0.9627	0.3176	0.5018	0.058*
C7	0.9953 (2)	0.47195 (19)	0.31466 (18)	0.0397 (4)
H7	1.1000	0.4723	0.3180	0.048*
C8	0.57443 (18)	0.69824 (19)	0.02012 (16)	0.0313 (3)
H8A	0.5715	0.5940	0.0184	0.038*
H8B	0.5908	0.7566	-0.0808	0.038*
C11	0.40093 (17)	0.80188 (16)	0.11250 (15)	0.0270 (3)
C12	0.24639 (18)	0.80968 (17)	0.09924 (15)	0.0274 (3)
C13	0.08497 (18)	0.90253 (18)	0.18424 (16)	0.0322 (3)
H13	-0.0200	0.9101	0.1733	0.039*
C14	0.0764 (2)	0.98409 (18)	0.28484 (16)	0.0341 (3)
H14	-0.0341	1.0448	0.3444	0.041*
C15	0.2284 (2)	0.97727 (18)	0.29875 (16)	0.0344 (3)
H15	0.2228	1.0335	0.3673	0.041*
C16	0.38896 (19)	0.88763 (17)	0.21170 (16)	0.0309 (3)
H16	0.4930	0.8848	0.2201	0.037*
C21	0.4166 (2)	0.9279 (2)	0.62694 (19)	0.0456 (4)
H21	0.3596	0.8781	0.7143	0.055*
C22	0.6494 (2)	0.9049 (2)	0.4094 (2)	0.0455 (4)
H22	0.7529	0.8387	0.3470	0.055*
C23	0.5668 (2)	0.8322 (2)	0.5354 (2)	0.0474 (4)
H23	0.6131	0.7161	0.5595	0.057*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0247 (5)	0.0495 (7)	0.0431 (6)	-0.0190 (5)	-0.0056 (4)	-0.0181 (5)
N1	0.0209 (6)	0.0305 (6)	0.0328 (6)	-0.0121 (5)	-0.0084 (5)	-0.0038 (5)
N2	0.0243 (6)	0.0380 (7)	0.0398 (7)	-0.0148 (5)	-0.0091 (5)	-0.0084 (5)
C1	0.0265 (7)	0.0340 (7)	0.0320 (7)	-0.0160 (6)	-0.0075 (6)	-0.0030 (6)
C2	0.0255 (7)	0.0274 (7)	0.0331 (7)	-0.0072 (5)	-0.0087 (6)	-0.0098 (6)
C3	0.0246 (7)	0.0246 (6)	0.0308 (7)	-0.0073 (5)	-0.0062 (5)	-0.0073 (5)
C4	0.0357 (8)	0.0307 (8)	0.0422 (9)	-0.0149 (6)	-0.0026 (7)	-0.0040 (6)
C5	0.0580 (11)	0.0309 (8)	0.0373 (9)	-0.0133 (8)	-0.0038 (8)	-0.0004 (7)
C6	0.0630 (12)	0.0327 (8)	0.0364 (9)	-0.0019 (8)	-0.0219 (8)	-0.0050 (7)
C7	0.0381 (8)	0.0359 (8)	0.0440 (9)	-0.0020 (7)	-0.0211 (7)	-0.0140 (7)
C8	0.0233 (7)	0.0378 (8)	0.0387 (8)	-0.0126 (6)	-0.0106 (6)	-0.0102 (6)
C11	0.0241 (7)	0.0272 (7)	0.0318 (7)	-0.0117 (5)	-0.0099 (5)	-0.0018 (5)
C12	0.0266 (7)	0.0298 (7)	0.0295 (7)	-0.0147 (6)	-0.0075 (5)	-0.0036 (5)
C13	0.0238 (7)	0.0357 (8)	0.0383 (8)	-0.0156 (6)	-0.0055 (6)	-0.0044 (6)
C14	0.0313 (8)	0.0318 (7)	0.0327 (8)	-0.0119 (6)	-0.0023 (6)	-0.0052 (6)
C15	0.0418 (8)	0.0294 (7)	0.0320 (7)	-0.0116 (6)	-0.0137 (6)	-0.0046 (6)
C16	0.0308 (7)	0.0294 (7)	0.0373 (8)	-0.0120 (6)	-0.0162 (6)	-0.0030 (6)
C21	0.0432 (9)	0.0642 (11)	0.0411 (9)	-0.0337 (9)	-0.0094 (7)	-0.0055 (8)
C22	0.0305 (8)	0.0586 (11)	0.0556 (10)	-0.0191 (8)	-0.0015 (7)	-0.0303 (9)

C23	0.0391 (9)	0.0384 (9)	0.0715 (12)	-0.0159 (7)	-0.0207 (8)	-0.0098 (8)
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Geometric parameters (Å, °)

O1—C12	1.3602 (17)	C8—H8A	0.9900
O1—H1	0.98 (2)	C8—H8B	0.9900
N1—C1	1.3531 (18)	C11—C16	1.390 (2)
N1—C3	1.3807 (19)	C11—C12	1.3999 (19)
N1—C8	1.4570 (17)	C12—C13	1.391 (2)
N2—C1	1.3101 (19)	C13—C14	1.386 (2)
N2—C2	1.390 (2)	C13—H13	0.9500
C1—H1A	0.9500	C14—C15	1.385 (2)
C2—C7	1.395 (2)	C14—H14	0.9500
C2—C3	1.398 (2)	C15—C16	1.387 (2)
C3—C4	1.390 (2)	C15—H15	0.9500
C4—C5	1.374 (3)	C16—H16	0.9500
C4—H4	0.9500	C21—C22 ⁱ	1.370 (3)
C5—C6	1.398 (3)	C21—C23	1.383 (3)
C5—H5	0.9500	C21—H21	0.9500
C6—C7	1.379 (3)	C22—C21 ⁱ	1.370 (3)
C6—H6	0.9500	C22—C23	1.375 (3)
C7—H7	0.9500	C22—H22	0.9500
C8—C11	1.5114 (19)	C23—H23	0.9500
C12—O1—H1	111.1 (12)	C11—C8—H8B	109.0
C1—N1—C3	106.30 (12)	H8A—C8—H8B	107.8
C1—N1—C8	126.83 (12)	C16—C11—C12	118.72 (13)
C3—N1—C8	126.86 (12)	C16—C11—C8	122.58 (12)
C1—N2—C2	104.48 (11)	C12—C11—C8	118.69 (12)
N2—C1—N1	114.07 (13)	O1—C12—C13	122.49 (12)
N2—C1—H1A	123.0	O1—C12—C11	117.60 (12)
N1—C1—H1A	123.0	C13—C12—C11	119.91 (13)
N2—C2—C7	130.19 (14)	C14—C13—C12	120.37 (13)
N2—C2—C3	109.62 (12)	C14—C13—H13	119.8
C7—C2—C3	120.19 (14)	C12—C13—H13	119.8
N1—C3—C4	131.74 (14)	C15—C14—C13	120.17 (13)
N1—C3—C2	105.52 (12)	C15—C14—H14	119.9
C4—C3—C2	122.74 (14)	C13—C14—H14	119.9
C5—C4—C3	116.22 (16)	C14—C15—C16	119.39 (13)
C5—C4—H4	121.9	C14—C15—H15	120.3
C3—C4—H4	121.9	C16—C15—H15	120.3
C4—C5—C6	121.83 (16)	C15—C16—C11	121.41 (13)
C4—C5—H5	119.1	C15—C16—H16	119.3
C6—C5—H5	119.1	C11—C16—H16	119.3
C7—C6—C5	121.91 (15)	C22 ⁱ —C21—C23	119.45 (16)
C7—C6—H6	119.0	C22 ⁱ —C21—H21	120.3
C5—C6—H6	119.0	C23—C21—H21	120.3
C6—C7—C2	117.10 (16)	C21 ⁱ —C22—C23	120.50 (16)

C6—C7—H7	121.4	C21 ⁱ —C22—H22	119.8
C2—C7—H7	121.4	C23—C22—H22	119.8
N1—C8—C11	112.97 (11)	C22—C23—C21	120.05 (17)
N1—C8—H8A	109.0	C22—C23—H23	120.0
C11—C8—H8A	109.0	C21—C23—H23	120.0
N1—C8—H8B	109.0		
C2—N2—C1—N1	-0.25 (16)	C3—C2—C7—C6	-0.1 (2)
C3—N1—C1—N2	0.43 (16)	C1—N1—C8—C11	-110.59 (16)
C8—N1—C1—N2	-179.40 (12)	C3—N1—C8—C11	69.62 (17)
C1—N2—C2—C7	-179.68 (15)	N1—C8—C11—C16	15.8 (2)
C1—N2—C2—C3	-0.02 (15)	N1—C8—C11—C12	-163.13 (12)
C1—N1—C3—C4	179.49 (15)	C16—C11—C12—O1	-179.84 (12)
C8—N1—C3—C4	-0.7 (2)	C8—C11—C12—O1	-0.84 (19)
C1—N1—C3—C2	-0.40 (14)	C16—C11—C12—C13	0.2 (2)
C8—N1—C3—C2	179.42 (12)	C8—C11—C12—C13	179.21 (13)
N2—C2—C3—N1	0.27 (15)	O1—C12—C13—C14	178.38 (13)
C7—C2—C3—N1	179.96 (12)	C11—C12—C13—C14	-1.7 (2)
N2—C2—C3—C4	-179.63 (12)	C12—C13—C14—C15	1.7 (2)
C7—C2—C3—C4	0.1 (2)	C13—C14—C15—C16	-0.3 (2)
N1—C3—C4—C5	-179.58 (14)	C14—C15—C16—C11	-1.2 (2)
C2—C3—C4—C5	0.3 (2)	C12—C11—C16—C15	1.2 (2)
C3—C4—C5—C6	-0.6 (2)	C8—C11—C16—C15	-177.73 (13)
C4—C5—C6—C7	0.6 (3)	C21 ⁱ —C22—C23—C21	-0.3 (3)
C5—C6—C7—C2	-0.2 (2)	C22 ⁱ —C21—C23—C22	0.3 (3)
N2—C2—C7—C6	179.51 (14)		

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

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

Cg1, Cg2, Cg3 and Cg4 are the centroids of the C2—C7, N1/N2/C1—C3, C21—C23/C21'—C23' and C11—C16 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots N2 ⁱⁱ	0.98 (2)	1.74 (2)	2.7200 (16)	174 (2)
C22—H22 \cdots Cg1	0.95	3.25	3.868	124
C22—H22 \cdots Cg2	0.95	3.10	3.844	137
C15—H15 \cdots Cg3	0.95	3.06	3.761	132
C16—H16 \cdots Cg3	0.95	3.30	3.883	122
C1—H1A \cdots Cg4 ⁱⁱⁱ	0.95	2.65	3.467	145
C5—H5 \cdots Cg4 ^{iv}	0.95	3.17	3.922	138

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