

2-[2-(4-Methoxyphenyl)-4,5-diphenyl-1H-imidazol-1-yl]ethanol

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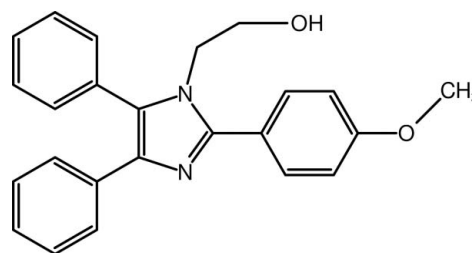
Received 7 February 2013; accepted 13 February 2013

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; disorder in main residue; R factor = 0.043; wR factor = 0.110; data-to-parameter ratio = 14.2.

In the title compound, $\text{C}_{24}\text{H}_{22}\text{N}_2\text{O}_2$, the central imidazole ring makes dihedral angles of 49.45 (8), 88.94 (9) and 19.43 (8) $^\circ$ with the benzene ring and the two phenyl rings, respectively. The dihedral angle between the phenyl rings is 77.86 (9) $^\circ$, and they form dihedral angles of 49.06 (9) and 67.31 (8) $^\circ$ with the benzene ring. In the crystal, molecules are linked by $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds, forming chains along the b axis. These chains are connected by $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, forming a two-dimensional network parallel to (100). In addition, $\text{C}-\text{H}\cdots\pi$ interactions are also observed. The terminal C and O atoms of the ethanol group are disordered over two sets of sites with an occupancy ratio of 0.801 (5):0.199 (5).

Related literature

For imidazole derivatives as anticancer agents, see, for example: Krezel (1998); Andreani *et al.* (2000). For related structures, see: Akkurt *et al.* (2012); Mohamed *et al.* (2012). For further biological applications of imidazoles, see: Maier *et al.* (1989*a,b*). For standard bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_{24}\text{H}_{22}\text{N}_2\text{O}_2$
 $M_r = 370.44$
 Monoclinic, $P2_1/c$
 $a = 14.3570$ (4) Å
 $b = 13.2820$ (4) Å
 $c = 10.7380$ (3) Å
 $\beta = 108.212$ (1) $^\circ$

$V = 1945.05$ (10) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 296$ K
 $0.30 \times 0.30 \times 0.30$ mm

Data collection

Bruker APEXII CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.976$, $T_{\max} = 0.976$

18622 measured reflections
 3822 independent reflections
 3046 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.110$
 $S = 1.04$
 3822 reflections
 269 parameters

2 restraints
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.16$ e Å⁻³
 $\Delta\rho_{\min} = -0.18$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, $^\circ$).

$Cg1$ is the centroid of the C4–C9 benzene ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1A}-\text{H1OA}\cdots\text{N2}^{\text{i}}$	0.82	2.01	2.829 (3)	175
$\text{C9}-\text{H9}\cdots\text{O1A}^{\text{ii}}$	0.93	2.58	3.452 (3)	156
$\text{C24}-\text{H24}\cdots\text{O1A}^{\text{iii}}$	0.93	2.53	3.448 (4)	170
$\text{C23}-\text{H23}\cdots\text{Cg1}^{\text{iii}}$	0.93	2.90	3.736 (2)	151

Symmetry codes: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (iii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$.

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012); software used to prepare material for publication: WinGX (Farrugia, 2012) and PLATON (Spek, 2009).

The authors are thankful to the National Academy of Sciences of Azerbaijan in collaboration with the Ministry of Higher Education of Egypt for funding this project. Manchester Metropolitan University, Erciyes University and Baku State University are gratefully acknowledged for supporting the study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2561).

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supplementary materials

Acta Cryst. (2013). E69, o474–o475 [doi:10.1107/S1600536813004285]

2-[2-(4-Methoxyphenyl)-4,5-diphenyl-1*H*-imidazol-1-yl]ethanol

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Comment

Heterocyclic compounds such as imidazoles have been a traditional focal point for the development of new bio-active molecules such as anticancer agents (Krezel, 1998; Andreani *et al.* 2000). Many of the substituted imidazoles are known as inhibitors of fungicides and herbicides, plant growth regulators and therapeutic agents (Maier *et al.* 1989*a,b*). As part of our on-going study to develop new routes for synthesis of tetra-substituted imidazole based amino alcohol compounds, we herein report the synthesis and crystal structure of the title compound.

In the title compound, Fig. 1, the central 1*H*-imidazole ring (N1/N2/C1—C3) makes dihedral angles of 49.45 (8), 88.94 (9) and 19.43 (8)°, with the benzene ring (C4–C9) and two phenyl rings (C13–C18 and C19–C24), respectively. The dihedral angle between the (C13–C18 and C19–C24) phenyl rings is 77.86 (9)°. The (C4–C9) benzene ring forms dihedral angles of 49.06 (9) and 67.31 (8)° with two the phenyl rings (C13–C18 and C19–C24), respectively. The N1–C11–C12A–O1A torsion angle is 46.6 (2)°. The values of the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges and are comparable to those reported for related structures (Akkurt *et al.*, 2012; Mohamed *et al.*, 2012).

In the crystal, O—H⋯N hydrogen bonds (Table 1 and Fig 2) connect the molecules to form chains along the *b* axis direction. These chains are linked by C—H⋯O hydrogen bonds forming a two-dimensional network parallel to the *bc* plane. There are also C—H⋯ π interactions present (Table 1).

Experimental

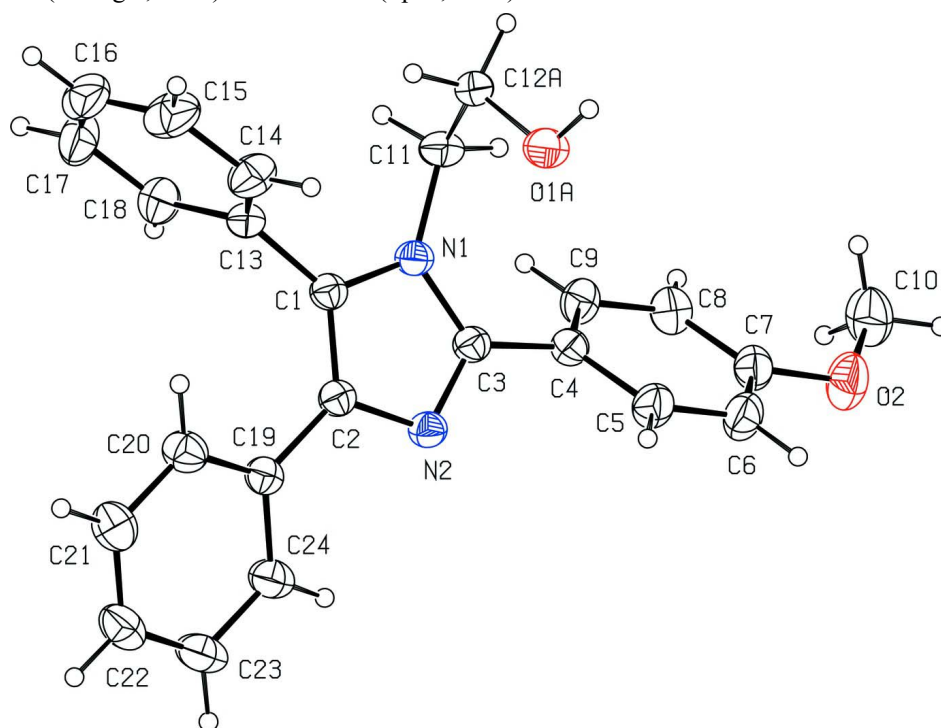
A mixture of 2.1 g (10 mmol) 1,2-diphenylethane-1,2-dione, 1.36 g (10 mmol) 4-methoxybenzaldehyde, 0.67 g (11 mmol) 2-aminoethanol and 0.77 g (10 mmol) ammonium acetate was added to 0.5 g (3 mmol) of a fresh prepared diethyl ammonium hydrogen sulfate as an ionic liquid. The reaction mixture was heated on oil bath at 373 K and monitored by TLC till completion after 30 min then poured on water. The obtained solid was filtered off, washed with cold ethanol and dried under vacuum. The crude product was crystallized from ethanol to afford colourless prisms (m.p. 460 – 462 K), by slow evaporation at room temperature, in excellent yield (95%).

Refinement

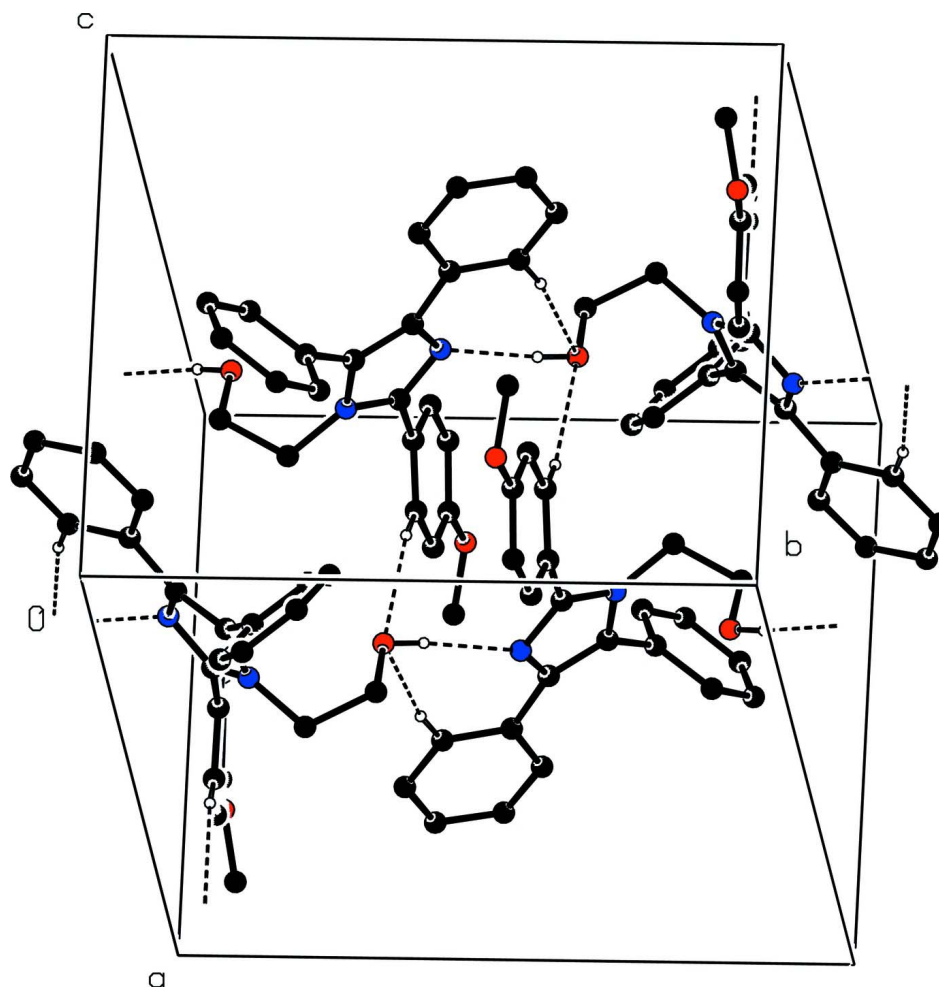
H atoms were positioned geometrically, with O—H = 0.82 Å, C—H = 0.93 Å (aromatic), 0.97 Å (methylene) and 0.98 Å (methine) H atoms, respectively, and refined as riding with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$ for hydroxyl H atoms, and = 1.2 $U_{\text{eq}}(\text{C})$ for other H atoms. Atoms C12 and O1 of the ethanol group are disordered over two sites (A and B), with occupancies of 0.801 (5):0.199 (5). Atoms O1A and O1B were refined with the EADP command.

Computing details

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus* (Bruker, 2001); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

**Figure 1**

A view of the molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level.


Figure 2

A partial view of the crystal packing of the title compound, showing the O—H...N and C—H...O hydrogen bonds (dashed lines; see Table 1 for details). H atoms not involved in hydrogen bonding have been omitted for clarity.

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Crystal data

$C_{24}H_{22}N_2O_2$

$M_r = 370.44$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 14.3570(4)\ \text{\AA}$

$b = 13.2820(4)\ \text{\AA}$

$c = 10.7380(3)\ \text{\AA}$

$\beta = 108.212(1)^\circ$

$V = 1945.05(10)\ \text{\AA}^3$

$Z = 4$

$F(000) = 784$

$D_x = 1.265\ \text{Mg m}^{-3}$

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

Cell parameters from 6445 reflections

$\theta = 2.5\text{--}28.1^\circ$

$\mu = 0.08\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Prism, colourless

$0.30 \times 0.30 \times 0.30\ \text{mm}$

Data collection

Bruker APEXII CCD diffractometer	18622 measured reflections
Radiation source: fine-focus sealed tube	3822 independent reflections
Graphite monochromator	3046 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.022$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 1.5^\circ$
$T_{\text{min}} = 0.976$, $T_{\text{max}} = 0.976$	$h = -17 \rightarrow 17$
	$k = -16 \rightarrow 16$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H-atom parameters constrained
$wR(F^2) = 0.110$	$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 0.4175P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
3822 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
269 parameters	$\Delta\rho_{\text{max}} = 0.16 \text{ e } \text{\AA}^{-3}$
2 restraints	$\Delta\rho_{\text{min}} = -0.18 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating $-R$ -factor-obs *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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
O1A	0.4684 (2)	0.37249 (19)	0.2105 (2)	0.0601 (7)	0.801 (5)
O2	0.85914 (8)	0.08118 (11)	0.17179 (13)	0.0735 (5)	
N1	0.39627 (8)	0.18785 (8)	0.09335 (11)	0.0404 (3)	
N2	0.43176 (8)	0.05860 (9)	0.22977 (11)	0.0417 (4)	
C1	0.31198 (10)	0.16540 (10)	0.12402 (13)	0.0392 (4)	
C2	0.33467 (10)	0.08474 (10)	0.20781 (13)	0.0386 (4)	
C3	0.46645 (10)	0.12152 (10)	0.16028 (14)	0.0400 (4)	
C4	0.56824 (10)	0.11574 (11)	0.15705 (14)	0.0426 (4)	
C5	0.64400 (12)	0.10619 (14)	0.27435 (16)	0.0554 (6)	
C6	0.73926 (12)	0.09378 (15)	0.27566 (17)	0.0621 (6)	
C7	0.76170 (11)	0.09152 (12)	0.16002 (17)	0.0523 (5)	
C8	0.68762 (12)	0.09900 (12)	0.04244 (16)	0.0518 (5)	
C9	0.59175 (11)	0.11052 (12)	0.04197 (15)	0.0496 (5)	
C10	0.88821 (14)	0.09847 (18)	0.0591 (2)	0.0797 (8)	
C11	0.40902 (12)	0.27268 (11)	0.01273 (15)	0.0507 (5)	
C12A	0.40758 (15)	0.37524 (14)	0.0781 (2)	0.0462 (7)	0.801 (5)
C13	0.21836 (10)	0.22019 (11)	0.06779 (14)	0.0428 (5)	

C14	0.19561 (13)	0.30302 (13)	0.13025 (18)	0.0605 (6)	
C15	0.10593 (15)	0.34991 (17)	0.0819 (2)	0.0764 (8)	
C16	0.03897 (14)	0.31534 (19)	-0.0294 (2)	0.0799 (8)	
C17	0.06034 (14)	0.23439 (19)	-0.0938 (2)	0.0808 (8)	
C18	0.15028 (12)	0.18658 (14)	-0.04567 (17)	0.0616 (6)	
C19	0.27150 (10)	0.02319 (10)	0.26213 (13)	0.0413 (4)	
C20	0.18141 (12)	0.05525 (13)	0.26891 (17)	0.0543 (6)	
C21	0.12225 (13)	-0.00802 (14)	0.31328 (18)	0.0628 (6)	
C22	0.15231 (14)	-0.10348 (14)	0.35442 (18)	0.0632 (7)	
C23	0.24208 (15)	-0.13547 (14)	0.3522 (2)	0.0707 (7)	
C24	0.30092 (13)	-0.07337 (12)	0.30620 (18)	0.0593 (6)	
O1B	0.4482 (10)	0.3797 (10)	0.1690 (11)	0.0601 (7)	0.199 (5)
C12B	0.4757 (6)	0.3448 (6)	0.0623 (8)	0.053 (3)	0.199 (5)
H6	0.78890	0.08690	0.35510	0.0750*	
H8	0.70200	0.09630	-0.03620	0.0620*	
H9	0.54190	0.11480	-0.03780	0.0600*	
H10A	0.86270	0.04600	-0.00370	0.1200*	
H10B	0.95850	0.09890	0.08350	0.1200*	
H10A	0.49500	0.42730	0.23080	0.0900*	0.801 (5)
H5	0.63000	0.10820	0.35320	0.0670*	
H11B	0.47090	0.26510	-0.00480	0.0610*	0.801 (5)
H12A	0.43070	0.42700	0.03120	0.0550*	0.801 (5)
H12B	0.34100	0.39170	0.07450	0.0550*	0.801 (5)
H14	0.24140	0.32750	0.20600	0.0730*	
H15	0.09120	0.40520	0.12540	0.0920*	
H16	-0.02160	0.34690	-0.06170	0.0960*	
H17	0.01440	0.21120	-0.17030	0.0970*	
H18	0.16470	0.13160	-0.09010	0.0740*	
H20	0.16040	0.12040	0.24320	0.0650*	
H21	0.06140	0.01450	0.31520	0.0750*	
H22	0.11210	-0.14610	0.38360	0.0760*	
H23	0.26370	-0.19970	0.38190	0.0850*	
H24	0.36160	-0.09670	0.30470	0.0710*	
H10C	0.86310	0.16230	0.02120	0.1200*	
H11A	0.35710	0.27100	-0.07060	0.0610*	0.801 (5)
H10B	0.47760	0.43200	0.19690	0.0900*	0.199 (5)
H11C	0.42580	0.24450	-0.06080	0.0610*	0.199 (5)
H11D	0.34540	0.30450	-0.02310	0.0610*	0.199 (5)
H12C	0.47170	0.39800	-0.00110	0.0640*	0.199 (5)
H12D	0.54170	0.31760	0.09060	0.0640*	0.199 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0760 (15)	0.0472 (8)	0.0422 (14)	-0.0150 (9)	-0.0031 (11)	0.0009 (10)
O2	0.0444 (6)	0.1058 (11)	0.0707 (8)	0.0008 (6)	0.0188 (6)	-0.0010 (7)
N1	0.0451 (6)	0.0354 (6)	0.0391 (6)	-0.0005 (5)	0.0107 (5)	0.0024 (5)
N2	0.0440 (7)	0.0361 (6)	0.0427 (7)	0.0011 (5)	0.0102 (5)	0.0016 (5)
C1	0.0428 (7)	0.0357 (7)	0.0378 (7)	-0.0013 (6)	0.0108 (6)	-0.0019 (6)

C2	0.0425 (7)	0.0345 (7)	0.0369 (7)	-0.0003 (6)	0.0099 (6)	-0.0029 (6)
C3	0.0437 (8)	0.0353 (7)	0.0384 (7)	-0.0007 (6)	0.0091 (6)	-0.0010 (6)
C4	0.0434 (8)	0.0378 (7)	0.0445 (8)	-0.0017 (6)	0.0106 (6)	-0.0002 (6)
C5	0.0494 (9)	0.0732 (11)	0.0426 (9)	-0.0019 (8)	0.0128 (7)	0.0073 (8)
C6	0.0453 (9)	0.0859 (13)	0.0487 (10)	-0.0025 (8)	0.0054 (7)	0.0085 (9)
C7	0.0424 (8)	0.0537 (9)	0.0595 (10)	-0.0027 (7)	0.0141 (7)	-0.0029 (7)
C8	0.0532 (9)	0.0559 (9)	0.0478 (9)	-0.0034 (7)	0.0179 (7)	-0.0124 (7)
C9	0.0471 (8)	0.0538 (9)	0.0434 (8)	-0.0008 (7)	0.0077 (7)	-0.0101 (7)
C10	0.0578 (11)	0.1018 (16)	0.0886 (15)	-0.0032 (10)	0.0361 (11)	-0.0036 (12)
C11	0.0593 (9)	0.0455 (9)	0.0474 (9)	0.0017 (7)	0.0170 (7)	0.0112 (7)
C12A	0.0448 (12)	0.0388 (10)	0.0489 (13)	-0.0008 (8)	0.0059 (10)	0.0084 (8)
C13	0.0429 (8)	0.0424 (8)	0.0421 (8)	-0.0005 (6)	0.0118 (6)	0.0086 (6)
C14	0.0619 (10)	0.0560 (10)	0.0594 (10)	0.0146 (8)	0.0130 (8)	0.0008 (8)
C15	0.0730 (13)	0.0769 (13)	0.0854 (15)	0.0310 (11)	0.0337 (12)	0.0189 (11)
C16	0.0457 (10)	0.1047 (17)	0.0919 (16)	0.0193 (11)	0.0254 (11)	0.0434 (14)
C17	0.0498 (11)	0.1072 (17)	0.0695 (13)	-0.0099 (11)	-0.0044 (9)	0.0164 (12)
C18	0.0567 (10)	0.0660 (11)	0.0535 (10)	-0.0065 (8)	0.0049 (8)	0.0003 (8)
C19	0.0475 (8)	0.0397 (8)	0.0350 (7)	-0.0050 (6)	0.0105 (6)	-0.0034 (6)
C20	0.0587 (10)	0.0475 (9)	0.0615 (10)	0.0017 (7)	0.0259 (8)	0.0015 (8)
C21	0.0595 (10)	0.0703 (12)	0.0669 (11)	-0.0057 (9)	0.0317 (9)	-0.0016 (9)
C22	0.0722 (12)	0.0628 (11)	0.0594 (11)	-0.0201 (9)	0.0277 (9)	0.0015 (9)
C23	0.0804 (13)	0.0481 (10)	0.0867 (14)	-0.0044 (9)	0.0308 (11)	0.0179 (9)
C24	0.0584 (10)	0.0467 (9)	0.0751 (12)	0.0015 (8)	0.0244 (9)	0.0127 (8)
O1B	0.0760 (15)	0.0472 (8)	0.0422 (14)	-0.0150 (9)	-0.0031 (11)	0.0009 (10)
C12B	0.051 (5)	0.053 (5)	0.058 (5)	-0.005 (4)	0.021 (4)	-0.007 (4)

Geometric parameters (Å, °)

O1A—C12A	1.417 (3)	C19—C24	1.386 (2)
O1B—C12B	1.402 (15)	C20—C21	1.381 (3)
O2—C10	1.417 (2)	C21—C22	1.367 (3)
O2—C7	1.372 (2)	C22—C23	1.364 (3)
O1A—H10A	0.8200	C23—C24	1.378 (3)
O1B—H10B	0.8200	C5—H5	0.9300
N1—C11	1.4668 (19)	C6—H6	0.9300
N1—C1	1.3824 (19)	C8—H8	0.9300
N1—C3	1.3621 (18)	C9—H9	0.9300
N2—C2	1.3834 (19)	C10—H10A	0.9600
N2—C3	1.3174 (18)	C10—H10C	0.9600
C1—C2	1.3712 (19)	C10—H10B	0.9600
C1—C13	1.481 (2)	C11—H11A	0.9700
C2—C19	1.470 (2)	C11—H11C	0.9700
C3—C4	1.475 (2)	C11—H11D	0.9700
C4—C9	1.381 (2)	C11—H11B	0.9700
C4—C5	1.389 (2)	C12A—H12A	0.9700
C5—C6	1.373 (3)	C12A—H12B	0.9700
C6—C7	1.377 (2)	C12B—H12C	0.9700
C7—C8	1.377 (2)	C12B—H12D	0.9700
C8—C9	1.383 (2)	C14—H14	0.9300
C11—C12B	1.341 (9)	C15—H15	0.9300

C11—C12A	1.536 (2)	C16—H16	0.9300
C13—C14	1.380 (2)	C17—H17	0.9300
C13—C18	1.377 (2)	C18—H18	0.9300
C14—C15	1.377 (3)	C20—H20	0.9300
C15—C16	1.358 (3)	C21—H21	0.9300
C16—C17	1.364 (3)	C22—H22	0.9300
C17—C18	1.386 (3)	C23—H23	0.9300
C19—C20	1.385 (2)	C24—H24	0.9300
C7—O2—C10	117.99 (15)	C9—C8—H8	120.00
C12A—O1A—H10A	109.00	C7—C8—H8	120.00
C12B—O1B—H10B	110.00	C4—C9—H9	119.00
C1—N1—C11	125.90 (12)	C8—C9—H9	119.00
C3—N1—C11	126.88 (13)	O2—C10—H10B	109.00
C1—N1—C3	107.04 (11)	O2—C10—H10C	109.00
C2—N2—C3	106.46 (12)	O2—C10—H10A	109.00
N1—C1—C2	106.18 (12)	H10A—C10—H10C	109.00
C2—C1—C13	130.59 (14)	H10B—C10—H10C	109.00
N1—C1—C13	123.19 (12)	H10A—C10—H10B	110.00
N2—C2—C1	109.15 (13)	N1—C11—H11A	109.00
C1—C2—C19	130.18 (14)	N1—C11—H11C	107.00
N2—C2—C19	120.43 (12)	N1—C11—H11D	107.00
N1—C3—N2	111.16 (13)	N1—C11—H11B	109.00
N1—C3—C4	126.61 (13)	C12A—C11—H11B	109.00
N2—C3—C4	122.22 (13)	H11A—C11—H11B	108.00
C3—C4—C9	123.02 (13)	C12B—C11—H11C	106.00
C5—C4—C9	117.76 (15)	C12B—C11—H11D	108.00
C3—C4—C5	118.97 (14)	H11C—C11—H11D	107.00
C4—C5—C6	121.02 (15)	C12A—C11—H11A	109.00
C5—C6—C7	120.42 (16)	O1A—C12A—H12B	110.00
O2—C7—C8	124.40 (16)	C11—C12A—H12A	110.00
O2—C7—C6	116.00 (15)	O1A—C12A—H12A	110.00
C6—C7—C8	119.60 (16)	H12A—C12A—H12B	108.00
C7—C8—C9	119.60 (15)	C11—C12A—H12B	110.00
C4—C9—C8	121.57 (15)	C11—C12B—H12D	111.00
N1—C11—C12B	121.3 (4)	O1B—C12B—H12C	111.00
N1—C11—C12A	112.93 (13)	H12C—C12B—H12D	109.00
O1A—C12A—C11	110.10 (17)	O1B—C12B—H12D	111.00
O1B—C12B—C11	102.2 (8)	C11—C12B—H12C	111.00
C1—C13—C14	121.08 (14)	C13—C14—H14	120.00
C14—C13—C18	118.58 (15)	C15—C14—H14	120.00
C1—C13—C18	120.29 (14)	C16—C15—H15	120.00
C13—C14—C15	120.84 (17)	C14—C15—H15	120.00
C14—C15—C16	120.0 (2)	C15—C16—H16	120.00
C15—C16—C17	120.2 (2)	C17—C16—H16	120.00
C16—C17—C18	120.20 (19)	C16—C17—H17	120.00
C13—C18—C17	120.17 (17)	C18—C17—H17	120.00
C2—C19—C20	123.49 (13)	C17—C18—H18	120.00
C2—C19—C24	119.33 (14)	C13—C18—H18	120.00

C20—C19—C24	117.15 (15)	C19—C20—H20	119.00
C19—C20—C21	121.07 (16)	C21—C20—H20	119.00
C20—C21—C22	120.64 (18)	C20—C21—H21	120.00
C21—C22—C23	119.18 (18)	C22—C21—H21	120.00
C22—C23—C24	120.54 (18)	C23—C22—H22	120.00
C19—C24—C23	121.37 (17)	C21—C22—H22	120.00
C6—C5—H5	119.00	C22—C23—H23	120.00
C4—C5—H5	119.00	C24—C23—H23	120.00
C5—C6—H6	120.00	C23—C24—H24	119.00
C7—C6—H6	120.00	C19—C24—H24	119.00
C10—O2—C7—C6	-167.65 (17)	N2—C3—C4—C5	-47.3 (2)
C10—O2—C7—C8	12.7 (3)	N2—C3—C4—C9	126.90 (16)
C3—N1—C1—C2	-0.76 (14)	C3—C4—C5—C6	175.61 (16)
C3—N1—C1—C13	-178.72 (13)	C9—C4—C5—C6	1.1 (3)
C11—N1—C1—C2	-176.05 (12)	C3—C4—C9—C8	-176.00 (14)
C11—N1—C1—C13	6.0 (2)	C5—C4—C9—C8	-1.8 (2)
C1—N1—C3—N2	0.55 (15)	C4—C5—C6—C7	0.6 (3)
C1—N1—C3—C4	179.26 (13)	C5—C6—C7—O2	178.52 (17)
C11—N1—C3—N2	175.78 (12)	C5—C6—C7—C8	-1.8 (3)
C11—N1—C3—C4	-5.5 (2)	O2—C7—C8—C9	-179.18 (15)
C1—N1—C11—C12A	67.64 (19)	C6—C7—C8—C9	1.2 (2)
C3—N1—C11—C12A	-106.74 (18)	C7—C8—C9—C4	0.6 (2)
C3—N2—C2—C1	-0.39 (15)	N1—C11—C12A—O1A	46.6 (2)
C3—N2—C2—C19	174.53 (12)	C1—C13—C14—C15	-175.92 (17)
C2—N2—C3—N1	-0.10 (16)	C18—C13—C14—C15	1.4 (3)
C2—N2—C3—C4	-178.89 (13)	C1—C13—C18—C17	176.12 (17)
N1—C1—C2—N2	0.71 (15)	C14—C13—C18—C17	-1.2 (3)
N1—C1—C2—C19	-173.56 (13)	C13—C14—C15—C16	-0.7 (3)
C13—C1—C2—N2	178.46 (13)	C14—C15—C16—C17	-0.2 (3)
C13—C1—C2—C19	4.2 (2)	C15—C16—C17—C18	0.4 (3)
N1—C1—C13—C14	-91.53 (18)	C16—C17—C18—C13	0.4 (3)
N1—C1—C13—C18	91.21 (18)	C2—C19—C20—C21	175.87 (15)
C2—C1—C13—C14	91.1 (2)	C24—C19—C20—C21	-2.3 (2)
C2—C1—C13—C18	-86.2 (2)	C2—C19—C24—C23	-176.95 (16)
N2—C2—C19—C20	165.59 (14)	C20—C19—C24—C23	1.3 (2)
N2—C2—C19—C24	-16.3 (2)	C19—C20—C21—C22	1.4 (3)
C1—C2—C19—C20	-20.7 (2)	C20—C21—C22—C23	0.5 (3)
C1—C2—C19—C24	157.46 (15)	C21—C22—C23—C24	-1.5 (3)
N1—C3—C4—C5	134.15 (16)	C22—C23—C24—C19	0.6 (3)
N1—C3—C4—C9	-51.7 (2)		

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

Cg1 is the centroid of the C4—C9 benzene ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1A—H1O A^i ...N2 i	0.82	2.01	2.829 (3)	175
C9—H9...O1A ii	0.93	2.58	3.452 (3)	156

C24—H24 \cdots O1A ⁱⁱⁱ	0.93	2.53	3.448 (4)	170
C23—H23 \cdots Cg1 ⁱⁱⁱ	0.93	2.90	3.736 (2)	151

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