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1*H*-Benzimidazol-2-ylmethyl phenyl ether

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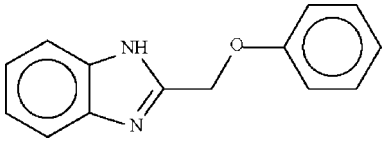
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.009 Å; R factor = 0.046; wR factor = 0.111; data-to-parameter ratio = 8.6.

There are two molecules in the asymmetric unit of the title compound, $C_{14}H_{10}N_2O$: the dihedral angles between their aromatic ring planes are 47.4 (4) and 46.8 (3)°. In the crystal structure, molecules are linked by N—H···N hydrogen bonds from the secondary nitrogen N—H donor to the tertiary N-atom acceptor of a symmetry-related neighbour, resulting in hydrogen-bonded chains. The two independent chains both propagate in [100].

Related literature

For related phenoxy-substituted *N*-heterocycles, see: Abdullah & Ng (2008); Hassan *et al.* (2008); Idris *et al.* (2009); Shah Bakhtiar *et al.* (2009).



Experimental

Crystal data

$C_{14}H_{12}N_2O$
M_r = 224.26
Orthorhombic, $Pca2_1$
a = 10.0299 (5) Å
b = 8.5391 (4) Å
c = 27.000 (1) Å
V = 2312.5 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 120 K
0.40 × 0.10 × 0.03 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: none
15022 measured reflections
2699 independent reflections
1783 reflections with $I > 2\sigma(I)$
R_{int} = 0.091

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.111
S = 1.00
2699 reflections
313 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 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
N1—H1···N2^{i}	0.88 (1)	2.03 (2)	2.879 (7)	163 (6)
N3—H3···N4^{ii}	0.88 (1)	1.97 (2)	2.845 (8)	172 (5)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank the University of Malaya for supporting this study (FS358/2008 A).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2923).

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supporting information

Acta Cryst. (2009). E**65**, o733 [doi:10.1107/S1600536809007922]

1*H*-Benzimidazol-2-ylmethyl phenyl ether

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S1. Experimental

Phenol (1.88 g, 20 mmol) was mixed with sodium hydroxide (0.08 g, 20 mmol) in several drops of water. The water was then evaporated. The paste was heated with 2-(chloromethyl)benzimidazole 3.30 g, 20 mmol) at 423–433 K for 6 h. The product was dissolved in water and the solution extracted with chloroform. The chloroform phase was dried over sodium sulfate; the evaporation of the solvent a brown product; this was purified by column chromatography with an ethyl acetate/hexane mixture. Crystals were grown from this solvent system gave well shaped colorless crystals along with some unidentified brown material.

S2. Refinement

Anomalous dispersion was negligible and Friedel pairs were merged before refinement.

The C-bound H-atoms were placed in calculated positions (C—H 0.95–98 Å) and refined as riding with U(H) = 1.2U_{eq}(C). The N-bound H atoms were located in a difference map, and were refined with a restraint of N–H 0.88±0.01 Å; their U_{iso} values were freely refined.

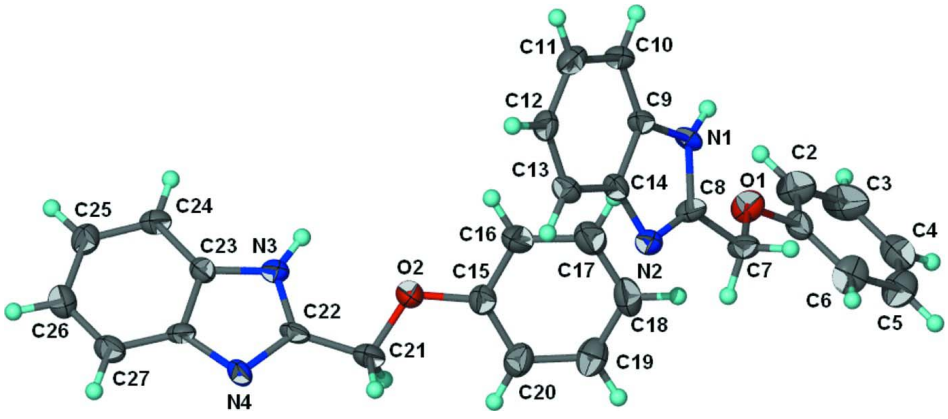

Figure 1

The molecular structure of (I) with displacement ellipsoids shown at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

1*H*-Benzimidazol-2-ylmethyl phenyl ether

Crystal data

$C_{14}H_{12}N_2O$
M_r = 224.26
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac

a = 10.0299 (5) Å
b = 8.5391 (4) Å
c = 27.000 (1) Å
V = 2312.5 (2) Å^3

$Z = 8$
$F(000) = 944$
$D_x = 1.288$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1070 reflections
$\theta = 2.8$–$21.3°$
$\mu = 0.08$ mm^{-1}
$T = 120$ K
Prism, colorless
0.40 × 0.10 × 0.03 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
15022 measured reflections
2699 independent reflections
1783 reflections with $I > 2\sigma(I)$
$R_{int} = 0.091$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.4°$
$h = -12 \rightarrow 12$
$k = -11 \rightarrow 10$
$l = -35 \rightarrow 34$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.111$
$S = 1.00$
2699 reflections
313 parameters
3 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.1971P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.0484 (3)	1.2098 (3)	0.50009 (13)	0.0299 (7)
O2	0.2955 (3)	0.7163 (3)	0.31456 (13)	0.0325 (7)
N1	0.0514 (5)	0.9631 (5)	0.5645 (2)	0.0218 (10)
H1	−0.030 (2)	0.991 (4)	0.557 (2)	0.026*
N2	0.2729 (4)	0.9563 (5)	0.56067 (17)	0.0248 (9)
N3	0.2988 (6)	0.4652 (5)	0.2512 (2)	0.0232 (11)
H3	0.2154 (18)	0.496 (4)	0.254 (2)	0.028*
N4	0.5228 (4)	0.4592 (5)	0.25497 (16)	0.0228 (9)
C1	0.0158 (8)	1.3554 (8)	0.4819 (3)	0.0241 (15)
C2	−0.0889 (9)	1.3564 (10)	0.4484 (3)	0.038 (2)
H2	−0.1315	1.2614	0.4392	0.046*
C3	−0.1303 (13)	1.4968 (6)	0.4286 (5)	0.046 (3)
H3A	−0.2025	1.4980	0.4059	0.055*
C4	−0.0687 (9)	1.6364 (10)	0.4412 (3)	0.0363 (19)
H4	−0.0977	1.7326	0.4271	0.044*
C5	0.0356 (9)	1.6329 (9)	0.4745 (3)	0.036 (2)
H5	0.0789	1.7276	0.4835	0.043*
C6	0.0775 (12)	1.4931 (5)	0.4947 (4)	0.031 (3)
H6	0.1494	1.4920	0.5177	0.037*
C7	0.1627 (4)	1.1991 (5)	0.53097 (18)	0.0251 (10)

H7A	0.1569	1.2759	0.5584	0.030*
H7B	0.2446	1.2206	0.5117	0.030*
C8	0.1653 (6)	1.0354 (7)	0.5510 (2)	0.0227 (13)
C9	0.0880 (4)	0.8244 (5)	0.58670 (16)	0.0207 (10)
C10	0.0147 (4)	0.7057 (5)	0.60944 (17)	0.0241 (9)
H10	−0.0799	0.7088	0.6108	0.029*
C11	0.0864 (4)	0.5826 (6)	0.63004 (18)	0.0266 (11)
H11	0.0403	0.5013	0.6469	0.032*
C12	0.2252 (4)	0.5768 (5)	0.62635 (17)	0.0241 (10)
H12	0.2713	0.4901	0.6403	0.029*
C13	0.2976 (4)	0.6931 (5)	0.60308 (15)	0.0239 (9)
H13	0.3919	0.6867	0.6003	0.029*
C14	0.2276 (4)	0.8200 (5)	0.58383 (16)	0.0219 (9)
C15	0.2627 (8)	0.8623 (8)	0.3334 (3)	0.0249 (15)
C16	0.1578 (8)	0.8609 (10)	0.3667 (3)	0.0348 (19)
H16	0.1140	0.7654	0.3744	0.042*
C17	0.1170 (12)	0.9988 (5)	0.3886 (4)	0.035 (3)
H17	0.0473	0.9978	0.4124	0.042*
C18	0.1780 (9)	1.1382 (10)	0.3759 (3)	0.0333 (18)
H18	0.1481	1.2340	0.3899	0.040*
C19	0.2824 (9)	1.1375 (9)	0.3427 (3)	0.0334 (19)
H19	0.3246	1.2337	0.3346	0.040*
C20	0.3278 (12)	0.9996 (4)	0.3207 (4)	0.030 (3)
H20	0.4002	0.9999	0.2980	0.036*
C21	0.4121 (4)	0.7020 (6)	0.28515 (19)	0.0288 (11)
H21A	0.4927	0.7198	0.3055	0.035*
H21B	0.4110	0.7797	0.2579	0.035*
C22	0.4117 (5)	0.5409 (7)	0.2650 (2)	0.0211 (12)
C23	0.3366 (4)	0.3256 (5)	0.22992 (16)	0.0201 (10)
C24	0.2635 (4)	0.2077 (5)	0.20763 (16)	0.0241 (9)
H24	0.1689	0.2108	0.2062	0.029*
C25	0.3346 (4)	0.0861 (6)	0.18773 (18)	0.0262 (11)
H25	0.2881	0.0041	0.1714	0.031*
C26	0.4741 (4)	0.0791 (5)	0.19069 (18)	0.0286 (10)
H26	0.5197	−0.0077	0.1766	0.034*
C27	0.5464 (4)	0.1960 (5)	0.21372 (16)	0.0260 (10)
H27	0.6408	0.1905	0.2162	0.031*
C28	0.4760 (4)	0.3219 (5)	0.23303 (16)	0.0203 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0255 (17)	0.0259 (16)	0.0382 (17)	0.0004 (14)	−0.0086 (14)	0.0034 (14)
O2	0.0274 (17)	0.0236 (16)	0.0465 (18)	−0.0025 (13)	0.0146 (15)	−0.0054 (14)
N1	0.007 (2)	0.0248 (18)	0.033 (3)	0.005 (2)	−0.0012 (19)	−0.001 (3)
N2	0.017 (2)	0.0212 (18)	0.037 (2)	0.000 (2)	0.002 (2)	−0.002 (2)
N3	0.015 (3)	0.0226 (18)	0.032 (3)	−0.001 (2)	0.002 (2)	−0.001 (3)
N4	0.014 (2)	0.0246 (19)	0.029 (2)	0.004 (2)	0.0014 (18)	−0.006 (2)

C1	0.023 (3)	0.021 (3)	0.027 (3)	0.006 (2)	0.003 (2)	0.004 (2)
C2	0.029 (4)	0.033 (4)	0.052 (4)	0.002 (3)	−0.006 (3)	0.011 (3)
C3	0.026 (7)	0.053 (8)	0.059 (8)	0.005 (2)	−0.011 (6)	0.015 (3)
C4	0.038 (4)	0.033 (4)	0.039 (3)	0.010 (3)	0.011 (3)	0.013 (3)
C5	0.045 (5)	0.029 (4)	0.032 (3)	−0.002 (3)	−0.002 (3)	0.006 (3)
C6	0.042 (7)	0.034 (5)	0.016 (4)	0.001 (2)	−0.010 (4)	0.0036 (17)
C7	0.016 (2)	0.024 (3)	0.036 (3)	−0.0022 (16)	−0.0023 (17)	0.004 (2)
C8	0.021 (3)	0.021 (2)	0.026 (3)	−0.006 (2)	0.000 (2)	0.003 (3)
C9	0.015 (2)	0.023 (2)	0.024 (2)	−0.0020 (17)	−0.0003 (17)	−0.0032 (19)
C10	0.016 (2)	0.025 (2)	0.031 (2)	−0.0027 (18)	0.0027 (18)	−0.001 (2)
C11	0.032 (3)	0.022 (3)	0.026 (2)	−0.0074 (19)	0.0008 (19)	−0.002 (2)
C12	0.025 (3)	0.018 (2)	0.030 (2)	0.0031 (19)	−0.0003 (19)	−0.0006 (19)
C13	0.016 (2)	0.026 (2)	0.029 (2)	0.0034 (17)	0.0003 (18)	0.0000 (18)
C14	0.017 (2)	0.023 (2)	0.025 (2)	0.0029 (18)	0.0011 (17)	−0.0022 (17)
C15	0.025 (3)	0.024 (3)	0.025 (3)	0.000 (2)	0.000 (2)	−0.004 (2)
C16	0.028 (4)	0.036 (4)	0.040 (4)	−0.007 (3)	0.012 (3)	−0.010 (3)
C17	0.029 (6)	0.040 (6)	0.037 (6)	−0.0004 (19)	0.003 (5)	−0.012 (2)
C18	0.033 (4)	0.035 (4)	0.032 (3)	0.009 (3)	−0.002 (3)	−0.012 (3)
C19	0.044 (4)	0.025 (3)	0.031 (3)	0.001 (3)	−0.004 (3)	0.002 (3)
C20	0.029 (6)	0.023 (5)	0.038 (5)	0.0021 (17)	−0.006 (4)	−0.0012 (18)
C21	0.018 (3)	0.033 (3)	0.036 (3)	−0.0038 (18)	0.0055 (18)	−0.004 (2)
C22	0.010 (3)	0.025 (2)	0.029 (3)	0.002 (2)	0.0020 (19)	0.005 (3)
C23	0.019 (2)	0.020 (2)	0.021 (2)	0.0017 (17)	0.0031 (17)	0.0017 (19)
C24	0.019 (2)	0.026 (2)	0.028 (2)	−0.0038 (18)	−0.0001 (17)	0.003 (2)
C25	0.028 (3)	0.025 (3)	0.026 (2)	−0.0021 (19)	−0.0023 (19)	−0.005 (2)
C26	0.029 (3)	0.027 (3)	0.030 (2)	0.004 (2)	0.001 (2)	−0.003 (2)
C27	0.019 (2)	0.028 (2)	0.032 (2)	0.0029 (18)	0.0016 (18)	0.0038 (19)
C28	0.014 (2)	0.020 (2)	0.026 (2)	−0.0038 (17)	0.0009 (17)	0.0047 (17)

Geometric parameters (Å, º)

O1—C1	1.376 (8)	C10—H10	0.9500
O1—C7	1.421 (5)	C11—C12	1.397 (6)
O2—C15	1.386 (8)	C11—H11	0.9500
O2—C21	1.419 (5)	C12—C13	1.381 (6)
N1—C8	1.349 (8)	C12—H12	0.9500
N1—C9	1.377 (6)	C13—C14	1.392 (5)
N1—H1	0.880 (10)	C13—H13	0.9500
N2—C8	1.299 (7)	C15—C16	1.383 (11)
N2—C14	1.397 (6)	C15—C20	1.385 (11)
N3—C22	1.357 (8)	C16—C17	1.380 (11)
N3—C23	1.376 (6)	C16—H16	0.9500
N3—H3	0.881 (10)	C17—C18	1.382 (11)
N4—C22	1.342 (7)	C17—H17	0.9500
N4—C28	1.395 (6)	C18—C19	1.377 (13)
C1—C6	1.373 (10)	C18—H18	0.9500
C1—C2	1.386 (12)	C19—C20	1.396 (11)
C2—C3	1.377 (11)	C19—H19	0.9500

C2—H2	0.9500	C20—H20	0.9500
C3—C4	1.384 (12)	C21—C22	1.480 (8)
C3—H3A	0.9500	C21—H21A	0.9900
C4—C5	1.381 (13)	C21—H21B	0.9900
C4—H4	0.9500	C23—C24	1.383 (6)
C5—C6	1.379 (10)	C23—C28	1.402 (5)
C5—H5	0.9500	C24—C25	1.369 (6)
C6—H6	0.9500	C24—H24	0.9500
C7—C8	1.500 (7)	C25—C26	1.402 (6)
C7—H7A	0.9900	C25—H25	0.9500
C7—H7B	0.9900	C26—C27	1.382 (6)
C9—C10	1.394 (6)	C26—H26	0.9500
C9—C14	1.403 (5)	C27—C28	1.387 (6)
C10—C11	1.389 (6)	C27—H27	0.9500

C1—O1—C7	117.3 (4)	C12—C13—H13	121.2
C15—O2—C21	118.5 (4)	C14—C13—H13	121.2
C8—N1—C9	106.6 (5)	C13—C14—N2	130.7 (4)
C8—N1—H1	127 (3)	C13—C14—C9	120.2 (4)
C9—N1—H1	126 (3)	N2—C14—C9	109.1 (3)
C8—N2—C14	104.6 (5)	C16—C15—C20	121.8 (8)
C22—N3—C23	107.3 (5)	C16—C15—O2	114.3 (6)
C22—N3—H3	129 (3)	C20—C15—O2	124.0 (7)
C23—N3—H3	124 (3)	C17—C16—C15	119.8 (8)
C22—N4—C28	104.1 (4)	C17—C16—H16	120.1
C6—C1—O1	125.2 (7)	C15—C16—H16	120.1
C6—C1—C2	120.1 (8)	C16—C17—C18	119.7 (10)
O1—C1—C2	114.7 (7)	C16—C17—H17	120.1
C3—C2—C1	119.1 (9)	C18—C17—H17	120.1
C3—C2—H2	120.4	C19—C18—C17	119.7 (8)
C1—C2—H2	120.4	C19—C18—H18	120.2
C2—C3—C4	121.4 (11)	C17—C18—H18	120.2
C2—C3—H3A	119.3	C18—C19—C20	121.9 (9)
C4—C3—H3A	119.3	C18—C19—H19	119.0
C5—C4—C3	118.6 (8)	C20—C19—H19	119.0
C5—C4—H4	120.7	C15—C20—C19	117.0 (11)
C3—C4—H4	120.7	C15—C20—H20	121.5
C6—C5—C4	120.6 (9)	C19—C20—H20	121.5
C6—C5—H5	119.7	O2—C21—C22	106.5 (4)
C4—C5—H5	119.7	O2—C21—H21A	110.4
C1—C6—C5	120.2 (10)	C22—C21—H21A	110.4
C1—C6—H6	119.9	O2—C21—H21B	110.4
C5—C6—H6	119.9	C22—C21—H21B	110.4
O1—C7—C8	106.6 (4)	H21A—C21—H21B	108.6
O1—C7—H7A	110.4	N4—C22—N3	113.0 (5)
C8—C7—H7A	110.4	N4—C22—C21	123.7 (5)
O1—C7—H7B	110.4	N3—C22—C21	123.1 (5)
C8—C7—H7B	110.4	N3—C23—C24	131.8 (4)

H7A—C7—H7B	108.6	N3—C23—C28	105.7 (4)
N2—C8—N1	114.3 (5)	C24—C23—C28	122.5 (4)
N2—C8—C7	124.8 (5)	C25—C24—C23	116.6 (4)
N1—C8—C7	120.6 (5)	C25—C24—H24	121.7
N1—C9—C10	132.6 (4)	C23—C24—H24	121.7
N1—C9—C14	105.3 (4)	C24—C25—C26	122.0 (4)
C10—C9—C14	122.1 (4)	C24—C25—H25	119.0
C11—C10—C9	117.0 (4)	C26—C25—H25	119.0
C11—C10—H10	121.5	C27—C26—C25	121.2 (4)
C9—C10—H10	121.5	C27—C26—H26	119.4
C10—C11—C12	120.9 (4)	C25—C26—H26	119.4
C10—C11—H11	119.5	C26—C27—C28	117.5 (4)
C12—C11—H11	119.5	C26—C27—H27	121.3
C13—C12—C11	122.0 (4)	C28—C27—H27	121.3
C13—C12—H12	119.0	C27—C28—N4	129.8 (4)
C11—C12—H12	119.0	C27—C28—C23	120.2 (4)
C12—C13—C14	117.7 (4)	N4—C28—C23	110.0 (3)

C7—O1—C1—C6	−6.1 (11)	C21—O2—C15—C16	−172.0 (6)
C7—O1—C1—C2	174.2 (6)	C21—O2—C15—C20	7.9 (10)
C6—C1—C2—C3	−0.5 (15)	C20—C15—C16—C17	−0.9 (14)
O1—C1—C2—C3	179.1 (8)	O2—C15—C16—C17	179.0 (8)
C1—C2—C3—C4	0.6 (18)	C15—C16—C17—C18	2.4 (16)
C2—C3—C4—C5	−0.4 (18)	C16—C17—C18—C19	−2.4 (16)
C3—C4—C5—C6	0.0 (15)	C17—C18—C19—C20	1.1 (14)
O1—C1—C6—C5	−179.4 (6)	C16—C15—C20—C19	−0.4 (15)
C2—C1—C6—C5	0.2 (16)	O2—C15—C20—C19	179.6 (6)
C4—C5—C6—C1	0.1 (16)	C18—C19—C20—C15	0.4 (15)
C1—O1—C7—C8	172.5 (5)	C15—O2—C21—C22	−172.6 (5)
C14—N2—C8—N1	−1.5 (7)	C28—N4—C22—N3	0.2 (7)
C14—N2—C8—C7	173.1 (5)	C28—N4—C22—C21	−175.0 (5)
C9—N1—C8—N2	2.0 (8)	C23—N3—C22—N4	−1.0 (7)
C9—N1—C8—C7	−172.9 (5)	C23—N3—C22—C21	174.3 (5)
O1—C7—C8—N2	146.8 (6)	O2—C21—C22—N4	−149.1 (5)
O1—C7—C8—N1	−39.0 (7)	O2—C21—C22—N3	36.1 (7)
C8—N1—C9—C10	177.0 (5)	C22—N3—C23—C24	−176.6 (5)
C8—N1—C9—C14	−1.6 (6)	C22—N3—C23—C28	1.3 (6)
N1—C9—C10—C11	−177.4 (5)	N3—C23—C24—C25	176.7 (5)
C14—C9—C10—C11	1.0 (6)	C28—C23—C24—C25	−1.0 (6)
C9—C10—C11—C12	−2.2 (6)	C23—C24—C25—C26	1.5 (7)
C10—C11—C12—C13	1.2 (6)	C24—C25—C26—C27	−0.5 (7)
C11—C12—C13—C14	1.1 (6)	C25—C26—C27—C28	−1.1 (6)
C12—C13—C14—N2	176.8 (4)	C26—C27—C28—N4	−175.4 (4)
C12—C13—C14—C9	−2.3 (5)	C26—C27—C28—C23	1.5 (6)
C8—N2—C14—C13	−178.8 (5)	C22—N4—C28—C27	177.8 (5)
C8—N2—C14—C9	0.4 (6)	C22—N4—C28—C23	0.7 (5)
N1—C9—C14—C13	−179.9 (4)	N3—C23—C28—C27	−178.7 (4)
C10—C9—C14—C13	1.3 (6)	C24—C23—C28—C27	−0.5 (6)

N1—C9—C14—N2	0.7 (5)	N3—C23—C28—N4	−1.3 (5)
C10—C9—C14—N2	−178.0 (4)	C24—C23—C28—N4	176.9 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2^{i}	0.88 (1)	2.03 (2)	2.879 (7)	163 (6)
N3—H3···N4^{ii}	0.88 (1)	1.97 (2)	2.845 (8)	172 (5)

Symmetry codes: (i) *x*−1/2, −*y*+2, *z*; (ii) *x*−1/2, −*y*+1, *z*.