Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis{2-[1-(8-hydroxy-2-quinolylmethyl)-1*H*-benzimidazol-2-yl]quinolin-8-ol} toluene solvate

Hui-Li Chen,[a]* Qi Ma[a,b] and Qing-Ming Wang[a]

[a]Institute of Molecular Science, Key Laboratory of Chemical Biology and Molecular, Engineering of the Education Ministry, Shanxi University, Taiyuan, Shanxi 030006, People's Republic of China, and [b]College of Chemistry and Chemical Engineering , Shanxi Datong University, Datong, Shanxi 037009, People's Republic of China
Correspondence e-mail: huilichen@sxu.edu.cn

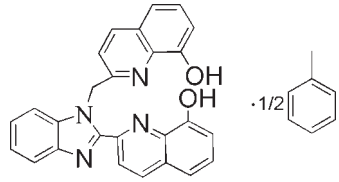
Received 9 December 2009; accepted 7 February 2010

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; H-atom completeness 98%; disorder in solvent or counterion; R factor = 0.051; wR factor = 0.156; data-to-parameter ratio = 12.4.

Crystals of the title compound, $2C_{26}H_{18}N_4O_2\cdot C_7H_8$, were obtained from the reaction of 8-hydroxyquinoline with 1,2-phenylenediamine in methanol and recrystallized from toluene. The compound contains three essentially planar ring systems: the benzimidazole ring (r.m.s. deviation = 0.039 Å) and two 8-hydroxyquinoline rings (r.m.s. deviations of 0.0056 Å in both rings). The benzimidazole ring and one 8-hydroxyquinoline ring are almost co-planar, forming a dihdral angle of 3.1 (2)°. The other 8-hydroxyquinoline ring is almost perpendicular to the benzimidazole plane with a dihedral angle of 86.2 (2)°. Intramolecular O—H···N contacts are present. The crystal structure is stabilized by intermolecular O—H···N interactions. The complete toluene molecule is generated by crystallographic inversion symmetry; therefore its methyl group is disordered over two sites of equal occupancy.

Related literature

For the use of the reaction of *o*-phenylenediamine with excess aldehyde without an oxidant to produce a Shiff base compound containing two —N=CH— bonds, see: Chen & Martell (1987); Wang *et al.* (1994). Similar benzimidazole derivatives have been obtained, see: Dege *et al.* (2006); Yang *et al.* (2004). For the preparation of benzimidazole, see: Boufatah *et al.* (2004); Grimmet (1997); Kumar *et al.* (1981); Srivastava & Venkataramair (1988).



Experimental

Crystal data

$2C_{26}H_{18}N_4O_2\cdot C_7H_8$
M_r = 929.02
Triclinic, $P\overline{1}$
a = 8.014 (7) Å
b = 12.669 (11) Å
c = 12.727 (11) Å
α = 112.979 (10)°
β = 90.881 (11)°
γ = 100.966 (11)°
V = 1162.1 (17) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 K
0.30 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.975, T_{max} = 0.987
6333 measured reflections
4077 independent reflections
3049 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.156
S = 1.03
4077 reflections
329 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	2.29	2.745 (3)	116
O1—H1···N4	0.82	2.47	3.131 (3)	139
O2—H2···N4	0.82	2.27	2.722 (3)	116
O2—H2···N2^{i}	0.82	2.55	3.145 (3)	131

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL/PC* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL/PC*.

The authors acknowledge financial support from the National Natural Science Foundation of China (grant No. 20601018) and the Province Natural Science Foundation of Shanxi Province of China (grant No. 2009021006–3).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2138).

References

Boufatah, N., Gellis, A., Maldonado, J. & Vanelle, P. (2004). *Tetrahedron*, **60**, 9131–9137.

Bruker (2000). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Chen, D. & Martell, A. E. (1987). *Inorg. Chem.* **26**, 1026–1030.

Dege, N., Şekerci, M., Servi, S., Dinçer, M. & Demirbaş, Ü. (2006). *Turk J. Chem.* **30**, 103–108.

Grimmet, M. R. (1997). *Imidazole and Benzimidazole Synthesis*. London: Academic Press.

Kumar, S., Kansal, V. & Bhaduri, A. (1981). *Indian J. Chem. Sect. B*, **20**, 254–256.

Sheldrick, G. M. (2001). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Srivastava, R. G. & Venkataramair, P. S. (1988). *Synth. Commun.* **18**, 1537–1544.

Wang, H., Li, S.-L., Liu, D.-X., Cui, X.-G. & Li, X.-Y. (1994). *Acta Chim. Sin.* **52**, 676–682.

Yang, H.-W., Yue, F., Feng, S., Wang, J.-D., Liu, A.-H., Chen, H.-M. & Yu, K.-B. (2004). *Chin. J. Org. Chem.* **24**, 792–796.

supporting information

Acta Cryst. (2010). E**66**, o671–o672 [doi:10.1107/S1600536810004794]

Bis{2-[1-(8-hydroxy-2-quinolylmethyl)-1*H*-benzimidazol-2-yl]quinolin-8-ol} toluene solvate

Hui-Li Chen, Qi Ma and Qing-Ming Wang

S1. Comment

In most cases, without oxidant, the reaction of *o*-phenylenediamine with excess aldehyde produces a Shiff-base compound containing two —N═CH— bonds (Chen *et al.*,1987; Wang *et al.*,1994). However, in our case, the reaction of *o*-phenylenediamine with 3 equivalents of 8-hydroxyquinoline-2-aldehyde did not form the desired compound. Instead, the reaction produced a novel 2-substituted benzimidazole. Similar benzimidazole derivatives were also obtained by Dege and Yang (Dege *et al.*, 2006; Yang *et al.*, 2004). Usually, one of the general routes for synthesis of benzimidazole involves the reaction of a carboxylic acid with *o*-phenylenediamine in the presence of a strong acid (Grimmet *et al.*, 1997; Boufatah *et al.*, 2004). Another typical procedure involves heating *o*-phenylenediamine with an aldehyde in the presence of oxidant, such as $Pb(OAc)_4$ (Kumar *et al.*, 1981), $BaMnO_4$ (Srivastava *et al.*, 1988).

The molecular structure and a packing diagram of the title compound are illustrated in Figs 1 and 2, respectively. Selected geometric parameters are listed in Table 1.The compound contains 3 planar rings. One is the benzimidazole ring (N2, N3, C10—C16); the others are the 8-hydroxyquinoline rings. The 8-hydroxyquinoline ring [A(N1,O1,C1—C9)] attached to C10, is almost coplanar with the benzimidazole ring (with a dihedral angle of 3.1 (2)°). The other 8-hydroxyquinoline group [B(N4,O2,C18—C26)], was attached to the C17 methylene group almost perpendicular to the benzimidazole plane (with a dihedral angle of 93.8 (2)°). Two 8-hydroxyquinoline rings (A and B) form a dihedral angle of 96.5 (2)°. The C17—C18,C17—N3 and N2—C10 bond distances are 1.513 (3), 1.462 (3) and 1.327 (3) Å, which are similar to the corresponding bond lengths in 1-(thiophen-2-ylmethyl)-2-(thiophen-2-yl)-1*H*-benzimidazole (1.501 (3), 1.452 (3) and 1.315 (3) Å) (Dege *et al.*, 2006). There is a strong intermolecular between O2—H2···N2(x + 1,y,z), with a H2···N2 distance of 2.55 Å (Figure 2, Table 2).

S2. Experimental

A solution of 1,2-diaminobenzene (0.001 mol) in absolute methanol (20 ml) was added in small portions to a solution of 8-hydroxyquinoline-2-aldehyde (0.003 mol) in absolute methanol (30 ml). The reaction mixture was maintained at 348 K for 2 h,and was monitored by TLC. The resulting precipitation was washed with methanol, dried and recrystallized from toluene. ^{1}H NMR(d6-DMSO):9.46(s,1*H*),9.33(s,1*H*),8.56(d,1*H*),8.47(d,1*H*),8.15(d,1*H*), 7.82–7.85(m,2*H*),7.42–7.48(m,2*H*),7.08–7.40(m,7*H*),6.73(s,2*H*).

S3. Refinement

Toluene molecule is located at a symmetrical center, so 4-H of toluene is not present. H atoms attached to C atoms were placed in geometrically idealized positions with Csp^2—H = 0.93 Å and Csp^3—H = 0.96 Å, and were constrained to ride on their parent atoms.

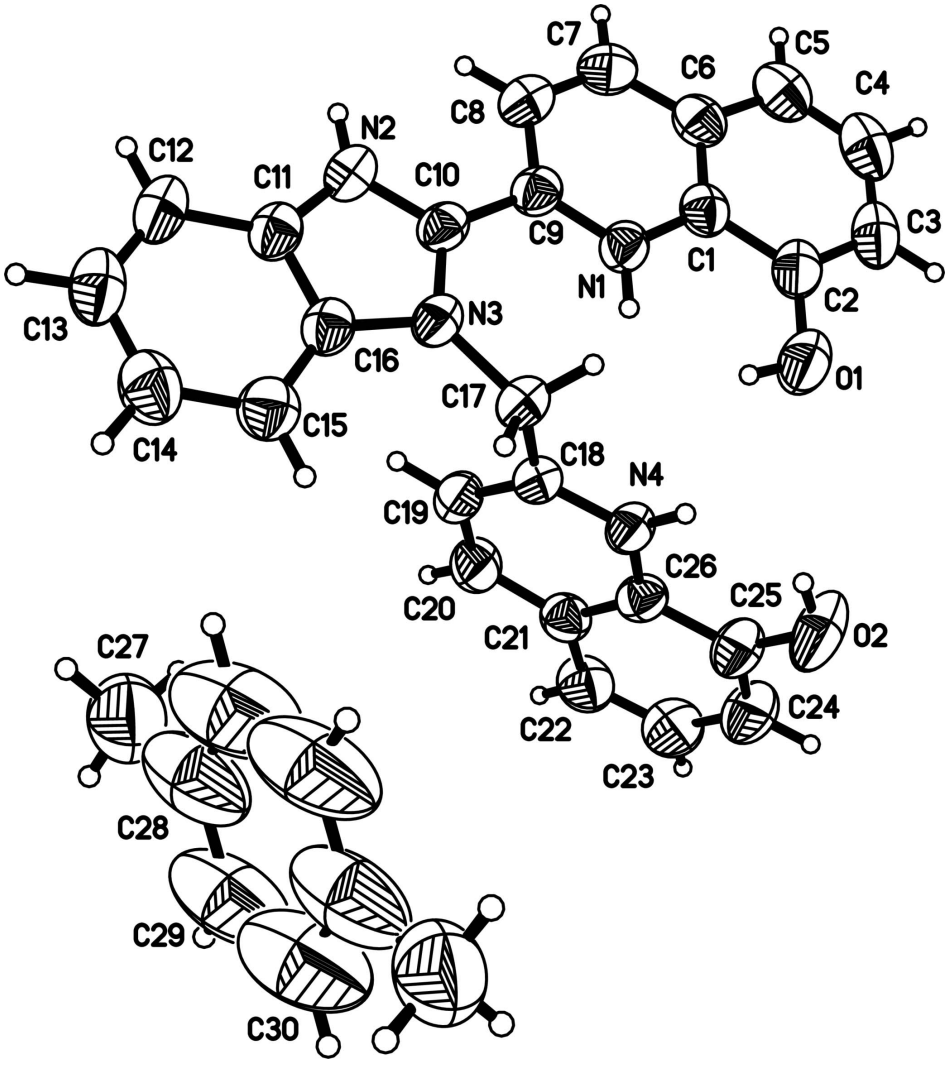


Figure 1

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

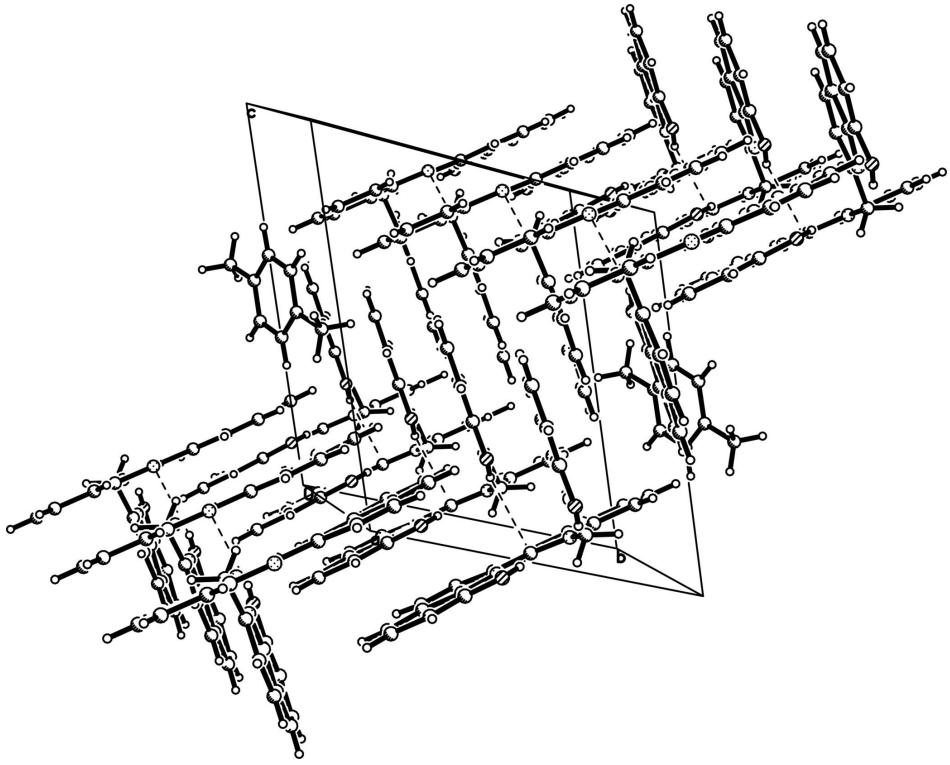


Figure 2

The packing view of the title compound.

Bis{2-[1-(8-hydroxy-2-quinolylmethyl)-1*H*-benzimidazol-2-yl]quinolin- 8-ol} toluene solvate

Crystal data

$2C_{26}H_{18}N_4O_2\cdot C_7H_8$
$M_r = 929.02$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.014\ (7)$ Å
$b = 12.669\ (11)$ Å
$c = 12.727\ (11)$ Å
$\alpha = 112.979\ (10)°$
$\beta = 90.881\ (11)°$
$\gamma = 100.966\ (11)°$
$V = 1162.1\ (17)$ Å^3
$Z = 1$
$F(000) = 486$
$D_x = 1.327$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2466 reflections
$\theta = 3.0–25.9°$
$\mu = 0.09$ mm^{-1}
$T = 295$ K
Block, yellow
0.30 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{min} = 0.975$, $T_{max} = 0.987$
6333 measured reflections
4077 independent reflections
3049 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 25.1°$, $\theta_{min} = 1.8°$
$h = -9\rightarrow7$
$k = -15\rightarrow14$
$l = -12\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.156$
$S = 1.03$
4077 reflections
329 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0768P)^2 + 0.2872P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.033 (4)

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.

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 $F^2 > \sigma(F^2)$ 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}	Occ. (<1)
C1	0.5707 (3)	0.12196 (18)	−0.05782 (17)	0.0455 (5)	
C2	0.7346 (3)	0.0952 (2)	−0.0469 (2)	0.0535 (6)	
C3	0.7601 (3)	−0.0148 (2)	−0.1092 (2)	0.0624 (6)	
H3	0.8668	−0.0316	−0.1027	0.075*	
C4	0.6260 (4)	−0.1028 (2)	−0.1830 (2)	0.0676 (7)	
H4	0.6453	−0.1773	−0.2248	0.081*	
C5	0.4679 (3)	−0.0808 (2)	−0.1944 (2)	0.0633 (6)	
H5	0.3807	−0.1402	−0.2435	0.076*	
C6	0.4366 (3)	0.03220 (19)	−0.13169 (18)	0.0509 (5)	
C7	0.2767 (3)	0.0626 (2)	−0.13557 (19)	0.0556 (6)	
H7	0.1833	0.0059	−0.1805	0.067*	
C8	0.2582 (3)	0.17396 (19)	−0.07426 (19)	0.0524 (6)	
H8	0.1532	0.1942	−0.0774	0.063*	
C9	0.4018 (2)	0.25868 (18)	−0.00545 (17)	0.0434 (5)	
C10	0.3807 (2)	0.37994 (17)	0.05742 (16)	0.0421 (5)	
C11	0.2623 (3)	0.52959 (18)	0.12008 (18)	0.0462 (5)	
C12	0.1518 (3)	0.6075 (2)	0.1430 (2)	0.0554 (6)	
H12	0.0394	0.5825	0.1100	0.066*	
C13	0.2159 (3)	0.7227 (2)	0.2162 (2)	0.0625 (6)	
H13	0.1452	0.7763	0.2325	0.075*	
C14	0.3845 (3)	0.7607 (2)	0.2665 (2)	0.0652 (7)	
H14	0.4228	0.8390	0.3160	0.078*	
C15	0.4960 (3)	0.6855 (2)	0.2448 (2)	0.0569 (6)	

H15	0.6081	0.7112	0.2783	0.068*	
C16	0.4318 (2)	0.56921 (18)	0.16998 (17)	0.0441 (5)	
C17	0.6860 (2)	0.47670 (18)	0.15656 (18)	0.0437 (5)	
H17A	0.7497	0.5569	0.1811	0.052*	
H17B	0.7314	0.4293	0.0878	0.052*	
C18	0.7154 (2)	0.43377 (16)	0.24939 (16)	0.0411 (5)	
C19	0.5972 (3)	0.43317 (19)	0.33017 (18)	0.0511 (5)	
H19	0.4935	0.4545	0.3249	0.061*	
C20	0.6374 (3)	0.4007 (2)	0.41619 (19)	0.0557 (6)	
H20	0.5605	0.4004	0.4701	0.067*	
C21	0.7938 (3)	0.36783 (18)	0.42466 (17)	0.0481 (5)	
C22	0.8471 (3)	0.3341 (2)	0.5118 (2)	0.0632 (6)	
H22	0.7776	0.3338	0.5695	0.076*	
C23	1.0006 (4)	0.3022 (2)	0.5104 (2)	0.0702 (7)	
H23	1.0346	0.2799	0.5675	0.084*	
C24	1.1081 (3)	0.3024 (2)	0.4245 (2)	0.0680 (7)	
H24	1.2123	0.2804	0.4252	0.082*	
C25	1.0602 (3)	0.3348 (2)	0.3397 (2)	0.0556 (6)	
C26	0.9023 (2)	0.36878 (17)	0.33817 (17)	0.0440 (5)	
C27	0.6666 (8)	0.9326 (7)	0.5448 (6)	0.109 (2)	0.50
H27A	0.6352	0.8484	0.5116	0.163*	0.50
H27B	0.5904	0.9635	0.5112	0.163*	0.50
H27C	0.6590	0.9610	0.6260	0.163*	0.50
C28	0.8398 (8)	0.9701 (3)	0.5231 (4)	0.1311 (17)	
C29	0.8662 (8)	0.9652 (4)	0.4163 (4)	0.151 (2)	
H29	0.7753	0.9409	0.3601	0.181*	
C30	1.0280 (8)	0.9965 (4)	0.3939 (4)	0.141 (2)	
H30	1.0493	0.9953	0.3219	0.169*	
N1	0.5530 (2)	0.23373 (15)	0.00443 (14)	0.0448 (4)	
N2	0.2332 (2)	0.41096 (15)	0.05066 (15)	0.0486 (5)	
N3	0.5069 (2)	0.47278 (14)	0.12805 (14)	0.0426 (4)	
N4	0.8615 (2)	0.40046 (14)	0.25095 (14)	0.0437 (4)	
O1	0.8628 (2)	0.17832 (16)	0.02683 (16)	0.0740 (5)	
H1	0.8293	0.2394	0.0589	0.111*	
O2	1.1662 (2)	0.3371 (2)	0.25782 (18)	0.0811 (6)	
H2	1.1174	0.3512	0.2093	0.122*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0529 (12)	0.0487 (12)	0.0422 (12)	0.0166 (9)	0.0120 (9)	0.0232 (10)
C2	0.0539 (13)	0.0595 (14)	0.0556 (14)	0.0219 (11)	0.0143 (10)	0.0271 (11)
C3	0.0682 (16)	0.0667 (16)	0.0672 (16)	0.0343 (13)	0.0272 (12)	0.0325 (13)
C4	0.091 (2)	0.0566 (15)	0.0625 (16)	0.0302 (14)	0.0287 (14)	0.0244 (12)
C5	0.0789 (17)	0.0514 (14)	0.0552 (14)	0.0112 (12)	0.0127 (12)	0.0176 (11)
C6	0.0610 (14)	0.0511 (13)	0.0430 (12)	0.0117 (10)	0.0097 (10)	0.0214 (10)
C7	0.0552 (13)	0.0541 (14)	0.0526 (13)	0.0027 (10)	−0.0015 (10)	0.0204 (11)
C8	0.0441 (12)	0.0589 (14)	0.0560 (13)	0.0092 (10)	−0.0010 (10)	0.0260 (11)

C9	0.0438 (11)	0.0506 (12)	0.0424 (11)	0.0128 (9)	0.0048 (8)	0.0243 (9)
C10	0.0395 (11)	0.0515 (12)	0.0420 (11)	0.0120 (9)	0.0034 (8)	0.0249 (9)
C11	0.0455 (11)	0.0545 (13)	0.0492 (12)	0.0162 (9)	0.0099 (9)	0.0291 (10)
C12	0.0471 (12)	0.0673 (15)	0.0682 (15)	0.0250 (11)	0.0153 (10)	0.0383 (13)
C13	0.0691 (16)	0.0657 (16)	0.0717 (16)	0.0334 (13)	0.0234 (12)	0.0382 (13)
C14	0.0793 (17)	0.0525 (14)	0.0670 (16)	0.0222 (12)	0.0132 (13)	0.0236 (12)
C15	0.0582 (14)	0.0547 (14)	0.0584 (14)	0.0136 (11)	0.0034 (11)	0.0227 (11)
C16	0.0465 (11)	0.0502 (12)	0.0455 (12)	0.0166 (9)	0.0089 (9)	0.0267 (10)
C17	0.0359 (10)	0.0505 (12)	0.0486 (12)	0.0099 (8)	0.0023 (8)	0.0236 (9)
C18	0.0375 (10)	0.0424 (11)	0.0410 (11)	0.0084 (8)	0.0008 (8)	0.0142 (9)
C19	0.0423 (11)	0.0665 (14)	0.0477 (13)	0.0199 (10)	0.0052 (9)	0.0225 (11)
C20	0.0548 (13)	0.0716 (15)	0.0456 (13)	0.0202 (11)	0.0140 (10)	0.0254 (11)
C21	0.0557 (13)	0.0482 (12)	0.0412 (12)	0.0143 (10)	0.0029 (9)	0.0173 (9)
C22	0.0791 (17)	0.0717 (16)	0.0489 (14)	0.0247 (13)	0.0084 (12)	0.0309 (12)
C23	0.0856 (19)	0.0767 (17)	0.0633 (16)	0.0304 (14)	−0.0019 (13)	0.0381 (14)
C24	0.0625 (15)	0.0780 (17)	0.0804 (18)	0.0291 (13)	0.0023 (13)	0.0431 (14)
C25	0.0489 (13)	0.0634 (14)	0.0669 (15)	0.0196 (11)	0.0063 (11)	0.0357 (12)
C26	0.0437 (11)	0.0418 (11)	0.0466 (12)	0.0084 (9)	−0.0012 (9)	0.0184 (9)
C27	0.126 (6)	0.111 (6)	0.093 (5)	0.052 (5)	0.008 (5)	0.033 (4)
C28	0.243 (5)	0.064 (2)	0.083 (3)	0.045 (3)	−0.029 (3)	0.0222 (18)
C29	0.262 (7)	0.096 (3)	0.094 (3)	0.027 (4)	−0.041 (4)	0.044 (2)
C30	0.268 (7)	0.085 (3)	0.069 (3)	0.036 (4)	−0.027 (4)	0.031 (2)
N1	0.0448 (10)	0.0504 (10)	0.0444 (10)	0.0156 (8)	0.0062 (7)	0.0220 (8)
N2	0.0403 (9)	0.0540 (11)	0.0579 (11)	0.0146 (8)	0.0035 (8)	0.0270 (9)
N3	0.0383 (9)	0.0491 (10)	0.0464 (10)	0.0136 (7)	0.0035 (7)	0.0237 (8)
N4	0.0381 (9)	0.0495 (10)	0.0473 (10)	0.0131 (7)	0.0031 (7)	0.0217 (8)
O1	0.0539 (10)	0.0736 (12)	0.0870 (13)	0.0276 (9)	0.0027 (9)	0.0180 (10)
O2	0.0540 (10)	0.1300 (17)	0.1009 (15)	0.0461 (11)	0.0256 (10)	0.0773 (13)

Geometric parameters (Å, º)

C1—N1	1.363 (3)	C17—C18	1.513 (3)
C1—C6	1.415 (3)	C17—H17A	0.9700
C1—C2	1.435 (3)	C17—H17B	0.9700
C2—O1	1.354 (3)	C18—N4	1.320 (3)
C2—C3	1.365 (3)	C18—C19	1.410 (3)
C3—C4	1.406 (4)	C19—C20	1.365 (3)
C3—H3	0.9300	C19—H19	0.9300
C4—C5	1.365 (4)	C20—C21	1.409 (3)
C4—H4	0.9300	C20—H20	0.9300
C5—C6	1.414 (3)	C21—C26	1.416 (3)
C5—H5	0.9300	C21—C22	1.421 (3)
C6—C7	1.411 (3)	C22—C23	1.365 (4)
C7—C8	1.358 (3)	C22—H22	0.9300
C7—H7	0.9300	C23—C24	1.403 (4)
C8—C9	1.418 (3)	C23—H23	0.9300
C8—H8	0.9300	C24—C25	1.369 (3)
C9—N1	1.325 (3)	C24—H24	0.9300

C9—C10	1.474 (3)	C25—O2	1.361 (3)
C10—N2	1.327 (3)	C25—C26	1.414 (3)
C10—N3	1.381 (3)	C26—N4	1.374 (3)
C11—N2	1.385 (3)	C27—C28	1.4463 (15)
C11—C12	1.400 (3)	C27—H27A	0.9600
C11—C16	1.402 (3)	C27—H27B	0.9600
C12—C13	1.378 (4)	C27—H27C	0.9600
C12—H12	0.9300	C28—C29	1.358 (6)
C13—C14	1.398 (4)	C28—C30^{i}	1.365 (6)
C13—H13	0.9300	C29—C30	1.351 (9)
C14—C15	1.381 (3)	C29—H29	0.9300
C14—H14	0.9300	C30—C28^{i}	1.365 (6)
C15—C16	1.394 (3)	C30—H30	0.9300
C15—H15	0.9300	O1—H1	0.8200
C16—N3	1.385 (3)	O2—H2	0.8200
C17—N3	1.462 (3)		

N1—C1—C6	123.4 (2)	C18—C17—H17B	108.7
N1—C1—C2	117.63 (19)	H17A—C17—H17B	107.6
C6—C1—C2	119.0 (2)	N4—C18—C19	122.82 (19)
O1—C2—C3	120.0 (2)	N4—C18—C17	115.06 (17)
O1—C2—C1	120.0 (2)	C19—C18—C17	122.09 (18)
C3—C2—C1	120.0 (2)	C20—C19—C18	118.8 (2)
C2—C3—C4	120.4 (2)	C20—C19—H19	120.6
C2—C3—H3	119.8	C18—C19—H19	120.6
C4—C3—H3	119.8	C19—C20—C21	121.0 (2)
C5—C4—C3	121.2 (2)	C19—C20—H20	119.5
C5—C4—H4	119.4	C21—C20—H20	119.5
C3—C4—H4	119.4	C20—C21—C26	115.94 (19)
C4—C5—C6	120.1 (2)	C20—C21—C22	124.9 (2)
C4—C5—H5	119.9	C26—C21—C22	119.2 (2)
C6—C5—H5	119.9	C23—C22—C21	119.8 (2)
C7—C6—C5	124.3 (2)	C23—C22—H22	120.1
C7—C6—C1	116.4 (2)	C21—C22—H22	120.1
C5—C6—C1	119.3 (2)	C22—C23—C24	121.2 (2)
C8—C7—C6	120.6 (2)	C22—C23—H23	119.4
C8—C7—H7	119.7	C24—C23—H23	119.4
C6—C7—H7	119.7	C25—C24—C23	120.2 (2)
C7—C8—C9	118.8 (2)	C25—C24—H24	119.9
C7—C8—H8	120.6	C23—C24—H24	119.9
C9—C8—H8	120.6	O2—C25—C24	120.1 (2)
N1—C9—C8	123.0 (2)	O2—C25—C26	119.5 (2)
N1—C9—C10	118.97 (18)	C24—C25—C26	120.3 (2)
C8—C9—C10	117.98 (18)	N4—C26—C25	117.61 (19)
N2—C10—N3	112.54 (18)	N4—C26—C21	123.14 (19)
N2—C10—C9	122.02 (18)	C25—C26—C21	119.2 (2)
N3—C10—C9	125.44 (17)	C28—C27—H27A	109.5
N2—C11—C12	129.9 (2)	C28—C27—H27B	109.5

N2—C11—C16	109.73 (17)	H27A—C27—H27B	109.5
C12—C11—C16	120.4 (2)	C28—C27—H27C	109.5
C13—C12—C11	117.5 (2)	H27A—C27—H27C	109.5
C13—C12—H12	121.2	H27B—C27—H27C	109.5
C11—C12—H12	121.2	C29—C28—C30^{i}	121.6 (5)
C12—C13—C14	121.5 (2)	C29—C28—C27	117.7 (6)
C12—C13—H13	119.2	C30^{i}—C28—C27	120.6 (6)
C14—C13—H13	119.2	C30—C29—C28	118.3 (5)
C15—C14—C13	121.9 (2)	C30—C29—H29	120.9
C15—C14—H14	119.0	C28—C29—H29	120.9
C13—C14—H14	119.0	C29—C30—C28^{i}	120.1 (5)
C14—C15—C16	116.6 (2)	C29—C30—H30	120.0
C14—C15—H15	121.7	C28^{i}—C30—H30	120.0
C16—C15—H15	121.7	C9—N1—C1	117.77 (18)
N3—C16—C15	132.0 (2)	C10—N2—C11	105.48 (17)
N3—C16—C11	106.02 (18)	C10—N3—C16	106.21 (16)
C15—C16—C11	122.00 (19)	C10—N3—C17	129.92 (17)
N3—C17—C18	114.36 (16)	C16—N3—C17	123.86 (16)
N3—C17—H17A	108.7	C18—N4—C26	118.16 (17)
C18—C17—H17A	108.7	C2—O1—H1	109.5
N3—C17—H17B	108.7	C25—O2—H2	109.5

N1—C1—C2—O1	2.7 (3)	C19—C20—C21—C22	179.3 (2)
C6—C1—C2—O1	−177.24 (19)	C20—C21—C22—C23	179.0 (2)
N1—C1—C2—C3	−178.68 (19)	C26—C21—C22—C23	−0.6 (3)
C6—C1—C2—C3	1.4 (3)	C21—C22—C23—C24	0.3 (4)
O1—C2—C3—C4	177.8 (2)	C22—C23—C24—C25	−0.1 (4)
C1—C2—C3—C4	−0.8 (3)	C23—C24—C25—O2	178.7 (2)
C2—C3—C4—C5	0.0 (4)	C23—C24—C25—C26	0.2 (4)
C3—C4—C5—C6	0.2 (4)	O2—C25—C26—N4	1.5 (3)
C4—C5—C6—C7	−178.4 (2)	C24—C25—C26—N4	179.9 (2)
C4—C5—C6—C1	0.4 (3)	O2—C25—C26—C21	−179.1 (2)
N1—C1—C6—C7	−2.3 (3)	C24—C25—C26—C21	−0.6 (3)
C2—C1—C6—C7	177.70 (19)	C20—C21—C26—N4	0.6 (3)
N1—C1—C6—C5	178.91 (19)	C22—C21—C26—N4	−179.78 (19)
C2—C1—C6—C5	−1.1 (3)	C20—C21—C26—C25	−178.89 (19)
C5—C6—C7—C8	−178.7 (2)	C22—C21—C26—C25	0.8 (3)
C1—C6—C7—C8	2.5 (3)	C30^{i}—C28—C29—C30	−1.2 (8)
C6—C7—C8—C9	−0.7 (3)	C27—C28—C29—C30	−178.0 (5)
C7—C8—C9—N1	−1.8 (3)	C28—C29—C30—C28^{i}	1.2 (8)
C7—C8—C9—C10	178.01 (19)	C8—C9—N1—C1	2.2 (3)
N1—C9—C10—N2	179.53 (18)	C10—C9—N1—C1	−177.69 (17)
C8—C9—C10—N2	−0.3 (3)	C6—C1—N1—C9	0.0 (3)
N1—C9—C10—N3	−0.2 (3)	C2—C1—N1—C9	180.00 (18)
C8—C9—C10—N3	179.92 (18)	N3—C10—N2—C11	−0.2 (2)
N2—C11—C12—C13	−179.8 (2)	C9—C10—N2—C11	−179.95 (17)
C16—C11—C12—C13	−0.5 (3)	C12—C11—N2—C10	178.8 (2)
C11—C12—C13—C14	−0.3 (3)	C16—C11—N2—C10	−0.6 (2)

C12—C13—C14—C15	0.6 (4)	N2—C10—N3—C16	0.8 (2)
C13—C14—C15—C16	−0.1 (4)	C9—C10—N3—C16	−179.41 (18)
C14—C15—C16—N3	178.5 (2)	N2—C10—N3—C17	−178.58 (18)
C14—C15—C16—C11	−0.8 (3)	C9—C10—N3—C17	1.2 (3)
N2—C11—C16—N3	1.0 (2)	C15—C16—N3—C10	179.6 (2)
C12—C11—C16—N3	−178.36 (18)	C11—C16—N3—C10	−1.1 (2)
N2—C11—C16—C15	−179.55 (19)	C15—C16—N3—C17	−1.0 (3)
C12—C11—C16—C15	1.1 (3)	C11—C16—N3—C17	178.35 (17)
N3—C17—C18—N4	158.92 (17)	C18—C17—N3—C10	−81.6 (3)
N3—C17—C18—C19	−23.0 (3)	C18—C17—N3—C16	99.1 (2)
N4—C18—C19—C20	2.3 (3)	C19—C18—N4—C26	−2.8 (3)
C17—C18—C19—C20	−175.59 (19)	C17—C18—N4—C26	175.22 (16)
C18—C19—C20—C21	−0.3 (3)	C25—C26—N4—C18	−179.18 (18)
C19—C20—C21—C26	−1.1 (3)	C21—C26—N4—C18	1.4 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	2.29	2.745 (3)	116
O1—H1···N4	0.82	2.47	3.131 (3)	139
O2—H2···N4	0.82	2.27	2.722 (3)	116
O2—H2···N2^{ii}	0.82	2.55	3.145 (3)	131

Symmetry code: (ii) *x*+1, *y*, *z*.