Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Terephthalic acid–2,2′-dimethyl-1,1′-(butane-1,4-diyl)dibenzimidazole (2/3)

Hui Jiang and Xian-Wu Dong*

Department of Chemistry, Jilin Agriculture Science and Technology College, Jilin 132101, People's Republic of China
Correspondence e-mail: jiangh_468@yahoo.com.cn

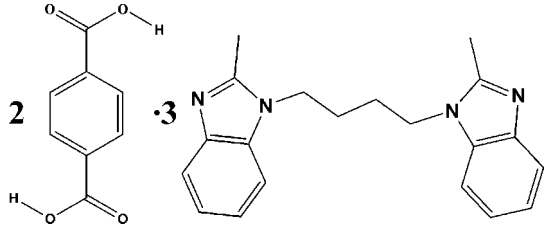
Received 22 November 2007; accepted 8 April 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.071; wR factor = 0.164; data-to-parameter ratio = 17.3.

In the crystal structure of the title compound, $2C_8H_6O_4\cdot 3C_{20}H_{22}N_4$, there are three independent 2,2′-dimethyl-1,1′-(butane-1,4-diyl)dibenzimidazole molecules, each of which lies on an inversion centre. The terephthalic acid molecules are linked to adjacent 2,2′-dimethyl-1,1′-(butane-1,4-diyl)dibenzimidazole molecules *via* O—H···N hydrogen bonds.

Related literature

For related literature, see: Dale & Elsegood (2004); Ma *et al.* (2000).



Experimental

Crystal data

$2C_8H_6O_4\cdot 3C_{20}H_{22}N_4$
M_r = 1286.88
Triclinic, $P\overline{1}$
a = 9.225 (5) Å
b = 12.298 (8) Å
c = 14.883 (7) Å
α = 87.17 (2)°
β = 87.768 (16)°
γ = 89.33 (2)°
V = 1685.0 (16) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.49 × 0.38 × 0.26 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.963, T_{max} = 0.977
16449 measured reflections
7573 independent reflections
3739 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.163
S = 1.01
7573 reflections
437 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.82	1.83	2.609 (3)	157
O3—H3A···N3^{ii}	0.82	1.87	2.668 (3)	165

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL-Plus* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The authors thank the Analysis and Testing Foundation of Northeast Normal University for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CS2066).

References

Dale, S. H. & Elsegood, M. R. J. (2004). *Acta Cryst.* C**60**, o444–o448.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Ma, J.-F., Liu, J.-F., Liu, Y.-C., Xing, Y., Jia, H.-Q. & Lin, Y.-H. (2000). *New J. Chem.* **24**, 759–763.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

  doi:10.1107/S1600536808009665

supporting information

Acta Cryst. (2008). E**64**, o838 [doi:10.1107/S1600536808009665]

Terephthalic acid–2,2′-dimethyl-1,1′-(butane-1,4-diyl)dibenzimidazole (2/3)

Hui Jiang and Xian-Wu Dong

S1. Comment

The title compound is composed of terephthalic acid and 2,2′-dimethyl-1,1′-(butane-1,4-diyl)dibenzimidazole (Fig. 1). The bond distances and angles are normal (Dale & Elsegood, 2004; Ma *et al.*, 2000). There are three independent 2,2′-dimethyl-1,1′-(butane-1,4-diyl)dibenzimidazole molecules, which extend in different directions, sitting around independent symmetry centres. The terephthalic acids are hydrogen bonded to the 2,2′-dimethyl-1,1′-(butane-1,4-diyl)dibenzimidazole (Table 1) *via* O—H···N hydrogen bonds into the chains (Fig. 2).

S2. Experimental

A mixture of terephthalic acid (0.033 g, 0.2 mmol), 2,2′-dimethyl-1,1′-(butane-1,4-diyl)dibenzimidazole (0.064 g, 0.2 mmol) in 1:4 (*v*/*v*) EtOH/H_2O (10 ml) was placed in a Teflon-lined autoclave. The mixture was heated at 430 K for 1 days, and then it was gradually cooled to room temperature at a rate of 10 $K.h^{-1}$. Colorless single crystals of the title compound were obtained.

S3. Refinement

All H-atoms bound to carbon were refined using a riding model with d(C—H) = 0.93 Å, $U_{iso} = 1.2U_{eq}$ (C) for aromatic, 0.97 Å, $U_{iso} = 1.5U_{eq}$ (C) for CH_2 atoms and 0.96 Å, $U_{iso} = 1.5U_{eq}$ (C) for CH_3 atoms. Hydroxyl H atoms were refined using a riding model with d(O—H) = 0.82 Å, $U_{iso} = 1.5U_{eq}$ (O).

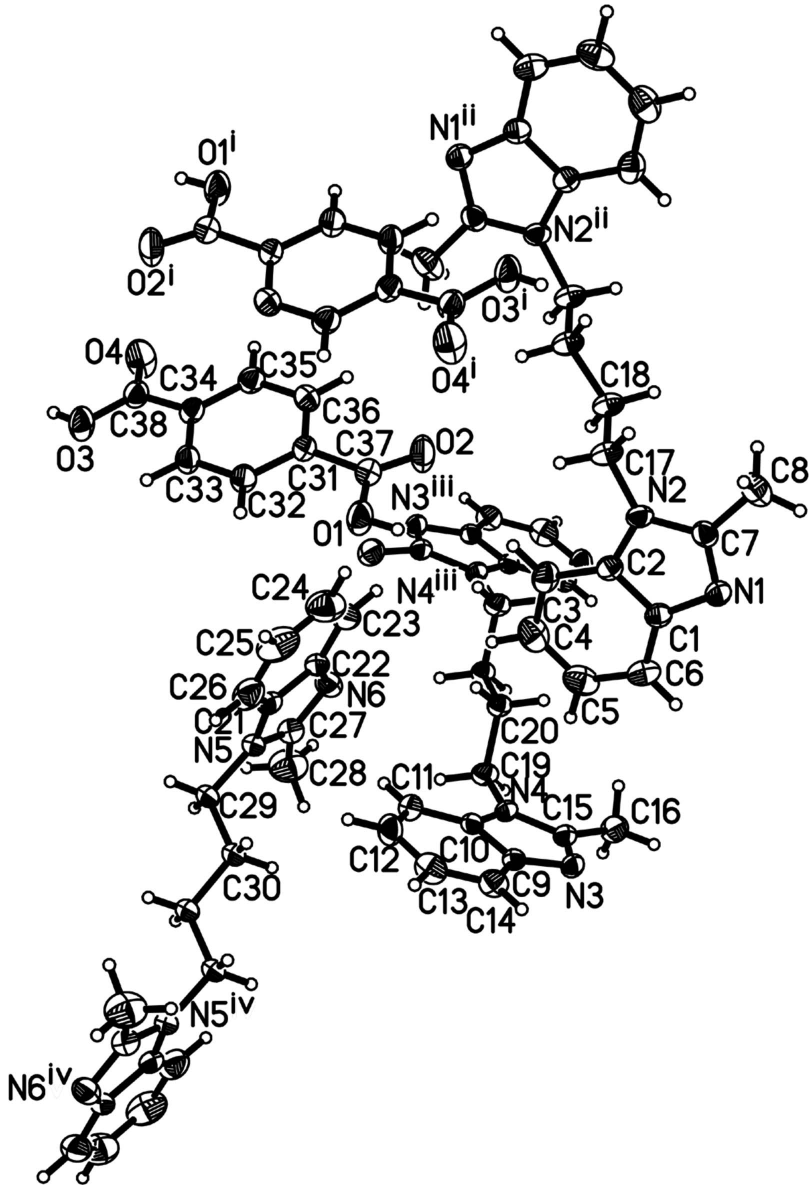


Figure 1

A view of the title clathrate. The displacement ellipsoids are drawn at the 30% probability level.(i) -*x*, -*y*, -*z* + 1. (ii) -*x*, -*y* + 1, -*z* + 1. (iii) -*x* + 1, -*y* + 1, -*z*. (iv) -*x* + 2, -*y*, -*z*.

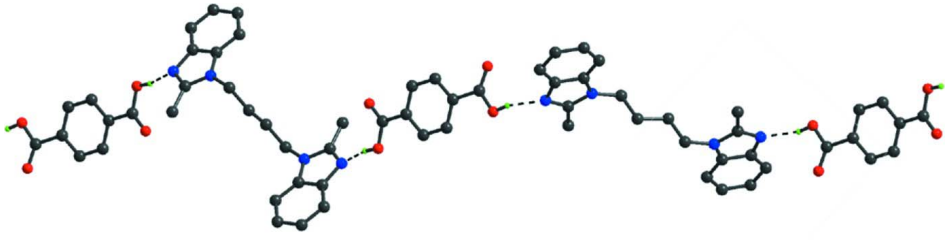


Figure 2

A one-dimensional chain linked by hydrogen bonds. The H-bonds are shown as dashed lines.

Terephthalic acid–2,2′-dimethyl-1,1′-(butane-1,4-diyl)dibenzimidazole (2/3)

Crystal data

$2C_8H_6O_4 \cdot 3C_{20}H_{22}N_4$
$M_r = 1286.88$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.225$ (5) Å
$b = 12.298$ (8) Å
$c = 14.883$ (7) Å
$\alpha = 87.17$ (2)°
$\beta = 87.768$ (16)°
$\gamma = 89.33$ (2)°
$V = 1685.0$ (16) Å^3
$Z = 1$
$F(000) = 682$
$D_x = 1.268$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 7573 reflections
$\theta = 3.0$–27.5°
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Plate, colourless
0.49 × 0.38 × 0.26 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: rotation-anode tube
Graphite monochromator
Detector resolution: 10.0 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.963$, $T_{max} = 0.977$
16449 measured reflections
7573 independent reflections
3739 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -11 \rightarrow 10$
$k = -15 \rightarrow 15$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.071$
$wR(F^2) = 0.163$
$S = 1.01$
7573 reflections
437 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
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0674P)^2 + 0.1144P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0101 (15)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.4952 (3)	0.6452 (2)	0.39701 (16)	0.0443 (6)
C2	0.4004 (3)	0.5588 (2)	0.41249 (16)	0.0436 (6)
C3	0.4031 (3)	0.4701 (2)	0.35876 (18)	0.0565 (7)
H3	0.3405	0.4119	0.3701	0.068*
C4	0.5025 (4)	0.4726 (3)	0.2882 (2)	0.0728 (10)
H4	0.5074	0.4144	0.2505	0.087*
C5	0.5956 (4)	0.5585 (3)	0.2710 (2)	0.0713 (9)
H5	0.6609	0.5570	0.2218	0.086*
C6	0.5948 (3)	0.6460 (3)	0.32422 (18)	0.0592 (8)
H6	0.6581	0.7037	0.3123	0.071*

C7	0.3629 (3)	0.6799 (2)	0.51495 (18)	0.0481 (7)
C8	0.2974 (3)	0.7342 (3)	0.5937 (2)	0.0756 (10)
H8A	0.3136	0.6901	0.6475	0.113*
H8B	0.1949	0.7435	0.5864	0.113*
H8C	0.3410	0.8041	0.5982	0.113*
C9	0.9763 (2)	0.4712 (2)	0.16737 (16)	0.0383 (6)
C10	0.8777 (2)	0.4183 (2)	0.11664 (15)	0.0368 (6)
C11	0.8522 (3)	0.3085 (2)	0.12836 (18)	0.0521 (7)
H11	0.7845	0.2741	0.0951	0.063*
C12	0.9318 (3)	0.2525 (2)	0.1917 (2)	0.0611 (8)
H12	0.9170	0.1782	0.2021	0.073*
C13	1.0343 (3)	0.3039 (3)	0.24080 (18)	0.0621 (8)
H13	1.0883	0.2627	0.2819	0.074*
C14	1.0571 (3)	0.4128 (2)	0.22996 (17)	0.0529 (7)
H14	1.1247	0.4469	0.2635	0.063*
C15	0.8801 (2)	0.5945 (2)	0.08040 (16)	0.0416 (6)
C16	0.8408 (3)	0.7004 (2)	0.0362 (2)	0.0604 (8)
H16A	0.8748	0.7024	−0.0256	0.091*
H16B	0.8848	0.7580	0.0664	0.091*
H16C	0.7373	0.7096	0.0392	0.091*
C17	0.1997 (2)	0.5149 (2)	0.52713 (18)	0.0519 (7)
H17A	0.1880	0.5270	0.5909	0.062*
H17B	0.2251	0.4388	0.5207	0.062*
C18	0.0580 (2)	0.5394 (2)	0.48259 (17)	0.0511 (7)
H18A	0.0717	0.5344	0.4180	0.061*
H18B	0.0269	0.6132	0.4944	0.061*
C19	0.7073 (2)	0.4862 (2)	−0.00500 (16)	0.0469 (7)
H19A	0.7158	0.4139	−0.0281	0.056*
H19B	0.7226	0.5386	−0.0553	0.056*
C20	0.5564 (2)	0.5015 (2)	0.03514 (15)	0.0410 (6)
H20A	0.5369	0.4444	0.0812	0.049*
H20B	0.5502	0.5708	0.0635	0.049*
C21	0.6099 (3)	0.0780 (2)	0.09565 (19)	0.0499 (7)
C22	0.5086 (3)	0.1624 (2)	0.08891 (18)	0.0463 (6)
C23	0.4243 (3)	0.1903 (3)	0.1628 (2)	0.0667 (8)
H23	0.3561	0.2464	0.1585	0.080*
C24	0.4434 (4)	0.1336 (4)	0.2417 (3)	0.0917 (12)
H24	0.3872	0.1516	0.2922	0.110*
C25	0.5439 (5)	0.0499 (4)	0.2497 (3)	0.0946 (13)
H25	0.5544	0.0133	0.3053	0.114*
C26	0.6290 (4)	0.0197 (3)	0.1766 (3)	0.0764 (10)
H26	0.6960	−0.0372	0.1814	0.092*
C27	0.6126 (3)	0.1528 (2)	−0.0416 (2)	0.0569 (7)
C28	0.6558 (4)	0.1745 (4)	−0.1375 (2)	0.0991 (13)
H28A	0.7523	0.2031	−0.1420	0.149*
H28B	0.5899	0.2266	−0.1641	0.149*
H28C	0.6531	0.1081	−0.1685	0.149*
C29	0.7922 (3)	−0.0014 (3)	−0.0138 (3)	0.0739 (10)

H29A	0.7951	−0.0081	−0.0785	0.089*
H29B	0.7731	−0.0729	0.0143	0.089*
C30	0.9373 (3)	0.0365 (2)	0.0140 (3)	0.0741 (10)
H30A	0.9350	0.0407	0.0790	0.089*
H30B	0.9541	0.1093	−0.0121	0.089*
C31	0.1777 (3)	0.0473 (2)	0.42478 (16)	0.0420 (6)
C32	0.2506 (3)	−0.0499 (2)	0.41235 (17)	0.0493 (7)
H32	0.3417	−0.0616	0.4358	0.059*
C33	0.1875 (3)	−0.1296 (2)	0.36497 (17)	0.0490 (7)
H33	0.2373	−0.1947	0.3563	0.059*
C34	0.0517 (3)	−0.1139 (2)	0.33031 (16)	0.0449 (6)
C35	−0.0224 (3)	−0.0178 (2)	0.34588 (18)	0.0504 (7)
H35	−0.1151	−0.0069	0.3245	0.060*
C36	0.0403 (3)	0.0617 (2)	0.39292 (17)	0.0507 (7)
H36	−0.0107	0.1258	0.4033	0.061*
C37	0.2471 (3)	0.1394 (2)	0.46745 (18)	0.0497 (7)
C38	−0.0130 (3)	−0.1938 (2)	0.27258 (19)	0.0518 (7)
N1	0.4693 (2)	0.72048 (18)	0.46235 (15)	0.0498 (6)
N2	0.3174 (2)	0.58270 (18)	0.48811 (13)	0.0442 (5)
N3	0.9751 (2)	0.58143 (17)	0.14404 (14)	0.0445 (5)
N4	0.81999 (19)	0.49945 (16)	0.05991 (13)	0.0393 (5)
N5	0.6745 (2)	0.07253 (18)	0.01097 (17)	0.0530 (6)
N6	0.5129 (2)	0.20832 (19)	0.00184 (15)	0.0567 (6)
O1	0.3721 (2)	0.11390 (16)	0.50186 (14)	0.0674 (6)
H1	0.4049	0.1675	0.5244	0.081*
O2	0.1950 (2)	0.22979 (17)	0.46676 (16)	0.0793 (7)
O3	0.0626 (2)	−0.28314 (16)	0.26517 (13)	0.0667 (6)
H3A	0.0214	−0.3237	0.2325	0.080*
O4	−0.1239 (2)	−0.17682 (18)	0.23391 (17)	0.0881 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0354 (13)	0.0509 (17)	0.0473 (14)	−0.0004 (12)	−0.0090 (12)	−0.0023 (12)
C2	0.0352 (13)	0.0505 (17)	0.0462 (14)	−0.0008 (12)	−0.0111 (12)	−0.0054 (12)
C3	0.0593 (17)	0.0555 (19)	0.0567 (17)	−0.0048 (14)	−0.0188 (15)	−0.0092 (14)
C4	0.086 (2)	0.082 (3)	0.0530 (18)	0.008 (2)	−0.0140 (18)	−0.0234 (17)
C5	0.067 (2)	0.101 (3)	0.0458 (16)	0.007 (2)	0.0036 (15)	−0.0110 (18)
C6	0.0447 (15)	0.077 (2)	0.0550 (17)	−0.0084 (14)	−0.0038 (14)	0.0042 (16)
C7	0.0386 (14)	0.0508 (18)	0.0563 (16)	0.0061 (13)	−0.0086 (13)	−0.0128 (13)
C8	0.073 (2)	0.083 (3)	0.073 (2)	0.0173 (18)	−0.0005 (18)	−0.0272 (18)
C9	0.0306 (12)	0.0401 (15)	0.0448 (13)	0.0012 (10)	−0.0050 (11)	−0.0063 (11)
C10	0.0303 (11)	0.0393 (15)	0.0413 (13)	0.0020 (10)	−0.0022 (11)	−0.0058 (11)
C11	0.0502 (15)	0.0467 (18)	0.0603 (16)	−0.0047 (13)	−0.0004 (14)	−0.0116 (13)
C12	0.074 (2)	0.0376 (17)	0.0702 (19)	0.0023 (15)	0.0017 (17)	0.0047 (14)
C13	0.0659 (19)	0.064 (2)	0.0545 (17)	0.0139 (16)	−0.0068 (15)	0.0121 (15)
C14	0.0465 (15)	0.062 (2)	0.0512 (15)	0.0058 (14)	−0.0139 (13)	−0.0031 (14)
C15	0.0321 (12)	0.0407 (15)	0.0520 (14)	−0.0006 (11)	−0.0035 (12)	−0.0019 (12)

C16	0.0524 (16)	0.0495 (18)	0.079 (2)	0.0006 (13)	−0.0095 (16)	0.0099 (15)
C17	0.0347 (13)	0.067 (2)	0.0529 (15)	−0.0090 (13)	−0.0040 (12)	0.0059 (13)
C18	0.0348 (13)	0.0659 (19)	0.0522 (15)	−0.0069 (12)	−0.0052 (12)	0.0051 (13)
C19	0.0336 (13)	0.0634 (19)	0.0452 (14)	−0.0010 (12)	−0.0112 (12)	−0.0094 (12)
C20	0.0348 (12)	0.0491 (16)	0.0399 (13)	−0.0020 (11)	−0.0075 (11)	−0.0051 (11)
C21	0.0346 (13)	0.0450 (17)	0.0704 (19)	−0.0064 (11)	−0.0049 (14)	−0.0025 (14)
C22	0.0335 (13)	0.0458 (16)	0.0601 (17)	−0.0004 (11)	−0.0031 (13)	−0.0071 (13)
C23	0.0556 (18)	0.074 (2)	0.071 (2)	0.0005 (16)	0.0074 (17)	−0.0108 (17)
C24	0.081 (3)	0.118 (4)	0.075 (3)	−0.013 (2)	0.014 (2)	−0.008 (2)
C25	0.092 (3)	0.117 (4)	0.073 (2)	−0.026 (3)	−0.008 (2)	0.029 (2)
C26	0.064 (2)	0.060 (2)	0.104 (3)	−0.0069 (16)	−0.018 (2)	0.021 (2)
C27	0.0495 (16)	0.0558 (19)	0.0654 (18)	−0.0039 (14)	0.0031 (15)	−0.0061 (15)
C28	0.099 (3)	0.130 (4)	0.068 (2)	−0.011 (3)	0.016 (2)	−0.008 (2)
C29	0.0360 (14)	0.053 (2)	0.135 (3)	0.0018 (13)	0.0092 (17)	−0.0380 (19)
C30	0.0364 (14)	0.053 (2)	0.135 (3)	−0.0005 (13)	0.0082 (17)	−0.0372 (19)
C31	0.0445 (14)	0.0370 (15)	0.0443 (14)	−0.0032 (11)	−0.0018 (12)	0.0001 (11)
C32	0.0450 (14)	0.0439 (17)	0.0599 (16)	0.0015 (12)	−0.0139 (13)	−0.0032 (13)
C33	0.0487 (15)	0.0383 (16)	0.0607 (16)	0.0024 (12)	−0.0113 (14)	−0.0041 (12)
C34	0.0452 (14)	0.0405 (15)	0.0488 (14)	−0.0043 (12)	−0.0051 (12)	0.0039 (12)
C35	0.0419 (14)	0.0489 (18)	0.0606 (16)	−0.0020 (12)	−0.0092 (13)	0.0005 (13)
C36	0.0465 (15)	0.0448 (17)	0.0608 (16)	0.0066 (12)	−0.0019 (14)	−0.0033 (13)
C37	0.0494 (15)	0.0449 (18)	0.0549 (16)	−0.0024 (13)	−0.0004 (14)	−0.0028 (13)
C38	0.0482 (15)	0.0445 (17)	0.0636 (17)	−0.0044 (13)	−0.0095 (14)	−0.0044 (13)
N1	0.0382 (12)	0.0499 (14)	0.0623 (14)	−0.0034 (10)	−0.0078 (11)	−0.0085 (11)
N2	0.0304 (10)	0.0540 (14)	0.0484 (12)	−0.0042 (10)	−0.0031 (10)	−0.0044 (10)
N3	0.0361 (11)	0.0408 (13)	0.0579 (13)	−0.0021 (9)	−0.0122 (10)	−0.0067 (10)
N4	0.0298 (10)	0.0412 (13)	0.0478 (11)	−0.0028 (9)	−0.0090 (9)	−0.0061 (9)
N5	0.0352 (11)	0.0444 (14)	0.0801 (16)	−0.0001 (10)	0.0049 (12)	−0.0153 (12)
N6	0.0486 (13)	0.0566 (16)	0.0644 (15)	0.0090 (11)	−0.0013 (12)	−0.0023 (12)
O1	0.0630 (12)	0.0492 (13)	0.0933 (15)	−0.0026 (10)	−0.0258 (12)	−0.0187 (10)
O2	0.0744 (14)	0.0431 (13)	0.1239 (19)	0.0057 (11)	−0.0263 (13)	−0.0218 (12)
O3	0.0662 (12)	0.0494 (13)	0.0883 (14)	0.0003 (10)	−0.0303 (11)	−0.0199 (11)
O4	0.0714 (14)	0.0772 (17)	0.1216 (19)	0.0137 (12)	−0.0481 (15)	−0.0336 (14)

Geometric parameters (Å, º)

C1—N1	1.388 (3)	C20—C20^{ii}	1.506 (4)
C1—C2	1.388 (4)	C20—H20A	0.9700
C1—C6	1.393 (4)	C20—H20B	0.9700
C2—N2	1.378 (3)	C21—N5	1.377 (3)
C2—C3	1.384 (4)	C21—C26	1.387 (4)
C3—C4	1.367 (4)	C21—C22	1.392 (3)
C3—H3	0.9300	C22—C23	1.377 (4)
C4—C5	1.377 (5)	C22—N6	1.387 (3)
C4—H4	0.9300	C23—C24	1.353 (5)
C5—C6	1.367 (4)	C23—H23	0.9300
C5—H5	0.9300	C24—C25	1.381 (5)
C6—H6	0.9300	C24—H24	0.9300

C7—N1	1.319 (3)	C25—C26	1.380 (5)
C7—N2	1.355 (3)	C25—H25	0.9300
C7—C8	1.482 (4)	C26—H26	0.9300
C8—H8A	0.9600	C27—N6	1.308 (3)
C8—H8B	0.9600	C27—N5	1.363 (3)
C8—H8C	0.9600	C27—C28	1.479 (4)
C9—N3	1.382 (3)	C28—H28A	0.9600
C9—C14	1.384 (3)	C28—H28B	0.9600
C9—C10	1.391 (3)	C28—H28C	0.9600
C10—C11	1.375 (4)	C29—N5	1.456 (3)
C10—N4	1.390 (3)	C29—C30	1.502 (4)
C11—C12	1.371 (4)	C29—H29A	0.9700
C11—H11	0.9300	C29—H29B	0.9700
C12—C13	1.393 (4)	C30—C30^{iii}	1.515 (5)
C12—H12	0.9300	C30—H30A	0.9700
C13—C14	1.359 (4)	C30—H30B	0.9700
C13—H13	0.9300	C31—C36	1.377 (3)
C14—H14	0.9300	C31—C32	1.381 (3)
C15—N3	1.318 (3)	C31—C37	1.488 (4)
C15—N4	1.353 (3)	C32—C33	1.382 (4)
C15—C16	1.477 (4)	C32—H32	0.9300
C16—H16A	0.9600	C33—C34	1.382 (3)
C16—H16B	0.9600	C33—H33	0.9300
C16—H16C	0.9600	C34—C35	1.383 (4)
C17—N2	1.462 (3)	C34—C38	1.482 (4)
C17—C18	1.510 (3)	C35—C36	1.376 (4)
C17—H17A	0.9700	C35—H35	0.9300
C17—H17B	0.9700	C36—H36	0.9300
C18—C18^{i}	1.511 (5)	C37—O2	1.206 (3)
C18—H18A	0.9700	C37—O1	1.308 (3)
C18—H18B	0.9700	C38—O4	1.205 (3)
C19—N4	1.463 (3)	C38—O3	1.301 (3)
C19—C20	1.507 (3)	O1—H1	0.8199
C19—H19A	0.9700	O3—H3A	0.8197
C19—H19B	0.9700		

N1—C1—C2	109.2 (2)	N5—C21—C26	133.3 (3)
N1—C1—C6	130.6 (3)	N5—C21—C22	105.5 (2)
C2—C1—C6	120.2 (3)	C26—C21—C22	121.2 (3)
N2—C2—C3	132.0 (3)	C23—C22—N6	129.6 (2)
N2—C2—C1	105.9 (2)	C23—C22—C21	120.7 (3)
C3—C2—C1	122.1 (3)	N6—C22—C21	109.7 (2)
C4—C3—C2	116.5 (3)	C24—C23—C22	118.1 (3)
C4—C3—H3	121.8	C24—C23—H23	121.0
C2—C3—H3	121.8	C22—C23—H23	121.0
C3—C4—C5	122.1 (3)	C23—C24—C25	122.0 (4)
C3—C4—H4	118.9	C23—C24—H24	119.0
C5—C4—H4	118.9	C25—C24—H24	119.0

C6—C5—C4	121.8 (3)	C26—C25—C24	121.1 (3)
C6—C5—H5	119.1	C26—C25—H25	119.4
C4—C5—H5	119.1	C24—C25—H25	119.4
C5—C6—C1	117.2 (3)	C25—C26—C21	117.0 (3)
C5—C6—H6	121.4	C25—C26—H26	121.5
C1—C6—H6	121.4	C21—C26—H26	121.5
N1—C7—N2	112.3 (2)	N6—C27—N5	113.0 (3)
N1—C7—C8	124.5 (3)	N6—C27—C28	124.1 (3)
N2—C7—C8	123.2 (3)	N5—C27—C28	122.9 (3)
C7—C8—H8A	109.5	C27—C28—H28A	109.5
C7—C8—H8B	109.5	C27—C28—H28B	109.5
H8A—C8—H8B	109.5	H28A—C28—H28B	109.5
C7—C8—H8C	109.5	C27—C28—H28C	109.5
H8A—C8—H8C	109.5	H28A—C28—H28C	109.5
H8B—C8—H8C	109.5	H28B—C28—H28C	109.5
N3—C9—C14	130.0 (2)	N5—C29—C30	112.6 (2)
N3—C9—C10	109.79 (19)	N5—C29—H29A	109.1
C14—C9—C10	120.2 (2)	C30—C29—H29A	109.1
C11—C10—N4	132.6 (2)	N5—C29—H29B	109.1
C11—C10—C9	122.3 (2)	C30—C29—H29B	109.1
N4—C10—C9	105.0 (2)	H29A—C29—H29B	107.8
C12—C11—C10	116.4 (2)	C29—C30—C30^{iii}	113.8 (3)
C12—C11—H11	121.8	C29—C30—H30A	108.8
C10—C11—H11	121.8	C30^{iii}—C30—H30A	108.8
C11—C12—C13	121.8 (3)	C29—C30—H30B	108.8
C11—C12—H12	119.1	C30^{iii}—C30—H30B	108.8
C13—C12—H12	119.1	H30A—C30—H30B	107.7
C14—C13—C12	121.4 (2)	C36—C31—C32	119.4 (2)
C14—C13—H13	119.3	C36—C31—C37	119.0 (2)
C12—C13—H13	119.3	C32—C31—C37	121.6 (2)
C13—C14—C9	117.8 (2)	C31—C32—C33	119.8 (2)
C13—C14—H14	121.1	C31—C32—H32	120.1
C9—C14—H14	121.1	C33—C32—H32	120.1
N3—C15—N4	112.5 (2)	C34—C33—C32	120.9 (2)
N3—C15—C16	124.6 (2)	C34—C33—H33	119.6
N4—C15—C16	122.9 (2)	C32—C33—H33	119.6
C15—C16—H16A	109.5	C33—C34—C35	118.8 (2)
C15—C16—H16B	109.5	C33—C34—C38	122.0 (2)
H16A—C16—H16B	109.5	C35—C34—C38	119.1 (2)
C15—C16—H16C	109.5	C36—C35—C34	120.3 (2)
H16A—C16—H16C	109.5	C36—C35—H35	119.8
H16B—C16—H16C	109.5	C34—C35—H35	119.8
N2—C17—C18	112.0 (2)	C35—C36—C31	120.7 (2)
N2—C17—H17A	109.2	C35—C36—H36	119.6
C18—C17—H17A	109.2	C31—C36—H36	119.6
N2—C17—H17B	109.2	O2—C37—O1	123.6 (3)
C18—C17—H17B	109.2	O2—C37—C31	122.7 (2)
H17A—C17—H17B	107.9	O1—C37—C31	113.7 (2)

C17—C18—C18^{i}	110.9 (3)	O4—C38—O3	122.7 (3)
C17—C18—H18A	109.5	O4—C38—C34	123.2 (3)
C18^{i}—C18—H18A	109.5	O3—C38—C34	114.1 (2)
C17—C18—H18B	109.5	C7—N1—C1	105.6 (2)
C18^{i}—C18—H18B	109.5	C7—N2—C2	107.1 (2)
H18A—C18—H18B	108.0	C7—N2—C17	128.4 (2)
N4—C19—C20	112.81 (19)	C2—N2—C17	124.5 (2)
N4—C19—H19A	109.0	C15—N3—C9	105.54 (19)
C20—C19—H19A	109.0	C15—N4—C10	107.14 (18)
N4—C19—H19B	109.0	C15—N4—C19	126.2 (2)
C20—C19—H19B	109.0	C10—N4—C19	126.5 (2)
H19A—C19—H19B	107.8	C27—N5—C21	106.6 (2)
C20^{ii}—C20—C19	111.6 (2)	C27—N5—C29	127.9 (3)
C20^{ii}—C20—H20A	109.3	C21—N5—C29	125.4 (3)
C19—C20—H20A	109.3	C27—N6—C22	105.1 (2)
C20^{ii}—C20—H20B	109.3	C37—O1—H1	109.3
C19—C20—H20B	109.3	C38—O3—H3A	109.4
H20A—C20—H20B	108.0		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{iv}	0.82	1.83	2.609 (3)	157
O3—H3*A*···N3^{v}	0.82	1.87	2.668 (3)	165

Symmetry codes: (iv) −*x*+1, −*y*+1, −*z*+1; (v) *x*−1, *y*−1, *z*.