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2-[4-(Dimethylamino)phenyl]-4,5-diphenyl-1*H*-imidazole isopropanol solvate

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Key indicators

Single-crystal X-ray study
T = 393 K
Mean σ(C–C) = 0.004 Å
R factor = 0.047
wR factor = 0.119
Data-to-parameter ratio = 15.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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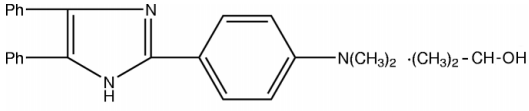
The title compound, $C_{23}H_{21}N_3\cdot C_3H_8O$, crystallizes with two independent molecules and two solvent molecules in the asymmetric unit. These are connected through hydrogen bonds between the NH group of the imidazole ring and the O atom of the isopropanol solvent molecule, as well as between the N atom of the imidazole ring and the OH group of the isopropanol solvent molecule.

Comment

Microwave-assisted organic synthesis (MAOS) has been used extensively since the mid-1990s due to the availability of commercial microwave equipment and the continuing development of solvent-free reaction techniques. Different types of organic compounds have been synthesized using MAOS (Lidström *et al.*, 2001). Usyatinsky & Khmelnitsky (2000) have reported the use of this technique in the preparation of 2,4,5-substituted imidazoles. Their synthetic procedure involved the condensation of 1,2-diaryethandienones with aldehydes and ammonium acetate as the source of ammonia with an acidic support (acidic silica) in a microwave oven. We attempted to synthesize 2-[4-(dimethylamino)phenyl]-4,5-diphenyl-1*H*-imidazole using a similar technique in the absence of the acidic support media. Recrystallization of the reaction product from isopropanol afforded compound (I), as shown by single-crystal X-ray structure determination.



(I)

Compound (I) crystallizes with two independent molecules, *A* and *B* (Fig. 1), as well as two solvent molecules, in the asymmetric unit. The general conformation of the two molecules is similar, as shown by the dihedral angles between the imidazole ring (C1 to N2 and C26 to N4, ring 1) and the three benzene rings (C4–C9 and C27–C32, ring 2; C12–C17 and C35–C40, ring 3; C18–C23 and C41–C46, ring 4). In molecule *A*, 1/2 = 7.42°, 1/3 = 36.71° and 1/4 = 45.49 °; in molecule *B*, 1/2 = 8.79°, 1/3 = 40.34 ° and 1/4 = 43.84 °.

A comparison of the bond distances of the imidazole ring of (I) (Table 1) and the mean values of the distances found in similar structures reported in the Cambridge Structural Database (Version 5.25 of October 2003; Allen, 2002) shows that the bond distance N1—C2 (N5—C25 for molecule *B*) is 0.010 Å smaller, the rest of the bond distances being practically the same.

In the crystal structure, the molecules are connected through hydrogen bonds (Table 2) between the NH group of

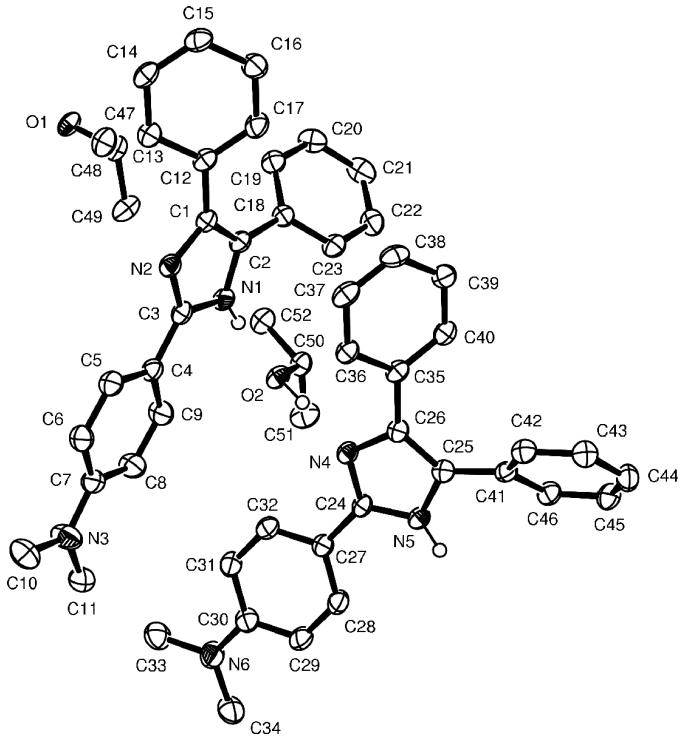


Figure 1
The molecular structure of (I), showing the atom labelling and 50% probability ellipsoids. H atoms have been omitted for clarity, except for the H atom of the NH group and the solvent OH group. Molecule *A* is on the left and molecule *B* is on the right.

the imidazole ring and the O atom of the isopropanol solvent molecule and between the N atom of the imidazole ring and the OH group of the isopropanol solvent molecule. There are short contacts between C9—H9 and O2 and between C28—H28 and O1($x-1, y+1, z$).

Experimental

A mixture of 0.525 g (2.5 mmol) of benzil, 0.372 g (2.5 mmol) of dimethylaminobenzaldehyde and 7 g of ammonium acetate was irradiated with a microwave power of 262 W for 10 min. The reaction product was treated with 20 ml of diethyl ether and filtered. The solid residue was crystallized from isopropanol (m.p. 530–531 K).

Crystal data

$C_{23}H_{21}N_3{\cdot}C_3H_8O$
$M_r = 399.52$
Triclinic, $P\overline{1}$
$a = 8.764\ (12)$ Å
$b = 12.087\ (14)$ Å
$c = 21.07\ (4)$ Å
$\alpha = 97.48\ (9)^\circ$
$\beta = 93.12\ (10)^\circ$
$\gamma = 91.89\ (10)^\circ$
$V = 2208\ (6)$ Å^3
$Z = 4$
$D_x = 1.202$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1567 reflections
$\theta = 2.6$–25.4°
$\mu = 0.07$ mm^{-1}
$T = 393\ (2)$ K
Plate, colourless
0.45 × 0.24 × 0.02 mm

Data collection

Bruker SMART CCD 1K area-detector diffractometer
ω scans
Absorption correction: none
15473 measured reflections
8644 independent reflections
5245 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 26.0^\circ$
$h = -8 \rightarrow 10$
$k = -14 \rightarrow 14$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.119$
$S = 0.85$
8644 reflections
565 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0679P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C3	1.362 (3)	N4—C26	1.379 (3)
N1—C2	1.370 (3)	N5—C24	1.361 (3)
N2—C3	1.326 (3)	N5—C25	1.369 (3)
N2—C1	1.379 (3)	C1—C2	1.384 (3)
N4—C24	1.333 (3)	C25—C26	1.381 (3)
C3—N1—C2	108.75 (19)	N1—C2—C1	104.56 (19)
C3—N2—C1	105.67 (18)	N2—C3—N1	110.58 (19)
C24—N4—C26	104.97 (18)	N4—C24—N5	111.13 (19)
C24—N5—C25	108.19 (19)	N5—C25—C26	105.01 (19)
N2—C1—C2	110.44 (18)	N4—C26—C25	110.69 (17)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.85 (2)	1.95 (2)	2.797 (4)	173 (2)
N5—H2···O1^{i}	0.92 (2)	1.92 (2)	2.840 (4)	173 (2)
O1—H3···N2^{ii}	0.84 (3)	1.97 (3)	2.814 (4)	174 (2)
O2—H4···N4	0.95 (3)	1.86 (3)	2.814 (4)	176 (2)
C9—H9···O2	0.93	2.47	3.329 (7)	155
C28—H28···O1^{i}	0.93	2.44	3.294 (7)	153

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

All H atoms were placed in ideal positions and refined as riding [C—H = 0.93 Å or 0.96 Å (methyl H atoms); U(H) = 1.2 or 1.5 (methyl H atoms) times U_{eq}(parent atrom)], except for the H atoms linked to the N and O atoms, which were located in difference Fourier maps and refined freely.

Data collection: *SMART-NT* (Bruker, 1998); cell refinement: *SAINT-NT* (Bruker, 1998); data reduction: *SAINT-NT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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Acta Cryst. (2004). E**60**, o1229–o1230 [https://doi.org/10.1107/S1600536804014503]

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2-[4-(Dimethylamino)phenyl]-4,5-diphenyl-1*H*-imidazole isopropyl alcohol solvate

Crystal data

$C_{23}H_{21}N_3·C_3H_8O$
$M_r = 399.52$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.764$ (12) Å
$b = 12.087$ (14) Å
$c = 21.07$ (4) Å
$\alpha = 97.48$ (9)°
$\beta = 93.12$ (10)°
$\gamma = 91.89$ (10)°
$V = 2208$ (6) Å^3
$Z = 4$
$F(000) = 856$
$D_x = 1.202$ Mg m^{-3}
Melting point: 530 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1567 reflections
$\theta = 2.6$–25.4°
$\mu = 0.07$ mm^{-1}
$T = 393$ K
Plates, colourless
0.45 × 0.24 × 0.02 mm

Data collection

Bruker SMART CCD 1K area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8 pixels mm^{-1}
ω scans
15473 measured reflections
8644 independent reflections
5245 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.7°$
$h = -8 \rightarrow 10$
$k = -14 \rightarrow 14$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.119$
$S = 0.85$
8644 reflections
565 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0679P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.00326 (16)	0.04421 (11)	0.27669 (7)	0.0290 (3)
O2	0.45391 (15)	0.55282 (10)	0.27837 (6)	0.0275 (3)

N1	0.39415 (18)	0.32183 (13)	0.26143 (7)	0.0246 (4)
N2	0.28727 (17)	0.15892 (12)	0.27476 (7)	0.0249 (3)
N3	0.1504 (2)	0.43948 (15)	0.54869 (8)	0.0438 (5)
N4	0.17083 (17)	0.65444 (12)	0.26835 (7)	0.0244 (3)
N5	0.05680 (17)	0.81224 (13)	0.25548 (7)	0.0248 (4)
N6	0.3556 (2)	0.93704 (15)	0.54645 (8)	0.0442 (5)
C1	0.3505 (2)	0.15053 (14)	0.21588 (8)	0.0235 (4)
C2	0.4176 (2)	0.25195 (14)	0.20654 (8)	0.0234 (4)
C3	0.3166 (2)	0.26353 (14)	0.30146 (9)	0.0245 (4)
C4	0.2756 (2)	0.30913 (15)	0.36510 (9)	0.0251 (4)
C5	0.1855 (2)	0.24683 (15)	0.40157 (9)	0.0290 (4)
H5	0.1511	0.1751	0.3842	0.035*
C6	0.1460 (2)	0.28791 (16)	0.46209 (9)	0.0312 (4)
H6	0.0861	0.2439	0.4849	0.037*
C7	0.1955 (2)	0.39577 (16)	0.48963 (9)	0.0309 (4)
C8	0.2901 (2)	0.45655 (16)	0.45402 (9)	0.0366 (5)
H8	0.3285	0.5270	0.4720	0.044*
C9	0.3279 (2)	0.41510 (16)	0.39340 (9)	0.0331 (5)
H9	0.3895	0.4584	0.3709	0.040*
C10	0.0514 (2)	0.37587 (19)	0.58397 (10)	0.0422 (6)
H10A	−0.0398	0.3517	0.5579	0.063*
H10B	0.0248	0.4216	0.6222	0.063*
H10C	0.1032	0.3119	0.5954	0.063*
C11	0.1962 (3)	0.55307 (17)	0.57435 (10)	0.0426 (6)
H11A	0.3043	0.5579	0.5851	0.064*
H11B	0.1424	0.5752	0.6121	0.064*
H11C	0.1724	0.6016	0.5429	0.064*
C12	0.3421 (2)	0.04430 (14)	0.17335 (9)	0.0246 (4)
C13	0.3557 (2)	−0.05649 (15)	0.19911 (9)	0.0268 (4)
H13	0.3667	−0.0555	0.2433	0.032*
C14	0.3532 (2)	−0.15685 (15)	0.15979 (9)	0.0300 (4)
H14	0.3622	−0.2232	0.1773	0.036*
C15	0.3372 (2)	−0.15840 (15)	0.09443 (9)	0.0319 (5)
H15	0.3371	−0.2259	0.0676	0.038*
C16	0.3212 (2)	−0.05876 (16)	0.06826 (9)	0.0335 (5)
H16	0.3090	−0.0601	0.0240	0.040*
C17	0.3234 (2)	0.04103 (15)	0.10756 (9)	0.0306 (4)
H17	0.3122	0.1071	0.0898	0.037*
C18	0.5004 (2)	0.29155 (15)	0.15409 (8)	0.0246 (4)
C19	0.6144 (2)	0.22881 (16)	0.12475 (9)	0.0291 (4)
H19	0.6363	0.1597	0.1371	0.035*
C20	0.6953 (2)	0.26938 (17)	0.07715 (9)	0.0347 (5)
H20	0.7718	0.2275	0.0581	0.042*
C21	0.6626 (2)	0.37232 (17)	0.05767 (10)	0.0375 (5)
H21	0.7174	0.3993	0.0259	0.045*
C22	0.5487 (2)	0.43389 (16)	0.08572 (9)	0.0331 (5)
H22	0.5260	0.5022	0.0725	0.040*
C23	0.4675 (2)	0.39464 (15)	0.13373 (9)	0.0280 (4)

H23	0.3911	0.4370	0.1524	0.034*
C24	0.1455 (2)	0.75769 (14)	0.29539 (8)	0.0231 (4)
C25	0.0222 (2)	0.74141 (14)	0.20004 (8)	0.0239 (4)
C26	0.0936 (2)	0.64401 (14)	0.20894 (8)	0.0242 (4)
C27	0.1997 (2)	0.80486 (15)	0.36001 (9)	0.0256 (4)
C28	0.1483 (2)	0.90582 (16)	0.38895 (9)	0.0329 (5)
H28	0.0797	0.9451	0.3661	0.040*
C29	0.1965 (2)	0.94830 (16)	0.45018 (9)	0.0359 (5)
H29	0.1590	1.0154	0.4685	0.043*
C30	0.3021 (2)	0.89234 (16)	0.48613 (9)	0.0313 (5)
C31	0.3506 (2)	0.78913 (16)	0.45744 (9)	0.0320 (5)
H31	0.4175	0.7488	0.4804	0.038*
C32	0.3008 (2)	0.74725 (15)	0.39625 (9)	0.0293 (4)
H32	0.3349	0.6788	0.3782	0.035*
C33	0.4602 (3)	0.87672 (19)	0.58327 (10)	0.0437 (6)
H33A	0.4099	0.8093	0.5924	0.065*
H33B	0.4924	0.9224	0.6228	0.065*
H33C	0.5478	0.8584	0.5591	0.065*
C34	0.3093 (3)	1.04585 (17)	0.57312 (10)	0.0442 (6)
H34A	0.3251	1.0978	0.5431	0.066*
H34B	0.3690	1.0703	0.6123	0.066*
H34C	0.2030	1.0418	0.5818	0.066*
C35	0.0936 (2)	0.53774 (14)	0.16620 (9)	0.0245 (4)
C36	0.0803 (2)	0.43579 (14)	0.19121 (9)	0.0263 (4)
H36	0.0721	0.4360	0.2350	0.032*
C37	0.0794 (2)	0.33573 (16)	0.15178 (10)	0.0318 (5)
H37	0.0702	0.2688	0.1688	0.038*
C38	0.0924 (2)	0.33508 (16)	0.08669 (10)	0.0322 (5)
H38	0.0924	0.2676	0.0599	0.039*
C39	0.1055 (2)	0.43529 (16)	0.06125 (9)	0.0311 (5)
H39	0.1141	0.4345	0.0174	0.037*
C40	0.1059 (2)	0.53566 (15)	0.10049 (9)	0.0283 (4)
H40	0.1144	0.6023	0.0830	0.034*
C41	−0.0746 (2)	0.77615 (14)	0.14765 (8)	0.0245 (4)
C42	−0.1915 (2)	0.70540 (15)	0.11677 (9)	0.0283 (4)
H42	−0.2061	0.6342	0.1282	0.034*
C43	−0.2860 (2)	0.73993 (16)	0.06927 (9)	0.0321 (5)
H43	−0.3630	0.6914	0.0485	0.038*
C44	−0.2670 (2)	0.84716 (17)	0.05203 (9)	0.0340 (5)
H44	−0.3331	0.8707	0.0209	0.041*
C45	−0.1502 (2)	0.91767 (16)	0.08133 (9)	0.0341 (5)
H45	−0.1352	0.9884	0.0694	0.041*
C46	−0.0546 (2)	0.88250 (15)	0.12891 (9)	0.0294 (4)
H46	0.0242	0.9304	0.1487	0.035*
C47	0.8794 (2)	0.10395 (15)	0.25164 (10)	0.0291 (4)
H47	0.8974	0.1138	0.2072	0.035*
C48	0.7361 (2)	0.03045 (17)	0.25227 (10)	0.0358 (5)
H48A	0.7446	−0.0374	0.2236	0.054*

H48B	0.6488	0.0692	0.2387	0.054*
H48C	0.7241	0.0130	0.2949	0.054*
C49	0.8656 (2)	0.21699 (16)	0.28979 (11)	0.0400 (5)
H49A	0.8422	0.2081	0.3329	0.060*
H49B	0.7853	0.2557	0.2704	0.060*
H49C	0.9605	0.2593	0.2904	0.060*
C50	0.5789 (2)	0.61192 (15)	0.25372 (9)	0.0280 (4)
H50	0.5531	0.6206	0.2089	0.034*
C51	0.6079 (2)	0.72532 (16)	0.29192 (10)	0.0401 (5)
H51A	0.5167	0.7670	0.2903	0.060*
H51B	0.6892	0.7642	0.2742	0.060*
H51C	0.6361	0.7171	0.3357	0.060*
C52	0.7165 (2)	0.53920 (16)	0.25709 (10)	0.0339 (5)
H52A	0.7347	0.5231	0.3002	0.051*
H52B	0.8048	0.5779	0.2443	0.051*
H52C	0.6969	0.4706	0.2288	0.051*
H1	0.420 (2)	0.3907 (18)	0.2680 (9)	0.036 (6)*
H2	0.031 (2)	0.8860 (19)	0.2619 (10)	0.046 (6)*
H3	1.089 (3)	0.080 (2)	0.2791 (12)	0.060 (8)*
H4	0.361 (3)	0.590 (2)	0.2741 (11)	0.060 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0269 (7)	0.0180 (6)	0.0426 (8)	−0.0012 (6)	0.0000 (6)	0.0078 (6)
O2	0.0266 (7)	0.0178 (6)	0.0391 (7)	−0.0014 (6)	0.0050 (6)	0.0067 (6)
N1	0.0288 (9)	0.0153 (8)	0.0301 (8)	−0.0035 (7)	0.0031 (7)	0.0044 (7)
N2	0.0278 (8)	0.0191 (8)	0.0286 (8)	−0.0003 (7)	0.0023 (7)	0.0058 (7)
N3	0.0601 (12)	0.0339 (10)	0.0372 (10)	−0.0066 (9)	0.0196 (9)	−0.0004 (8)
N4	0.0271 (8)	0.0184 (8)	0.0282 (8)	−0.0006 (7)	0.0022 (7)	0.0057 (7)
N5	0.0280 (8)	0.0161 (8)	0.0306 (8)	−0.0015 (7)	0.0019 (7)	0.0046 (7)
N6	0.0615 (13)	0.0339 (10)	0.0344 (9)	0.0075 (9)	−0.0127 (9)	−0.0005 (8)
C1	0.0236 (9)	0.0202 (9)	0.0276 (9)	0.0015 (8)	0.0017 (8)	0.0058 (8)
C2	0.0242 (9)	0.0178 (9)	0.0282 (9)	−0.0007 (7)	0.0006 (8)	0.0035 (8)
C3	0.0246 (9)	0.0194 (9)	0.0307 (10)	−0.0005 (8)	0.0016 (8)	0.0077 (8)
C4	0.0270 (10)	0.0206 (9)	0.0289 (10)	0.0010 (8)	0.0035 (8)	0.0063 (8)
C5	0.0324 (11)	0.0218 (9)	0.0332 (10)	−0.0036 (8)	0.0037 (9)	0.0051 (8)
C6	0.0346 (11)	0.0280 (10)	0.0324 (10)	−0.0029 (9)	0.0069 (9)	0.0086 (9)
C7	0.0365 (11)	0.0266 (10)	0.0309 (10)	0.0027 (9)	0.0067 (9)	0.0057 (9)
C8	0.0518 (13)	0.0224 (10)	0.0349 (11)	−0.0067 (10)	0.0085 (10)	0.0010 (9)
C9	0.0424 (12)	0.0250 (10)	0.0327 (10)	−0.0058 (9)	0.0093 (9)	0.0060 (9)
C10	0.0394 (12)	0.0533 (14)	0.0335 (11)	−0.0055 (11)	0.0066 (10)	0.0050 (11)
C11	0.0632 (15)	0.0324 (12)	0.0325 (11)	0.0072 (11)	0.0074 (11)	0.0020 (10)
C12	0.0224 (9)	0.0189 (9)	0.0328 (10)	−0.0019 (8)	0.0027 (8)	0.0041 (8)
C13	0.0252 (10)	0.0239 (10)	0.0316 (10)	−0.0033 (8)	0.0018 (8)	0.0057 (8)
C14	0.0307 (10)	0.0181 (9)	0.0424 (11)	−0.0005 (8)	0.0033 (9)	0.0083 (9)
C15	0.0366 (11)	0.0193 (9)	0.0389 (11)	−0.0020 (8)	0.0043 (10)	0.0001 (9)
C16	0.0428 (12)	0.0274 (11)	0.0301 (10)	−0.0033 (9)	0.0040 (9)	0.0031 (9)

C17	0.0365 (11)	0.0208 (10)	0.0352 (11)	−0.0023 (9)	0.0014 (9)	0.0079 (9)
C18	0.0269 (10)	0.0205 (9)	0.0260 (9)	−0.0036 (8)	0.0011 (8)	0.0031 (8)
C19	0.0301 (10)	0.0241 (10)	0.0330 (10)	−0.0020 (8)	0.0023 (9)	0.0037 (9)
C20	0.0311 (11)	0.0346 (11)	0.0372 (11)	−0.0046 (9)	0.0086 (9)	−0.0011 (10)
C21	0.0401 (12)	0.0375 (12)	0.0338 (11)	−0.0144 (10)	0.0097 (10)	0.0021 (10)
C22	0.0423 (12)	0.0242 (10)	0.0329 (10)	−0.0096 (9)	0.0001 (10)	0.0081 (9)
C23	0.0297 (10)	0.0207 (9)	0.0331 (10)	−0.0030 (8)	0.0009 (9)	0.0034 (8)
C24	0.0236 (9)	0.0185 (9)	0.0283 (9)	−0.0009 (8)	0.0022 (8)	0.0078 (8)
C25	0.0247 (9)	0.0192 (9)	0.0279 (9)	−0.0045 (8)	0.0031 (8)	0.0047 (8)
C26	0.0252 (10)	0.0203 (9)	0.0277 (9)	−0.0030 (8)	0.0023 (8)	0.0061 (8)
C27	0.0298 (10)	0.0189 (9)	0.0286 (10)	−0.0022 (8)	0.0031 (8)	0.0056 (8)
C28	0.0421 (12)	0.0247 (10)	0.0322 (10)	0.0057 (9)	−0.0039 (9)	0.0061 (9)
C29	0.0488 (13)	0.0214 (10)	0.0365 (11)	0.0065 (9)	−0.0024 (10)	0.0014 (9)
C30	0.0362 (11)	0.0260 (10)	0.0313 (10)	−0.0029 (9)	−0.0004 (9)	0.0037 (9)
C31	0.0340 (11)	0.0300 (11)	0.0326 (10)	0.0028 (9)	−0.0017 (9)	0.0076 (9)
C32	0.0340 (11)	0.0208 (9)	0.0335 (10)	0.0018 (8)	0.0019 (9)	0.0042 (8)
C33	0.0416 (13)	0.0527 (14)	0.0352 (11)	0.0029 (11)	−0.0041 (10)	0.0026 (11)
C34	0.0642 (16)	0.0322 (12)	0.0336 (11)	−0.0054 (11)	−0.0028 (11)	−0.0006 (10)
C35	0.0221 (9)	0.0193 (9)	0.0320 (10)	−0.0007 (8)	0.0013 (8)	0.0039 (8)
C36	0.0267 (10)	0.0211 (9)	0.0318 (10)	−0.0004 (8)	0.0027 (8)	0.0061 (8)
C37	0.0291 (10)	0.0188 (9)	0.0480 (12)	−0.0016 (8)	0.0036 (9)	0.0063 (9)
C38	0.0302 (10)	0.0227 (10)	0.0406 (11)	0.0000 (8)	−0.0002 (9)	−0.0060 (9)
C39	0.0327 (11)	0.0286 (10)	0.0314 (10)	0.0040 (9)	0.0000 (9)	0.0020 (9)
C40	0.0289 (10)	0.0227 (10)	0.0341 (10)	0.0012 (8)	0.0015 (9)	0.0073 (8)
C41	0.0271 (10)	0.0196 (9)	0.0274 (9)	0.0027 (8)	0.0047 (8)	0.0035 (8)
C42	0.0302 (10)	0.0222 (10)	0.0327 (10)	−0.0024 (8)	0.0039 (9)	0.0043 (8)
C43	0.0311 (11)	0.0320 (11)	0.0328 (10)	−0.0013 (9)	0.0003 (9)	0.0048 (9)
C44	0.0355 (11)	0.0388 (12)	0.0299 (10)	0.0065 (10)	0.0018 (9)	0.0120 (9)
C45	0.0423 (12)	0.0248 (10)	0.0373 (11)	0.0033 (9)	0.0038 (10)	0.0114 (9)
C46	0.0351 (11)	0.0204 (9)	0.0327 (10)	−0.0004 (8)	0.0011 (9)	0.0046 (8)
C47	0.0261 (10)	0.0258 (10)	0.0371 (11)	0.0018 (8)	0.0014 (9)	0.0110 (9)
C48	0.0301 (11)	0.0326 (11)	0.0466 (12)	−0.0023 (9)	0.0017 (10)	0.0133 (10)
C49	0.0375 (12)	0.0260 (10)	0.0561 (13)	0.0055 (9)	−0.0018 (11)	0.0044 (10)
C50	0.0294 (10)	0.0229 (10)	0.0331 (10)	−0.0032 (8)	0.0039 (9)	0.0095 (8)
C51	0.0413 (12)	0.0241 (10)	0.0543 (13)	−0.0075 (9)	0.0069 (11)	0.0030 (10)
C52	0.0292 (11)	0.0307 (11)	0.0425 (11)	−0.0012 (9)	0.0028 (9)	0.0084 (9)

Geometric parameters (Å, º)

O1—C47	1.438 (3)	C23—H23	0.9300
O1—H3	0.84 (3)	C24—C27	1.454 (4)
O2—C50	1.444 (3)	C25—C26	1.381 (3)
O2—H4	0.95 (3)	C25—C41	1.469 (3)
N1—C3	1.362 (3)	C26—C35	1.470 (3)
N1—C2	1.370 (3)	C27—C28	1.392 (3)
N1—H1	0.85 (2)	C27—C32	1.399 (3)
N2—C3	1.326 (3)	C28—C29	1.364 (4)
N2—C1	1.379 (3)	C28—H28	0.9300

N3—C7	1.371 (3)	C29—C30	1.410 (3)
N3—C10	1.439 (3)	C29—H29	0.9300
N3—C11	1.444 (3)	C30—C31	1.403 (3)
N4—C24	1.333 (3)	C31—C32	1.365 (4)
N4—C26	1.379 (3)	C31—H31	0.9300
N5—C24	1.361 (3)	C32—H32	0.9300
N5—C25	1.369 (3)	C33—H33A	0.9600
N5—H2	0.92 (2)	C33—H33B	0.9600
N6—C30	1.366 (3)	C33—H33C	0.9600
N6—C34	1.441 (3)	C34—H34A	0.9600
N6—C33	1.445 (3)	C34—H34B	0.9600
C1—C2	1.384 (3)	C34—H34C	0.9600
C1—C12	1.464 (3)	C35—C40	1.392 (4)
C2—C18	1.476 (3)	C35—C36	1.406 (3)
C3—C4	1.451 (4)	C36—C37	1.375 (3)
C4—C9	1.393 (3)	C36—H36	0.9300
C4—C5	1.400 (3)	C37—C38	1.381 (4)
C5—C6	1.374 (4)	C37—H37	0.9300
C5—H5	0.9300	C38—C39	1.391 (3)
C6—C7	1.401 (3)	C38—H38	0.9300
C6—H6	0.9300	C39—C40	1.376 (3)
C7—C8	1.401 (3)	C39—H39	0.9300
C8—C9	1.372 (4)	C40—H40	0.9300
C8—H8	0.9300	C41—C42	1.389 (3)
C9—H9	0.9300	C41—C46	1.401 (3)
C10—H10A	0.9600	C42—C43	1.380 (3)
C10—H10B	0.9600	C42—H42	0.9300
C10—H10C	0.9600	C43—C44	1.398 (3)
C11—H11A	0.9600	C43—H43	0.9300
C11—H11B	0.9600	C44—C45	1.376 (3)
C11—H11C	0.9600	C44—H44	0.9300
C12—C17	1.382 (4)	C45—C46	1.390 (3)
C12—C13	1.403 (3)	C45—H45	0.9300
C13—C14	1.376 (3)	C46—H46	0.9300
C13—H13	0.9300	C47—C49	1.504 (3)
C14—C15	1.375 (4)	C47—C48	1.516 (3)
C14—H14	0.9300	C47—H47	0.9800
C15—C16	1.396 (3)	C48—H48A	0.9600
C15—H15	0.9300	C48—H48B	0.9600
C16—C17	1.370 (3)	C48—H48C	0.9600
C16—H16	0.9300	C49—H49A	0.9600
C17—H17	0.9300	C49—H49B	0.9600
C18—C19	1.397 (3)	C49—H49C	0.9600
C18—C23	1.403 (3)	C50—C51	1.503 (3)
C19—C20	1.390 (3)	C50—C52	1.520 (3)
C19—H19	0.9300	C50—H50	0.9800
C20—C21	1.394 (3)	C51—H51A	0.9600
C20—H20	0.9300	C51—H51B	0.9600

C21—C22	1.378 (3)	C51—H51C	0.9600
C21—H21	0.9300	C52—H52A	0.9600
C22—C23	1.391 (3)	C52—H52B	0.9600
C22—H22	0.9300	C52—H52C	0.9600
C47—O1—H3	113.5 (17)	C28—C27—C24	121.49 (19)
C50—O2—H4	111.6 (15)	C32—C27—C24	120.72 (19)
C3—N1—C2	108.75 (19)	C29—C28—C27	121.3 (2)
C3—N1—H1	126.3 (14)	C29—C28—H28	119.4
C2—N1—H1	124.9 (14)	C27—C28—H28	119.4
C3—N2—C1	105.67 (18)	C28—C29—C30	121.2 (2)
C7—N3—C10	120.9 (2)	C28—C29—H29	119.4
C7—N3—C11	119.5 (2)	C30—C29—H29	119.4
C10—N3—C11	119.45 (19)	N6—C30—C31	121.3 (2)
C24—N4—C26	104.97 (18)	N6—C30—C29	121.3 (2)
C24—N5—C25	108.19 (19)	C31—C30—C29	117.4 (2)
C24—N5—H2	127.1 (13)	C32—C31—C30	120.8 (2)
C25—N5—H2	124.4 (13)	C32—C31—H31	119.6
C30—N6—C34	119.8 (2)	C30—C31—H31	119.6
C30—N6—C33	120.4 (2)	C31—C32—C27	121.6 (2)
C34—N6—C33	119.8 (2)	C31—C32—H32	119.2
N2—C1—C2	110.44 (18)	C27—C32—H32	119.2
N2—C1—C12	120.57 (18)	N6—C33—H33A	109.5
C2—C1—C12	128.99 (19)	N6—C33—H33B	109.5
N1—C2—C1	104.56 (19)	H33A—C33—H33B	109.5
N1—C2—C18	121.24 (18)	N6—C33—H33C	109.5
C1—C2—C18	134.20 (17)	H33A—C33—H33C	109.5
N2—C3—N1	110.58 (19)	H33B—C33—H33C	109.5
N2—C3—C4	124.89 (19)	N6—C34—H34A	109.5
N1—C3—C4	124.51 (19)	N6—C34—H34B	109.5
C9—C4—C5	117.1 (2)	H34A—C34—H34B	109.5
C9—C4—C3	121.64 (19)	N6—C34—H34C	109.5
C5—C4—C3	121.26 (19)	H34A—C34—H34C	109.5
C6—C5—C4	122.3 (2)	H34B—C34—H34C	109.5
C6—C5—H5	118.8	C40—C35—C36	118.69 (19)
C4—C5—H5	118.8	C40—C35—C26	121.03 (19)
C5—C6—C7	120.3 (2)	C36—C35—C26	120.3 (2)
C5—C6—H6	119.8	C37—C36—C35	120.9 (2)
C7—C6—H6	119.8	C37—C36—H36	119.5
N3—C7—C8	122.0 (2)	C35—C36—H36	119.5
N3—C7—C6	120.7 (2)	C36—C37—C38	119.7 (2)
C8—C7—C6	117.3 (2)	C36—C37—H37	120.2
C9—C8—C7	121.9 (2)	C38—C37—H37	120.2
C9—C8—H8	119.1	C37—C38—C39	120.05 (19)
C7—C8—H8	119.1	C37—C38—H38	120.0
C8—C9—C4	121.0 (2)	C39—C38—H38	120.0
C8—C9—H9	119.5	C40—C39—C38	120.5 (2)
C4—C9—H9	119.5	C40—C39—H39	119.8

N3—C10—H10A	109.5	C38—C39—H39	119.8
N3—C10—H10B	109.5	C39—C40—C35	120.2 (2)
H10A—C10—H10B	109.5	C39—C40—H40	119.9
N3—C10—H10C	109.5	C35—C40—H40	119.9
H10A—C10—H10C	109.5	C42—C41—C46	118.4 (2)
H10B—C10—H10C	109.5	C42—C41—C25	120.65 (19)
N3—C11—H11A	109.5	C46—C41—C25	120.95 (19)
N3—C11—H11B	109.5	C43—C42—C41	120.5 (2)
H11A—C11—H11B	109.5	C43—C42—H42	119.8
N3—C11—H11C	109.5	C41—C42—H42	119.8
H11A—C11—H11C	109.5	C42—C43—C44	120.6 (2)
H11B—C11—H11C	109.5	C42—C43—H43	119.7
C17—C12—C13	118.78 (19)	C44—C43—H43	119.7
C17—C12—C1	121.19 (19)	C45—C44—C43	119.7 (2)
C13—C12—C1	120.0 (2)	C45—C44—H44	120.2
C14—C13—C12	120.8 (2)	C43—C44—H44	120.2
C14—C13—H13	119.6	C44—C45—C46	119.6 (2)
C12—C13—H13	119.6	C44—C45—H45	120.2
C15—C14—C13	119.6 (2)	C46—C45—H45	120.2
C15—C14—H14	120.2	C45—C46—C41	121.2 (2)
C13—C14—H14	120.2	C45—C46—H46	119.4
C14—C15—C16	120.07 (19)	C41—C46—H46	119.4
C14—C15—H15	120.0	O1—C47—C49	111.91 (19)
C16—C15—H15	120.0	O1—C47—C48	106.41 (19)
C17—C16—C15	120.2 (2)	C49—C47—C48	112.0 (2)
C17—C16—H16	119.9	O1—C47—H47	108.8
C15—C16—H16	119.9	C49—C47—H47	108.8
C16—C17—C12	120.5 (2)	C48—C47—H47	108.8
C16—C17—H17	119.7	C47—C48—H48A	109.5
C12—C17—H17	119.7	C47—C48—H48B	109.5
C19—C18—C23	118.8 (2)	H48A—C48—H48B	109.5
C19—C18—C2	120.99 (19)	C47—C48—H48C	109.5
C23—C18—C2	120.19 (18)	H48A—C48—H48C	109.5
C20—C19—C18	120.2 (2)	H48B—C48—H48C	109.5
C20—C19—H19	119.9	C47—C49—H49A	109.5
C18—C19—H19	119.9	C47—C49—H49B	109.5
C19—C20—C21	120.5 (2)	H49A—C49—H49B	109.5
C19—C20—H20	119.7	C47—C49—H49C	109.5
C21—C20—H20	119.7	H49A—C49—H49C	109.5
C22—C21—C20	119.6 (2)	H49B—C49—H49C	109.5
C22—C21—H21	120.2	O2—C50—C51	110.52 (19)
C20—C21—H21	120.2	O2—C50—C52	106.50 (18)
C21—C22—C23	120.5 (2)	C51—C50—C52	112.19 (19)
C21—C22—H22	119.7	O2—C50—H50	109.2
C23—C22—H22	119.7	C51—C50—H50	109.2
C22—C23—C18	120.4 (2)	C52—C50—H50	109.2
C22—C23—H23	119.8	C50—C51—H51A	109.5
C18—C23—H23	119.8	C50—C51—H51B	109.5

N4—C24—N5	111.13 (19)	H51A—C51—H51B	109.5
N4—C24—C27	124.73 (18)	C50—C51—H51C	109.5
N5—C24—C27	124.09 (18)	H51A—C51—H51C	109.5
N5—C25—C26	105.01 (19)	H51B—C51—H51C	109.5
N5—C25—C41	121.03 (19)	C50—C52—H52A	109.5
C26—C25—C41	133.95 (18)	C50—C52—H52B	109.5
N4—C26—C25	110.69 (17)	H52A—C52—H52B	109.5
N4—C26—C35	119.68 (19)	C50—C52—H52C	109.5
C25—C26—C35	129.61 (19)	H52A—C52—H52C	109.5
C28—C27—C32	117.7 (2)	H52B—C52—H52C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.85 (2)	1.95 (2)	2.797 (4)	173 (2)
N5—H2···O1^{i}	0.92 (2)	1.92 (2)	2.840 (4)	173 (2)
O1—H3···N2^{ii}	0.84 (3)	1.97 (3)	2.814 (4)	174 (2)
O2—H4···N4	0.95 (3)	1.86 (3)	2.814 (4)	176 (2)
C9—H9···O2	0.93	2.47	3.329 (7)	155
C28—H28···O1^{i}	0.93	2.44	3.294 (7)	153

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