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2-{[(2-Methoxynaphthalen-1-yl)methyl]amino}-phenol

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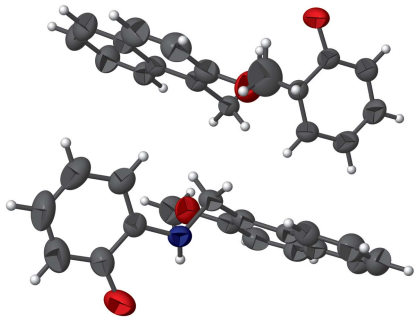
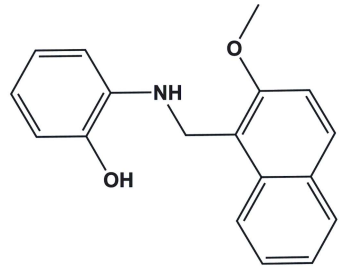
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{18}H_{17}NO_2$, contains two independent molecules (*A* and *B*). The dihedral angle between the naphthalene ring system and the benzene ring is 74.67 (10)° in molecule *A* and 78.81 (9)° in molecule *B*. In the crystal, molecules are linked by a series of C—H···π interactions, forming sheets parallel to the *ab* plane.

3D view



Chemical scheme



Structure description

Aromatic amines and aminophenols, are of considerable importance for their industrial, toxicological and pharmaceutical aspects (Kirk-Othmer, 1979). In view of this interest we have synthesized the title amino-phenol derivative, which was obtained by reduction of the initially prepared Schiff base, and report herein on its crystal structure.

The title compound, Fig. 1, crystallized with two independent molecules (*A* and *B*) in the asymmetric unit. The naphthalene ring system and the benzene ring are inclined to one another by 74.67 (10)° in molecule *A* and 78.81 (9)° in molecule *B*. The bridging C—N bond lengths are single bonds as confirmed by their bond lengths; C7—N1 = 1.464 (2) Å in molecule *A*, and C25—N2 = 1.462 (2) Å in molecule *B*.

In the crystal, molecules are linked by a series of C—H···π interactions (Table 1) forming sheets lying parallel to (001); see Fig. 2. There are no other significant intermolecular interactions present.

Synthesis and crystallization

A mixture of 2-aminophenol (3 mmol) and 2-methoxy-1-naphthaldehyde (3 mmol) in methanol (10 mmol) was stirred at room temperature for 24 h. On completion of this

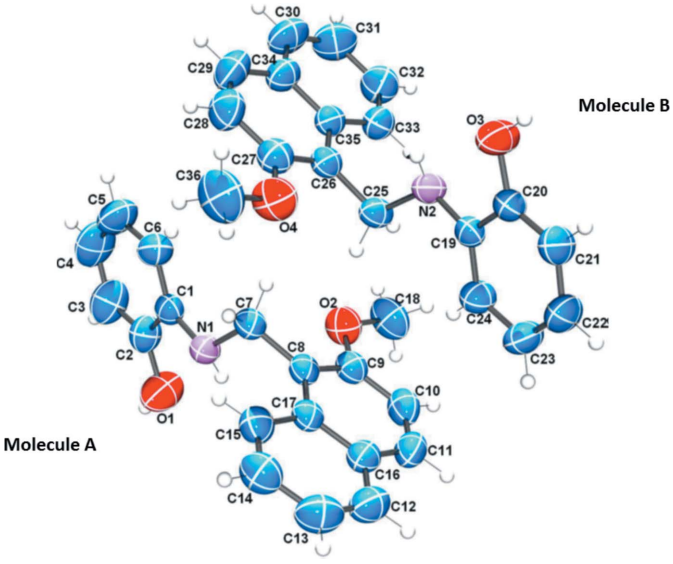


Figure 1
View of the molecular structure of the two independent molecules (*A* and *B*) of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

condensation reaction (monitored by thin layer chromatography), $NaBH_3CN$ (4.5 mmol) was added and stirring was continued for 24 h. On completion of the reaction (monitored by thin layer chromatography), the mixture was poured over ice–water. The resulting precipitate was filtered, washed with water and dried. The resulting light-brown fine powder of the title compound was obtained in very high purity with excellent yield.

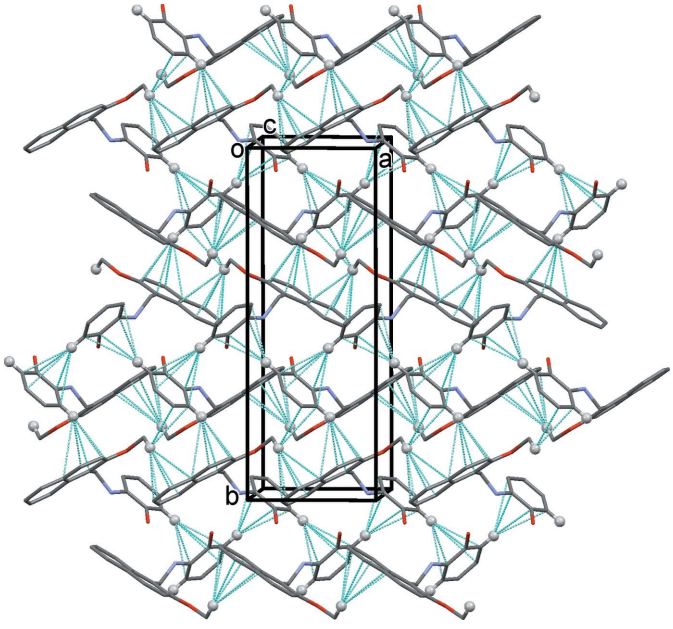


Figure 2
A view along the *c* axis of the crystal packing of the title compound. The C—H···π interactions are illustrated by dashed lines, and for clarity only the H atoms involved (grey balls) have been included (see Table 1 for details).

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

*Cg*1, *Cg*2, *Cg*3, *Cg*5 and *Cg*7 are the centroids of rings C1–C6, C8–C11/C16/C17, C12–C17, C19–C24 and C30–C35, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···*Cg*5^{i}	0.93	2.93	3.826 (3)	162
C18—H18*A*···*Cg*3^{ii}	0.96	2.81	3.637 (3)	144
C21—H21···*Cg*1^{iii}	0.93	2.99	3.890 (3)	165
C24—H24···*Cg*2	0.93	2.97	3.753 (2)	143
C36—H36*B*···*Cg*7^{iv}	0.96	2.98	3.814 (3)	146

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{16}NO_2$
M_r	278.32
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, *b*, *c* (Å)	7.1402 (5), 19.3384 (14), 22.0655 (17)
β (°)	96.874 (4)
V (Å^3)	3024.9 (4)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.03 × 0.02 × 0.01
Data collection	
Diffractometer	Bruker APEXII CCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19509, 5337, 3608
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.053, 0.167, 1.02
No. of reflections	5337
No. of parameters	390
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.22

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

Spectroscopic data: IR (KBr,cm^{-1}) ν: 3476; 3418; 1601; 1258. ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.04 (*d*, *J* = 8.6 Hz, 1*H*); 7.88 (*d*, *J* = 9.1 Hz, 1*H*); 7.84 (*d*,*J* = 8.6 Hz, 1*H*); 7.51 (*t*, *J* = 7.7 Hz, 1*H*); 7.39 (*t*, *J* = 7.5 Hz, 1*H*); 7.34 (*d*, *J* = 9.1 Hz, 1H); 7.04 (*d*, *J* = 7.9 Hz, 1*H*); 6.96 (*t*, *J* = 7.5 Hz, 1*H*); 6.81–6.72 (*m*, 2*H*); 4.71 (*s*, 2*H*); 3.99 (*s*, 2*H*). ^{13}CNMR (101 MHz, $CDCl_3$) δ 155.26; 145.11; 137.23; 133.28; 129.71; 129.20; 128.49; 127.04; 123.59; 123.11; 121.42;119.48; 119.00;114.45;114.33; 113.32; 56.72; 39.49. HRMS: $(M+Na)^+$, found 302.1180,$C_{18}H_{17}NO_2Na$ requires 302.1157.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Three reflections (031, 002, 013), affected by the backstop were omitted from the final cycles of refinement.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161160 [https://doi.org/10.1107/S2414314616011603]

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Crystal data

$C_{18}H_{16}NO_2$
M_r = 278.32
Monoclinic, $P2_1/c$
a = 7.1402 (5) Å
b = 19.3384 (14) Å
c = 22.0655 (17) Å
β = 96.874 (4)°
V = 3024.9 (4) Å^3
Z = 8
$F(000)$ = 1176
D_x = 1.222 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8065 reflections
θ = 3.1–25.5°
μ = 0.08 mm^{-1}
T = 293 K
Block, orange
0.03 × 0.02 × 0.01 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: Bruker–Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 18.4 pixels mm^{-1}
φ and ω scans
19509 measured reflections
5337 independent reflections
3608 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.0°, θ_{min} = 2.1°
h = −5→8
k = −22→21
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.167
S = 1.02
5337 reflections
390 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0903P)^2 + 0.6386P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0053 (12)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.1871 (3)	0.57240 (10)	0.20335 (8)	0.0911 (6)
O2	−0.0327 (2)	0.36826 (8)	0.29552 (7)	0.0677 (5)
N1	0.0977 (2)	0.48913 (8)	0.21416 (8)	0.0485 (4)
H34	0.036 (3)	0.5017 (11)	0.2456 (11)	0.065 (7)*
C1	−0.0168 (3)	0.48804 (10)	0.15803 (9)	0.0479 (5)
C2	−0.1693 (3)	0.53455 (13)	0.15179 (10)	0.0626 (6)
C3	−0.2816 (4)	0.54052 (17)	0.09782 (13)	0.0850 (8)
H3	−0.3818	0.5716	0.0939	0.102*
C4	−0.2460 (4)	0.50012 (19)	0.04878 (13)	0.0938 (10)
H4	−0.3229	0.5041	0.0118	0.113*
C5	−0.0975 (4)	0.45394 (16)	0.05404 (11)	0.0854 (8)
H5	−0.0751	0.4269	0.0208	0.103*
C6	0.0185 (3)	0.44792 (12)	0.10900 (10)	0.0628 (6)
H6	0.1191	0.4171	0.1127	0.075*
C7	0.2195 (3)	0.43007 (10)	0.23271 (9)	0.0497 (5)
H7A	0.3384	0.4350	0.2160	0.060*
H7B	0.1597	0.3878	0.2166	0.060*
C8	0.2561 (3)	0.42537 (9)	0.30118 (9)	0.0460 (5)
C9	0.1217 (3)	0.39253 (10)	0.33156 (9)	0.0510 (5)
C10	0.1471 (3)	0.38502 (11)	0.39523 (10)	0.0610 (6)
H10	0.0549	0.3635	0.4149	0.073*
C11	0.3070 (3)	0.40930 (12)	0.42812 (10)	0.0633 (6)
H11	0.3242	0.4029	0.4702	0.076*
C12	0.6122 (3)	0.47032 (13)	0.43392 (11)	0.0691 (7)
H12	0.6322	0.4629	0.4758	0.083*
C13	0.7428 (4)	0.50649 (14)	0.40637 (13)	0.0779 (7)
H13	0.8501	0.5239	0.4294	0.094*
C14	0.7139 (3)	0.51724 (13)	0.34319 (12)	0.0718 (7)
H14	0.8017	0.5425	0.3245	0.086*
C15	0.5591 (3)	0.49120 (11)	0.30879 (10)	0.0576 (6)
H15	0.5441	0.4984	0.2668	0.069*
C16	0.4474 (3)	0.44400 (10)	0.39997 (9)	0.0538 (5)
C17	0.4198 (3)	0.45330 (10)	0.33556 (9)	0.0469 (5)
C18	−0.1706 (4)	0.32928 (14)	0.32310 (13)	0.0824 (8)
H18A	−0.2216	0.3573	0.3531	0.124*
H18B	−0.1124	0.2889	0.3423	0.124*
H18C	−0.2702	0.3156	0.2923	0.124*
O3	0.6832 (3)	0.10351 (9)	0.29302 (7)	0.0796 (5)
O4	0.5217 (2)	0.30583 (9)	0.17915 (8)	0.0802 (5)
N2	0.4025 (2)	0.18845 (8)	0.27327 (8)	0.0505 (4)
H35	0.465 (3)	0.1718 (11)	0.2442 (10)	0.061 (7)*
C19	0.5112 (3)	0.19270 (9)	0.33008 (8)	0.0434 (4)
C20	0.6598 (3)	0.14551 (10)	0.34137 (9)	0.0519 (5)
C21	0.7683 (3)	0.14390 (12)	0.39699 (10)	0.0660 (6)
H21	0.8673	0.1126	0.4041	0.079*

C22	0.7296 (4)	0.18927 (13)	0.44263 (10)	0.0733 (7)
H22	0.8024	0.1881	0.4805	0.088*
C23	0.5849 (4)	0.23555 (13)	0.43210 (10)	0.0711 (7)
H23	0.5603	0.2661	0.4627	0.085*
C24	0.4743 (3)	0.23732 (11)	0.37598 (9)	0.0562 (5)
H24	0.3751	0.2686	0.3693	0.067*
C25	0.2839 (3)	0.24647 (10)	0.24990 (9)	0.0499 (5)
H25A	0.3471	0.2896	0.2618	0.060*
H25B	0.1659	0.2453	0.2676	0.060*
C26	0.2444 (3)	0.24313 (10)	0.18170 (9)	0.0482 (5)
C27	0.3695 (3)	0.27438 (12)	0.14705 (10)	0.0592 (6)
C28	0.3399 (4)	0.27346 (14)	0.08317 (11)	0.0731 (7)
H28	0.4241	0.2958	0.0607	0.088*
C29	0.1871 (4)	0.23974 (15)	0.05396 (11)	0.0753 (7)
H29	0.1690	0.2390	0.0115	0.090*
C30	−0.1031 (4)	0.17011 (15)	0.05697 (11)	0.0787 (8)
H30	−0.1222	0.1687	0.0145	0.094*
C31	−0.2272 (4)	0.13796 (15)	0.08931 (13)	0.0841 (8)
H31	−0.3311	0.1151	0.0691	0.101*
C32	−0.1988 (3)	0.13913 (14)	0.15317 (12)	0.0732 (7)
H32	−0.2838	0.1166	0.1752	0.088*
C33	−0.0489 (3)	0.17276 (11)	0.18333 (10)	0.0575 (6)
H33	−0.0331	0.1729	0.2258	0.069*
C34	0.0559 (3)	0.20595 (12)	0.08671 (9)	0.0592 (6)
C35	0.0839 (3)	0.20765 (10)	0.15160 (9)	0.0484 (5)
C36	0.6600 (4)	0.33821 (17)	0.14691 (15)	0.1022 (10)
H36A	0.6016	0.3742	0.1213	0.153*
H36B	0.7138	0.3045	0.1221	0.153*
H36C	0.7575	0.3577	0.1756	0.153*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1044 (14)	0.0957 (14)	0.0720 (12)	0.0467 (11)	0.0064 (10)	−0.0047 (10)
O2	0.0568 (9)	0.0696 (10)	0.0770 (11)	−0.0108 (8)	0.0097 (8)	0.0033 (8)
N1	0.0571 (10)	0.0414 (9)	0.0465 (10)	0.0043 (8)	0.0043 (8)	−0.0019 (7)
C1	0.0505 (11)	0.0438 (11)	0.0491 (11)	−0.0077 (9)	0.0041 (9)	0.0028 (9)
C2	0.0565 (13)	0.0701 (15)	0.0598 (14)	0.0024 (11)	0.0013 (11)	0.0110 (11)
C3	0.0667 (16)	0.111 (2)	0.0745 (18)	0.0090 (15)	−0.0030 (14)	0.0142 (16)
C4	0.0795 (19)	0.127 (3)	0.0678 (18)	−0.0158 (19)	−0.0209 (15)	0.0121 (17)
C5	0.099 (2)	0.099 (2)	0.0555 (15)	−0.0185 (18)	0.0002 (14)	−0.0131 (14)
C6	0.0702 (14)	0.0609 (14)	0.0567 (13)	−0.0064 (11)	0.0053 (11)	−0.0063 (11)
C7	0.0540 (12)	0.0430 (11)	0.0527 (12)	0.0063 (9)	0.0089 (9)	0.0002 (9)
C8	0.0494 (11)	0.0389 (10)	0.0507 (11)	0.0081 (9)	0.0095 (9)	0.0021 (8)
C9	0.0507 (12)	0.0441 (11)	0.0591 (13)	0.0049 (9)	0.0111 (10)	0.0012 (9)
C10	0.0671 (15)	0.0565 (13)	0.0635 (14)	0.0050 (11)	0.0246 (12)	0.0077 (11)
C11	0.0817 (16)	0.0606 (14)	0.0493 (12)	0.0118 (12)	0.0153 (12)	0.0035 (10)
C12	0.0743 (16)	0.0722 (16)	0.0583 (14)	0.0082 (13)	−0.0020 (12)	−0.0083 (12)

C13	0.0675 (16)	0.0799 (18)	0.0830 (19)	−0.0028 (14)	−0.0052 (14)	−0.0174 (14)
C14	0.0628 (15)	0.0678 (16)	0.0856 (18)	−0.0075 (12)	0.0126 (13)	−0.0021 (13)
C15	0.0577 (13)	0.0556 (13)	0.0599 (13)	0.0023 (10)	0.0086 (10)	0.0036 (10)
C16	0.0616 (13)	0.0477 (12)	0.0522 (12)	0.0085 (10)	0.0070 (10)	−0.0027 (9)
C17	0.0508 (11)	0.0391 (10)	0.0512 (12)	0.0092 (9)	0.0081 (9)	0.0002 (8)
C18	0.0679 (16)	0.0728 (17)	0.109 (2)	−0.0173 (13)	0.0211 (15)	0.0093 (15)
O3	0.1055 (13)	0.0722 (11)	0.0563 (9)	0.0390 (10)	−0.0105 (9)	−0.0142 (8)
O4	0.0653 (10)	0.0875 (12)	0.0884 (12)	−0.0206 (9)	0.0123 (9)	−0.0064 (10)
N2	0.0565 (10)	0.0452 (10)	0.0478 (10)	0.0052 (8)	−0.0023 (8)	−0.0056 (8)
C19	0.0473 (11)	0.0378 (10)	0.0445 (10)	−0.0024 (8)	0.0031 (8)	0.0008 (8)
C20	0.0644 (13)	0.0432 (11)	0.0467 (11)	0.0040 (10)	0.0008 (10)	0.0004 (9)
C21	0.0757 (15)	0.0593 (14)	0.0594 (14)	0.0150 (12)	−0.0068 (12)	0.0027 (11)
C22	0.0942 (18)	0.0718 (16)	0.0484 (13)	0.0101 (14)	−0.0144 (12)	−0.0019 (12)
C23	0.0920 (18)	0.0707 (16)	0.0488 (13)	0.0123 (14)	0.0014 (12)	−0.0127 (11)
C24	0.0600 (13)	0.0543 (13)	0.0537 (12)	0.0075 (10)	0.0044 (10)	−0.0056 (10)
C25	0.0513 (11)	0.0456 (11)	0.0511 (12)	0.0075 (9)	−0.0010 (9)	−0.0047 (9)
C26	0.0499 (11)	0.0429 (11)	0.0512 (11)	0.0081 (9)	0.0038 (9)	0.0007 (9)
C27	0.0569 (13)	0.0569 (13)	0.0644 (14)	0.0042 (11)	0.0096 (11)	−0.0017 (11)
C28	0.0769 (17)	0.0784 (17)	0.0675 (16)	0.0005 (14)	0.0235 (13)	0.0088 (13)
C29	0.0848 (18)	0.0942 (19)	0.0476 (13)	0.0106 (15)	0.0113 (13)	0.0050 (12)
C30	0.0834 (18)	0.096 (2)	0.0524 (14)	0.0044 (15)	−0.0083 (13)	−0.0116 (13)
C31	0.0751 (17)	0.093 (2)	0.0795 (18)	−0.0124 (15)	−0.0106 (15)	−0.0173 (15)
C32	0.0689 (15)	0.0786 (17)	0.0711 (16)	−0.0131 (13)	0.0044 (13)	−0.0021 (13)
C33	0.0617 (13)	0.0588 (13)	0.0506 (12)	0.0016 (11)	0.0007 (10)	0.0011 (10)
C34	0.0645 (14)	0.0640 (14)	0.0478 (12)	0.0099 (11)	0.0011 (10)	−0.0017 (10)
C35	0.0517 (11)	0.0459 (11)	0.0464 (11)	0.0102 (9)	0.0003 (9)	0.0002 (9)
C36	0.0808 (19)	0.102 (2)	0.127 (3)	−0.0285 (17)	0.0257 (18)	0.0137 (19)

Geometric parameters (Å, º)

O1—C2	1.371 (3)	O3—C20	1.367 (2)
O2—C9	1.363 (3)	O4—C27	1.367 (3)
O2—C18	1.432 (3)	O4—C36	1.429 (3)
N1—C1	1.400 (3)	N2—C19	1.395 (2)
N1—C7	1.464 (2)	N2—C25	1.462 (2)
N1—H34	0.90 (2)	N2—H35	0.88 (2)
C1—C6	1.379 (3)	C19—C24	1.380 (3)
C1—C2	1.407 (3)	C19—C20	1.399 (3)
C2—C3	1.359 (3)	C20—C21	1.371 (3)
C3—C4	1.383 (4)	C21—C22	1.388 (3)
C3—H3	0.9300	C21—H21	0.9300
C4—C5	1.381 (4)	C22—C23	1.366 (3)
C4—H4	0.9300	C22—H22	0.9300
C5—C6	1.389 (3)	C23—C24	1.387 (3)
C5—H5	0.9300	C23—H23	0.9300
C6—H6	0.9300	C24—H24	0.9300
C7—C8	1.505 (3)	C25—C26	1.499 (3)
C7—H7A	0.9700	C25—H25A	0.9700

C7—H7B	0.9700	C25—H25B	0.9700
C8—C9	1.388 (3)	C26—C27	1.383 (3)
C8—C17	1.422 (3)	C26—C35	1.429 (3)
C9—C10	1.402 (3)	C27—C28	1.400 (3)
C10—C11	1.361 (3)	C28—C29	1.365 (4)
C10—H10	0.9300	C28—H28	0.9300
C11—C16	1.411 (3)	C29—C34	1.410 (3)
C11—H11	0.9300	C29—H29	0.9300
C12—C13	1.365 (4)	C30—C31	1.354 (4)
C12—C16	1.412 (3)	C30—C34	1.422 (3)
C12—H12	0.9300	C30—H30	0.9300
C13—C14	1.400 (4)	C31—C32	1.400 (4)
C13—H13	0.9300	C31—H31	0.9300
C14—C15	1.360 (3)	C32—C33	1.357 (3)
C14—H14	0.9300	C32—H32	0.9300
C15—C17	1.420 (3)	C33—C35	1.415 (3)
C15—H15	0.9300	C33—H33	0.9300
C16—C17	1.423 (3)	C34—C35	1.422 (3)
C18—H18A	0.9600	C36—H36A	0.9600
C18—H18B	0.9600	C36—H36B	0.9600
C18—H18C	0.9600	C36—H36C	0.9600

C9—O2—C18	118.85 (18)	C27—O4—C36	119.4 (2)
C1—N1—C7	120.01 (16)	C19—N2—C25	120.54 (16)
C1—N1—H34	113.4 (14)	C19—N2—H35	113.6 (14)
C7—N1—H34	109.0 (14)	C25—N2—H35	110.1 (14)
C6—C1—N1	124.09 (19)	C24—C19—N2	124.18 (18)
C6—C1—C2	119.7 (2)	C24—C19—C20	118.99 (18)
N1—C1—C2	116.13 (18)	N2—C19—C20	116.73 (17)
C3—C2—O1	125.3 (2)	O3—C20—C21	125.2 (2)
C3—C2—C1	120.6 (2)	O3—C20—C19	114.18 (17)
O1—C2—C1	114.05 (19)	C21—C20—C19	120.63 (19)
C2—C3—C4	119.6 (3)	C20—C21—C22	119.7 (2)
C2—C3—H3	120.2	C20—C21—H21	120.2
C4—C3—H3	120.2	C22—C21—H21	120.2
C5—C4—C3	120.7 (3)	C23—C22—C21	120.2 (2)
C5—C4—H4	119.6	C23—C22—H22	119.9
C3—C4—H4	119.6	C21—C22—H22	119.9
C4—C5—C6	119.9 (3)	C22—C23—C24	120.4 (2)
C4—C5—H5	120.0	C22—C23—H23	119.8
C6—C5—H5	120.0	C24—C23—H23	119.8
C1—C6—C5	119.5 (2)	C19—C24—C23	120.1 (2)
C1—C6—H6	120.3	C19—C24—H24	119.9
C5—C6—H6	120.3	C23—C24—H24	119.9
N1—C7—C8	110.71 (15)	N2—C25—C26	110.65 (16)
N1—C7—H7A	109.5	N2—C25—H25A	109.5
C8—C7—H7A	109.5	C26—C25—H25A	109.5
N1—C7—H7B	109.5	N2—C25—H25B	109.5

C8—C7—H7B	109.5	C26—C25—H25B	109.5
H7A—C7—H7B	108.1	H25A—C25—H25B	108.1
C9—C8—C17	119.19 (18)	C27—C26—C35	119.22 (19)
C9—C8—C7	117.74 (18)	C27—C26—C25	118.67 (19)
C17—C8—C7	123.07 (17)	C35—C26—C25	122.11 (18)
O2—C9—C8	115.68 (18)	O4—C27—C26	115.7 (2)
O2—C9—C10	123.19 (19)	O4—C27—C28	122.9 (2)
C8—C9—C10	121.1 (2)	C26—C27—C28	121.4 (2)
C11—C10—C9	119.9 (2)	C29—C28—C27	119.8 (2)
C11—C10—H10	120.1	C29—C28—H28	120.1
C9—C10—H10	120.1	C27—C28—H28	120.1
C10—C11—C16	121.6 (2)	C28—C29—C34	121.5 (2)
C10—C11—H11	119.2	C28—C29—H29	119.3
C16—C11—H11	119.2	C34—C29—H29	119.3
C13—C12—C16	121.2 (2)	C31—C30—C34	121.2 (2)
C13—C12—H12	119.4	C31—C30—H30	119.4
C16—C12—H12	119.4	C34—C30—H30	119.4
C12—C13—C14	119.5 (2)	C30—C31—C32	119.9 (2)
C12—C13—H13	120.2	C30—C31—H31	120.1
C14—C13—H13	120.2	C32—C31—H31	120.1
C15—C14—C13	120.9 (2)	C33—C32—C31	120.8 (2)
C15—C14—H14	119.6	C33—C32—H32	119.6
C13—C14—H14	119.6	C31—C32—H32	119.6
C14—C15—C17	121.5 (2)	C32—C33—C35	121.4 (2)
C14—C15—H15	119.3	C32—C33—H33	119.3
C17—C15—H15	119.3	C35—C33—H33	119.3
C11—C16—C12	121.9 (2)	C29—C34—C35	118.9 (2)
C11—C16—C17	118.6 (2)	C29—C34—C30	122.1 (2)
C12—C16—C17	119.4 (2)	C35—C34—C30	119.0 (2)
C15—C17—C8	123.10 (18)	C33—C35—C34	117.73 (19)
C15—C17—C16	117.43 (19)	C33—C35—C26	123.11 (18)
C8—C17—C16	119.47 (18)	C34—C35—C26	119.15 (19)
O2—C18—H18A	109.5	O4—C36—H36A	109.5
O2—C18—H18B	109.5	O4—C36—H36B	109.5
H18A—C18—H18B	109.5	H36A—C36—H36B	109.5
O2—C18—H18C	109.5	O4—C36—H36C	109.5
H18A—C18—H18C	109.5	H36A—C36—H36C	109.5
H18B—C18—H18C	109.5	H36B—C36—H36C	109.5

C7—N1—C1—C6	−23.4 (3)	C25—N2—C19—C24	22.2 (3)
C7—N1—C1—C2	160.56 (18)	C25—N2—C19—C20	−161.57 (18)
C6—C1—C2—C3	−0.3 (3)	C24—C19—C20—O3	179.58 (19)
N1—C1—C2—C3	175.9 (2)	N2—C19—C20—O3	3.1 (3)
C6—C1—C2—O1	−178.7 (2)	C24—C19—C20—C21	−0.5 (3)
N1—C1—C2—O1	−2.6 (3)	N2—C19—C20—C21	−177.0 (2)
O1—C2—C3—C4	178.6 (3)	O3—C20—C21—C22	−179.8 (2)
C1—C2—C3—C4	0.4 (4)	C19—C20—C21—C22	0.4 (4)
C2—C3—C4—C5	−0.1 (4)	C20—C21—C22—C23	−0.4 (4)

C3—C4—C5—C6	−0.3 (4)	C21—C22—C23—C24	0.5 (4)
N1—C1—C6—C5	−175.9 (2)	N2—C19—C24—C23	176.8 (2)
C2—C1—C6—C5	−0.1 (3)	C20—C19—C24—C23	0.7 (3)
C4—C5—C6—C1	0.4 (4)	C22—C23—C24—C19	−0.7 (4)
C1—N1—C7—C8	−153.22 (18)	C19—N2—C25—C26	157.18 (18)
N1—C7—C8—C9	83.4 (2)	N2—C25—C26—C27	−88.3 (2)
N1—C7—C8—C17	−96.1 (2)	N2—C25—C26—C35	90.5 (2)
C18—O2—C9—C8	175.37 (19)	C36—O4—C27—C26	178.8 (2)
C18—O2—C9—C10	−4.2 (3)	C36—O4—C27—C28	−1.3 (4)
C17—C8—C9—O2	178.85 (16)	C35—C26—C27—O4	−178.50 (17)
C7—C8—C9—O2	−0.7 (3)	C25—C26—C27—O4	0.3 (3)
C17—C8—C9—C10	−1.6 (3)	C35—C26—C27—C28	1.6 (3)
C7—C8—C9—C10	178.88 (18)	C25—C26—C27—C28	−179.6 (2)
O2—C9—C10—C11	178.6 (2)	O4—C27—C28—C29	178.5 (2)
C8—C9—C10—C11	−0.9 (3)	C26—C27—C28—C29	−1.6 (4)
C9—C10—C11—C16	1.9 (3)	C27—C28—C29—C34	0.6 (4)
C16—C12—C13—C14	−0.6 (4)	C34—C30—C31—C32	−0.6 (4)
C12—C13—C14—C15	−1.1 (4)	C30—C31—C32—C33	0.6 (4)
C13—C14—C15—C17	1.1 (4)	C31—C32—C33—C35	−0.1 (4)
C10—C11—C16—C12	178.9 (2)	C28—C29—C34—C35	0.4 (4)
C10—C11—C16—C17	−0.2 (3)	C28—C29—C34—C30	−179.5 (2)
C13—C12—C16—C11	−177.0 (2)	C31—C30—C34—C29	179.9 (3)
C13—C12—C16—C17	2.1 (3)	C31—C30—C34—C35	0.1 (4)
C14—C15—C17—C8	179.9 (2)	C32—C33—C35—C34	−0.4 (3)
C14—C15—C17—C16	0.5 (3)	C32—C33—C35—C26	−179.5 (2)
C9—C8—C17—C15	−176.21 (18)	C29—C34—C35—C33	−179.4 (2)
C7—C8—C17—C15	3.3 (3)	C30—C34—C35—C33	0.4 (3)
C9—C8—C17—C16	3.2 (3)	C29—C34—C35—C26	−0.4 (3)
C7—C8—C17—C16	−177.29 (17)	C30—C34—C35—C26	179.5 (2)
C11—C16—C17—C15	177.13 (18)	C27—C26—C35—C33	178.39 (19)
C12—C16—C17—C15	−2.0 (3)	C25—C26—C35—C33	−0.4 (3)
C11—C16—C17—C8	−2.3 (3)	C27—C26—C35—C34	−0.6 (3)
C12—C16—C17—C8	178.50 (18)	C25—C26—C35—C34	−179.40 (17)

Hydrogen-bond geometry (Å, º)

*Cg*1, *Cg*2, *Cg*3, *Cg*5 and *Cg*7 are the centroids of rings C1–C6, C8–C11/C16/C17, C12–C17, C19–C24 and C30–C35, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···*Cg*5^{i}	0.93	2.93	3.826 (3)	162
C18—H18*A*···*Cg*3^{ii}	0.96	2.81	3.637 (3)	144
C21—H21···*Cg*1^{iii}	0.93	2.99	3.890 (3)	165
C24—H24···*Cg*2	0.93	2.97	3.753 (2)	143
C36—H36*B*···*Cg*7^{iv}	0.96	2.98	3.814 (3)	146

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