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(*E*)-1-(4-Aminophenyl)-3-[4-(benzyloxy)phenyl]-prop-2-en-1-one

T. Hannah Clara,[a] Johanan Christian Prasana,[a] D. Reuben Jonathan,[b] B. K. Revathi[c] and G. Usha[d]*

[a]Department of Physics, Madras Christian College, Chennai 600 059, Tamilnadu, India, [b]Department of Chemistry, Madras Christian College, Chennai 600 059, Tamilnadu, India, [c]Department of Physics, Jerusalem College of Engineering, Chennai 100, Tamilnadu, India, and [d]PG and Research Department of Physics, Queen Mary's College, Chennai-4, Tamilnadu, India. *Correspondence e-mail: guqmc@yahoo.com

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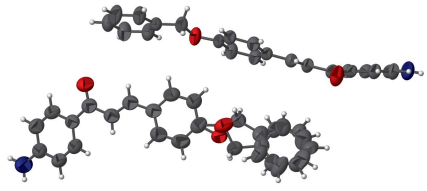
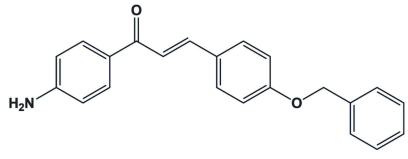
The title compound, $C_{22}H_{19}NO_2$, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. The benzyloxy ring in molecule *A* is disordered over two sets of sites, with a refined occupancy ratio of 0.665 (6):0.335 (6). Both molecules have an *E* conformation about the C=C bond of the prop-2-en-1-one unit. In the major component of molecule *A*, the aminobenzene and benzyloxy rings are inclined to the central benzene ring by 20.12 (16) and 36.2 (3)°, respectively, and by 55.6 (3)° to one another. In molecule *B*, the corresponding dihedral angles are 23.65 (12), 10.24 (14) and 23.07 (14)°, respectively. In the crystal, the two molecules are linked by an N—H···O hydrogen bond. These *A*–*B* units are linked by N—H···π and C—H···π interactions, forming undulating sheets parallel to the *ab* plane.

3D view



Chemical scheme



Structure description

Chalcones, members of the flavonoid family, constitute an important group of natural products owing to their wide range of pharmocological activities such as anti- inflammatory, antifungal, antiviral, antimicrobial, anticancer and antitumor activities (Hamada & Sharshira, 2011; Kumar *et al.*, 2003). Flavonoids are effectively exploited for their insecticidal and enzyme-inhibitory properties (Won *et al.*, 2005; Churkin *et al.*, 1982). In our efforts to study the biological activities of chalcone derivatives, we synthesized the title compound and report herein on its crystal structure.

The asymmetric unit of the title compound (Fig. 1), contains two crystallographically independent molecules (*A* and *B*). The benzyloxy ring in molecule *A* (O2/C16–C22) is disordered over two sets of sites. Both molecules have an *E* conformation about the C=C

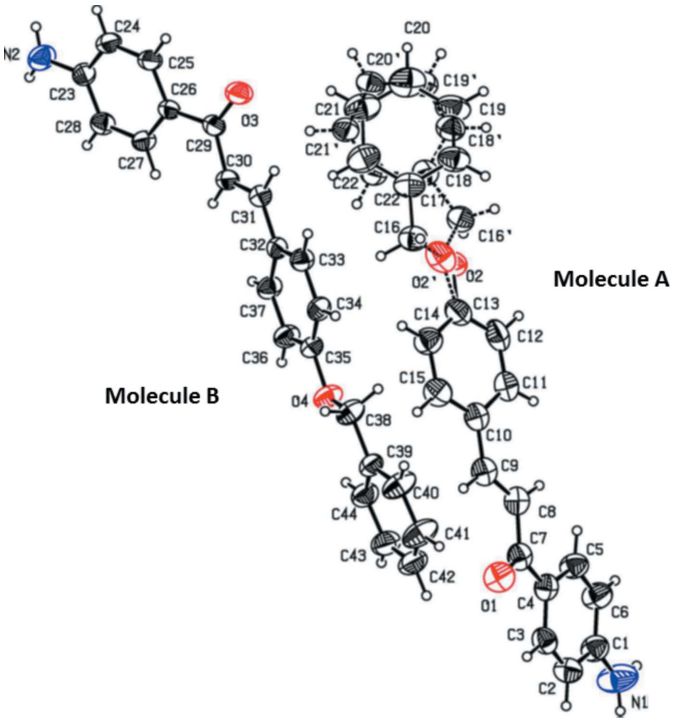


Figure 1
The molecular structure of the two independent molecules (*A* and *B*) of the title compound, with the atom labelling. Displacement ellipsoids drawn at the 30% probability level.

bond of the prop-2-en-1-one unit. In the major component of molecule *A*, the aminobenzene (C1–C6) and benzyloxy (C17–C22) rings are inclined to the central benzene (C10–C15) ring by 20.12 (16) and 36.2 (3)°, respectively, and by 55.6 (3)° to one another. The corresponding dihedral angles in molecule *B* differ quite considerably from those in molecule *A*, with the aminobenzene (C23–C28) and benzyloxy (C39–C44) rings inclined to the central benzene (C32–C37) ring by 23.65 (12) and 10.24 (14)°, and by only 23.07 (14)° to one another. The conformation of molecule *B* is similar to that of the 4-hydroxyphenyl analogue, (*E*)-3-[4-(benzyloxy)phenyl]-1-(4-hydroxyphenyl)prop-2-en-1-one (Ramkumar *et al.*, 2013) in which the corresponding dihedral angles are 24.7 (2), 9.6 (2) and 33.1 (2)°, respectively.

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

*Cg*1, *Cg*2 and *Cg*5 are the centroids of rings C1–C6, C10–C15 and C23–C28, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···O1^{i}	0.93 (4)	2.14 (4)	3.070 (5)	177 (3)
N1—H1*A*···*Cg*5^{ii}	0.84 (5)	2.81 (4)	3.619 (5)	166 (4)
C2—H2···*Cg*1^{iii}	0.93	2.97	3.699 (3)	136
C18—H18···*Cg*2^{iv}	0.93	2.98	3.661 (7)	131
C40—H40···*Cg*5^{v}	0.93	2.92	3.683 (3)	141
C16′—H16*D*···*Cg*2^{iv}	0.97	2.87	3.757 (10)	152

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $-x+1, -y+1, -z+2$; (iii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iv) $x, y+1, z$; (v) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{5}{2}$.

In the crystal, the two molecules are linked by an N—H···O hydrogen bond (Table 1). These *A*–*B* units are linked by N—H···π and C—H···π interactions, forming undulating sheets parallel to the *ab* plane (Table 1 and Figs. 2 and 3).

Synthesis and crystallization

In a 250 ml round-bottomed flask 120 ml of absolute alcohol was added to 4-aminoacetophenone (0.01 mol) and 4-benzyloxybenzaldehyde (0.01 mol), and the mixture stirred at room temperature. A 10% sodium hydroxide solution was added and the mixture stirred for a further 2 h. In order to precipitate the formed product the mixture was poured into 500 ml of ice-cold water. The precipitate was filtered, washed with distilled water and dried. It was purified by repeated recrys-

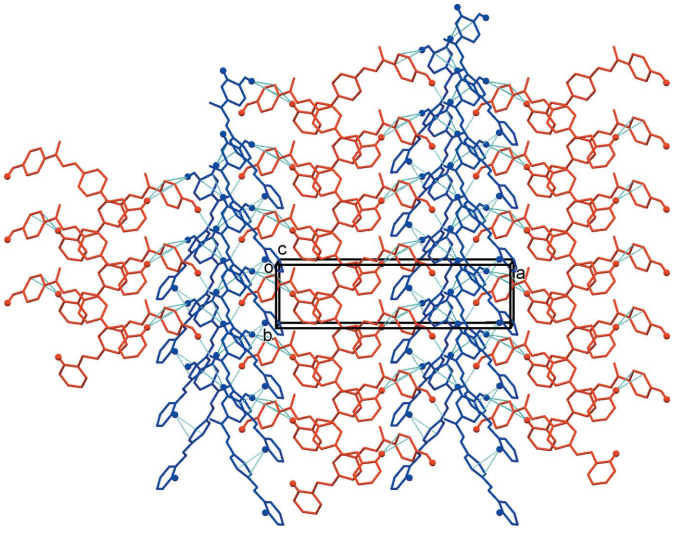


Figure 2
The crystal packing of the title compound, viewed along the *c* axis (major component of molecule *A* blue, molecule *B* red). The dashed lines indicate the hydrogen bonds and the N—H···π and C—H···π interactions (see Table 1). For clarity, only H atoms (shown as balls) involved in these interactions have been included.

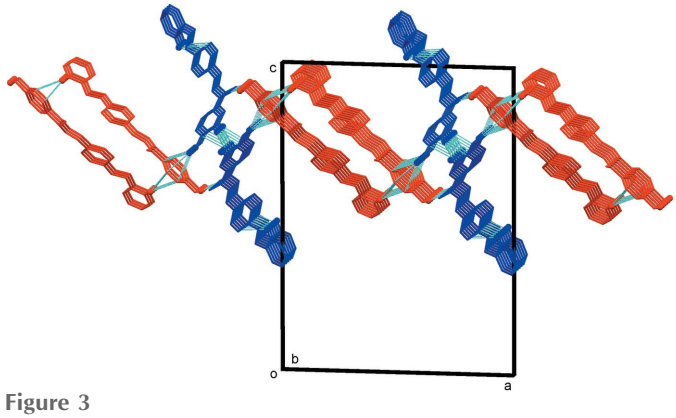


Figure 3
A partial view along the *b* axis, of the crystal packing of the title compound (major component of molecule *A* blue, molecule *B* red). The dashed lines indicate the hydrogen bonds and the N—H···π and C—H···π interactions (see Table 1). For clarity, only H atoms (shown as balls) involved in these interactions have been included.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{19}NO_2$
M_r	329.38
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	293
a, b, c (Å)	21.3428 (8), 5.7635 (2), 28.2870 (11)
β (°)	91.634 (1)
V (Å^3)	3478.1 (2)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.30 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.976, 0.984
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	36876, 6128, 3471
R_{int}	0.036
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.191, 1.02
No. of reflections	6128
No. of parameters	541
No. of restraints	134
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.19

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2004), *SIR92* (Altomare *et al.*, 1993), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008).

tallization in absolute ethanol, giving yellow block-like crystals of the title compound (yield 97%).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The benzyloxy ring in molecule *A* is disordered over two sets of sites (O2/C16–C22 and O2′/C16′–C22′), with a refined occupancy ratio of 0.665 (6):0.335 (6).

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161371 [doi:10.1107/S2414314616013717]

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Crystal data

$C_{22}H_{19}NO_2$
M_r = 329.38
Monoclinic, $P2_1/n$
a = 21.3428 (8) Å
b = 5.7635 (2) Å
c = 28.2870 (11) Å
β = 91.634 (1)°
V = 3478.1 (2) Å^3
Z = 8
$F(000)$ = 1392
D_x = 1.258 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8554 reflections
θ = 2.4–21.9°
μ = 0.08 mm^{-1}
T = 293 K
Block, yellow
0.30 × 0.25 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.976, T_{max} = 0.984
36876 measured reflections
6128 independent reflections
3471 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 25.0°, θ_{min} = 2.4°
h = −25→24
k = −6→6
l = −26→33

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.191
S = 1.02
6128 reflections
541 parameters
134 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
$w = 1/[\sigma^2(F_o^2) + (0.0963P)^2 + 0.9188P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0029 (7)

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}	Occ. (<1)
C1	0.66578 (15)	−0.2791 (6)	0.76246 (11)	0.0842 (9)	
C2	0.71650 (15)	−0.3689 (6)	0.78799 (11)	0.0846 (9)	
H2	0.7346	−0.5074	0.7784	0.102*	
C3	0.74027 (13)	−0.2569 (6)	0.82699 (11)	0.0761 (8)	
H3	0.7744	−0.3210	0.8434	0.091*	
C4	0.71491 (12)	−0.0492 (5)	0.84300 (10)	0.0694 (8)	
C5	0.66439 (14)	0.0399 (6)	0.81634 (11)	0.0840 (9)	
H5	0.6466	0.1801	0.8252	0.101*	
C6	0.64038 (15)	−0.0739 (6)	0.77743 (12)	0.0918 (10)	
H6	0.6062	−0.0111	0.7608	0.110*	
C7	0.74135 (14)	0.0647 (5)	0.88568 (11)	0.0742 (8)	
C8	0.70887 (13)	0.2667 (5)	0.90498 (11)	0.0770 (8)	
H8	0.6796	0.3432	0.8856	0.092*	
C9	0.71895 (13)	0.3453 (5)	0.94832 (11)	0.0746 (8)	
H9	0.7496	0.2680	0.9662	0.089*	
C10	0.68838 (13)	0.5370 (5)	0.97165 (11)	0.0712 (8)	
C11	0.64444 (15)	0.6768 (6)	0.94886 (12)	0.0862 (9)	
H11	0.6348	0.6510	0.9170	0.103*	
C12	0.61492 (17)	0.8505 (7)	0.97172 (13)	0.0977 (11)	
H12	0.5856	0.9417	0.9554	0.117*	
C13	0.62783 (15)	0.8934 (6)	1.01877 (13)	0.0855 (9)	
C14	0.67269 (15)	0.7612 (6)	1.04260 (12)	0.0879 (9)	
H14	0.6830	0.7906	1.0742	0.105*	
C15	0.70157 (14)	0.5862 (6)	1.01876 (12)	0.0838 (9)	
H15	0.7314	0.4964	1.0350	0.101*	
C23	0.40931 (11)	1.0076 (5)	1.39037 (9)	0.0613 (7)	
C24	0.43961 (13)	1.2218 (5)	1.39056 (10)	0.0702 (8)	
H24	0.4290	1.3331	1.4127	0.084*	
C25	0.48466 (12)	1.2709 (4)	1.35868 (9)	0.0642 (7)	
H25	0.5042	1.4152	1.3597	0.077*	
C26	0.50210 (11)	1.1101 (4)	1.32472 (8)	0.0536 (6)	
C27	0.47235 (11)	0.8958 (5)	1.32505 (9)	0.0595 (7)	
H27	0.4836	0.7832	1.3033	0.071*	
C28	0.42673 (11)	0.8464 (5)	1.35673 (9)	0.0620 (7)	
H28	0.4071	0.7023	1.3557	0.074*	
C29	0.55081 (12)	1.1757 (5)	1.29130 (9)	0.0611 (7)	
C30	0.58160 (12)	0.9971 (4)	1.26320 (8)	0.0590 (7)	
H30	0.5641	0.8495	1.2610	0.071*	
C31	0.63412 (12)	1.0435 (5)	1.24088 (8)	0.0596 (7)	
H31	0.6490	1.1946	1.2438	0.071*	
C32	0.67115 (11)	0.8876 (4)	1.21254 (8)	0.0541 (6)	
C33	0.73159 (12)	0.9480 (5)	1.20084 (9)	0.0628 (7)	
H33	0.7479	1.0887	1.2116	0.075*	
C34	0.76849 (12)	0.8051 (5)	1.17363 (8)	0.0621 (7)	
H34	0.8092	0.8483	1.1667	0.075*	

C35	0.74420 (12)	0.5989 (5)	1.15706 (8)	0.0585 (6)	
C36	0.68406 (13)	0.5352 (5)	1.16836 (10)	0.0705 (8)	
H36	0.6675	0.3956	1.1572	0.085*	
C37	0.64855 (12)	0.6769 (5)	1.19594 (9)	0.0650 (7)	
H37	0.6084	0.6303	1.2036	0.078*	
C38	0.83712 (13)	0.4868 (6)	1.11791 (10)	0.0782 (9)	
H38A	0.8632	0.4729	1.1464	0.094*	
H38B	0.8415	0.6434	1.1058	0.094*	
C39	0.85833 (12)	0.3169 (5)	1.08190 (8)	0.0635 (7)	
C40	0.91657 (14)	0.3446 (7)	1.06354 (11)	0.0968 (11)	
H40	0.9422	0.4653	1.0742	0.116*	
C41	0.93766 (16)	0.1951 (8)	1.02936 (13)	0.1127 (13)	
H41	0.9771	0.2169	1.0170	0.135*	
C42	0.90094 (17)	0.0153 (6)	1.01360 (11)	0.0917 (10)	
H42	0.9155	−0.0872	0.9910	0.110*	
C43	0.84347 (17)	−0.0118 (6)	1.03113 (11)	0.0911 (10)	
H43	0.8178	−0.1318	1.0201	0.109*	
C44	0.82232 (15)	0.1370 (6)	1.06529 (10)	0.0816 (9)	
H44	0.7827	0.1145	1.0773	0.098*	
O1	0.78887 (10)	−0.0107 (4)	0.90580 (8)	0.0962 (7)	
O3	0.56699 (10)	1.3799 (4)	1.28826 (8)	0.0923 (7)	
O4	0.77438 (8)	0.4456 (3)	1.12854 (7)	0.0783 (6)	
N1	0.6416 (2)	−0.3944 (9)	0.72373 (14)	0.1351 (15)	
N2	0.36548 (13)	0.9551 (7)	1.42293 (11)	0.0857 (8)	
O2	0.5882 (2)	1.0498 (8)	1.03545 (17)	0.0858 (16)	0.665 (6)
C16	0.5999 (3)	1.1013 (11)	1.0832 (2)	0.0804 (17)	0.665 (6)
H16A	0.6424	1.1591	1.0875	0.097*	0.665 (6)
H16B	0.5959	0.9617	1.1020	0.097*	0.665 (6)
C17	0.5551 (3)	1.2776 (12)	1.0990 (3)	0.0810 (19)	0.665 (6)
C18	0.5384 (3)	1.4543 (16)	1.0683 (2)	0.0926 (18)	0.665 (6)
H18	0.5536	1.4542	1.0378	0.111*	0.665 (6)
C19	0.4992 (4)	1.6319 (15)	1.0822 (4)	0.113 (3)	0.665 (6)
H19	0.4887	1.7499	1.0610	0.136*	0.665 (6)
C20	0.4758 (5)	1.636 (2)	1.1268 (4)	0.116 (3)	0.665 (6)
H20	0.4512	1.7602	1.1363	0.139*	0.665 (6)
C21	0.4889 (4)	1.4579 (19)	1.1573 (3)	0.113 (3)	0.665 (6)
H21	0.4718	1.4552	1.1872	0.136*	0.665 (6)
C22	0.5281 (5)	1.2815 (18)	1.1432 (3)	0.102 (3)	0.665 (6)
H22	0.5368	1.1604	1.1641	0.123*	0.665 (6)
O2′	0.6126 (5)	1.0846 (17)	1.0544 (4)	0.098 (4)	0.335 (6)
C16′	0.5607 (4)	1.2296 (18)	1.0416 (3)	0.077 (3)	0.335 (6)
H16C	0.5288	1.1385	1.0251	0.093*	0.335 (6)
H16D	0.5743	1.3509	1.0204	0.093*	0.335 (6)
C17′	0.5334 (7)	1.338 (3)	1.0855 (5)	0.072 (3)	0.335 (6)
C18′	0.5086 (10)	1.551 (3)	1.0777 (5)	0.090 (4)	0.335 (6)
H18′	0.5133	1.6235	1.0487	0.108*	0.335 (6)
C19′	0.4767 (11)	1.660 (4)	1.1125 (5)	0.090 (5)	0.335 (6)
H19′	0.4574	1.8024	1.1063	0.108*	0.335 (6)

C20′	0.4730 (6)	1.560 (2)	1.1568 (5)	0.078 (3)	0.335 (6)
H20′	0.4540	1.6388	1.1813	0.094*	0.335 (6)
C21′	0.4980 (6)	1.341 (2)	1.1640 (5)	0.076 (3)	0.335 (6)
H21′	0.4934	1.2653	1.1928	0.091*	0.335 (6)
C22′	0.5295 (8)	1.236 (3)	1.1285 (6)	0.076 (4)	0.335 (6)
H22′	0.5484	1.0924	1.1338	0.091*	0.335 (6)
H2B	0.3414 (18)	0.822 (7)	1.4189 (12)	0.120 (14)*	
H2A	0.3524 (16)	1.065 (6)	1.4385 (11)	0.094 (12)*	
H1B	0.663 (2)	−0.508 (8)	0.7123 (16)	0.16 (2)*	
H1A	0.614 (2)	−0.334 (8)	0.7064 (16)	0.149 (19)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.077 (2)	0.094 (2)	0.081 (2)	0.0092 (19)	0.0012 (17)	−0.0071 (18)
C2	0.083 (2)	0.077 (2)	0.094 (2)	0.0092 (17)	−0.0007 (18)	−0.0057 (18)
C3	0.0641 (17)	0.078 (2)	0.086 (2)	0.0053 (16)	0.0022 (15)	0.0134 (17)
C4	0.0538 (15)	0.084 (2)	0.0705 (17)	−0.0048 (15)	0.0055 (13)	0.0057 (16)
C5	0.0740 (19)	0.091 (2)	0.087 (2)	0.0158 (17)	0.0017 (17)	−0.0099 (18)
C6	0.079 (2)	0.109 (3)	0.087 (2)	0.025 (2)	−0.0114 (17)	−0.013 (2)
C7	0.0586 (17)	0.082 (2)	0.082 (2)	−0.0061 (16)	0.0072 (15)	0.0090 (17)
C8	0.0682 (18)	0.086 (2)	0.077 (2)	−0.0092 (17)	−0.0022 (15)	0.0050 (17)
C9	0.0534 (15)	0.085 (2)	0.086 (2)	−0.0113 (15)	0.0024 (14)	0.0078 (17)
C10	0.0564 (16)	0.077 (2)	0.080 (2)	−0.0132 (15)	−0.0011 (14)	0.0099 (16)
C11	0.090 (2)	0.087 (2)	0.082 (2)	−0.0034 (19)	0.0016 (18)	0.0185 (19)
C12	0.103 (3)	0.095 (3)	0.094 (3)	0.009 (2)	−0.004 (2)	0.038 (2)
C13	0.078 (2)	0.071 (2)	0.108 (3)	0.0054 (19)	0.0155 (19)	0.017 (2)
C14	0.080 (2)	0.095 (2)	0.089 (2)	0.0084 (19)	0.0006 (17)	−0.0047 (19)
C15	0.0643 (18)	0.093 (2)	0.093 (2)	0.0051 (17)	−0.0096 (16)	0.0028 (19)
C23	0.0545 (15)	0.0652 (18)	0.0647 (15)	0.0071 (14)	0.0103 (13)	0.0026 (13)
C24	0.0787 (18)	0.0602 (18)	0.0727 (17)	0.0078 (15)	0.0204 (14)	−0.0115 (14)
C25	0.0714 (17)	0.0479 (15)	0.0739 (17)	0.0054 (13)	0.0139 (14)	−0.0048 (13)
C26	0.0561 (14)	0.0448 (15)	0.0601 (14)	0.0094 (12)	0.0074 (11)	0.0012 (12)
C27	0.0592 (15)	0.0558 (16)	0.0638 (15)	0.0068 (13)	0.0076 (12)	−0.0071 (13)
C28	0.0554 (15)	0.0574 (17)	0.0733 (16)	0.0000 (13)	0.0052 (13)	−0.0026 (14)
C29	0.0667 (16)	0.0485 (17)	0.0685 (16)	0.0057 (13)	0.0107 (13)	0.0042 (13)
C30	0.0637 (15)	0.0500 (15)	0.0639 (15)	0.0053 (12)	0.0119 (13)	−0.0040 (12)
C31	0.0624 (16)	0.0576 (16)	0.0590 (14)	0.0040 (13)	0.0077 (12)	−0.0010 (12)
C32	0.0542 (14)	0.0547 (16)	0.0539 (13)	0.0027 (12)	0.0076 (11)	0.0037 (12)
C33	0.0611 (16)	0.0611 (17)	0.0667 (15)	−0.0035 (14)	0.0078 (13)	−0.0041 (13)
C34	0.0511 (14)	0.0730 (19)	0.0627 (15)	−0.0017 (14)	0.0106 (12)	−0.0022 (14)
C35	0.0590 (15)	0.0612 (17)	0.0558 (14)	0.0055 (14)	0.0124 (12)	−0.0047 (13)
C36	0.0688 (17)	0.0647 (18)	0.0789 (18)	−0.0086 (15)	0.0198 (15)	−0.0128 (14)
C37	0.0549 (15)	0.0676 (18)	0.0736 (17)	−0.0047 (14)	0.0195 (13)	−0.0070 (14)
C38	0.0608 (17)	0.099 (2)	0.0758 (18)	0.0015 (16)	0.0149 (14)	−0.0189 (16)
C39	0.0597 (16)	0.0779 (19)	0.0533 (14)	0.0109 (15)	0.0064 (12)	−0.0071 (13)
C40	0.0656 (19)	0.130 (3)	0.095 (2)	−0.0030 (19)	0.0168 (17)	−0.042 (2)
C41	0.072 (2)	0.153 (4)	0.115 (3)	0.006 (2)	0.0342 (19)	−0.041 (3)

C42	0.098 (3)	0.098 (3)	0.080 (2)	0.016 (2)	0.0201 (19)	−0.0204 (18)
C43	0.101 (2)	0.079 (2)	0.095 (2)	−0.0058 (19)	0.0249 (19)	−0.0207 (18)
C44	0.079 (2)	0.083 (2)	0.084 (2)	0.0018 (18)	0.0268 (16)	−0.0106 (18)
O1	0.0700 (13)	0.1152 (18)	0.1026 (16)	0.0058 (13)	−0.0122 (12)	−0.0056 (13)
O3	0.1107 (16)	0.0543 (13)	0.1147 (16)	0.0020 (12)	0.0530 (13)	0.0015 (11)
O4	0.0680 (12)	0.0818 (13)	0.0867 (13)	−0.0025 (10)	0.0275 (10)	−0.0225 (11)
N1	0.130 (3)	0.150 (4)	0.123 (3)	0.046 (3)	−0.045 (2)	−0.058 (3)
N2	0.0801 (18)	0.085 (2)	0.0938 (19)	−0.0027 (17)	0.0346 (15)	−0.0080 (17)
O2	0.090 (3)	0.080 (3)	0.086 (3)	0.017 (3)	−0.018 (2)	−0.0083 (18)
C16	0.079 (3)	0.077 (3)	0.084 (3)	0.004 (3)	−0.014 (3)	−0.014 (3)
C17	0.067 (3)	0.073 (3)	0.102 (4)	−0.006 (2)	−0.009 (3)	−0.022 (2)
C18	0.070 (3)	0.083 (4)	0.126 (4)	0.011 (3)	0.012 (3)	−0.008 (3)
C19	0.084 (4)	0.086 (5)	0.171 (6)	0.016 (4)	0.037 (4)	−0.002 (4)
C20	0.068 (5)	0.116 (6)	0.165 (7)	−0.006 (4)	0.028 (5)	−0.019 (5)
C21	0.093 (5)	0.107 (6)	0.139 (6)	−0.012 (4)	0.015 (4)	−0.035 (4)
C22	0.092 (5)	0.112 (5)	0.103 (4)	−0.004 (3)	−0.001 (4)	−0.027 (3)
O2′	0.066 (5)	0.100 (7)	0.129 (11)	0.008 (4)	−0.003 (5)	0.024 (7)
C16′	0.069 (4)	0.078 (6)	0.084 (5)	0.005 (4)	−0.004 (3)	0.001 (4)
C17′	0.068 (7)	0.063 (6)	0.087 (5)	−0.017 (5)	0.006 (4)	−0.004 (4)
C18′	0.101 (10)	0.068 (6)	0.102 (6)	−0.003 (5)	0.008 (5)	−0.006 (4)
C19′	0.099 (11)	0.079 (7)	0.091 (5)	0.016 (7)	−0.006 (5)	−0.004 (4)
C20′	0.070 (7)	0.071 (6)	0.092 (5)	0.010 (5)	−0.013 (4)	−0.005 (4)
C21′	0.069 (6)	0.075 (6)	0.082 (5)	0.015 (5)	0.003 (4)	0.000 (4)
C22′	0.074 (7)	0.064 (6)	0.091 (5)	0.000 (5)	0.014 (5)	−0.002 (4)

Geometric parameters (Å, º)

C1—N1	1.370 (5)	C35—O4	1.370 (3)
C1—C6	1.373 (4)	C35—C36	1.381 (4)
C1—C2	1.384 (4)	C36—C37	1.373 (3)
C2—C3	1.363 (4)	C36—H36	0.9300
C2—H2	0.9300	C37—H37	0.9300
C3—C4	1.395 (4)	C38—O4	1.401 (3)
C3—H3	0.9300	C38—C39	1.493 (4)
C4—C5	1.396 (4)	C38—H38A	0.9700
C4—C7	1.472 (4)	C38—H38B	0.9700
C5—C6	1.368 (4)	C39—C44	1.366 (4)
C5—H5	0.9300	C39—C40	1.370 (4)
C6—H6	0.9300	C40—C41	1.380 (4)
C7—O1	1.228 (3)	C40—H40	0.9300
C7—C8	1.468 (4)	C41—C42	1.366 (5)
C8—C9	1.319 (4)	C41—H41	0.9300
C8—H8	0.9300	C42—C43	1.345 (4)
C9—C10	1.451 (4)	C42—H42	0.9300
C9—H9	0.9300	C43—C44	1.378 (4)
C10—C11	1.382 (4)	C43—H43	0.9300
C10—C15	1.383 (4)	C44—H44	0.9300
C11—C12	1.357 (5)	N1—H1B	0.87 (5)

C11—H11	0.9300	N1—H1A	0.84 (5)
C12—C13	1.374 (5)	N2—H2B	0.93 (4)
C12—H12	0.9300	N2—H2A	0.83 (3)
C13—O2	1.332 (5)	O2—C16	1.397 (7)
C13—C14	1.384 (4)	C16—C17	1.474 (8)
C13—O2′	1.534 (11)	C16—H16A	0.9700
C14—C15	1.370 (4)	C16—H16B	0.9700
C14—H14	0.9300	C17—C18	1.379 (8)
C15—H15	0.9300	C17—C22	1.393 (8)
C23—N2	1.365 (4)	C18—C19	1.386 (8)
C23—C28	1.388 (3)	C18—H18	0.9300
C23—C24	1.394 (4)	C19—C20	1.371 (9)
C24—C25	1.367 (4)	C19—H19	0.9300
C24—H24	0.9300	C20—C21	1.367 (11)
C25—C26	1.393 (3)	C20—H20	0.9300
C25—H25	0.9300	C21—C22	1.382 (10)
C26—C27	1.389 (4)	C21—H21	0.9300
C26—C29	1.475 (3)	C22—H22	0.9300
C27—C28	1.372 (3)	O2′—C16′	1.425 (11)
C27—H27	0.9300	C16′—C17′	1.523 (15)
C28—H28	0.9300	C16′—H16C	0.9700
C29—O3	1.230 (3)	C16′—H16D	0.9700
C29—C30	1.467 (3)	C17′—C18′	1.352 (14)
C30—C31	1.329 (3)	C17′—C22′	1.356 (13)
C30—H30	0.9300	C18′—C19′	1.366 (14)
C31—C32	1.453 (3)	C18′—H18′	0.9300
C31—H31	0.9300	C19′—C20′	1.385 (13)
C32—C37	1.383 (4)	C19′—H19′	0.9300
C32—C33	1.385 (3)	C20′—C21′	1.387 (13)
C33—C34	1.388 (3)	C20′—H20′	0.9300
C33—H33	0.9300	C21′—C22′	1.365 (12)
C34—C35	1.373 (4)	C21′—H21′	0.9300
C34—H34	0.9300	C22′—H22′	0.9300

N1—C1—C6	121.4 (3)	C37—C36—H36	119.8
N1—C1—C2	120.5 (4)	C35—C36—H36	119.8
C6—C1—C2	118.1 (3)	C36—C37—C32	121.5 (2)
C3—C2—C1	120.8 (3)	C36—C37—H37	119.3
C3—C2—H2	119.6	C32—C37—H37	119.3
C1—C2—H2	119.6	O4—C38—C39	110.2 (2)
C2—C3—C4	122.0 (3)	O4—C38—H38A	109.6
C2—C3—H3	119.0	C39—C38—H38A	109.6
C4—C3—H3	119.0	O4—C38—H38B	109.6
C3—C4—C5	116.2 (3)	C39—C38—H38B	109.6
C3—C4—C7	120.4 (3)	H38A—C38—H38B	108.1
C5—C4—C7	123.5 (3)	C44—C39—C40	117.8 (3)
C6—C5—C4	121.6 (3)	C44—C39—C38	123.6 (2)
C6—C5—H5	119.2	C40—C39—C38	118.6 (3)

C4—C5—H5	119.2	C39—C40—C41	120.7 (3)
C5—C6—C1	121.3 (3)	C39—C40—H40	119.7
C5—C6—H6	119.4	C41—C40—H40	119.7
C1—C6—H6	119.4	C42—C41—C40	120.4 (3)
O1—C7—C8	120.1 (3)	C42—C41—H41	119.8
O1—C7—C4	121.0 (3)	C40—C41—H41	119.8
C8—C7—C4	119.0 (3)	C43—C42—C41	119.2 (3)
C9—C8—C7	123.5 (3)	C43—C42—H42	120.4
C9—C8—H8	118.2	C41—C42—H42	120.4
C7—C8—H8	118.2	C42—C43—C44	120.4 (3)
C8—C9—C10	128.4 (3)	C42—C43—H43	119.8
C8—C9—H9	115.8	C44—C43—H43	119.8
C10—C9—H9	115.8	C39—C44—C43	121.4 (3)
C11—C10—C15	116.5 (3)	C39—C44—H44	119.3
C11—C10—C9	122.6 (3)	C43—C44—H44	119.3
C15—C10—C9	120.8 (3)	C35—O4—C38	119.0 (2)
C12—C11—C10	121.7 (3)	C1—N1—H1B	118 (3)
C12—C11—H11	119.1	C1—N1—H1A	121 (3)
C10—C11—H11	119.1	H1B—N1—H1A	118 (4)
C11—C12—C13	120.8 (3)	C23—N2—H2B	119 (2)
C11—C12—H12	119.6	C23—N2—H2A	116 (2)
C13—C12—H12	119.6	H2B—N2—H2A	120 (3)
O2—C13—C12	110.7 (4)	C13—O2—C16	112.8 (4)
O2—C13—C14	129.6 (4)	O2—C16—C17	109.8 (5)
C12—C13—C14	119.3 (3)	O2—C16—H16A	109.7
C12—C13—O2′	136.4 (5)	C17—C16—H16A	109.7
C14—C13—O2′	103.5 (5)	O2—C16—H16B	109.7
C15—C14—C13	118.7 (3)	C17—C16—H16B	109.7
C15—C14—H14	120.6	H16A—C16—H16B	108.2
C13—C14—H14	120.6	C18—C17—C22	116.6 (7)
C14—C15—C10	122.9 (3)	C18—C17—C16	118.5 (7)
C14—C15—H15	118.6	C22—C17—C16	124.9 (9)
C10—C15—H15	118.6	C17—C18—C19	120.9 (7)
N2—C23—C28	121.1 (3)	C17—C18—H18	119.6
N2—C23—C24	121.4 (3)	C19—C18—H18	119.6
C28—C23—C24	117.5 (2)	C20—C19—C18	121.0 (9)
C25—C24—C23	121.1 (2)	C20—C19—H19	119.5
C25—C24—H24	119.5	C18—C19—H19	119.5
C23—C24—H24	119.5	C21—C20—C19	119.6 (10)
C24—C25—C26	121.6 (3)	C21—C20—H20	120.2
C24—C25—H25	119.2	C19—C20—H20	120.2
C26—C25—H25	119.2	C20—C21—C22	119.1 (9)
C27—C26—C25	117.1 (2)	C20—C21—H21	120.5
C27—C26—C29	124.3 (2)	C22—C21—H21	120.5
C25—C26—C29	118.6 (2)	C21—C22—C17	122.7 (9)
C28—C27—C26	121.4 (2)	C21—C22—H22	118.6
C28—C27—H27	119.3	C17—C22—H22	118.6
C26—C27—H27	119.3	C16′—O2′—C13	115.6 (9)

C27—C28—C23	121.2 (2)	O2′—C16′—C17′	110.3 (10)
C27—C28—H28	119.4	O2′—C16′—H16C	109.6
C23—C28—H28	119.4	C17′—C16′—H16C	109.6
O3—C29—C30	120.2 (2)	O2′—C16′—H16D	109.6
O3—C29—C26	119.6 (2)	C17′—C16′—H16D	109.6
C30—C29—C26	120.1 (2)	H16C—C16′—H16D	108.1
C31—C30—C29	120.9 (2)	C18′—C17′—C22′	120.5 (13)
C31—C30—H30	119.6	C18′—C17′—C16′	113.4 (14)
C29—C30—H30	119.6	C22′—C17′—C16′	126.0 (15)
C30—C31—C32	128.1 (3)	C17′—C18′—C19′	120.1 (15)
C30—C31—H31	115.9	C17′—C18′—H18′	119.9
C32—C31—H31	115.9	C19′—C18′—H18′	119.9
C37—C32—C33	117.2 (2)	C18′—C19′—C20′	120.1 (16)
C37—C32—C31	122.7 (2)	C18′—C19′—H19′	120.0
C33—C32—C31	120.1 (2)	C20′—C19′—H19′	120.0
C32—C33—C34	122.0 (3)	C19′—C20′—C21′	118.9 (14)
C32—C33—H33	119.0	C19′—C20′—H20′	120.6
C34—C33—H33	119.0	C21′—C20′—H20′	120.6
C35—C34—C33	119.2 (2)	C22′—C21′—C20′	119.4 (13)
C35—C34—H34	120.4	C22′—C21′—H21′	120.3
C33—C34—H34	120.4	C20′—C21′—H21′	120.3
O4—C35—C34	125.4 (2)	C17′—C22′—C21′	120.7 (14)
O4—C35—C36	114.9 (2)	C17′—C22′—H22′	119.6
C34—C35—C36	119.7 (2)	C21′—C22′—H22′	119.6
C37—C36—C35	120.3 (3)		

N1—C1—C2—C3	−179.0 (4)	C37—C32—C33—C34	0.0 (4)
C6—C1—C2—C3	0.3 (5)	C31—C32—C33—C34	−179.6 (2)
C1—C2—C3—C4	0.2 (5)	C32—C33—C34—C35	1.1 (4)
C2—C3—C4—C5	−1.1 (4)	C33—C34—C35—O4	177.5 (2)
C2—C3—C4—C7	179.1 (3)	C33—C34—C35—C36	−1.1 (4)
C3—C4—C5—C6	1.6 (4)	O4—C35—C36—C37	−178.7 (2)
C7—C4—C5—C6	−178.6 (3)	C34—C35—C36—C37	0.1 (4)
C4—C5—C6—C1	−1.2 (5)	C35—C36—C37—C32	1.0 (4)
N1—C1—C6—C5	179.5 (4)	C33—C32—C37—C36	−1.1 (4)
C2—C1—C6—C5	0.2 (5)	C31—C32—C37—C36	178.6 (2)
C3—C4—C7—O1	5.6 (4)	O4—C38—C39—C44	−5.0 (4)
C5—C4—C7—O1	−174.2 (3)	O4—C38—C39—C40	173.5 (3)
C3—C4—C7—C8	−172.4 (2)	C44—C39—C40—C41	0.1 (5)
C5—C4—C7—C8	7.8 (4)	C38—C39—C40—C41	−178.5 (3)
O1—C7—C8—C9	−15.3 (4)	C39—C40—C41—C42	−0.7 (6)
C4—C7—C8—C9	162.7 (3)	C40—C41—C42—C43	1.3 (6)
C7—C8—C9—C10	−177.7 (3)	C41—C42—C43—C44	−1.3 (5)
C8—C9—C10—C11	−3.7 (5)	C40—C39—C44—C43	−0.2 (5)
C8—C9—C10—C15	175.3 (3)	C38—C39—C44—C43	178.3 (3)
C15—C10—C11—C12	−1.1 (4)	C42—C43—C44—C39	0.8 (5)
C9—C10—C11—C12	177.9 (3)	C34—C35—O4—C38	5.8 (4)
C10—C11—C12—C13	−0.1 (5)	C36—C35—O4—C38	−175.5 (2)

C11—C12—C13—O2	−171.9 (4)	C39—C38—O4—C35	−173.0 (2)
C11—C12—C13—C14	1.7 (5)	C12—C13—O2—C16	−179.3 (5)
C11—C12—C13—O2′	169.7 (7)	C14—C13—O2—C16	7.9 (7)
O2—C13—C14—C15	170.3 (4)	C13—O2—C16—C17	179.1 (6)
C12—C13—C14—C15	−2.0 (5)	O2—C16—C17—C18	−38.3 (8)
O2′—C13—C14—C15	−173.5 (5)	O2—C16—C17—C22	142.2 (7)
C13—C14—C15—C10	0.7 (5)	C22—C17—C18—C19	3.3 (9)
C11—C10—C15—C14	0.8 (5)	C16—C17—C18—C19	−176.2 (7)
C9—C10—C15—C14	−178.2 (3)	C17—C18—C19—C20	−0.3 (11)
N2—C23—C24—C25	178.2 (3)	C18—C19—C20—C21	−2.9 (13)
C28—C23—C24—C25	0.2 (4)	C19—C20—C21—C22	3.0 (13)
C23—C24—C25—C26	0.1 (4)	C20—C21—C22—C17	0.1 (13)
C24—C25—C26—C27	−0.9 (4)	C18—C17—C22—C21	−3.2 (11)
C24—C25—C26—C29	179.6 (2)	C16—C17—C22—C21	176.2 (8)
C25—C26—C27—C28	1.5 (4)	C12—C13—O2′—C16′	19.2 (13)
C29—C26—C27—C28	−179.1 (2)	C14—C13—O2′—C16′	−171.5 (8)
C26—C27—C28—C23	−1.2 (4)	C13—O2′—C16′—C17′	156.4 (9)
N2—C23—C28—C27	−177.7 (3)	O2′—C16′—C17′—C18′	148.4 (13)
C24—C23—C28—C27	0.4 (4)	O2′—C16′—C17′—C22′	−35.4 (17)
C27—C26—C29—O3	167.8 (3)	C22′—C17′—C18′—C19′	−3 (2)
C25—C26—C29—O3	−12.8 (4)	C16′—C17′—C18′—C19′	173.3 (15)
C27—C26—C29—C30	−14.6 (4)	C17′—C18′—C19′—C20′	4 (3)
C25—C26—C29—C30	164.7 (2)	C18′—C19′—C20′—C21′	−5 (2)
O3—C29—C30—C31	12.2 (4)	C19′—C20′—C21′—C22′	4.6 (18)
C26—C29—C30—C31	−165.3 (2)	C18′—C17′—C22′—C21′	3 (2)
C29—C30—C31—C32	178.7 (2)	C16′—C17′—C22′—C21′	−173.0 (13)
C30—C31—C32—C37	15.2 (4)	C20′—C21′—C22′—C17′	−4 (2)
C30—C31—C32—C33	−165.2 (3)		

Hydrogen-bond geometry (Å, º)

Cg1, Cg2 and Cg5 are the centroids of rings C1–C6, C10–C15 and C23–C28, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···O1^{i}	0.93 (4)	2.14 (4)	3.070 (5)	177 (3)
N1—H1*A*···*Cg*5^{ii}	0.84 (5)	2.81 (4)	3.619 (5)	166 (4)
C2—H2···*Cg*1^{iii}	0.93	2.97	3.699 (3)	136
C18—H18···*Cg*2^{iv}	0.93	2.98	3.661 (7)	131
C40—H40···*Cg*5^{v}	0.93	2.92	3.683 (3)	141
C16′—H16*D*···*Cg*2^{iv}	0.97	2.87	3.757 (10)	152

Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*+1/2; (ii) −*x*+1, −*y*+1, −*z*+2; (iii) −*x*+3/2, *y*−1/2, −*z*+3/2; (iv) *x*, *y*+1, *z*; (v) −*x*+3/2, *y*−1/2, −*z*+5/2.