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Crystal structure of 26-(4-methylphenyl)-8,11,14,17-tetraoxa-28-azatetracyclo-[22.3.1.$0^{2,7}$.$0^{18,23}$]hexacosa-2,4,6,18(23),19,21,24(1),25,27-nonaene

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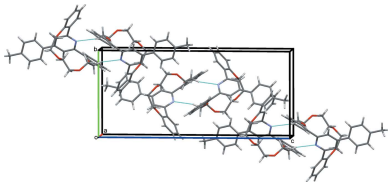
The title compound, $C_{30}H_{29}NO_4$, is a tetracyclic system containing a 4-arylpyridine fragment, two benzene rings and an aza-17-crown-5 ether moiety, in a bowl-like arrangement. The pyridine ring is inclined to the 4-methylphenyl ring by 26.64 (6)°, and by 57.43 (6) and 56.81 (6)° to the benzene rings. The benzene rings are inclined to one another by 88.32 (6)°. In the crystal, molecules are linked by pairs of C—H···N hydrogen bonds, forming inversion dimers with an $R_2^2(14)$ ring motif. The dimers are linked *via* a number of C—H···π interactions, forming a three-dimensional architecture.

1. Chemical context

Over the last decades, there has been considerable interest in pyridino-fused azacrown ethers owing to their great theoretical and practical potential (Bradshaw *et al.*, 1993). Among them, pyridinocrownophanes containing a benzo subunit show high effectiveness as complexating ligands in metal-ion capture and separation (Pedersen, 1988). They are also of interest as phase-transfer catalysts, as membrane ion transporting vehicles (Gokel & Murillo, 1996), as active components useful in environmental chemistry (Bradshaw & Izatt, 1997), in design technology for the construction of organic sensors (Costero *et al.*, 2005) and as nanosized on–off switches and other molecular electronic devices (Natali & Giordani, 2012). It has also been shown that the family of pyridinoaza-crown compounds can possess antibacterial (An *et al.*, 1998) and anticancer properties (Artiemenko *et al.*, 2002; Le *et al.*, 2015).

Recently, we have proposed a new efficient one-step Chichibabin method for the preparation of a series of



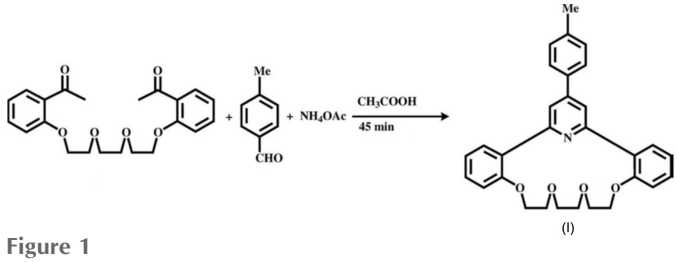


Figure 1
Chichibabin-type condensation of 1,8-bis(2-acetylphenoxy)-3,6-dioxaoctane with 4-methylbenzaldehyde and ammonium acetate to produce the title compound (I).

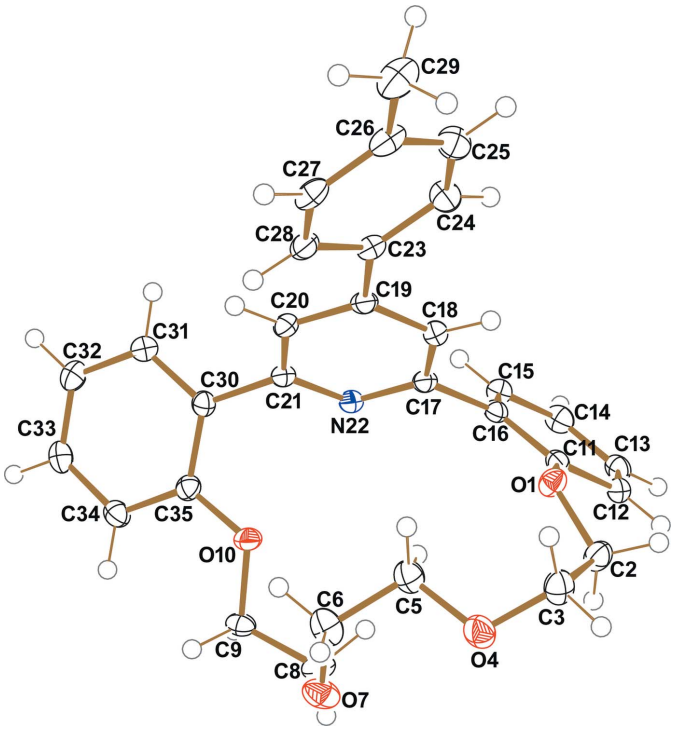
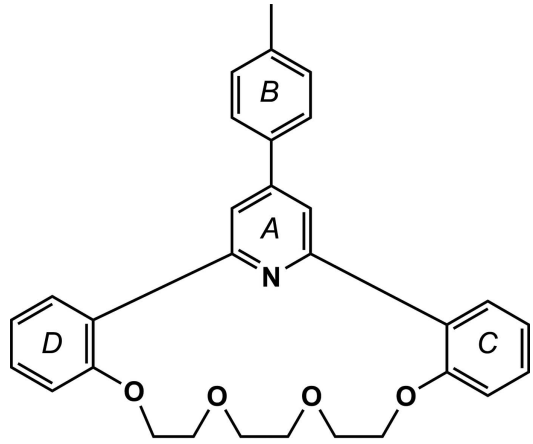


Figure 2
Molecular structure of the title compound (I), with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

pyridinocrownophanes incorporating a 14-crown-4 ether moiety (Le *et al.*, 2014, 2015; Anh *et al.*, 2008; Levov *et al.*, 2008). During the course of our attempts to develop the chemistry of these azacrown systems and obtain macrocyclic ligands which include more extended macro-heterocycles, namely the 17-crown-5 ether moiety, we have studied the Chichibabin-type condensation of 1,8-bis(2-acetylphenoxy)-3,6-dioxaoctane with 4-methylbenzaldehyde and ammonium acetate in acetic acid. This reaction (Fig. 1) proceeds smoothly under heating of the multicomponent mixture to give the expected azacrown with reasonable yield (30%). Herein, we report on the synthesis and crystal structure of this new azacrown compound (I).



2. Structural commentary

The molecule of the title compound, (I), is a tetracyclic system containing a 4-arylpyridine fragment (rings *A* = N22/C17–C22 and *B* = C23–C28), two benzene rings (*C* = C11–C16 and *D* = C30–C35), and an aza-17-crown-5 ether moiety, and has a bowl-like arrangement (Fig. 2). While the dihedral angles between the benzene rings and the pyridine ring are *A*/*D* = 56.81 (6)° and *A*/*C* = 57.43 (6)°, the dihedral angle between the 4-methylphenyl ring (*B*) and the pyridine ring (*A*) in the 4-arylpyridine fragment is only 26.64 (6)°. The distances from the center of the macrocycle cavity, defined as the centroid of

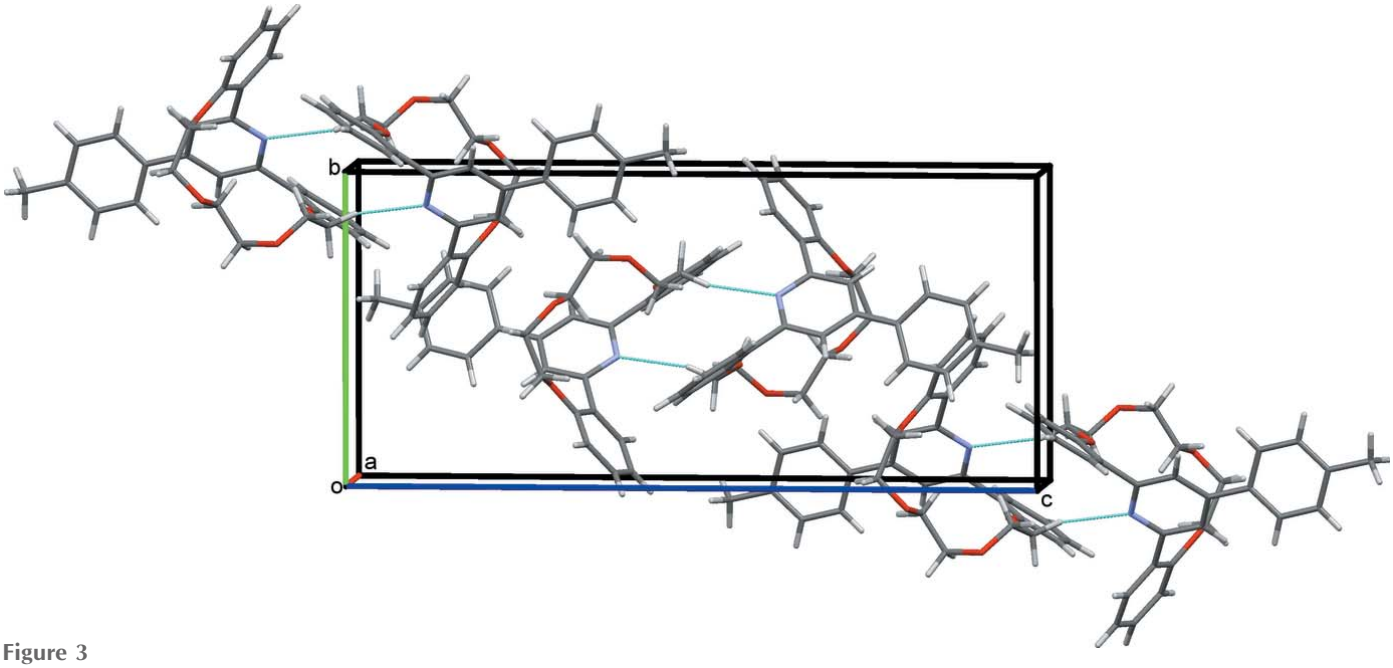


Figure 3
A view along the *a* axis of the crystal packing of the title compound (I). The C—H···N hydrogen bonds are shown as dashed lines (see Table 1).

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

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of rings *A* (N22/C17–C21), *C* (C11–C16), *B* (C23–C28) and *D* (C30–C35), respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*A*···N22^{i}	0.99	2.55	3.4606 (15)	152
C3—H3*B*···*Cg*2^{ii}	0.99	2.75	3.6182 (15)	146
C12—H12···*Cg*3^{iii}	0.95	2.93	3.7281 (13)	142
C25—H25···*Cg*4^{iv}	0.95	2.86	3.6987 (15)	148
C27—H27···*Cg*1^{v}	0.95	2.99	3.7685 (14)	140
C34—H34···*Cg*2^{i}	0.95	2.77	3.5912 (13)	146

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

atoms O1/O4/O7/O10/N22, to the individual atoms O1, O4, O7, O10 and N22 are 2.813 (2), 2.549 (2), 2.588 (2), 2.517 (2) and 2.825 (2) Å, respectively.

3. Supramolecular features

In the crystal, molecules are linked by pairs of C—H···N hydrogen bonds, forming inversion dimers with an $R_2^2(14)$ ring motif (Table 1 and Fig. 3). The dimers are linked *via* a number of C—H···π interactions, forming a three-dimensional structure (Table 1).

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.38, update February 2016; Groom *et al.*, 2016) for the macrocyclic substructure **S1**, illustrated in Fig. 4, gave three hits, *viz*. 2,4,15,17,20-pentamethyl-6,7,9,10,12,13,20,21-octahydro-19*H*-dibenzo[*k*,*p*][1,4,7,10,14]tetraoxazacycloheptadecine (DORPOQ; Rungsimanon *et al.*, 2008), 25,27-dimethyl-8,11,14,17-tetraoxa-28-azatetracyclo(22.3.1.0^{2,7}.0^{18,23})octacosa-2,4,6,18 (23),19,21-hexen-26-one (EFIJEV; Levov *et al.*, 2008), and 20-cyclohexyl-2,4,15,17-tetramethyl-6,7,9,10,12,13,20,21-octahydro-19*H*-dibenzo[*k*,*p*][1,4,7,10,14]-tetraoxazacycloheptadecine (KUFWIS; Chirachanchai *et al.*, 2009), also illustrated in Fig. 4. The two benzene rings are inclined to one another by 50.41 (6)° in DORPOQ, 88.28 (9)° in EFIJEV and 74.3 (9)° in KUGWIS. The corresponding dihedral angle in the title compound [*D*/*C* = 88.32 (6)°] is similar to that observed in EFIJEV.

5. Synthesis and crystallization

The synthesis of the title compound (I), is illustrated in Fig. 1. Ammonium acetate (10.0 g, 130 mmol) was added to a solution of 1,8-bis(2-acetylphenoxy)-3,6-dioxaoctane (0.50 g, 1.30 mmol) and *p*-methylbenzaldehyde (0.155 g, 1.30 mmol) in acetic acid (10 ml). The reaction mixture was then refluxed for 45 min (monitored by TLC until disappearance of the starting diketone spot). At the end of the reaction, the reaction mixture was left to cool to room temperature, neutralized with Na_2CO_3 and extracted with ethyl acetate. The extract was purified by column chromatography on silica gel to give colourless crystals of the title compound (I) [yield 0.18 g, 30%; m.p. 471–472 K]. IR (KBr), ν cm^{-1}: C═N$_{pyridine}$ (1607), C═C$_{aromatic}$ (1545, 1514, 1492), C—O—C (1182, 1120, 1058, 1029). ^{1}H NMR ($CDCl_3$, 500 MHz, 300 K): *d* = 2.42 (*s*, 3H, CH_3), 3.18 (*s*, 4H, H_{ether}), 3.62 and 4.11 (both *t*, 4H each, H_{ether}, *J* = 8 Hz each), 7.0–6.98 (*d*, 2H, H_{arom}), 7.13–7.10 (*m*, 2H, H_{arom}), 7.30–7.29 (*d*, 2H, H_{arom}), 7.37–7.34 (*m*, 2H, H_{arom}), 7.66–7.62 (*m*, 4H, H_{arom}), 7.75 (*s*, 2H, $H_{25,\ 27}$). ESI–MS: $[M+H]^+$ = 468.2. Analysis calculated for $C_{30}H_{29}NO_4$: C, 77.07; H, 6.25; N, 3.00. Found: C, 77.22; H, 6.05; N, 3.12.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The H atoms were placed in calculated positions and refined as riding atoms: C—H = 0.95–

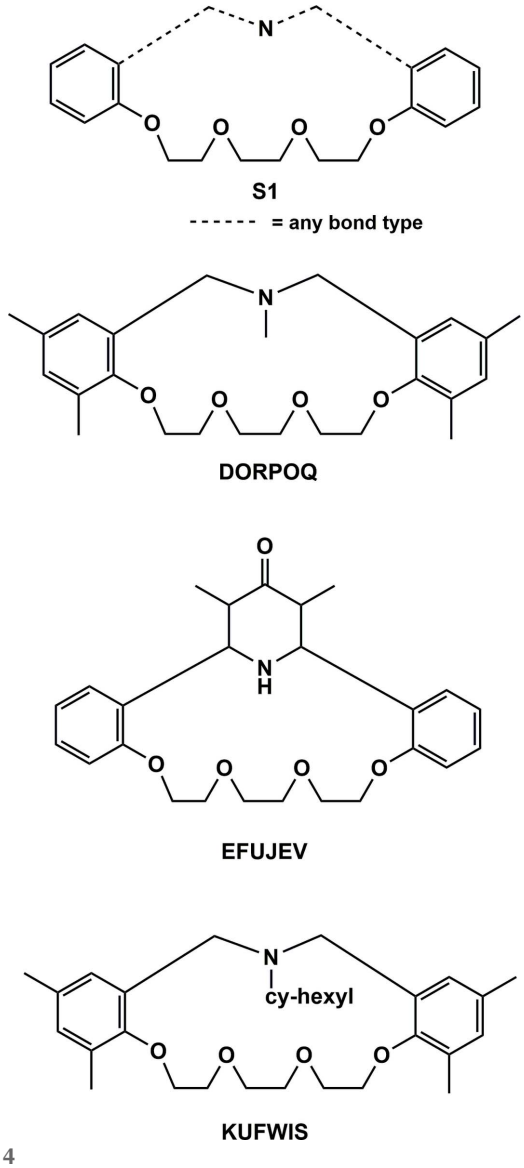


Figure 4
Database search substructure **S1**, and results.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{30}H_{29}NO_4$
M_r	467.54
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, b, c (Å)	10.0819 (4), 10.4531 (4), 23.6016 (9)
β (°)	100.607 (1)
V (Å^3)	2444.80 (16)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.14 × 0.12 × 0.12
Data collection	
Diffractometer	D8 Quest Bruker CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.695, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	77012, 5825, 4706
R_{int}	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.658
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.099, 1.01
No. of reflections	5825
No. of parameters	317
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.31, −0.20

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

0.99 Å with U_{iso}(H) = 1.5U_{eq}(C-methyl) and 1.2U_{eq}(C) for other H atoms.

Acknowledgements

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supporting information

Acta Cryst. (2016). E**72**, 663-666 [doi:10.1107/S2056989016005752]

Crystal structure of 26-(4-methylphenyl)-8,11,14,17-tetraoxa-28-azatetracyclo-[22.3.1.$0^{2,7}$.$0^{18,23}$]hexacosa-2,4,6,18(23),19,21,24(1),25,27-nonaene

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Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: SHELXT2014 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009) and *PLATON* (Spek, 2009).

26-(4-Methylphenyl)-8,11,14,17-tetraoxa-28-azatetracyclo[22.3.1.$0^{2,7}$.$0^{18,23}$]hexacosa-2,4,6,18 (23),19,21,24 (1),25,27-nonaene

Crystal data

$C_{30}H_{29}NO_4$
M_r = 467.54
Monoclinic, $P2_1/n$
a = 10.0819 (4) Å
b = 10.4531 (4) Å
c = 23.6016 (9) Å
β = 100.607 (1)°
V = 2444.80 (16) Å^3
Z = 4
$F(000)$ = 992
D_x = 1.270 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9281 reflections
θ = 2.9–28.3°
μ = 0.08 mm^{-1}
T = 100 K
Block, colourless
0.14 × 0.12 × 0.12 mm

Data collection

D8 Quest Bruker CMOS diffractometer
Detector resolution: 0.5 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)
T_{min} = 0.695, T_{max} = 0.746
77012 measured reflections
5825 independent reflections
4706 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 27.9°, θ_{min} = 2.8°
h = −13→13
k = −13→13
l = −31→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.099
S = 1.01
5825 reflections
317 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0422P)^2 + 1.1744P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

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	0.76598 (8)	0.67651 (8)	0.70887 (4)	0.02073 (19)
C2	0.90811 (12)	0.64977 (12)	0.71765 (6)	0.0236 (3)
H2A	0.9585	0.7123	0.7450	0.028*
H2B	0.9407	0.6561	0.6807	0.028*
C3	0.93002 (13)	0.51576 (13)	0.74174 (6)	0.0260 (3)
H3A	1.0261	0.5060	0.7600	0.031*
H3B	0.8752	0.5042	0.7721	0.031*
O4	0.89565 (10)	0.41796 (9)	0.69952 (4)	0.0283 (2)
C5	0.75342 (13)	0.40022 (13)	0.68115 (6)	0.0254 (3)
H5A	0.7148	0.4735	0.6570	0.030*
H5B	0.7088	0.3956	0.7151	0.030*
C6	0.72925 (15)	0.27780 (13)	0.64690 (6)	0.0276 (3)
H6A	0.7722	0.2065	0.6712	0.033*
H6B	0.6310	0.2610	0.6382	0.033*
O7	0.77874 (10)	0.27738 (9)	0.59417 (4)	0.0294 (2)
C8	0.71355 (13)	0.36342 (13)	0.55114 (5)	0.0240 (3)
H8A	0.7674	0.3683	0.5201	0.029*
H8B	0.7137	0.4497	0.5685	0.029*
C9	0.57024 (12)	0.32947 (12)	0.52436 (5)	0.0191 (2)
H9A	0.5462	0.3679	0.4855	0.023*
H9B	0.5602	0.2355	0.5206	0.023*
O10	0.48389 (8)	0.37838 (9)	0.56118 (4)	0.0226 (2)
C11	0.71707 (12)	0.77257 (11)	0.67121 (5)	0.0169 (2)
C12	0.79826 (12)	0.86832 (12)	0.65433 (5)	0.0202 (2)
H12	0.8924	0.8694	0.6694	0.024*
C13	0.74163 (13)	0.96191 (12)	0.61564 (5)	0.0216 (3)
H13	0.7973	1.0267	0.6041	0.026*
C14	0.60453 (13)	0.96142 (12)	0.59371 (5)	0.0223 (3)
H14	0.5656	1.0261	0.5675	0.027*
C15	0.52418 (12)	0.86528 (12)	0.61036 (5)	0.0200 (2)
H15	0.4303	0.8646	0.5949	0.024*
C16	0.57788 (12)	0.77018 (11)	0.64904 (5)	0.0167 (2)
C17	0.48787 (11)	0.66625 (11)	0.66367 (5)	0.0164 (2)
C18	0.47440 (12)	0.64112 (11)	0.72038 (5)	0.0177 (2)
H18	0.5257	0.6882	0.7513	0.021*
C19	0.38500 (11)	0.54616 (11)	0.73144 (5)	0.0173 (2)

C20	0.31490 (12)	0.47876 (11)	0.68404 (5)	0.0182 (2)
H20	0.2526	0.4137	0.6895	0.022*
C21	0.33672 (11)	0.50726 (11)	0.62894 (5)	0.0170 (2)
N22	0.41964 (10)	0.60176 (9)	0.61821 (4)	0.0168 (2)
C23	0.36716 (11)	0.51592 (12)	0.79121 (5)	0.0182 (2)
C24	0.39161 (13)	0.60818 (13)	0.83481 (5)	0.0233 (3)
H24	0.4182	0.6920	0.8261	0.028*
C25	0.37740 (14)	0.57841 (14)	0.89078 (5)	0.0264 (3)
H25	0.3930	0.6428	0.9196	0.032*
C26	0.34073 (12)	0.45582 (14)	0.90541 (5)	0.0243 (3)
C27	0.31736 (12)	0.36405 (13)	0.86220 (6)	0.0231 (3)
H27	0.2930	0.2797	0.8713	0.028*
C28	0.32895 (12)	0.39334 (12)	0.80585 (5)	0.0207 (3)
H28	0.3107	0.3293	0.7769	0.025*
C29	0.32647 (14)	0.42573 (16)	0.96669 (6)	0.0331 (3)
H29A	0.4159	0.4246	0.9914	0.050*
H29B	0.2837	0.3418	0.9679	0.050*
H29C	0.2705	0.4913	0.9804	0.050*
C30	0.26916 (12)	0.43182 (11)	0.57809 (5)	0.0177 (2)
C31	0.12989 (13)	0.42073 (12)	0.56426 (6)	0.0241 (3)
H31	0.0755	0.4597	0.5883	0.029*
C32	0.06873 (13)	0.35301 (13)	0.51548 (6)	0.0279 (3)
H32	−0.0268	0.3469	0.5062	0.034*
C33	0.14684 (13)	0.29501 (12)	0.48079 (6)	0.0240 (3)
H33	0.1047	0.2502	0.4473	0.029*
C34	0.28687 (13)	0.30147 (12)	0.49435 (5)	0.0208 (3)
H34	0.3404	0.2600	0.4707	0.025*
C35	0.34786 (12)	0.36931 (11)	0.54301 (5)	0.0180 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0174 (4)	0.0189 (4)	0.0258 (4)	−0.0004 (3)	0.0037 (3)	0.0035 (3)
C2	0.0177 (6)	0.0225 (6)	0.0299 (7)	−0.0001 (5)	0.0023 (5)	0.0013 (5)
C3	0.0239 (6)	0.0238 (7)	0.0276 (7)	0.0010 (5)	−0.0024 (5)	0.0017 (5)
O4	0.0277 (5)	0.0221 (5)	0.0332 (5)	0.0041 (4)	0.0006 (4)	−0.0031 (4)
C5	0.0277 (7)	0.0229 (6)	0.0242 (6)	0.0009 (5)	0.0012 (5)	−0.0007 (5)
C6	0.0370 (8)	0.0201 (6)	0.0235 (6)	0.0021 (6)	−0.0002 (5)	0.0027 (5)
O7	0.0303 (5)	0.0283 (5)	0.0280 (5)	0.0122 (4)	0.0016 (4)	−0.0012 (4)
C8	0.0213 (6)	0.0281 (7)	0.0244 (6)	0.0036 (5)	0.0092 (5)	0.0040 (5)
C9	0.0227 (6)	0.0193 (6)	0.0174 (5)	0.0030 (5)	0.0090 (5)	0.0013 (5)
O10	0.0162 (4)	0.0311 (5)	0.0214 (4)	0.0001 (4)	0.0057 (3)	−0.0089 (4)
C11	0.0196 (6)	0.0140 (5)	0.0176 (5)	−0.0007 (4)	0.0050 (4)	−0.0024 (4)
C12	0.0189 (6)	0.0180 (6)	0.0247 (6)	−0.0031 (5)	0.0067 (5)	−0.0046 (5)
C13	0.0281 (6)	0.0150 (6)	0.0245 (6)	−0.0049 (5)	0.0120 (5)	−0.0021 (5)
C14	0.0288 (7)	0.0174 (6)	0.0216 (6)	0.0010 (5)	0.0071 (5)	0.0030 (5)
C15	0.0198 (6)	0.0202 (6)	0.0205 (6)	−0.0005 (5)	0.0046 (5)	−0.0015 (5)
C16	0.0195 (6)	0.0156 (5)	0.0167 (5)	−0.0021 (4)	0.0075 (4)	−0.0029 (4)

C17	0.0148 (5)	0.0156 (5)	0.0195 (6)	0.0008 (4)	0.0052 (4)	−0.0008 (4)
C18	0.0173 (5)	0.0180 (6)	0.0179 (5)	−0.0012 (4)	0.0040 (4)	−0.0019 (4)
C19	0.0153 (5)	0.0181 (6)	0.0195 (6)	0.0017 (4)	0.0060 (4)	−0.0002 (4)
C20	0.0163 (5)	0.0172 (6)	0.0229 (6)	−0.0023 (4)	0.0078 (4)	−0.0012 (5)
C21	0.0146 (5)	0.0165 (6)	0.0207 (6)	0.0006 (4)	0.0055 (4)	−0.0019 (4)
N22	0.0159 (5)	0.0166 (5)	0.0188 (5)	−0.0002 (4)	0.0055 (4)	−0.0014 (4)
C23	0.0141 (5)	0.0219 (6)	0.0191 (6)	0.0009 (4)	0.0047 (4)	0.0020 (5)
C24	0.0280 (7)	0.0218 (6)	0.0208 (6)	−0.0014 (5)	0.0064 (5)	0.0016 (5)
C25	0.0297 (7)	0.0312 (7)	0.0186 (6)	−0.0020 (6)	0.0050 (5)	−0.0008 (5)
C26	0.0160 (6)	0.0366 (7)	0.0204 (6)	0.0007 (5)	0.0037 (5)	0.0076 (5)
C27	0.0167 (6)	0.0256 (6)	0.0282 (7)	−0.0015 (5)	0.0069 (5)	0.0082 (5)
C28	0.0158 (6)	0.0223 (6)	0.0252 (6)	−0.0015 (5)	0.0063 (5)	0.0006 (5)
C29	0.0280 (7)	0.0489 (9)	0.0219 (7)	−0.0044 (6)	0.0034 (5)	0.0117 (6)
C30	0.0188 (6)	0.0154 (5)	0.0193 (6)	−0.0021 (4)	0.0047 (4)	−0.0008 (4)
C31	0.0199 (6)	0.0240 (6)	0.0298 (7)	−0.0015 (5)	0.0083 (5)	−0.0059 (5)
C32	0.0171 (6)	0.0302 (7)	0.0351 (7)	−0.0035 (5)	0.0013 (5)	−0.0064 (6)
C33	0.0257 (6)	0.0225 (6)	0.0223 (6)	−0.0050 (5)	0.0004 (5)	−0.0042 (5)
C34	0.0247 (6)	0.0195 (6)	0.0190 (6)	−0.0009 (5)	0.0061 (5)	−0.0020 (5)
C35	0.0180 (6)	0.0183 (6)	0.0183 (6)	−0.0019 (4)	0.0049 (4)	0.0008 (4)

Geometric parameters (Å, º)

O1—C2	1.4370 (15)	C18—C19	1.3973 (16)
O1—C11	1.3712 (14)	C19—C20	1.3987 (17)
C2—C3	1.5126 (18)	C19—C23	1.4886 (16)
C3—O4	1.4251 (16)	C20—C21	1.3905 (16)
O4—C5	1.4317 (16)	C21—N22	1.3479 (15)
C5—C6	1.5093 (18)	C21—C30	1.4917 (16)
C6—O7	1.4236 (17)	C23—C24	1.3987 (17)
O7—C8	1.4235 (15)	C23—C28	1.3995 (17)
C8—C9	1.5089 (17)	C24—C25	1.3900 (17)
C9—O10	1.4329 (14)	C25—C26	1.3946 (19)
O10—C35	1.3628 (14)	C26—C27	1.3883 (19)
C11—C12	1.3966 (16)	C26—C29	1.5125 (17)
C11—C16	1.4047 (16)	C27—C28	1.3905 (17)
C12—C13	1.3874 (18)	C30—C31	1.3867 (17)
C13—C14	1.3839 (18)	C30—C35	1.4084 (16)
C14—C15	1.3921 (17)	C31—C32	1.3947 (18)
C15—C16	1.3901 (17)	C32—C33	1.3768 (19)
C16—C17	1.4962 (16)	C33—C34	1.3906 (18)
C17—C18	1.3948 (16)	C34—C35	1.3928 (17)
C17—N22	1.3444 (15)		

C11—O1—C2	117.77 (9)	C20—C19—C23	121.31 (11)
O1—C2—C3	107.88 (10)	C21—C20—C19	119.77 (11)
O4—C3—C2	113.69 (11)	C20—C21—C30	120.79 (10)
C3—O4—C5	113.93 (10)	N22—C21—C20	122.89 (11)
O4—C5—C6	109.02 (11)	N22—C21—C30	116.32 (10)

O7—C6—C5	115.01 (11)	C17—N22—C21	117.48 (10)
C8—O7—C6	115.57 (10)	C24—C23—C19	121.01 (11)
O7—C8—C9	115.53 (11)	C24—C23—C28	117.96 (11)
O10—C9—C8	107.68 (10)	C28—C23—C19	121.01 (11)
C35—O10—C9	118.22 (9)	C25—C24—C23	120.65 (12)
O1—C11—C12	123.37 (11)	C24—C25—C26	121.29 (12)
O1—C11—C16	116.35 (10)	C25—C26—C29	120.26 (13)
C12—C11—C16	120.28 (11)	C27—C26—C25	118.03 (12)
C13—C12—C11	120.08 (11)	C27—C26—C29	121.71 (13)
C14—C13—C12	120.35 (11)	C26—C27—C28	121.18 (12)
C13—C14—C15	119.34 (11)	C27—C28—C23	120.87 (12)
C16—C15—C14	121.68 (11)	C31—C30—C21	121.75 (11)
C11—C16—C17	122.26 (10)	C31—C30—C35	118.58 (11)
C15—C16—C11	118.26 (11)	C35—C30—C21	119.67 (10)
C15—C16—C17	119.43 (11)	C30—C31—C32	120.76 (12)
C18—C17—C16	121.91 (10)	C33—C32—C31	120.00 (12)
N22—C17—C16	115.01 (10)	C32—C33—C34	120.62 (12)
N22—C17—C18	123.06 (11)	C33—C34—C35	119.34 (11)
C17—C18—C19	119.54 (11)	O10—C35—C30	115.21 (10)
C18—C19—C20	117.18 (11)	O10—C35—C34	124.11 (11)
C18—C19—C23	121.50 (11)	C34—C35—C30	120.66 (11)

Hydrogen-bond geometry (Å, º)

Cg1, Cg2, Cg3 and Cg4 are the centroids of rings *A* (N22/C17–C21), *C* (C11–C16), *B* (C23–C28) and *D* (C30–C35), respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*A*···N22^{i}	0.99	2.55	3.4606 (15)	152
C3—H3*B*···*Cg*2^{ii}	0.99	2.75	3.6182 (15)	146
C12—H12···*Cg*3^{iii}	0.95	2.93	3.7281 (13)	142
C25—H25···*Cg*4^{iv}	0.95	2.86	3.6987 (15)	148
C27—H27···*Cg*1^{v}	0.95	2.99	3.7685 (14)	140
C34—H34···*Cg*2^{i}	0.95	2.77	3.5912 (13)	146

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