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N-Benzyl-2-[3,5-bis(benzyloxy)-benzyloxy]benzamide

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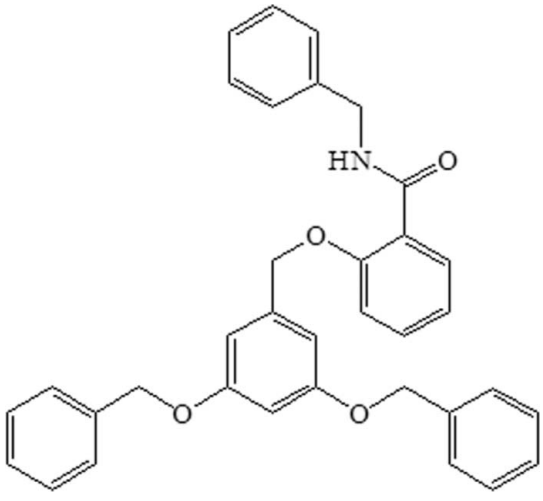
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.141; data-to-parameter ratio = 16.2.

The title compound, $C_{35}H_{31}NO_4$, which is a new amide podand ligand, contains an intramolecular hydrogen bond between the phenoxy O atom and the amide N atom. The packing is stabilized by weak C—H···O hydrogen-bonding interactions.

Related literature

For general background see: Renaud *et al.* (1999); Fujita *et al.* (1998); Su *et al.* (2002, 2003); Tümmler *et al.* (1979).



Experimental

Crystal data

$C_{35}H_{31}NO_4$
M_r = 529.61
Monoclinic, $P2_1/c$
a = 10.8413 (11) Å
b = 13.4524 (13) Å
c = 19.761 (2) Å
β = 98.749 (2)°
V = 2848.5 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 294 (2) K
0.31 × 0.26 × 0.25 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
15639 measured reflections
5853 independent reflections
3315 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.141
S = 1.03
5853 reflections
361 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.86	2.02	2.6702 (18)	132
C4—H4···O1^{i}	0.93	2.64	3.538 (2)	163
C22—H22···O1^{i}	0.93	2.63	3.531 (2)	163
C20—H20···O4^{ii}	0.93	2.61	3.491 (3)	159

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2200).

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supplementary materials

Acta Cryst. (2007). E**63**, o3283 [**doi:10.1107/S1600536807029406**]

N-Benzyl-2-[3,5-bis(benzyloxy)benzyloxy]benzamide

Z.-H. Tang, Y. Tang and X.-P. Cao

Comment

Podand-type ligands have drawn much attention in recent years, mainly due to their selective coordinating capacity, spherodial cavities and hard binding sites, thereby stabilizing their complexes, acquiring novel coordination structure and shielding the encapsulated ion from interaction with the surroundings (Renaud *et al.*, 1999). Among numerous podands which have demonstrated their potential use in functional supramolecular chemistry (Fujita *et al.*, 1998; Su *et al.*, 2002, 2003), amide-type podands are important for preparing rare earth complexes possessing strong luminescent properties. It is expected that the amide type podand ligands, which are flexible in structure and have 'terminal group effects' (Tümmler *et al.*, 1979), will shied the encapsulated rare earth ion from interaction with the surroundings, and thus to achieve strong luminescent properties. We report here the synthesis and structure of a new amide-type podand ligand, namely 2-[3,5-bis(benzyloxy)benzyloxy]-*N*-benzylbenzamide (I).

In the molecule (I) there is an intramolecular hydrogen bond between the phenoxy O atom and the amide N atom (Table 1, Fig. 1). The packing is stabilized by weak C—H···O hydrogen bonding interactions (Table 1).

Experimental

N-Benzylsalicylamide (0.91 g, 4.00 mmol), potassium carbonate (1.5 g, 7.2 mmol) and DMF (30 ml) were heated to *ca* 100 °C and 1,3-bis(benzyloxy)-5-(bromomethyl)benzene (1.53 g, 4.00 mmol) was added. The reaction mixture was stirred at 95–105 °C for 10 h. After cooling, the mixture was poured into water(100 ml). The resulted solid was subjected to column chromatography on silica gel [petroleum ether: ethyl acetate (5:1)] for separating the title compound (I), yield 89%. m. p. 84–86 °C; Analysis calculated for $C_{35}H_{31}N_1O_4$: C 79.37, H 5.90, N 2.64; Found: C 79.08, H 5.94, N 2.57. The crystal used for the data collection was obtained by slow evaporation of a saturated ethanol solution of (I) at room temperature.

Refinement

All H atoms attached to C atoms and N atom were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic) or 0.97 Å (methylene) and N—H = 0.86 Å with U_{iso}(H) = 1.2U_{eq}(C or N).

Figures

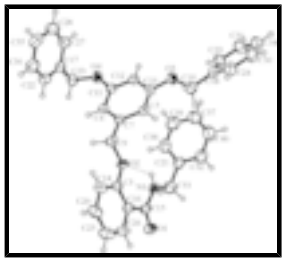


Fig. 1. Molecular view of (I), with the atom-numbering scheme. Ellipsoids are drawjn at the 30% probability level. H atoms are shown as small spheres of arbitrary radii. The intramolecular H bond is shown as dashed line.

N-Benzyl-2-[3,5-bis(benzyloxy)benzyloxy]benzamide

Crystal data

$C_{35}H_{31}NO_4$	F_{000} = 1120
M_r = 529.61	D_x = 1.235 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 85 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 10.8413 (11) Å	Cell parameters from 2898 reflections
b = 13.4524 (13) Å	θ = 2.5–22.7º
c = 19.761 (2) Å	μ = 0.08 mm^{-1}
β = 98.749 (2)º	T = 294 (2) K
V = 2848.5 (5) Å^3	Block, colorless
Z = 4	0.31 × 0.26 × 0.25 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3315 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.035
Monochromator: graphite	θ_{max} = 26.4º
T = 294(2) K	θ_{min} = 1.8º
φ and ω scans	h = −13→12
Absorption correction: none	k = −16→8
15639 measured reflections	l = −24→24
5853 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.049	H-atom parameters constrained
$wR(F^2)$ = 0.141	$w = 1/[\sigma^2(F_o^2) + (0.0646P)^2 + 0.0363P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
5853 reflections	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
361 parameters	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations

between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections.? The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement.? *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.46345 (11)	0.61754 (8)	0.14452 (6)	0.0577 (3)
O4	0.90358 (11)	0.42664 (9)	0.07570 (6)	0.0665 (4)
C3	0.35242 (16)	0.61863 (13)	0.16959 (8)	0.0514 (4)
C4	0.69374 (16)	0.48539 (13)	0.08748 (8)	0.0529 (4)
H4	0.6802	0.4331	0.1162	0.063*
C5	0.62291 (17)	0.63564 (13)	0.02773 (9)	0.0556 (5)
H5	0.5620	0.6841	0.0166	0.067*
O3	0.76385 (12)	0.71197 (9)	−0.04321 (7)	0.0737 (4)
C7	0.60291 (16)	0.55692 (12)	0.07024 (8)	0.0500 (4)
O1	0.41771 (14)	0.81493 (10)	0.29959 (7)	0.0822 (4)
C9	0.47838 (17)	0.54436 (13)	0.09333 (9)	0.0574 (5)
H9A	0.4125	0.5518	0.0546	0.069*
H9B	0.4723	0.4782	0.1121	0.069*
N1	0.52907 (16)	0.78273 (12)	0.21593 (8)	0.0726 (5)
H1	0.5343	0.7503	0.1790	0.087*
C11	0.80534 (16)	0.49229 (13)	0.06149 (8)	0.0525 (4)
C12	0.82580 (17)	0.57001 (13)	0.01907 (8)	0.0551 (4)
H12	0.9009	0.5745	0.0019	0.066*
C13	0.73461 (17)	0.64113 (13)	0.00210 (9)	0.0559 (5)
C14	0.25662 (17)	0.55232 (14)	0.14831 (9)	0.0629 (5)
H14	0.2673	0.5042	0.1159	0.075*
C15	0.43138 (19)	0.76671 (14)	0.24785 (9)	0.0616 (5)
C16	0.33748 (17)	0.69054 (13)	0.21937 (8)	0.0556 (5)
C17	0.80621 (18)	0.26532 (13)	0.04631 (9)	0.0576 (5)
C18	0.7242 (2)	0.85431 (13)	−0.11421 (9)	0.0618 (5)
C19	0.67362 (18)	0.78670 (14)	−0.06454 (10)	0.0698 (6)
H19A	0.6562	0.8244	−0.0252	0.084*
H19B	0.5965	0.7563	−0.0863	0.084*
C20	0.14600 (19)	0.55635 (17)	0.17428 (11)	0.0780 (6)
H20	0.0823	0.5117	0.1591	0.094*
C21	0.7162 (2)	0.86136 (16)	0.19042 (11)	0.0718 (6)
C22	0.6967 (2)	0.21968 (16)	0.05546 (11)	0.0738 (6)
H22	0.6639	0.2306	0.0957	0.089*
C23	0.87785 (19)	0.32944 (14)	0.10042 (10)	0.0673 (5)
H23A	0.8306	0.3363	0.1381	0.081*
H23B	0.9561	0.2970	0.1179	0.081*
C24	0.6429 (2)	0.90028 (16)	−0.16497 (10)	0.0756 (6)
H24	0.5578	0.8877	−0.1687	0.091*

C25	0.1297 (2)	0.6263 (2)	0.22263 (12)	0.0874 (7)
H25	0.0552	0.6294	0.2404	0.105*
C26	0.2237 (2)	0.69087 (17)	0.24419 (10)	0.0759 (6)
H26	0.2117	0.7377	0.2772	0.091*
C27	0.8518 (2)	0.24915 (17)	−0.01424 (10)	0.0778 (6)
H27	0.9253	0.2803	−0.0213	0.093*
C28	0.7915 (3)	0.1885 (2)	−0.06400 (12)	0.0921 (7)
H28	0.8242	0.1783	−0.1043	0.111*
C29	0.8491 (2)	0.87421 (16)	−0.10963 (11)	0.0774 (6)
H29	0.9054	0.8441	−0.0755	0.093*
C30	0.6860 (3)	0.96452 (18)	−0.21014 (11)	0.0941 (8)
H30	0.6300	0.9952	−0.2441	0.113*
C31	0.8925 (2)	0.93881 (18)	−0.15539 (13)	0.0927 (7)
H31	0.9775	0.9517	−0.1520	0.111*
C32	0.7090 (2)	0.93793 (18)	0.14453 (14)	0.0961 (7)
H32	0.6494	0.9873	0.1460	0.115*
C33	0.6274 (2)	0.85292 (17)	0.24101 (12)	0.0898 (7)
H33A	0.6716	0.8304	0.2847	0.108*
H33B	0.5913	0.9175	0.2477	0.108*
C34	0.8104 (3)	0.98351 (18)	−0.20541 (13)	0.1001 (8)
H34	0.8393	1.0268	−0.2362	0.120*
C35	0.6824 (3)	0.14280 (17)	−0.05429 (12)	0.0896 (7)
H35	0.6408	0.1017	−0.0881	0.107*
C36	0.6346 (2)	0.15801 (17)	0.00593 (14)	0.0876 (7)
H36	0.5611	0.1268	0.0129	0.105*
C37	0.8755 (3)	0.8733 (2)	0.09299 (14)	0.1003 (8)
H37	0.9291	0.8774	0.0606	0.120*
C38	0.8054 (3)	0.79057 (19)	0.18585 (14)	0.0987 (8)
H38	0.8129	0.7372	0.2161	0.118*
C39	0.8843 (3)	0.7965 (2)	0.13755 (16)	0.1099 (9)
H39	0.9440	0.7474	0.1356	0.132*
C40	0.7885 (3)	0.9438 (2)	0.09583 (14)	0.1065 (8)
H40	0.7816	0.9967	0.0651	0.128*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0573 (8)	0.0602 (8)	0.0600 (7)	−0.0018 (6)	0.0227 (6)	−0.0197 (6)
O4	0.0613 (8)	0.0577 (8)	0.0817 (9)	0.0075 (6)	0.0143 (6)	0.0125 (7)
C3	0.0518 (11)	0.0579 (12)	0.0463 (9)	0.0073 (8)	0.0135 (8)	0.0010 (8)
C4	0.0666 (12)	0.0483 (11)	0.0465 (9)	−0.0019 (9)	0.0170 (8)	−0.0023 (8)
C5	0.0610 (12)	0.0477 (11)	0.0613 (11)	0.0064 (8)	0.0192 (9)	−0.0050 (8)
O3	0.0757 (9)	0.0621 (9)	0.0892 (9)	0.0128 (7)	0.0310 (7)	0.0230 (7)
C7	0.0591 (11)	0.0470 (11)	0.0470 (9)	−0.0026 (8)	0.0176 (8)	−0.0111 (8)
O1	0.1151 (12)	0.0735 (10)	0.0637 (8)	0.0038 (8)	0.0320 (8)	−0.0208 (7)
C9	0.0674 (12)	0.0543 (12)	0.0545 (10)	−0.0039 (9)	0.0217 (9)	−0.0153 (8)
N1	0.0829 (12)	0.0725 (12)	0.0668 (10)	−0.0129 (9)	0.0257 (9)	−0.0278 (8)
C11	0.0564 (11)	0.0500 (11)	0.0515 (10)	0.0029 (8)	0.0096 (8)	−0.0033 (8)

C12	0.0555 (11)	0.0536 (12)	0.0584 (10)	−0.0004 (9)	0.0161 (8)	−0.0006 (9)
C13	0.0656 (12)	0.0470 (11)	0.0584 (11)	0.0002 (9)	0.0193 (9)	0.0029 (8)
C14	0.0578 (12)	0.0731 (14)	0.0593 (11)	0.0010 (10)	0.0136 (9)	−0.0044 (9)
C15	0.0799 (14)	0.0588 (12)	0.0491 (10)	0.0142 (10)	0.0193 (10)	−0.0041 (9)
C16	0.0626 (12)	0.0594 (12)	0.0468 (9)	0.0105 (9)	0.0150 (9)	−0.0013 (8)
C17	0.0651 (12)	0.0518 (11)	0.0574 (11)	0.0141 (9)	0.0137 (9)	0.0091 (9)
C18	0.0737 (14)	0.0493 (12)	0.0635 (11)	0.0004 (10)	0.0139 (10)	0.0020 (9)
C19	0.0677 (13)	0.0650 (14)	0.0788 (13)	0.0094 (10)	0.0181 (11)	0.0084 (10)
C20	0.0582 (13)	0.0972 (18)	0.0806 (14)	−0.0060 (11)	0.0173 (11)	0.0032 (13)
C21	0.0751 (15)	0.0579 (14)	0.0818 (14)	−0.0103 (11)	0.0101 (11)	−0.0148 (11)
C22	0.0752 (15)	0.0710 (15)	0.0797 (14)	0.0113 (11)	0.0262 (11)	−0.0053 (11)
C23	0.0769 (14)	0.0581 (13)	0.0669 (12)	0.0113 (10)	0.0113 (10)	0.0144 (10)
C24	0.0839 (15)	0.0666 (14)	0.0731 (13)	−0.0012 (11)	0.0015 (12)	0.0013 (11)
C25	0.0613 (14)	0.120 (2)	0.0862 (16)	0.0072 (14)	0.0293 (12)	−0.0013 (15)
C26	0.0739 (15)	0.0928 (17)	0.0668 (13)	0.0154 (12)	0.0293 (11)	−0.0109 (11)
C27	0.0935 (16)	0.0755 (15)	0.0686 (13)	0.0042 (12)	0.0260 (12)	0.0057 (12)
C28	0.114 (2)	0.0958 (19)	0.0684 (14)	0.0142 (16)	0.0213 (14)	−0.0034 (13)
C29	0.0805 (16)	0.0784 (16)	0.0747 (13)	0.0061 (12)	0.0158 (11)	0.0151 (11)
C30	0.130 (2)	0.0761 (17)	0.0725 (15)	0.0146 (16)	0.0022 (15)	0.0116 (12)
C31	0.0934 (18)	0.0916 (19)	0.0984 (17)	−0.0172 (14)	0.0320 (15)	0.0010 (15)
C32	0.0894 (18)	0.0799 (18)	0.121 (2)	0.0146 (13)	0.0235 (15)	0.0034 (15)
C33	0.1044 (18)	0.0791 (17)	0.0903 (16)	−0.0238 (13)	0.0287 (14)	−0.0321 (12)
C34	0.154 (3)	0.0682 (17)	0.0844 (17)	−0.0095 (17)	0.0377 (18)	0.0134 (13)
C35	0.104 (2)	0.0737 (16)	0.0845 (16)	0.0211 (14)	−0.0080 (15)	−0.0187 (12)
C36	0.0748 (16)	0.0753 (16)	0.1135 (19)	0.0021 (12)	0.0171 (14)	−0.0161 (14)
C37	0.091 (2)	0.111 (2)	0.1029 (19)	−0.0104 (17)	0.0266 (15)	−0.0028 (17)
C38	0.108 (2)	0.0773 (18)	0.114 (2)	0.0111 (15)	0.0293 (16)	0.0154 (14)
C39	0.098 (2)	0.096 (2)	0.140 (2)	0.0206 (15)	0.0325 (18)	0.0028 (19)
C40	0.104 (2)	0.101 (2)	0.117 (2)	0.0039 (17)	0.0244 (17)	0.0277 (16)

Geometric parameters (Å, °)

O2—C3	1.3696 (19)	C21—C32	1.367 (3)
O2—C9	1.4383 (18)	C21—C38	1.370 (3)
O4—C11	1.379 (2)	C21—C33	1.494 (3)
O4—C23	1.438 (2)	C22—C36	1.378 (3)
C3—C14	1.385 (2)	C22—H22	0.9300
C3—C16	1.406 (2)	C23—H23A	0.9700
C4—C7	1.382 (2)	C23—H23B	0.9700
C4—C11	1.387 (2)	C24—C30	1.374 (3)
C4—H4	0.9300	C24—H24	0.9300
C5—C13	1.384 (2)	C25—C26	1.358 (3)
C5—C7	1.389 (2)	C25—H25	0.9300
C5—H5	0.9300	C26—H26	0.9300
O3—C13	1.377 (2)	C27—C28	1.365 (3)
O3—C19	1.421 (2)	C27—H27	0.9300
C7—C9	1.499 (2)	C28—C35	1.372 (3)
O1—C15	1.239 (2)	C28—H28	0.9300
C9—H9A	0.9700	C29—C31	1.387 (3)

C9—H9B	0.9700	C29—H29	0.9300
N1—C15	1.330 (2)	C30—C34	1.362 (3)
N1—C33	1.454 (3)	C30—H30	0.9300
N1—H1	0.8600	C31—C34	1.365 (3)
C11—C12	1.379 (2)	C31—H31	0.9300
C12—C13	1.380 (2)	C32—C40	1.388 (3)
C12—H12	0.9300	C32—H32	0.9300
C14—C20	1.376 (3)	C33—H33A	0.9700
C14—H14	0.9300	C33—H33B	0.9700
C15—C16	1.493 (3)	C34—H34	0.9300
C16—C26	1.395 (3)	C35—C36	1.384 (3)
C17—C22	1.373 (3)	C35—H35	0.9300
C17—C27	1.379 (2)	C36—H36	0.9300
C17—C23	1.496 (3)	C37—C40	1.345 (3)
C18—C29	1.370 (3)	C37—C39	1.352 (3)
C18—C24	1.377 (3)	C37—H37	0.9300
C18—C19	1.502 (3)	C38—C39	1.378 (3)
C19—H19A	0.9700	C38—H38	0.9300
C19—H19B	0.9700	C39—H39	0.9300
C20—C25	1.371 (3)	C40—H40	0.9300
C20—H20	0.9300		
C3—O2—C9	117.44 (13)	C36—C22—H22	119.5
C11—O4—C23	117.89 (14)	O4—C23—C17	112.83 (15)
O2—C3—C14	122.89 (15)	O4—C23—H23A	109.0
O2—C3—C16	117.47 (16)	C17—C23—H23A	109.0
C14—C3—C16	119.64 (17)	O4—C23—H23B	109.0
C7—C4—C11	119.41 (16)	C17—C23—H23B	109.0
C7—C4—H4	120.3	H23A—C23—H23B	107.8
C11—C4—H4	120.3	C30—C24—C18	120.8 (2)
C13—C5—C7	119.20 (16)	C30—C24—H24	119.6
C13—C5—H5	120.4	C18—C24—H24	119.6
C7—C5—H5	120.4	C26—C25—C20	119.2 (2)
C13—O3—C19	117.79 (14)	C26—C25—H25	120.4
C4—C7—C5	120.60 (16)	C20—C25—H25	120.4
C4—C7—C9	119.18 (15)	C25—C26—C16	123.3 (2)
C5—C7—C9	120.05 (16)	C25—C26—H26	118.3
O2—C9—C7	109.86 (13)	C16—C26—H26	118.3
O2—C9—H9A	109.7	C28—C27—C17	121.6 (2)
C7—C9—H9A	109.7	C28—C27—H27	119.2
O2—C9—H9B	109.7	C17—C27—H27	119.2
C7—C9—H9B	109.7	C27—C28—C35	119.7 (2)
H9A—C9—H9B	108.2	C27—C28—H28	120.1
C15—N1—C33	122.63 (16)	C35—C28—H28	120.1
C15—N1—H1	118.7	C18—C29—C31	120.6 (2)
C33—N1—H1	118.7	C18—C29—H29	119.7
C12—C11—O4	114.75 (16)	C31—C29—H29	119.7
C12—C11—C4	120.37 (16)	C34—C30—C24	120.3 (2)
O4—C11—C4	124.87 (16)	C34—C30—H30	119.8
C11—C12—C13	119.86 (17)	C24—C30—H30	119.8

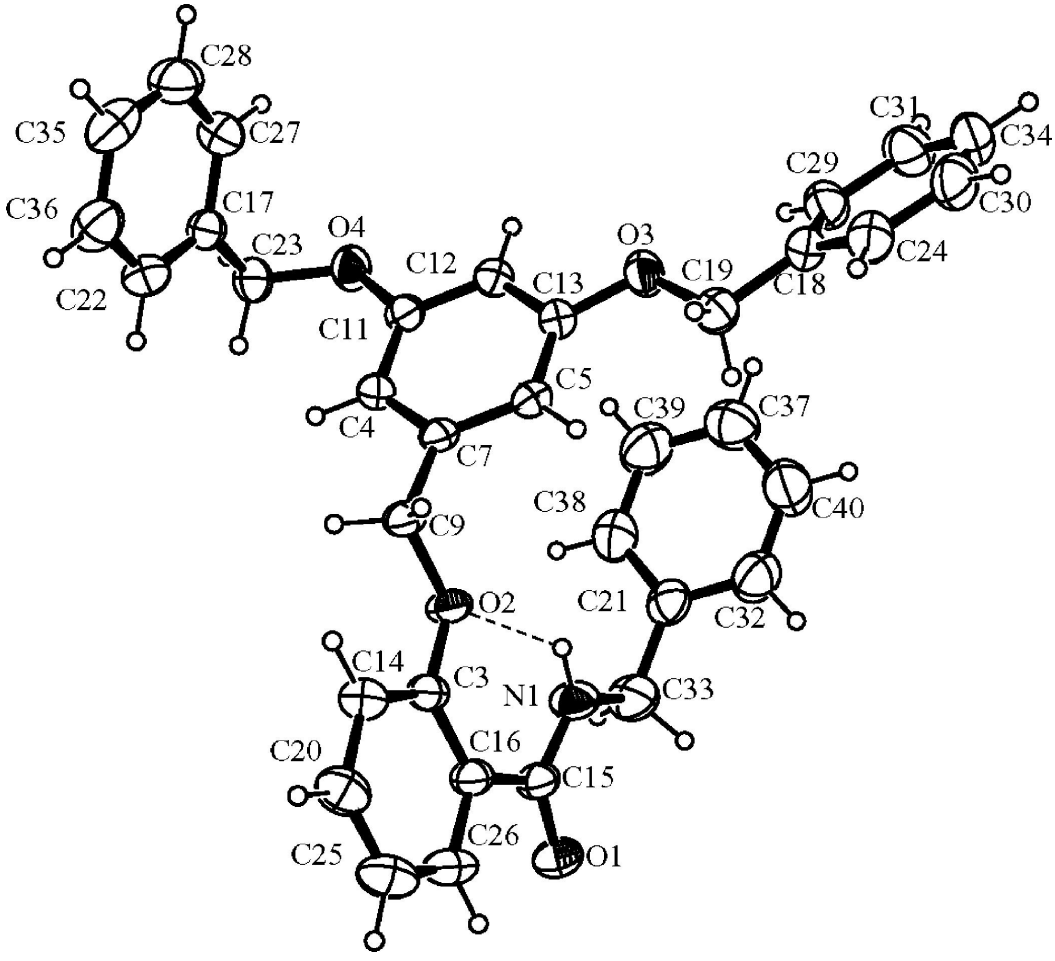
C11—C12—H12	120.1	C34—C31—C29	120.0 (2)
C13—C12—H12	120.1	C34—C31—H31	120.0
O3—C13—C12	114.24 (16)	C29—C31—H31	120.0
O3—C13—C5	125.15 (16)	C21—C32—C40	121.6 (2)
C12—C13—C5	120.56 (16)	C21—C32—H32	119.2
C20—C14—C3	121.16 (18)	C40—C32—H32	119.2
C20—C14—H14	119.4	N1—C33—C21	109.56 (16)
C3—C14—H14	119.4	N1—C33—H33A	109.8
O1—C15—N1	120.70 (19)	C21—C33—H33A	109.8
O1—C15—C16	120.68 (18)	N1—C33—H33B	109.8
N1—C15—C16	118.62 (15)	C21—C33—H33B	109.8
C26—C16—C3	116.76 (18)	H33A—C33—H33B	108.2
C26—C16—C15	117.00 (16)	C30—C34—C31	119.8 (2)
C3—C16—C15	126.25 (16)	C30—C34—H34	120.1
C22—C17—C27	118.34 (19)	C31—C34—H34	120.1
C22—C17—C23	121.94 (17)	C28—C35—C36	119.8 (2)
C27—C17—C23	119.70 (18)	C28—C35—H35	120.1
C29—C18—C24	118.50 (19)	C36—C35—H35	120.1
C29—C18—C19	122.06 (17)	C22—C36—C35	119.6 (2)
C24—C18—C19	119.42 (19)	C22—C36—H36	120.2
O3—C19—C18	108.60 (16)	C35—C36—H36	120.2
O3—C19—H19A	110.0	C40—C37—C39	119.5 (3)
C18—C19—H19A	110.0	C40—C37—H37	120.2
O3—C19—H19B	110.0	C39—C37—H37	120.2
C18—C19—H19B	110.0	C21—C38—C39	121.6 (2)
H19A—C19—H19B	108.4	C21—C38—H38	119.2
C25—C20—C14	119.9 (2)	C39—C38—H38	119.2
C25—C20—H20	120.0	C37—C39—C38	120.4 (3)
C14—C20—H20	120.0	C37—C39—H39	119.8
C32—C21—C38	116.7 (2)	C38—C39—H39	119.8
C32—C21—C33	121.6 (2)	C37—C40—C32	120.1 (3)
C38—C21—C33	121.6 (2)	C37—C40—H40	119.9
C17—C22—C36	120.9 (2)	C32—C40—H40	119.9
C17—C22—H22	119.5		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.86	2.02	2.6702 (18)	132
C4—H4···O1^{i}	0.93	2.64	3.538 (2)	163
C22—H22···O1^{i}	0.93	2.63	3.531 (2)	163
C20—H20···O4^{ii}	0.93	2.61	3.491 (3)	159

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

Fig. 1


C28
C35
C27
C36
C17
C23
O4
C12
C13
O3
C19
C18
C31
C34
C29
C30
C24
C22
C11
C5
C4
C7
C39
C37
C38
C40
C9
O2
C21
C32
C14
C3
N1
C33
C20
C16
C15
C26
C25
O1