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N,*N*′-Bis(2-methoxyphenyl)anthracene-1,8-dicarboxamide

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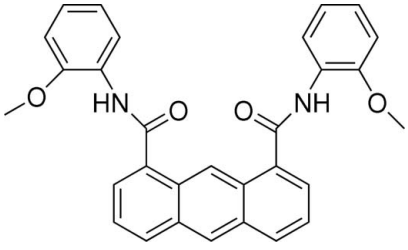
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.106; data-to-parameter ratio = 13.2.

In the title compound, $C_{30}H_{24}N_2O_4$, the anthracene system forms dihedral angles of 59.26 (5) and 82.83 (5)° with the benzene rings of the methoxyphenyl groups. Another feature of interest is the dihedral angle between the methoxyphenyl benzene rings, which is 42.62 (5)°. In the molecule, there are four very weak intramolecular C—H···O hydrogen bonds and the crystal packing is stabilized by weak C—H···O hydrogen bonds.

Related literature

For synthesis, see: Rogers & Averill (1986); Gunnlaugsson *et al.* (2005). For properties of anthracene-based molecules, see: Chen & Chen (2004); Gunnlaugsson *et al.* (2003).



Experimental

Crystal data

$C_{30}H_{24}N_2O_4$
M_r = 476.51
Monoclinic, $P2_1/c$
a = 13.131 (3) Å
b = 11.864 (2) Å
c = 14.911 (3) Å
β = 91.13 (3)°
V = 2322.4 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 153 (2) K
0.30 × 0.28 × 0.28 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: none
18982 measured reflections
4318 independent reflections
3977 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.107
S = 1.03
4318 reflections
328 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···O1	0.93	2.51	3.0581 (18)	118
C14—H14···O3	0.93	2.55	3.1012 (18)	119
C18—H18···O1	0.93	2.29	2.8870 (18)	122
C25—H25···O3	0.93	2.50	2.9084 (19)	107
N1—H1N···O2	0.86	2.20	2.6146 (15)	109
C5—H5···O4^{i}	0.93	2.58	3.4134 (19)	149
C30—H30B···O3^{ii}	0.96	2.42	3.254 (2)	145
C30—H30C···O1^{ii}	0.96	2.57	3.089 (2)	114

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

Data collection: *RAPID-AUTO* (Rigaku 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1994); 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: BH2130).

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supplementary materials

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N,*N*'-Bis(2-methoxyphenyl)anthracene-1,8-dicarboxamide

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Comment

Anthracene as well as its derivatives and analogs have been widely used as signaling subunits for both cation (Gunnlaugsson *et al.*, 2003) and anion (Chen & Chen, 2004) sensing, due to their well known photophysical properties and high fluorescence. We report here the crystal structure of the title compound, (I).

In the molecule, the anthracene ring system are slightly non-planar with a maximum deviation of ±0.036 Å. The anthracene group (C2···C15) and benzene group C17···C22 planes form a dihedral angle of 59.26 (5)°, and the phenyl ring, C24···C29 makes a dihedral angle of 82.83 (5)° with the anthracene group. The dihedral angle between the two benzene rings is 42.62 (5)° (Fig. 1). In the molecule, there are four very weak intramolecular C—H···O hydrogen bonds. The crystal structure is stabilized by weak intermolecular C—H···O hydrogen bonds.

Experimental

The title compound was prepared according to the reported procedure of Rogers & Averill (1986) and Gunnlaugsson *et al.* (2005). Yellow single crystals suitable for X-ray diffraction were obtained by recrystallization from dimethyl sulfoxide.

Refinement

All H atoms were placed in calculated positions with C—H = 0.93 (aromatic CH) or 0.96 Å (methyl CH_3) and N—H = 0.86 Å, and refined using a riding model approximation, with U_{iso}(H) = 1.2U_{eq}(carrier atom).

Figures

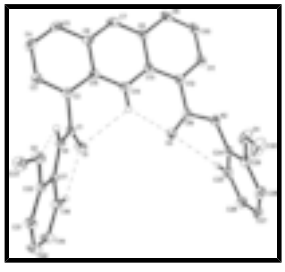


Fig. 1. The structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering. H atoms involved in an intramolecular hydrogen bond are shown, while other have been omitted.

N,*N*'-Bis(2-methoxyphenyl)anthracene-1,8-dicarboxamide

Crystal data

$C_{30}H_{24}N_2O_4$	F_{000} = 1000
M_r = 476.51	D_x = 1.363 Mg m^{-3}

Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 9633 reflections
$a = 13.131$ (3) Å	$\theta = 3.1$–27.5º
$b = 11.864$ (2) Å	$\mu = 0.09$ mm^{-1}
$c = 14.911$ (3) Å	$T = 153$ (2) K
$\beta = 91.13$ (3)º	Block, yellow
$V = 2322.4$ (8) Å^3	0.30 × 0.28 × 0.28 mm
$Z = 4$	

Data collection

Rigaku R-AXIS RAPID diffractometer	3977 reflections with $I > 2\sigma(I)$
Radiation source: Rotating Anode	$R_{int} = 0.016$
Monochromator: graphite	$\theta_{max} = 25.5$º
$T = 153(2)$ K	$\theta_{min} = 3.1$º
ω scans	$h = -15\rightarrow15$
Absorption correction: none	$k = -14\rightarrow14$
18982 measured reflections	$l = -17\rightarrow18$
4318 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.040$	$w = 1/[\sigma^2(F_o^2) + (0.0556P)^2 + 1.057P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.107$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.03$	$\Delta\rho_{max} = 0.45$ e Å^{-3}
4318 reflections	$\Delta\rho_{min} = -0.23$ e Å^{-3}
328 parameters	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0073 (9)
Secondary atom site location: difference Fourier map	

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.80682 (7)	0.43852 (9)	0.32771 (6)	0.0313 (2)
O2	0.92280 (7)	0.28470 (9)	0.61312 (6)	0.0292 (2)
O3	0.69131 (8)	0.75454 (9)	0.28542 (7)	0.0346 (3)
O4	0.71944 (10)	0.92830 (10)	0.55977 (7)	0.0415 (3)
N1	0.83860 (8)	0.35283 (9)	0.46228 (7)	0.0225 (2)
H1N	0.8081	0.3267	0.5084	0.027*
N2	0.64594 (9)	0.86852 (10)	0.40038 (8)	0.0275 (3)

H2N	0.5991	0.8824	0.4383	0.033*
C1	0.77717 (10)	0.38556 (11)	0.39246 (8)	0.0218 (3)
C2	0.66880 (10)	0.34690 (11)	0.39944 (8)	0.0231 (3)
C3	0.65052 (12)	0.23509 (13)	0.41266 (10)	0.0332 (3)
H3	0.7051	0.1865	0.4229	0.040*
C4	0.55002 (12)	0.19140 (13)	0.41107 (11)	0.0385 (4)
H4	0.5394	0.1145	0.4185	0.046*
C5	0.46969 (11)	0.26096 (13)	0.39878 (10)	0.0321 (3)
H5	0.4040	0.2316	0.3983	0.038*
C6	0.48431 (10)	0.37878 (12)	0.38651 (9)	0.0275 (3)
C7	0.40171 (10)	0.45152 (13)	0.37357 (9)	0.0302 (3)
H7	0.3361	0.4220	0.3739	0.036*
C8	0.41418 (10)	0.56646 (13)	0.36024 (9)	0.0282 (3)
C9	0.32907 (10)	0.63914 (14)	0.34815 (10)	0.0327 (3)
H9	0.2635	0.6095	0.3491	0.039*
C10	0.34224 (11)	0.75113 (15)	0.33527 (11)	0.0374 (4)
H10	0.2859	0.7975	0.3262	0.045*
C11	0.44143 (11)	0.79795 (13)	0.33559 (10)	0.0340 (3)
H11	0.4495	0.8753	0.3284	0.041*
C12	0.52564 (10)	0.73085 (12)	0.34629 (9)	0.0260 (3)
C13	0.51545 (10)	0.61194 (12)	0.35810 (9)	0.0251 (3)
C14	0.59885 (10)	0.53955 (12)	0.36966 (8)	0.0245 (3)
H14	0.6644	0.5689	0.3671	0.029*
C15	0.58584 (10)	0.42404 (12)	0.38492 (9)	0.0244 (3)
C16	0.62893 (10)	0.78344 (11)	0.34033 (9)	0.0252 (3)
C17	0.94581 (9)	0.35625 (11)	0.46862 (8)	0.0212 (3)
C18	1.00793 (10)	0.39188 (12)	0.40017 (9)	0.0273 (3)
H18	0.9794	0.4213	0.3476	0.033*
C19	1.11299 (11)	0.38351 (15)	0.41045 (10)	0.0368 (4)
H19	1.1546	0.4066	0.3642	0.044*
C20	1.15621 (11)	0.34135 (15)	0.48846 (10)	0.0371 (4)
H20	1.2267	0.3353	0.4942	0.045*
C21	1.09525 (11)	0.30789 (13)	0.55847 (10)	0.0299 (3)
H21	1.1245	0.2806	0.6115	0.036*
C22	0.99064 (10)	0.31554 (11)	0.54865 (9)	0.0230 (3)
C23	0.96345 (12)	0.23011 (13)	0.69133 (9)	0.0331 (3)
H23A	1.0000	0.1637	0.6740	0.040*
H23B	0.9088	0.2094	0.7299	0.040*
H23C	1.0089	0.2806	0.7227	0.040*
C24	0.73476 (10)	0.93539 (11)	0.40486 (9)	0.0247 (3)
C25	0.78309 (12)	0.97149 (12)	0.32848 (10)	0.0313 (3)
H25	0.7574	0.9509	0.2723	0.038*
C26	0.86950 (12)	1.03800 (13)	0.33509 (11)	0.0365 (4)
H26	0.9021	1.0614	0.2835	0.044*
C27	0.90712 (12)	1.06945 (12)	0.41811 (12)	0.0357 (4)
H27	0.9649	1.1145	0.4224	0.043*
C28	0.85948 (12)	1.03441 (12)	0.49528 (11)	0.0339 (3)
H28	0.8853	1.0559	0.5512	0.041*
C29	0.77318 (11)	0.96719 (11)	0.48910 (9)	0.0283 (3)

C30	0.76496 (18)	0.94020 (17)	0.64739 (11)	0.0562 (5)
H30A	0.8295	0.9023	0.6493	0.067*
H30B	0.7210	0.9076	0.6911	0.067*
H30C	0.7748	1.0187	0.6605	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0252 (5)	0.0426 (6)	0.0260 (5)	0.0029 (4)	−0.0006 (4)	0.0120 (4)
O2	0.0251 (5)	0.0380 (6)	0.0244 (5)	0.0034 (4)	−0.0023 (4)	0.0094 (4)
O3	0.0320 (6)	0.0323 (6)	0.0395 (6)	−0.0012 (4)	0.0045 (4)	−0.0114 (5)
O4	0.0618 (7)	0.0416 (6)	0.0211 (5)	−0.0214 (6)	−0.0003 (5)	−0.0019 (4)
N1	0.0200 (5)	0.0263 (6)	0.0211 (5)	0.0000 (4)	−0.0014 (4)	0.0042 (4)
N2	0.0291 (6)	0.0278 (6)	0.0256 (6)	−0.0028 (5)	0.0002 (5)	−0.0051 (5)
C1	0.0223 (6)	0.0217 (6)	0.0213 (6)	0.0036 (5)	−0.0018 (5)	−0.0004 (5)
C2	0.0236 (7)	0.0275 (7)	0.0179 (6)	−0.0005 (5)	−0.0041 (5)	0.0017 (5)
C3	0.0300 (8)	0.0293 (7)	0.0399 (8)	0.0003 (6)	−0.0076 (6)	0.0070 (6)
C4	0.0384 (9)	0.0278 (8)	0.0488 (9)	−0.0077 (6)	−0.0095 (7)	0.0106 (7)
C5	0.0263 (7)	0.0366 (8)	0.0330 (8)	−0.0109 (6)	−0.0056 (6)	0.0080 (6)
C6	0.0230 (7)	0.0334 (7)	0.0260 (7)	−0.0041 (6)	−0.0025 (5)	0.0013 (6)
C7	0.0214 (7)	0.0429 (8)	0.0262 (7)	−0.0058 (6)	−0.0021 (5)	0.0013 (6)
C8	0.0221 (7)	0.0366 (8)	0.0258 (7)	0.0008 (6)	−0.0023 (5)	−0.0052 (6)
C9	0.0189 (7)	0.0465 (9)	0.0324 (7)	0.0028 (6)	−0.0030 (5)	−0.0121 (7)
C10	0.0253 (7)	0.0446 (9)	0.0419 (8)	0.0114 (7)	−0.0076 (6)	−0.0073 (7)
C11	0.0323 (8)	0.0329 (8)	0.0366 (8)	0.0071 (6)	−0.0064 (6)	−0.0052 (6)
C12	0.0250 (7)	0.0298 (7)	0.0229 (6)	0.0028 (6)	−0.0044 (5)	−0.0076 (5)
C13	0.0218 (7)	0.0302 (7)	0.0232 (6)	0.0009 (5)	−0.0031 (5)	−0.0048 (5)
C14	0.0225 (6)	0.0308 (7)	0.0201 (6)	−0.0022 (5)	−0.0028 (5)	−0.0013 (5)
C15	0.0215 (6)	0.0294 (7)	0.0223 (6)	−0.0015 (5)	−0.0031 (5)	−0.0010 (5)
C16	0.0276 (7)	0.0229 (7)	0.0248 (7)	0.0033 (5)	−0.0055 (5)	−0.0019 (5)
C17	0.0203 (6)	0.0195 (6)	0.0237 (6)	0.0002 (5)	−0.0032 (5)	−0.0025 (5)
C18	0.0251 (7)	0.0331 (7)	0.0234 (6)	−0.0032 (6)	−0.0032 (5)	0.0009 (5)
C19	0.0237 (7)	0.0563 (10)	0.0306 (8)	−0.0059 (7)	0.0026 (6)	0.0024 (7)
C20	0.0181 (7)	0.0554 (10)	0.0378 (8)	0.0006 (7)	−0.0026 (6)	0.0000 (7)
C21	0.0256 (7)	0.0349 (8)	0.0289 (7)	0.0046 (6)	−0.0077 (5)	−0.0003 (6)
C22	0.0243 (6)	0.0212 (6)	0.0233 (6)	0.0014 (5)	−0.0012 (5)	−0.0011 (5)
C23	0.0354 (8)	0.0379 (8)	0.0257 (7)	0.0058 (6)	−0.0049 (6)	0.0092 (6)
C24	0.0289 (7)	0.0187 (6)	0.0264 (7)	0.0011 (5)	−0.0028 (5)	−0.0003 (5)
C25	0.0403 (8)	0.0271 (7)	0.0266 (7)	−0.0001 (6)	0.0000 (6)	0.0000 (6)
C26	0.0399 (9)	0.0279 (7)	0.0421 (9)	−0.0014 (6)	0.0104 (7)	0.0031 (6)
C27	0.0299 (8)	0.0223 (7)	0.0549 (10)	−0.0019 (6)	−0.0007 (7)	0.0007 (6)
C28	0.0393 (8)	0.0242 (7)	0.0378 (8)	−0.0020 (6)	−0.0126 (6)	−0.0020 (6)
C29	0.0380 (8)	0.0204 (6)	0.0263 (7)	−0.0016 (6)	−0.0037 (6)	0.0008 (5)
C30	0.0973 (16)	0.0474 (10)	0.0234 (8)	−0.0241 (10)	−0.0103 (9)	0.0007 (7)

Geometric parameters (Å, °)

O1—C1	1.2219 (16)	C11—H11	0.9300
O2—C22	1.3730 (17)	C12—C13	1.428 (2)

O2—C23	1.4283 (16)	C12—C16	1.4971 (19)
O3—C16	1.2187 (17)	C13—C14	1.3996 (19)
O4—C29	1.3603 (18)	C14—C15	1.400 (2)
O4—C30	1.433 (2)	C14—H14	0.9300
N1—C1	1.3610 (17)	C17—C18	1.3851 (19)
N1—C17	1.4096 (16)	C17—C22	1.4059 (18)
N1—H1N	0.8600	C18—C19	1.389 (2)
N2—C16	1.3647 (18)	C18—H18	0.9300
N2—C24	1.4110 (18)	C19—C20	1.378 (2)
N2—H2N	0.8600	C19—H19	0.9300
C1—C2	1.5007 (18)	C20—C21	1.386 (2)
C2—C3	1.363 (2)	C20—H20	0.9300
C2—C15	1.4359 (19)	C21—C22	1.381 (2)
C3—C4	1.418 (2)	C21—H21	0.9300
C3—H3	0.9300	C23—H23A	0.9600
C4—C5	1.349 (2)	C23—H23B	0.9600
C4—H4	0.9300	C23—H23C	0.9600
C5—C6	1.423 (2)	C24—C25	1.383 (2)
C5—H5	0.9300	C24—C29	1.3965 (19)
C6—C7	1.396 (2)	C25—C26	1.384 (2)
C6—C15	1.4379 (19)	C25—H25	0.9300
C7—C8	1.388 (2)	C26—C27	1.375 (2)
C7—H7	0.9300	C26—H26	0.9300
C8—C9	1.420 (2)	C27—C28	1.384 (2)
C8—C13	1.4361 (19)	C27—H27	0.9300
C9—C10	1.354 (2)	C28—C29	1.387 (2)
C9—H9	0.9300	C28—H28	0.9300
C10—C11	1.416 (2)	C30—H30A	0.9600
C10—H10	0.9300	C30—H30B	0.9600
C11—C12	1.369 (2)	C30—H30C	0.9600
C22—O2—C23	117.08 (11)	C2—C15—C6	117.41 (12)
C29—O4—C30	117.35 (13)	O3—C16—N2	123.05 (13)
C1—N1—C17	128.25 (11)	O3—C16—C12	122.97 (12)
C1—N1—H1N	115.9	N2—C16—C12	113.96 (12)
C17—N1—H1N	115.9	C18—C17—C22	119.18 (12)
C16—N2—C24	124.84 (12)	C18—C17—N1	124.14 (12)
C16—N2—H2N	117.6	C22—C17—N1	116.61 (12)
C24—N2—H2N	117.6	C17—C18—C19	119.67 (13)
O1—C1—N1	123.91 (12)	C17—C18—H18	120.2
O1—C1—C2	121.95 (11)	C19—C18—H18	120.2
N1—C1—C2	114.09 (11)	C20—C19—C18	120.72 (14)
C3—C2—C15	120.45 (13)	C20—C19—H19	119.6
C3—C2—C1	118.52 (12)	C18—C19—H19	119.6
C15—C2—C1	120.82 (12)	C19—C20—C21	120.35 (13)
C2—C3—C4	121.34 (14)	C19—C20—H20	119.8
C2—C3—H3	119.3	C21—C20—H20	119.8
C4—C3—H3	119.3	C22—C21—C20	119.29 (13)
C5—C4—C3	120.25 (14)	C22—C21—H21	120.4
C5—C4—H4	119.9	C20—C21—H21	120.4

C3—C4—H4	119.9	O2—C22—C21	124.46 (12)
C4—C5—C6	120.74 (13)	O2—C22—C17	114.78 (11)
C4—C5—H5	119.6	C21—C22—C17	120.76 (13)
C6—C5—H5	119.6	O2—C23—H23A	109.5
C7—C6—C5	121.22 (13)	O2—C23—H23B	109.5
C7—C6—C15	119.00 (13)	H23A—C23—H23B	109.5
C5—C6—C15	119.76 (13)	O2—C23—H23C	109.5
C8—C7—C6	122.23 (13)	H23A—C23—H23C	109.5
C8—C7—H7	118.9	H23B—C23—H23C	109.5
C6—C7—H7	118.9	C25—C24—C29	119.59 (13)
C7—C8—C9	121.32 (13)	C25—C24—N2	121.84 (12)
C7—C8—C13	118.96 (13)	C29—C24—N2	118.56 (12)
C9—C8—C13	119.72 (14)	C24—C25—C26	120.45 (14)
C10—C9—C8	120.75 (14)	C24—C25—H25	119.8
C10—C9—H9	119.6	C26—C25—H25	119.8
C8—C9—H9	119.6	C27—C26—C25	119.89 (14)
C9—C10—C11	120.31 (14)	C27—C26—H26	120.1
C9—C10—H10	119.8	C25—C26—H26	120.1
C11—C10—H10	119.8	C26—C27—C28	120.43 (14)
C12—C11—C10	120.86 (15)	C26—C27—H27	119.8
C12—C11—H11	119.6	C28—C27—H27	119.8
C10—C11—H11	119.6	C27—C28—C29	119.95 (14)
C11—C12—C13	120.74 (13)	C27—C28—H28	120.0
C11—C12—C16	118.76 (13)	C29—C28—H28	120.0
C13—C12—C16	120.41 (12)	O4—C29—C28	125.39 (13)
C14—C13—C12	123.11 (13)	O4—C29—C24	114.92 (12)
C14—C13—C8	119.30 (13)	C28—C29—C24	119.68 (13)
C12—C13—C8	117.57 (12)	O4—C30—H30A	109.5
C13—C14—C15	121.52 (13)	O4—C30—H30B	109.5
C13—C14—H14	119.2	H30A—C30—H30B	109.5
C15—C14—H14	119.2	O4—C30—H30C	109.5
C14—C15—C2	123.62 (12)	H30A—C30—H30C	109.5
C14—C15—C6	118.97 (12)	H30B—C30—H30C	109.5
C17—N1—C1—O1	−10.7 (2)	C5—C6—C15—C14	177.79 (13)
C17—N1—C1—C2	166.99 (12)	C7—C6—C15—C2	179.34 (12)
O1—C1—C2—C3	124.44 (15)	C5—C6—C15—C2	−2.30 (19)
N1—C1—C2—C3	−53.27 (17)	C24—N2—C16—O3	2.2 (2)
O1—C1—C2—C15	−50.30 (18)	C24—N2—C16—C12	−176.26 (12)
N1—C1—C2—C15	131.99 (12)	C11—C12—C16—O3	−120.69 (16)
C15—C2—C3—C4	1.0 (2)	C13—C12—C16—O3	55.99 (19)
C1—C2—C3—C4	−173.74 (13)	C11—C12—C16—N2	57.75 (17)
C2—C3—C4—C5	−1.8 (2)	C13—C12—C16—N2	−125.58 (13)
C3—C4—C5—C6	0.5 (2)	C1—N1—C17—C18	−2.3 (2)
C4—C5—C6—C7	179.89 (14)	C1—N1—C17—C22	−179.21 (12)
C4—C5—C6—C15	1.6 (2)	C22—C17—C18—C19	2.1 (2)
C5—C6—C7—C8	−179.09 (14)	N1—C17—C18—C19	−174.81 (14)
C15—C6—C7—C8	−0.8 (2)	C17—C18—C19—C20	−0.8 (2)
C6—C7—C8—C9	−179.33 (13)	C18—C19—C20—C21	−0.8 (3)
C6—C7—C8—C13	1.1 (2)	C19—C20—C21—C22	1.0 (2)

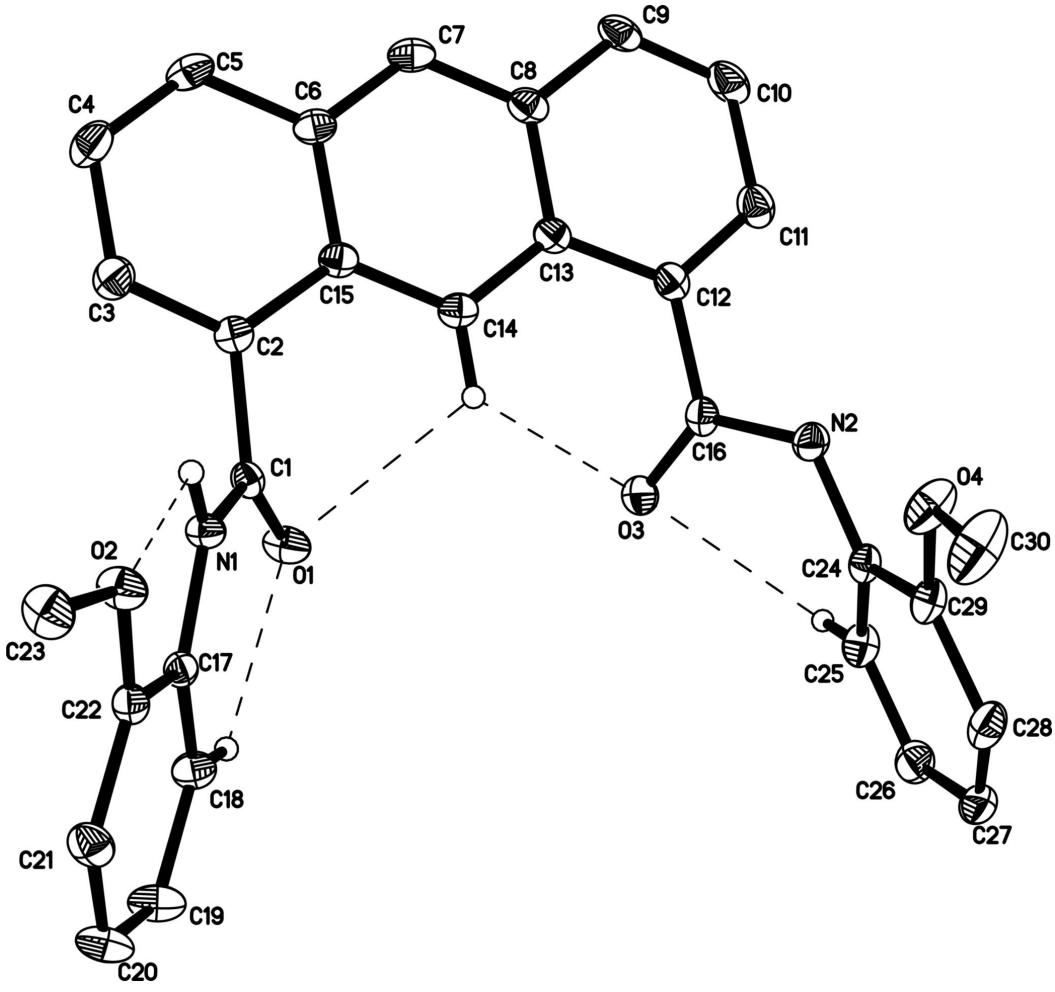
C7—C8—C9—C10	179.94 (14)	C23—O2—C22—C21	−7.0 (2)
C13—C8—C9—C10	−0.5 (2)	C23—O2—C22—C17	172.60 (12)
C8—C9—C10—C11	−1.4 (2)	C20—C21—C22—O2	179.81 (14)
C9—C10—C11—C12	1.9 (2)	C20—C21—C22—C17	0.3 (2)
C10—C11—C12—C13	−0.5 (2)	C18—C17—C22—O2	178.59 (12)
C10—C11—C12—C16	176.17 (13)	N1—C17—C22—O2	−4.31 (17)
C11—C12—C13—C14	−179.75 (13)	C18—C17—C22—C21	−1.8 (2)
C16—C12—C13—C14	3.6 (2)	N1—C17—C22—C21	175.27 (12)
C11—C12—C13—C8	−1.3 (2)	C16—N2—C24—C25	39.1 (2)
C16—C12—C13—C8	−177.93 (11)	C16—N2—C24—C29	−142.06 (14)
C7—C8—C13—C14	−0.12 (19)	C29—C24—C25—C26	0.5 (2)
C9—C8—C13—C14	−179.70 (12)	N2—C24—C25—C26	179.32 (13)
C7—C8—C13—C12	−178.62 (12)	C24—C25—C26—C27	−0.7 (2)
C9—C8—C13—C12	1.81 (19)	C25—C26—C27—C28	0.4 (2)
C12—C13—C14—C15	177.20 (12)	C26—C27—C28—C29	0.0 (2)
C8—C13—C14—C15	−1.20 (19)	C30—O4—C29—C28	−11.8 (2)
C13—C14—C15—C2	−178.36 (12)	C30—O4—C29—C24	168.75 (15)
C13—C14—C15—C6	1.54 (19)	C27—C28—C29—O4	−179.47 (14)
C3—C2—C15—C14	−179.08 (13)	C27—C28—C29—C24	−0.1 (2)
C1—C2—C15—C14	−4.43 (19)	C25—C24—C29—O4	179.30 (13)
C3—C2—C15—C6	1.03 (19)	N2—C24—C29—O4	0.46 (19)
C1—C2—C15—C6	175.67 (12)	C25—C24—C29—C28	−0.1 (2)
C7—C6—C15—C14	−0.56 (19)	N2—C24—C29—C28	−178.98 (13)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···O1	0.93	2.51	3.0581 (18)	118
C14—H14···O3	0.93	2.55	3.1012 (18)	119
C18—H18···O1	0.93	2.29	2.8870 (18)	122
C25—H25···O3	0.93	2.50	2.9084 (19)	107
N1—H1N···O2	0.86	2.20	2.6146 (15)	109
C5—H5···O4^{i}	0.93	2.58	3.4134 (19)	149
C30—H30B···O3^{ii}	0.96	2.42	3.254 (2)	145
C30—H30C···O1^{ii}	0.96	2.57	3.089 (2)	114

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

Fig. 1


C9
C7
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C16
C1
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C25
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C28
C18
C26
C21
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