Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4,6-Dibenzoylisophthalic acid pyridine disolvate

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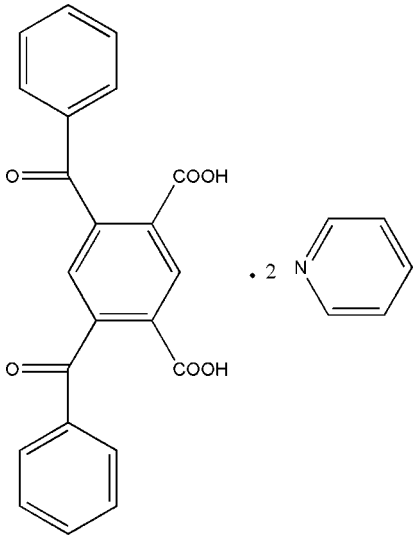
Received 29 May 2007; accepted 31 May 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.064; wR factor = 0.197; data-to-parameter ratio = 14.7.

The asymmetric unit of the title compound, $C_{22}H_{14}O_6\cdot 2C_5H_5N$, contains one 4,6-dibenzoylisophthalic acid (DBIA) and two pyridine molecules. The dihedral angles between the terminal phenyl rings and the central benzene ring are 73.3 (2) and 105.0 (3)°. In the crystal structure, there is an intramolecular C—H···O hydrogen bond; intermolecular O—H···N and C—H···O hydrogen bonds link the molecules to form a three-dimensional framework.

Related literature

For general background, see: Tonzola *et al.* (2003); Kolosov *et al.* (2002); Antoniadis *et al.* (1994); Allen *et al.* (1987). For related literature, see: Liu, Heng *et al.* (2006); Liu, Ji *et al.* (2006).



Experimental

Crystal data

$C_{22}H_{14}O_6\cdot 2C_5H_5N$
M_r = 532.53
Triclinic, $P\overline{1}$
a = 10.257 (2) Å
b = 11.228 (2) Å
c = 12.109 (2) Å
α = 101.37 (3)°
β = 97.17 (3)°
γ = 90.32 (3)°
V = 1355.8 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.40 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.935, T_{max} = 0.962
5635 measured reflections
5322 independent reflections
3172 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.197
S = 1.03
5322 reflections
361 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2B···N2	0.82	1.81	2.630 (4)	173
O4—H4A···N1^{i}	0.82	1.75	2.544 (4)	163
C10—H10A···O4	0.93	2.38	2.711 (4)	101
C22—H22A···O4^{ii}	0.93	2.44	3.241 (4)	144
C31—H31A···O1	0.93	2.56	3.209 (6)	127

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x, -y, -z+1$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

The authors thank the Center of Testing and Analysis, Nanjing University, for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2264).

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  doi:10.1107/S1600536807026657

supplementary materials

Acta Cryst. (2007). E**63**, o3110 [**doi:10.1107/S1600536807026657**]

4,6-Dibenzoylisophthalic acid pyridine disolvate

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Comment

4,6-Dibenzoylisophthalic acid (DBIA) and its isomer 2,5-Dibenzoylterephthalic acid (DBTA), can be utilized to synthesize organic semiconductors and conjugated polymers (Tonzola *et al.*, 2003), which are of wide current interest for applications in electronic and optoelectronic devices including light-emitting diodes (Kolosov *et al.*, 2002), thin film transistors, and photovoltaic cells (Antoniadis *et al.*, 1994). DBTA tetrasolvate has been reported recently (Liu, Heng *et al.*, 2006), and we herein report the crystal structure of the title compound, (I), which is of interest to us in the field of organic semiconductors.

The asymmetric unit of the title compound, (I), contains one DBIA and two pyridine molecules (Fig. 1), in which the bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

Rings A (C1—C6), B (C8—C13) and C (C17—C22) are, of course, planar and the dihedral angles between them are A/B = 73.3 (2)° and B/C = 105.0 (3)°.

In the crystal structure, intra- and intermolecular O—H···N and C—H···O hydrogen bonds (Table 1) link the molecules to form a three dimensional framework (Fig. 2), in which they may be effective in the stabilization of the structure.

Experimental

The title compound, (I) was prepared by the literature method (Liu, Ji *et al.*, 2006). The crystals were obtained by dissolving DBIA (1.5 g, 4.0 mmol) in pyridine (50 ml) and evaporating the solvent slowly at room temperature for about 15 d.

Refinement

H atoms were positioned geometrically, with O—H = 0.82 Å (for OH) and C—H = 0.93 Å for aromatic H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xUeq(C,*O*), where *x* = 1.5 for OH H, and *x* = 1.2 for aromatic H atoms.

Figures

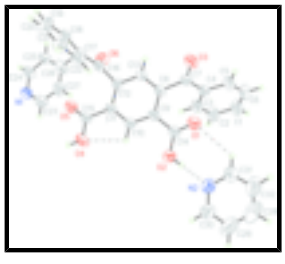

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. Hydrogen bonds are shown as dashed lines.

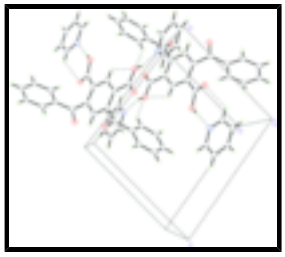

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

4,6-Dibenzoylisophthalic acid pyridine disolvate

Crystal data

$C_{22}H_{14}O_6 \cdot 2C_5H_5N$	$Z = 2$
$M_r = 532.53$	$F_{000} = 556$
Triclinic, $P\overline{1}$	$D_x = 1.304$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.257$ (2) Å	Cell parameters from 25 reflections
$b = 11.228$ (2) Å	$\theta = 10$–13°
$c = 12.109$ (2) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 101.37$ (3)°	$T = 298$ (2) K
$\beta = 97.17$ (3)°	Plate, colorless
$\gamma = 90.32$ (3)°	0.40 × 0.30 × 0.20 mm
$V = 1355.8$ (5) Å^3	

Data collection

Enraf-Nonius CAD-4 diffractometer	$R_{int} = 0.026$
Radiation source: fine-focus sealed tube	$\theta_{max} = 26.0^\circ$
Monochromator: graphite	$\theta_{min} = 1.7^\circ$
$T = 298(2)$ K	$h = -12 \rightarrow 12$
$\omega/2\theta$ scans	$k = -13 \rightarrow 13$
Absorption correction: ψ scan (North *et al.*, 1968)	$l = 0 \rightarrow 14$
$T_{min} = 0.935$, $T_{max} = 0.962$	3 standard reflections
5635 measured reflections	every 120 min
5322 independent reflections	intensity decay: 1%
3172 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.064$	H-atom parameters constrained
$wR(F^2) = 0.197$	$w = 1/[\sigma^2(F_o^2) + (0.06P)^2 + 1.5P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
5322 reflections	$\Delta\rho_{max} = 0.29$ e Å^{-3}
361 parameters	$\Delta\rho_{min} = -0.25$ 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}
O1	−0.3679 (3)	−0.3363 (2)	0.2543 (2)	0.0784 (9)
O2	−0.4109 (3)	−0.1895 (2)	0.3963 (2)	0.0687 (8)
H2B	−0.4594	−0.2424	0.4085	0.103*
O3	−0.2067 (3)	−0.3431 (2)	0.0336 (2)	0.0741 (8)
O4	−0.1013 (3)	0.1444 (2)	0.5193 (2)	0.0730 (8)
H4A	−0.0724	0.2065	0.5636	0.109*
O5	−0.0046 (3)	0.2261 (2)	0.3967 (2)	0.0708 (8)
O6	−0.0130 (3)	0.1521 (2)	0.1154 (2)	0.0663 (7)
N1	0.0531 (3)	0.6687 (3)	0.3228 (3)	0.0623 (8)
N2	−0.5820 (3)	−0.3480 (3)	0.4331 (3)	0.0675 (9)
C1	−0.6799 (4)	−0.2681 (4)	−0.0675 (4)	0.0854 (14)
H1A	−0.7676	−0.2688	−0.0986	0.102*
C2	−0.6243 (5)	−0.1657 (4)	0.0075 (4)	0.0809 (13)
H2A	−0.6742	−0.0974	0.0258	0.097*
C3	−0.4958 (4)	−0.1652 (3)	0.0546 (3)	0.0649 (10)
H3A	−0.4595	−0.0964	0.1054	0.078*
C4	−0.4187 (3)	−0.2652 (3)	0.0279 (3)	0.0490 (8)
C5	−0.4770 (4)	−0.3669 (3)	−0.0493 (3)	0.0587 (9)
H5A	−0.4274	−0.4350	−0.0695	0.070*
C6	−0.6067 (5)	−0.3673 (4)	−0.0955 (4)	0.0779 (13)
H6A	−0.6443	−0.4357	−0.1460	0.093*
C7	−0.2795 (4)	−0.2672 (3)	0.0743 (3)	0.0503 (8)
C8	−0.2242 (3)	−0.1645 (3)	0.1685 (3)	0.0466 (8)
C9	−0.2594 (3)	−0.1451 (3)	0.2787 (3)	0.0458 (8)
C10	−0.2073 (3)	−0.0454 (3)	0.3578 (3)	0.0446 (8)
H10A	−0.2332	−0.0317	0.4300	0.054*

C11	−0.1176 (3)	0.0352 (3)	0.3330 (2)	0.0434 (7)
C12	−0.0790 (3)	0.0147 (3)	0.2245 (3)	0.0459 (8)
C13	−0.1306 (3)	−0.0853 (3)	0.1442 (3)	0.0476 (8)
H13A	−0.1025	−0.1001	0.0727	0.057*
C14	−0.3510 (4)	−0.2336 (3)	0.3083 (3)	0.0527 (9)
C15	−0.0682 (3)	0.1453 (3)	0.4200 (3)	0.0458 (8)
C16	0.0225 (4)	0.0921 (3)	0.1880 (3)	0.0485 (8)
C17	0.1639 (3)	0.0816 (3)	0.2292 (3)	0.0435 (7)
C18	0.2573 (4)	0.1473 (3)	0.1907 (3)	0.0542 (9)
H18A	0.2316	0.1989	0.1411	0.065*
C19	0.3880 (4)	0.1357 (4)	0.2264 (3)	0.0645 (10)
H19A	0.4508	0.1799	0.2008	0.077*
C20	0.4278 (4)	0.0590 (4)	0.3000 (3)	0.0675 (11)
H20A	0.5166	0.0517	0.3238	0.081*
C21	0.3347 (4)	−0.0057 (4)	0.3371 (3)	0.0655 (10)
H21A	0.3608	−0.0576	0.3863	0.079*
C22	0.2039 (4)	0.0046 (3)	0.3030 (3)	0.0576 (9)
H22A	0.1418	−0.0399	0.3291	0.069*
C23	−0.0048 (5)	0.5690 (4)	0.3389 (4)	0.0759 (12)
H23A	−0.0385	0.5708	0.4070	0.091*
C24	0.1015 (5)	0.6645 (4)	0.2258 (3)	0.0703 (11)
H24A	0.1399	0.7350	0.2131	0.084*
C25	0.0979 (5)	0.5611 (4)	0.1431 (3)	0.0753 (12)
H25A	0.1363	0.5600	0.0773	0.090*
C26	0.0355 (5)	0.4595 (4)	0.1612 (4)	0.0797 (13)
H26A	0.0295	0.3883	0.1062	0.096*
C27	−0.0172 (5)	0.4627 (4)	0.2588 (4)	0.0798 (12)
H27A	−0.0607	0.3946	0.2713	0.096*
C28	−0.7248 (6)	−0.5425 (6)	0.4630 (7)	0.116 (2)
H28A	−0.7713	−0.6101	0.4730	0.139*
C29	−0.7039 (6)	−0.4422 (7)	0.5502 (5)	0.122 (2)
H29A	−0.7366	−0.4389	0.6190	0.146*
C30	−0.6308 (5)	−0.3460 (5)	0.5291 (4)	0.0898 (14)
H30A	−0.6156	−0.2766	0.5859	0.108*
C31	−0.6069 (5)	−0.4462 (4)	0.3544 (4)	0.0883 (14)
H31A	−0.5727	−0.4502	0.2861	0.106*
C32	−0.6802 (5)	−0.5432 (5)	0.3672 (6)	0.1088 (18)
H32A	−0.6982	−0.6095	0.3075	0.131*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.118 (2)	0.0478 (15)	0.0708 (18)	−0.0187 (15)	0.0389 (17)	0.0001 (13)
O2	0.0842 (19)	0.0604 (16)	0.0631 (16)	−0.0150 (14)	0.0312 (14)	0.0028 (13)
O3	0.0728 (18)	0.0655 (17)	0.0730 (18)	0.0103 (14)	0.0108 (14)	−0.0139 (14)
O4	0.119 (2)	0.0563 (16)	0.0420 (14)	−0.0208 (15)	0.0247 (14)	−0.0031 (12)
O5	0.103 (2)	0.0528 (15)	0.0559 (15)	−0.0217 (15)	0.0264 (15)	0.0002 (12)
O6	0.0717 (18)	0.0716 (17)	0.0627 (16)	−0.0037 (14)	0.0056 (13)	0.0328 (14)

N1	0.079 (2)	0.0567 (18)	0.0489 (17)	−0.0001 (16)	0.0137 (15)	0.0009 (14)
N2	0.068 (2)	0.067 (2)	0.069 (2)	−0.0097 (17)	0.0082 (17)	0.0155 (17)
C1	0.060 (3)	0.083 (3)	0.099 (4)	−0.005 (2)	−0.010 (2)	−0.003 (3)
C2	0.074 (3)	0.072 (3)	0.087 (3)	0.011 (2)	0.003 (2)	−0.003 (2)
C3	0.065 (3)	0.054 (2)	0.067 (2)	0.0021 (19)	0.008 (2)	−0.0087 (18)
C4	0.058 (2)	0.0468 (19)	0.0415 (18)	−0.0025 (16)	0.0085 (15)	0.0059 (15)
C5	0.071 (3)	0.047 (2)	0.053 (2)	−0.0035 (18)	0.0022 (18)	0.0011 (16)
C6	0.081 (3)	0.059 (3)	0.082 (3)	−0.016 (2)	−0.008 (2)	−0.002 (2)
C7	0.065 (2)	0.0440 (19)	0.0432 (18)	−0.0019 (17)	0.0182 (17)	0.0043 (15)
C8	0.057 (2)	0.0430 (18)	0.0377 (17)	−0.0001 (15)	0.0048 (15)	0.0037 (14)
C9	0.053 (2)	0.0407 (17)	0.0435 (18)	0.0023 (15)	0.0080 (15)	0.0058 (14)
C10	0.0514 (19)	0.0470 (18)	0.0356 (16)	−0.0001 (15)	0.0090 (14)	0.0066 (14)
C11	0.054 (2)	0.0428 (17)	0.0339 (16)	0.0024 (15)	0.0096 (14)	0.0062 (13)
C12	0.056 (2)	0.0410 (17)	0.0415 (17)	0.0003 (15)	0.0100 (15)	0.0080 (14)
C13	0.052 (2)	0.053 (2)	0.0372 (17)	0.0005 (16)	0.0118 (14)	0.0029 (15)
C14	0.065 (2)	0.049 (2)	0.0455 (19)	−0.0018 (17)	0.0131 (17)	0.0087 (16)
C15	0.055 (2)	0.0478 (19)	0.0354 (17)	−0.0005 (16)	0.0102 (14)	0.0084 (14)
C16	0.067 (2)	0.0433 (18)	0.0349 (17)	−0.0004 (16)	0.0075 (15)	0.0074 (14)
C17	0.0504 (19)	0.0414 (17)	0.0373 (16)	−0.0013 (14)	0.0079 (14)	0.0030 (13)
C18	0.063 (2)	0.051 (2)	0.048 (2)	−0.0081 (17)	0.0066 (17)	0.0084 (16)
C19	0.062 (3)	0.064 (2)	0.067 (2)	−0.0138 (19)	0.017 (2)	0.006 (2)
C20	0.060 (2)	0.070 (3)	0.068 (3)	0.001 (2)	0.013 (2)	0.002 (2)
C21	0.074 (3)	0.069 (3)	0.056 (2)	0.013 (2)	0.008 (2)	0.0183 (19)
C22	0.066 (3)	0.054 (2)	0.058 (2)	0.0003 (18)	0.0165 (18)	0.0176 (18)
C23	0.093 (3)	0.074 (3)	0.059 (2)	−0.010 (2)	0.018 (2)	0.004 (2)
C24	0.105 (3)	0.055 (2)	0.053 (2)	0.001 (2)	0.013 (2)	0.0112 (17)
C25	0.107 (3)	0.068 (3)	0.048 (2)	0.003 (2)	0.016 (2)	0.0007 (18)
C26	0.105 (3)	0.055 (2)	0.067 (3)	0.003 (2)	0.003 (2)	−0.009 (2)
C27	0.091 (3)	0.060 (2)	0.084 (3)	−0.012 (2)	0.008 (2)	0.007 (2)
C28	0.097 (4)	0.097 (4)	0.167 (5)	−0.015 (3)	0.007 (4)	0.066 (4)
C29	0.100 (4)	0.170 (5)	0.105 (4)	−0.043 (4)	0.011 (3)	0.055 (4)
C30	0.080 (3)	0.121 (4)	0.066 (3)	−0.027 (3)	0.008 (2)	0.014 (3)
C31	0.077 (3)	0.084 (3)	0.096 (3)	−0.015 (2)	0.016 (3)	−0.004 (3)
C32	0.086 (4)	0.074 (3)	0.155 (5)	−0.007 (3)	0.010 (3)	−0.002 (3)

Geometric parameters (Å, °)

O1—C14	1.208 (4)	C17—C18	1.386 (4)
O2—C14	1.310 (4)	C17—C22	1.390 (5)
O2—H2B	0.8200	C18—C19	1.371 (5)
O3—C7	1.208 (4)	C18—H18A	0.9300
O4—C15	1.292 (4)	C19—C20	1.384 (6)
O4—H4A	0.8200	C19—H19A	0.9300
O5—C15	1.212 (4)	C20—C21	1.368 (5)
O6—C16	1.231 (4)	C20—H20A	0.9300
C1—C6	1.358 (6)	C21—C22	1.365 (5)
C1—C2	1.387 (6)	C21—H21A	0.9300
C1—H1A	0.9300	C22—H22A	0.9300
C2—C3	1.369 (6)	N1—C24	1.324 (5)

C2—H2A	0.9300	N1—C23	1.324 (5)
C3—C4	1.386 (5)	N2—C31	1.308 (5)
C3—H3A	0.9300	N2—C30	1.318 (5)
C4—C5	1.403 (5)	C23—C27	1.376 (6)
C4—C7	1.470 (5)	C23—H23A	0.9300
C5—C6	1.377 (6)	C24—C25	1.372 (5)
C5—H5A	0.9300	C24—H24A	0.9300
C6—H6A	0.9300	C25—C26	1.373 (6)
C7—C8	1.506 (4)	C25—H25A	0.9300
C8—C9	1.402 (4)	C26—C27	1.354 (6)
C8—C13	1.401 (4)	C26—H26A	0.9300
C9—C10	1.378 (4)	C27—H27A	0.9300
C9—C14	1.487 (5)	C28—C32	1.298 (8)
C10—C11	1.386 (4)	C28—C29	1.379 (8)
C10—H10A	0.9300	C28—H28A	0.9300
C11—C12	1.395 (4)	C29—C30	1.392 (7)
C11—C15	1.497 (4)	C29—H29A	0.9300
C12—C13	1.386 (4)	C30—H30A	0.9300
C12—C16	1.514 (5)	C31—C32	1.364 (7)
C13—H13A	0.9300	C31—H31A	0.9300
C16—C17	1.487 (5)	C32—H32A	0.9300
C14—O2—H2B	109.5	C18—C17—C22	119.6 (3)
C15—O4—H4A	109.5	C18—C17—C16	119.2 (3)
C6—C1—C2	120.2 (4)	C22—C17—C16	121.2 (3)
C6—C1—H1A	119.9	C19—C18—C17	119.4 (3)
C2—C1—H1A	119.9	C19—C18—H18A	120.3
C3—C2—C1	119.9 (4)	C17—C18—H18A	120.3
C3—C2—H2A	120.0	C18—C19—C20	121.0 (4)
C1—C2—H2A	120.0	C18—C19—H19A	119.5
C2—C3—C4	121.2 (4)	C20—C19—H19A	119.5
C2—C3—H3A	119.4	C21—C20—C19	119.1 (4)
C4—C3—H3A	119.4	C21—C20—H20A	120.4
C5—C4—C3	117.7 (3)	C19—C20—H20A	120.4
C5—C4—C7	119.4 (3)	C22—C21—C20	121.0 (4)
C3—C4—C7	122.9 (3)	C22—C21—H21A	119.5
C6—C5—C4	120.9 (4)	C20—C21—H21A	119.5
C6—C5—H5A	119.6	C21—C22—C17	119.9 (3)
C4—C5—H5A	119.6	C21—C22—H22A	120.0
C1—C6—C5	120.2 (4)	C17—C22—H22A	120.0
C1—C6—H6A	119.9	C24—N1—C23	118.1 (3)
C5—C6—H6A	119.9	C31—N2—C30	116.7 (4)
O3—C7—C4	122.1 (3)	N1—C23—C27	122.6 (4)
O3—C7—C8	119.3 (3)	N1—C23—H23A	118.7
C4—C7—C8	118.3 (3)	C27—C23—H23A	118.7
C9—C8—C13	118.6 (3)	N1—C24—C25	123.2 (4)
C9—C8—C7	123.8 (3)	N1—C24—H24A	118.4
C13—C8—C7	117.6 (3)	C25—C24—H24A	118.4
C10—C9—C8	119.4 (3)	C24—C25—C26	117.5 (4)
C10—C9—C14	121.3 (3)	C24—C25—H25A	121.2

C8—C9—C14	119.3 (3)	C26—C25—H25A	121.2
C9—C10—C11	122.1 (3)	C27—C26—C25	120.2 (4)
C9—C10—H10A	119.0	C27—C26—H26A	119.9
C11—C10—H10A	119.0	C25—C26—H26A	119.9
C12—C11—C10	118.9 (3)	C26—C27—C23	118.4 (4)
C12—C11—C15	120.8 (3)	C26—C27—H27A	120.8
C10—C11—C15	120.2 (3)	C23—C27—H27A	120.8
C11—C12—C13	119.6 (3)	C32—C28—C29	120.5 (6)
C11—C12—C16	124.3 (3)	C32—C28—H28A	119.8
C13—C12—C16	116.0 (3)	C29—C28—H28A	119.8
C12—C13—C8	121.3 (3)	C30—C29—C28	116.0 (6)
C12—C13—H13A	119.4	C30—C29—H29A	122.0
C8—C13—H13A	119.4	C28—C29—H29A	122.0
O1—C14—O2	124.0 (3)	N2—C30—C29	123.6 (5)
O1—C14—C9	122.0 (3)	N2—C30—H30A	118.2
O2—C14—C9	114.0 (3)	C29—C30—H30A	118.2
O5—C15—O4	124.8 (3)	N2—C31—C32	123.4 (5)
O5—C15—C11	122.0 (3)	N2—C31—H31A	118.3
O4—C15—C11	113.2 (3)	C32—C31—H31A	118.3
O6—C16—C17	121.5 (3)	C28—C32—C31	119.8 (6)
O6—C16—C12	118.8 (3)	C28—C32—H32A	120.1
C17—C16—C12	119.2 (3)	C31—C32—H32A	120.1

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2B···N2	0.82	1.81	2.630 (4)	173
O4—H4A···N1^{i}	0.82	1.75	2.544 (4)	163
C10—H10A···O4	0.93	2.38	2.711 (4)	101
C22—H22A···O4^{ii}	0.93	2.44	3.241 (4)	144
C31—H31A···O1	0.93	2.56	3.209 (6)	127

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

Fig. 1

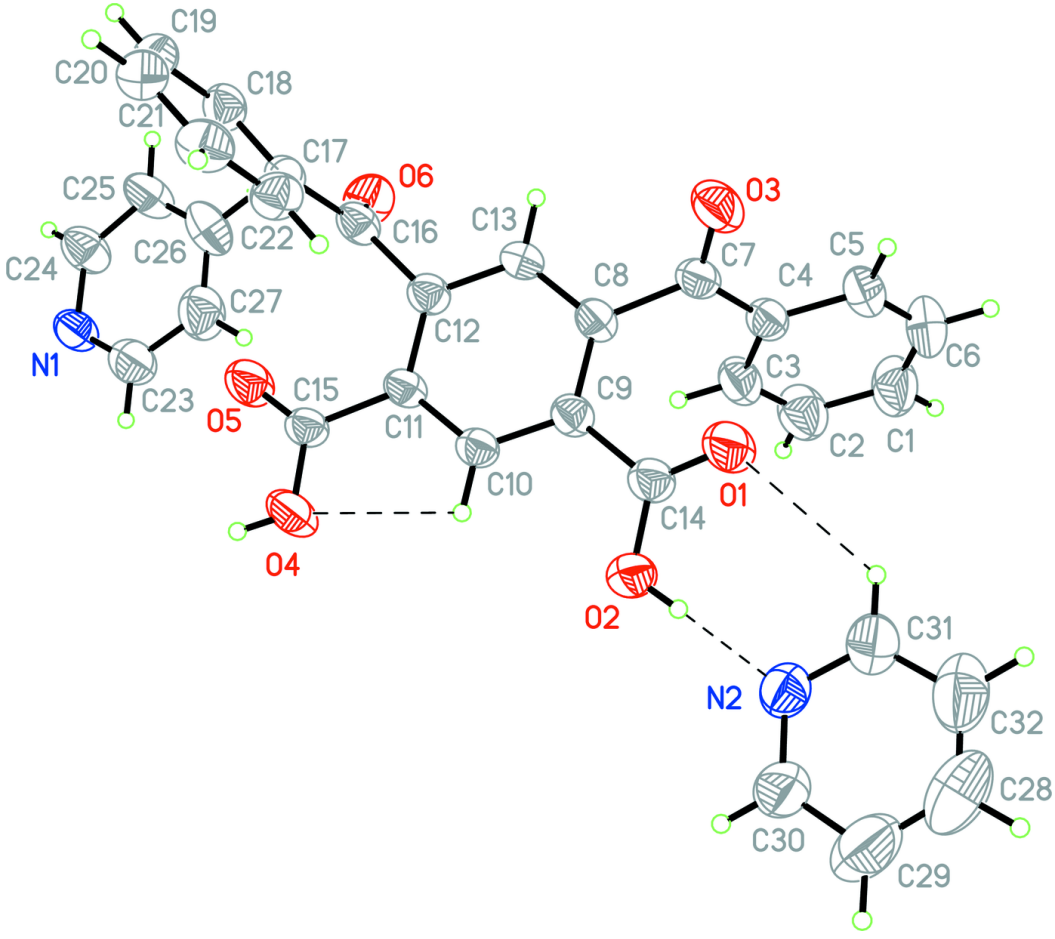
C19
C20
C18
C21
C17
O6
C25
C16
C13
O3
C22
C26
C24
C8
C7
C5
C4
C27
C12
N1
C3
C6
C23
O5
C15
C9
C11
C2
C1
C10
O1
C14
O4
O2
C31
N2
C32
C28
C30
C29

Fig. 2