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3-Allyl-1-{[3-(4-nitrophenyl)-4,5-dihydro-1,3-oxazol-5-yl]methyl}-1*H*-anthra[1,2-*d*]imidazole-2,6,11(3*H*)-trione

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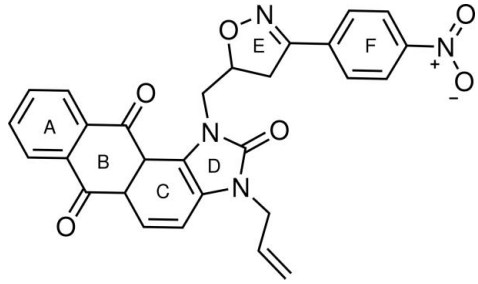
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.111; data-to-parameter ratio = 14.1.

The molecular structure of the title compound, $C_{28}H_{20}N_4O_6$, consists of three fused six-membered rings (*A*,*B*,*C*) and one five-membered ring (*D*). The latter is linked to an isoxazole ring (*E*) *via* a methylene unit. A 4-nitro-phenyl substituent (*F*) is attached to the isoxazole. The fused five and six-membered rings (*C*,*D*) are almost coplanar with an r.m.s. deviation of 0.0345 Å and make a dihedral angle of 9.40 (8)° with ring *A*. The isoxazole and 4-nitro-phenyl rings (*E*,*F*) are also almost coplanar with the imidazole and the fused adjacent ring (*C*,*D*), forming a dihedral angle of 11.4 (6)°. The crystal packing displays intermolecular C—H···O hydrogen bonding. An intramolecular C—H···O interaction also occurs.

Related literature

For the biological activity of anthraquinone derivatives, see: Agarwal *et al.* (2000); Barnard *et al.* (1995); Chen *et al.* (2007); Haug *et al.* (2003); Iizuka *et al.* (2004); Koyamaa *et al.* (2002); Su *et al.* (2005); Wu *et al.* (2005); Yen *et al.* (2000). For a derivative of the title compound, see: Afrakssou *et al.* (2010). For the use of related compounds as synthetic dyes, see: Simi *et al.* (1995). For puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{28}H_{20}N_4O_6$
M_r = 508.48
Monoclinic, $P2_1/n$
a = 10.0780 (3) Å
b = 22.7094 (6) Å
c = 11.2729 (3) Å
β = 113.809 (1)°
V = 2360.41 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.40 × 0.14 × 0.11 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*, Bruker, 2009)
T_{min} = 0.704, T_{max} = 0.745
47772 measured reflections
4828 independent reflections
2998 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.111
S = 1.00
4828 reflections
343 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 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
C7—H7···O1^{i}	0.93	2.60	3.516 (2)	169
C18—H18*B*···O2^{ii}	0.97	2.37	3.333 (2)	170
C26—H26*B*···O1^{i}	0.97	2.55	3.379 (3)	144
C16—H16*A*···O2	0.97	2.10	2.902 (2)	141

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT-Plus* (Bruker, 2009); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2283).

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supplementary materials

Acta Cryst. (2011). E**67**, o1363-o1364 [**doi:10.1107/S1600536811016606**]

3-Allyl-1-{[3-(4-nitrophenyl)-4,5-dihydro-1,3-oxazol-5-yl]methyl}-1*H*-anthra[1,2-*d*]imidazole-2,6,11(3*H*)-trione

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Comment

Recently, a number of pharmacological tests revealed that anthraquinone derivatives present various biological activities including antifungal (Agarwal *et al.*, 2000), antimicrobial (Wu *et al.*, 2005), anticancer (Koyamaa *et al.*, 2002; Su *et al.*, 2005; Chen *et al.*, 2007), antioxidant (Yen *et al.*, 2000; Iizuka *et al.*, 2004), and antihuman cytomegalovirus activity (Barnard *et al.*, 1995).

Aminoanthraquinone derivatives are a class of compounds largely used as phytotherapeutic drugs (laxatives, sedatives and antikidney and antibladder stones) and colouring agents (in the food, cosmetics and textile) (Simi *et al.*, 1995). Anthraquinone derivatives have also been utilized for the activation of human telomerase reverse transcriptase expression (Haug *et al.*, 2003), and they act as telomerase inhibitors or activators.

Due to their importance, in a previous study we have synthesized 1,3-diallyl-1*H*-anthra[1,2-*d*]imidazole-2,6,11(3*H*)-trione (Afrakssou *et al.*, 2010). Here we have focused on the reactivity of the exocyclic C=C bond of the allyl substituents towards nitriloxides. The latter are produced as intermediates in the dehydrohalogenation of 4-nitrobenzaldoxime by a solution of sodium hypochlorite. The oxime then reacts with 1,3-diallyl-1*H*-anthra[1,2-*d*] imidazole-2,6,11(3*H*)-trione in a biphasic medium (water-chloroform) at 0°C during 4 h to a unique cycloadduct 3-allyl-1-[3 -(4-nitro-phenyl)-4,5-dihydro-isoxazole-5-ylmethyl] -1,3-dihydro-anthra [1,2 d] imidazole-2,6,11-trione (Scheme 1). Due to this reaction sequence a racemate of the title compound which shows a stereogenic center at C(17) is formed.

Fig.1 shows the molecular plot of the crystal structure of the title compound. The isoxazole (E) adopts an envelope conformation on C(17) as indicated by the Cremer & Pople (1975) puckering parameters Q2 = 0.2117 (19) Å and φ2 = 141.6 (5)°. Moreover, ring (B) has a twisted conformation, with puckering parameters Q = 0.1480 (19) Å, θ = 114.6 (8) ° and φ = 139.7 (8) °, whereas all other rings are planar. The dihedral angles between fused five and six-membered rings (C,D) and the isoxazole ring (E) is 11.4 (6)°. The torsion angle between C27—C26—N2—C1 is 87.42 (0.22)°. In the crystal, adjacent molecules are linked by intermolecular C–H···O hydrogen bonding as shown in Fig. 2 and Table 1.

Experimental

To a solution of 1,3-diallyl-1*H*-anthra[1,2-*d*] imidazole-2,6,11(3*H*)-trione (0.3 g, 0.87 mmol) and 4-nitrobenzaldoxime (0.36 g, 2.17 mmol) in chloroform (16 ml) was added dropwise a 24% sodium hypochlorite solution (8 ml) at 273 K. Stirring was continued for 4 h. The organic layer was dried over Na_2SO_4 and the solvent was evaporated under reduced pressure. The residue was then purified by column chromatography on silica gel using a mixture of hexane/ethyl acetate (1/1) as eluent. The title compound is formed as a racemate (Yield: 35%). Orange crystals are isolated after the solvent was allowed to evaporate.

Refinement

All H atoms were located in a difference map and treated as riding with C—H = 0.93 Å for all aromatic H atoms, 0.97 Å for methylene and 0.98Å for methine with U_{iso}(H) = 1.2 U_{eq} aromatic, methylene and methine. The C-bound H atoms of the allyl group were positioned geometrically and treated as riding with C—H = 0.93 Å (H27, H28A and H28B) and 0.97 Å (methylene) with U_{iso}(H) = 1.2U_{eq}.

The reflections (0 2 0) and (0 1 1) were omitted because the difference between their calculated and observed intensities are very large. They are affected by the beamstop.

Figures

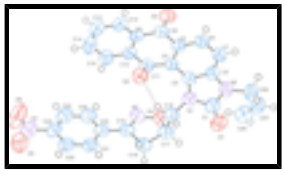

Fig. 1. : Molecular plot of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small circles.

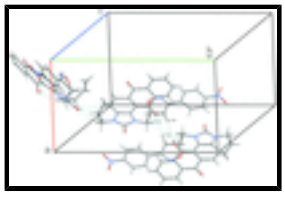

Fig. 2. : Partial packing view showing the intermolecular C–H···O interactions.

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Crystal data

$C_{28}H_{20}N_4O_6$	$F(000)$ = 1056
M_r = 508.48	D_x = 1.431 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 471 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 10.0780 (3) Å	Cell parameters from 7395 reflections
b = 22.7094 (6) Å	θ = 2.4–21.5°
c = 11.2729 (3) Å	μ = 0.10 mm^{-1}
β = 113.809 (1)°	T = 296 K
V = 2360.41 (11) Å^3	Prism, yellow
Z = 4	0.40 × 0.14 × 0.11 mm

Data collection

Bruker APEXII CCD diffractometer	4828 independent reflections
Radiation source: fine-focus sealed tube	2998 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.048
φ and ω scans	θ_{max} = 26.4°, θ_{min} = 2.5°

Absorption correction: multi-scan (*SADABS*, Bruker, 2009)	$h = -12 \rightarrow 12$
$T_{min} = 0.704$, $T_{max} = 0.745$	$k = -28 \rightarrow 28$
47772 measured reflections	$l = -12 \rightarrow 14$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.040$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.111$	H-atom parameters constrained
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 0.4447P]$ where $P = (F_o^2 + 2F_c^2)/3$
4828 reflections	$(\Delta/\sigma)_{max} = 0.001$
343 parameters	$\Delta\rho_{max} = 0.12$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.15$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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}
C1	0.6321 (2)	0.82375 (9)	0.19097 (19)	0.0612 (5)
C2	0.85135 (19)	0.84194 (8)	0.35084 (17)	0.0552 (4)
C3	0.81023 (17)	0.89317 (8)	0.27367 (15)	0.0502 (4)
C4	0.90411 (17)	0.94182 (7)	0.30538 (15)	0.0475 (4)
C5	1.04177 (18)	0.93398 (7)	0.40936 (15)	0.0505 (4)
C6	1.0776 (2)	0.88249 (8)	0.48157 (16)	0.0593 (5)
H6	1.1683	0.8794	0.5498	0.071*
C7	0.9829 (2)	0.83582 (8)	0.45530 (17)	0.0622 (5)
H7	1.0064	0.8018	0.5055	0.075*
C8	1.1555 (2)	0.97997 (8)	0.44241 (17)	0.0574 (4)
C9	1.1231 (2)	1.03401 (8)	0.36364 (17)	0.0556 (4)
C10	0.98508 (19)	1.04342 (7)	0.26723 (16)	0.0527 (4)
C11	0.86591 (19)	1.00068 (8)	0.24546 (16)	0.0524 (4)
C12	1.2303 (2)	1.07627 (9)	0.3858 (2)	0.0712 (5)

H12	1.3224	1.0703	0.4505	0.085*
C13	1.2012 (3)	1.12668 (10)	0.3127 (2)	0.0793 (6)
H13	1.2730	1.1550	0.3292	0.095*
C14	1.0663 (3)	1.13554 (9)	0.2151 (2)	0.0754 (6)
H14	1.0482	1.1692	0.1641	0.090*
C15	0.9574 (2)	1.09440 (8)	0.19255 (19)	0.0651 (5)
H15	0.8658	1.1008	0.1275	0.078*
C16	0.59135 (18)	0.91052 (8)	0.05248 (16)	0.0576 (5)
H16A	0.5982	0.9527	0.0669	0.069*
H16B	0.4900	0.8995	0.0226	0.069*
C17	0.64489 (18)	0.89559 (9)	−0.05152 (17)	0.0588 (5)
H17	0.6223	0.8546	−0.0797	0.071*
C18	0.58172 (18)	0.93738 (8)	−0.16582 (17)	0.0617 (5)
H18A	0.5628	0.9177	−0.2474	0.074*
H18B	0.4935	0.9560	−0.1695	0.074*
C19	0.70447 (18)	0.98060 (8)	−0.13153 (16)	0.0553 (4)
C20	0.69973 (18)	1.03873 (8)	−0.18912 (16)	0.0546 (4)
C21	0.5711 (2)	1.06028 (9)	−0.28290 (18)	0.0640 (5)
H21	0.4882	1.0370	−0.3120	0.077*
C22	0.5655 (2)	1.11605 (9)	−0.33315 (19)	0.0701 (5)
H22	0.4792	1.1305	−0.3955	0.084*
C23	0.6886 (2)	1.15008 (8)	−0.2904 (2)	0.0662 (5)
C24	0.8184 (2)	1.12962 (10)	−0.1991 (2)	0.0727 (6)
H24	0.9011	1.1530	−0.1718	0.087*
C25	0.8234 (2)	1.07410 (9)	−0.14903 (19)	0.0655 (5)
H25	0.9106	1.0599	−0.0875	0.079*
C26	0.7429 (2)	0.74050 (9)	0.3414 (2)	0.0749 (6)
H26A	0.6442	0.7270	0.3176	0.090*
H26B	0.7923	0.7385	0.4351	0.090*
C27	0.8169 (2)	0.70030 (9)	0.2829 (2)	0.0776 (6)
H27	0.8222	0.6608	0.3062	0.093*
C28	0.8743 (3)	0.71473 (12)	0.2031 (3)	0.0922 (7)
H28A	0.8718	0.7537	0.1768	0.111*
H28B	0.9182	0.6862	0.1720	0.111*
N1	0.67395 (14)	0.88059 (7)	0.17487 (13)	0.0554 (4)
N2	0.73969 (16)	0.80148 (7)	0.30080 (15)	0.0633 (4)
N3	0.82302 (15)	0.96221 (7)	−0.04143 (14)	0.0606 (4)
N4	0.6801 (3)	1.20974 (9)	−0.3438 (2)	0.0907 (6)
O1	0.52115 (15)	0.79872 (6)	0.12021 (14)	0.0768 (4)
O2	0.73990 (14)	1.01619 (6)	0.18463 (13)	0.0677 (4)
O3	1.27476 (15)	0.97262 (6)	0.53085 (13)	0.0835 (4)
O4	0.80057 (12)	0.90603 (6)	0.00001 (12)	0.0663 (4)
O5	0.5638 (2)	1.22624 (8)	−0.4262 (2)	0.1111 (6)
O6	0.7864 (2)	1.24061 (9)	−0.3026 (3)	0.1445 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

C1	0.0496 (11)	0.0657 (13)	0.0690 (12)	−0.0039 (10)	0.0245 (10)	−0.0025 (10)
C2	0.0513 (11)	0.0581 (11)	0.0572 (10)	−0.0025 (9)	0.0231 (9)	−0.0016 (8)
C3	0.0439 (10)	0.0582 (11)	0.0491 (9)	0.0041 (8)	0.0193 (8)	−0.0003 (8)
C4	0.0464 (10)	0.0516 (10)	0.0463 (9)	0.0034 (8)	0.0204 (8)	−0.0033 (7)
C5	0.0488 (10)	0.0559 (10)	0.0464 (9)	0.0008 (8)	0.0188 (8)	−0.0058 (8)
C6	0.0528 (11)	0.0668 (12)	0.0495 (9)	0.0057 (9)	0.0115 (8)	0.0018 (9)
C7	0.0623 (12)	0.0614 (12)	0.0578 (11)	0.0031 (10)	0.0190 (9)	0.0077 (9)
C8	0.0540 (11)	0.0654 (12)	0.0470 (9)	−0.0015 (9)	0.0145 (9)	−0.0099 (8)
C9	0.0584 (11)	0.0547 (11)	0.0557 (10)	−0.0037 (9)	0.0251 (9)	−0.0144 (8)
C10	0.0584 (11)	0.0489 (10)	0.0569 (10)	0.0057 (8)	0.0294 (9)	−0.0085 (8)
C11	0.0495 (11)	0.0581 (11)	0.0513 (9)	0.0077 (9)	0.0219 (8)	−0.0055 (8)
C12	0.0700 (13)	0.0670 (13)	0.0737 (13)	−0.0131 (11)	0.0258 (11)	−0.0153 (10)
C13	0.0819 (16)	0.0621 (14)	0.1010 (17)	−0.0139 (12)	0.0444 (14)	−0.0140 (12)
C14	0.0913 (17)	0.0502 (11)	0.0998 (16)	0.0048 (11)	0.0543 (14)	0.0004 (11)
C15	0.0718 (13)	0.0559 (11)	0.0748 (12)	0.0107 (10)	0.0371 (11)	−0.0013 (9)
C16	0.0391 (9)	0.0674 (11)	0.0611 (11)	0.0029 (8)	0.0147 (8)	0.0008 (9)
C17	0.0413 (10)	0.0693 (12)	0.0606 (10)	0.0026 (9)	0.0151 (8)	−0.0027 (9)
C18	0.0412 (10)	0.0799 (13)	0.0575 (10)	0.0015 (9)	0.0131 (8)	−0.0025 (9)
C19	0.0377 (10)	0.0742 (12)	0.0508 (9)	0.0038 (9)	0.0147 (8)	−0.0049 (9)
C20	0.0420 (10)	0.0692 (12)	0.0507 (9)	0.0026 (8)	0.0168 (8)	−0.0098 (8)
C21	0.0500 (11)	0.0681 (13)	0.0609 (11)	−0.0024 (9)	0.0090 (9)	−0.0084 (9)
C22	0.0600 (13)	0.0716 (13)	0.0649 (12)	0.0062 (11)	0.0109 (10)	−0.0085 (10)
C23	0.0684 (14)	0.0582 (12)	0.0739 (12)	0.0016 (10)	0.0309 (11)	−0.0113 (10)
C24	0.0553 (13)	0.0743 (14)	0.0889 (14)	−0.0077 (11)	0.0293 (11)	−0.0138 (12)
C25	0.0417 (10)	0.0818 (14)	0.0683 (12)	−0.0003 (10)	0.0174 (9)	−0.0063 (10)
C26	0.0668 (13)	0.0692 (13)	0.0855 (14)	−0.0114 (11)	0.0273 (11)	0.0125 (11)
C27	0.0647 (14)	0.0634 (13)	0.0915 (16)	−0.0019 (11)	0.0179 (12)	0.0047 (11)
C28	0.0823 (16)	0.0928 (17)	0.1015 (18)	−0.0009 (14)	0.0369 (15)	−0.0112 (14)
N1	0.0402 (8)	0.0646 (10)	0.0581 (8)	−0.0012 (7)	0.0164 (7)	0.0008 (7)
N2	0.0554 (10)	0.0604 (10)	0.0703 (10)	−0.0051 (8)	0.0216 (8)	0.0070 (8)
N3	0.0408 (8)	0.0796 (11)	0.0598 (9)	0.0054 (8)	0.0188 (7)	0.0010 (8)
N4	0.0901 (16)	0.0661 (13)	0.1166 (17)	0.0044 (12)	0.0426 (14)	−0.0096 (12)
O1	0.0551 (8)	0.0801 (10)	0.0868 (9)	−0.0157 (7)	0.0197 (7)	−0.0064 (7)
O2	0.0528 (8)	0.0662 (8)	0.0803 (9)	0.0133 (6)	0.0230 (7)	0.0037 (6)
O3	0.0639 (9)	0.0907 (11)	0.0692 (8)	−0.0144 (8)	−0.0008 (7)	0.0015 (7)
O4	0.0420 (7)	0.0861 (10)	0.0672 (8)	0.0113 (6)	0.0182 (6)	0.0102 (7)
O5	0.1209 (16)	0.0787 (12)	0.1199 (14)	0.0141 (11)	0.0344 (13)	0.0101 (10)
O6	0.1056 (16)	0.0775 (12)	0.233 (3)	−0.0174 (11)	0.0507 (16)	0.0068 (14)

Geometric parameters (Å, °)

C1—O1	1.221 (2)	C16—H16B	0.9700
C1—N2	1.371 (2)	C17—O4	1.456 (2)
C1—N1	1.392 (2)	C17—C18	1.518 (2)
C2—C7	1.379 (2)	C17—H17	0.9800
C2—N2	1.384 (2)	C18—C19	1.502 (2)
C2—C3	1.411 (2)	C18—H18A	0.9700
C3—C4	1.404 (2)	C18—H18B	0.9700
C3—N1	1.405 (2)	C19—N3	1.286 (2)

C4—C5	1.420 (2)	C19—C20	1.463 (3)
C4—C11	1.477 (2)	C20—C21	1.390 (2)
C5—C6	1.387 (2)	C20—C25	1.396 (2)
C5—C8	1.483 (2)	C21—C22	1.379 (3)
C6—C7	1.376 (2)	C21—H21	0.9300
C6—H6	0.9300	C22—C23	1.373 (3)
C7—H7	0.9300	C22—H22	0.9300
C8—O3	1.224 (2)	C23—C24	1.378 (3)
C8—C9	1.472 (3)	C23—N4	1.471 (3)
C9—C12	1.390 (3)	C24—C25	1.374 (3)
C9—C10	1.393 (2)	C24—H24	0.9300
C10—C15	1.392 (2)	C25—H25	0.9300
C10—C11	1.486 (2)	C26—N2	1.455 (2)
C11—O2	1.2264 (19)	C26—C27	1.490 (3)
C12—C13	1.371 (3)	C26—H26A	0.9700
C12—H12	0.9300	C26—H26B	0.9700
C13—C14	1.375 (3)	C27—C28	1.294 (3)
C13—H13	0.9300	C27—H27	0.9300
C14—C15	1.384 (3)	C28—H28A	0.9300
C14—H14	0.9300	C28—H28B	0.9300
C15—H15	0.9300	N3—O4	1.408 (2)
C16—N1	1.460 (2)	N4—O6	1.206 (3)
C16—C17	1.514 (2)	N4—O5	1.224 (2)
C16—H16A	0.9700		
O1—C1—N2	126.88 (18)	O4—C17—H17	110.8
O1—C1—N1	126.32 (18)	C16—C17—H17	110.8
N2—C1—N1	106.80 (16)	C18—C17—H17	110.8
C7—C2—N2	128.61 (17)	C19—C18—C17	99.82 (14)
C7—C2—C3	123.44 (17)	C19—C18—H18A	111.8
N2—C2—C3	107.93 (15)	C17—C18—H18A	111.8
C4—C3—N1	134.81 (15)	C19—C18—H18B	111.8
C4—C3—C2	119.47 (15)	C17—C18—H18B	111.8
N1—C3—C2	105.71 (15)	H18A—C18—H18B	109.5
C3—C4—C5	116.42 (15)	N3—C19—C20	119.80 (16)
C3—C4—C11	124.85 (15)	N3—C19—C18	113.39 (16)
C5—C4—C11	118.57 (15)	C20—C19—C18	126.82 (15)
C6—C5—C4	121.74 (16)	C21—C20—C25	118.73 (18)
C6—C5—C8	117.06 (16)	C21—C20—C19	120.55 (17)
C4—C5—C8	121.17 (15)	C25—C20—C19	120.70 (16)
C7—C6—C5	121.98 (16)	C22—C21—C20	120.41 (18)
C7—C6—H6	119.0	C22—C21—H21	119.8
C5—C6—H6	119.0	C20—C21—H21	119.8
C6—C7—C2	116.76 (17)	C23—C22—C21	119.46 (19)
C6—C7—H7	121.6	C23—C22—H22	120.3
C2—C7—H7	121.6	C21—C22—H22	120.3
O3—C8—C9	120.70 (17)	C22—C23—C24	121.52 (19)
O3—C8—C5	120.92 (17)	C22—C23—N4	118.7 (2)
C9—C8—C5	118.36 (16)	C24—C23—N4	119.8 (2)
C12—C9—C10	119.54 (18)	C25—C24—C23	118.87 (19)

C12—C9—C8	120.01 (17)	C25—C24—H24	120.6
C10—C9—C8	120.45 (16)	C23—C24—H24	120.6
C15—C10—C9	119.50 (17)	C24—C25—C20	120.99 (18)
C15—C10—C11	119.50 (17)	C24—C25—H25	119.5
C9—C10—C11	120.97 (16)	C20—C25—H25	119.5
O2—C11—C4	122.39 (16)	N2—C26—C27	113.34 (18)
O2—C11—C10	119.36 (16)	N2—C26—H26A	108.9
C4—C11—C10	118.15 (15)	C27—C26—H26A	108.9
C13—C12—C9	120.4 (2)	N2—C26—H26B	108.9
C13—C12—H12	119.8	C27—C26—H26B	108.9
C9—C12—H12	119.8	H26A—C26—H26B	107.7
C12—C13—C14	120.4 (2)	C28—C27—C26	126.6 (2)
C12—C13—H13	119.8	C28—C27—H27	116.7
C14—C13—H13	119.8	C26—C27—H27	116.7
C13—C14—C15	120.2 (2)	C27—C28—H28A	120.0
C13—C14—H14	119.9	C27—C28—H28B	120.0
C15—C14—H14	119.9	H28A—C28—H28B	120.0
C14—C15—C10	120.0 (2)	C1—N1—C3	109.62 (14)
C14—C15—H15	120.0	C1—N1—C16	117.89 (14)
C10—C15—H15	120.0	C3—N1—C16	131.04 (15)
N1—C16—C17	112.46 (14)	C1—N2—C2	109.85 (15)
N1—C16—H16A	109.1	C1—N2—C26	122.97 (16)
C17—C16—H16A	109.1	C2—N2—C26	126.32 (16)
N1—C16—H16B	109.1	C19—N3—O4	109.50 (14)
C17—C16—H16B	109.1	O6—N4—O5	123.0 (2)
H16A—C16—H16B	107.8	O6—N4—C23	118.8 (2)
O4—C17—C16	108.55 (14)	O5—N4—C23	118.2 (2)
O4—C17—C18	104.60 (14)	N3—O4—C17	107.87 (12)
C16—C17—C18	111.04 (15)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1^{i}	0.93	2.60	3.516 (2)	169
C18—H18B···O2^{ii}	0.97	2.37	3.333 (2)	170
C26—H26B···O1^{i}	0.97	2.55	3.379 (3)	144
C16—H16A···O2	0.97	2.10	2.902 (2)	141

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

Fig. 1

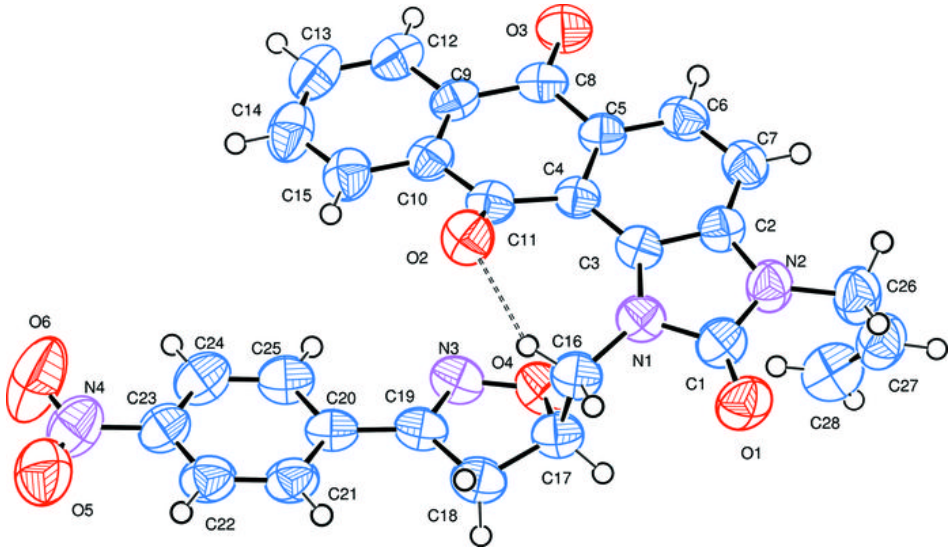
C13
C12
O3
C9
C8
C14
C5
C6
C7
C4
C15
C10
C11
C2
O2
C3
N2
C26
O6
C24
C25
N3
O4
C16
N1
C1
C27
N4
C23
C20
C19
C28
O1
O5
C22
C21
C18
C17

Fig. 2