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Benzyl 4-ethyl-3-methyl-5-(phthalimidomethyl)pyrrole-2-carboxylate

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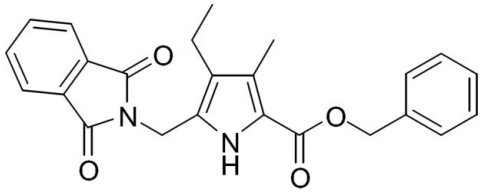
Key indicators: single-crystal X-ray study; T = 130 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.118; data-to-parameter ratio = 16.7.

The title compound, $C_{24}H_{22}N_2O_4$, forms weak inter- and intramolecular N—H···O hydrogen bonds. Additional intermolecular C—H···O interactions give rise to a three-dimensional network in the crystal structure.

Related literature

For related literature, see: Senge (2000, 2005); Senge & Smith (2005). The compound was prepared as described by Terry *et al.* (1965) and Kenner *et al.* (1977); crystals were handled as described by Hope (1994). The hydrogen-bonding analysis followed the criteria set out by Steiner (1997).



Experimental

Crystal data

$C_{24}H_{22}N_2O_4$
M_r = 402.44
Monoclinic, $P2_1/c$
a = 19.322 (6) Å
b = 7.482 (4) Å
c = 14.104 (3) Å
β = 98.27 (2)°
V = 2017.8 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 130 (2) K
0.50 × 0.44 × 0.40 mm

Data collection

Siemens $R3m/V$ diffractometer
Absorption correction: none
5193 measured reflections
4631 independent reflections
3592 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
2 standard reflections
every 198 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.118
S = 1.01
4631 reflections
277 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.851 (18)	2.506 (17)	3.0130 (18)	119.1 (15)
N1—H1···O2^{i}	0.851 (18)	2.520 (19)	3.201 (2)	137.8 (15)
C24—H24···O3^{ii}	0.95	2.48	3.293 (2)	144
C27—H27···O1^{iii}	0.95	2.30	3.193 (2)	157
C41—H41A···O4	0.98	2.56	2.979 (2)	106
C52—H52A···O2^{iv}	0.99	2.40	3.3857 (19)	175

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

Data collection: *P3/PC* (Siemens, 1995*a*); cell refinement: *P3/PC*; data reduction: *XDISK* (Siemens, 1995*b*); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1995*b*); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2022).

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supplementary materials

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Benzyl 4-ethyl-3-methyl-5-(phthalimidomethyl)pyrrole-2-carboxylate

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Comment

In continuation of studies on the hydrogen bonding pattern in pyrroles (Senge & Smith, 2005), dipyrromethanes (Senge, 2005) and porphyrins (Senge, 2000) the title compound was investigated for N–H···O and C–H···O interactions using the criteria put forward by Steiner (1997).

The structure is characterized by an intramolecular hydrogen bond between the pyrrole hydrogen and O1 from the phthalimido group [N1–H1···O1, 2.506 (17) Å, 119.1 (15)°]. The pyrrole hydrogen atom is also involved in intermolecular hydrogen bond, which is formed with the carbonyl oxygen atom (O2) of the phthalimido group not involved in the intramolecular hydrogen bond [N1–H1···O2, 2.520 (19) Å, 137.8 (15)°]. As indicated by their bond lenghts, both hydrogen bonds are relatively weak. The phthalimido group also participates in C–H···O interactions. Atom O1 is in close contact with an aromatic C–H unit [C27–H27···O1 = 2.30 (2) Å], while O2 is in close contact to an aliphatic CH_2-group [C52–H52···O2 = 2.40 (2) Å]. The benzylic ester group is only involved in a contact to another aromatic C–H unit [C24–H24···O3 = 2.48 (2) Å]. Thus, arrangement of the molecules in the crystal is dominated by intermolecular contacts involving the phthalimido groups. These arrange in parallel layers with the benzylester groups forming an outer rim of this ladder-type arrangement.

Experimental

Crystals were handled as described by Hope (1994). The compound was prepared as described by Terry *et al.* (1965) and Kenner *et al.* (1977) and was crystallized from CH_2Cl_2/*n*-hexane.

Refinement

H atoms were mostly placed in geometrically idealized positions and constrained to ride on their parent atoms with C–H distances in the range of 0.95–1.00 Å and U_{iso} (H) = 1.2 U_{eq} (C) for CH– and CH_2-groups and U_{iso} (H) = 1.5 U_{eq} (C) for methyl groups. The pyrrole hydrogen atom was refined with isotropic thermal parameters.

Figures

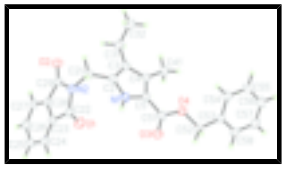

Fig. 1. The molecular structure and numbering scheme of title compound. Displacement ellipsoids for the non-hydrogen atoms are drawn at the 50% probability level.

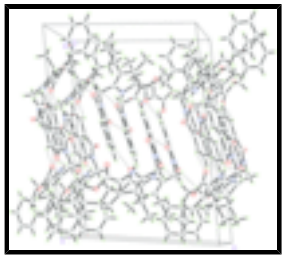

Fig. 2. View of the molecular arrangement in the crystal (down *b* axis). Dashed lines indicate indicate intermolecular C–H···O and N–H···O contacts.

Benzyl 4-ethyl-3-methyl-5-(phthalimidomethyl)pyrrole-2-carboxylate

Crystal data

$C_{24}H_{22}N_2O_4$	F_{000} = 848
M_r = 402.44	D_x = 1.325 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 33 reflections
a = 19.322 (6) Å	θ = 19–23º
b = 7.482 (4) Å	μ = 0.09 mm^{-1}
c = 14.104 (3) Å	*T* = 130 (2) K
β = 98.27 (2)º	Block, colorless
V = 2017.8 (13) Å^3	0.50 × 0.44 × 0.40 mm
Z = 4	

Data collection

Siemens R3m/V diffractometer	R_{int} = 0.037
Radiation source: fine-focus sealed tube	θ_{max} = 27.5º
Monochromator: graphite	θ_{min} = 2.1º
T = 130(2) K	*h* = −25→24
ω scans	*k* = 0→9
Absorption correction: none	*l* = 0→18
5193 measured reflections	2 standard reflections
4631 independent reflections	every 198 reflections
3592 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.044	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.118	$w = 1/[\sigma^2(F_o^2) + (0.0622P)^2 + 0.3895P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.002

4631 reflections	$\Delta\rho_{max} = 0.27$ e Å^{-3}
277 parameters	$\Delta\rho_{min} = -0.22$ 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 $F^2 > 2\sigma(F^2)$ 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}
N1	0.30261 (6)	0.37224 (17)	0.56068 (8)	0.0268 (3)
H1	0.3356 (9)	0.439 (3)	0.5864 (13)	0.042 (5)*
C2	0.28084 (7)	0.21436 (19)	0.59395 (10)	0.0278 (3)
C3	0.22269 (7)	0.15625 (19)	0.53190 (10)	0.0279 (3)
C4	0.20900 (7)	0.28679 (19)	0.45834 (10)	0.0267 (3)
C5	0.25936 (7)	0.41963 (19)	0.47815 (10)	0.0261 (3)
N2	0.38371 (6)	0.04176 (16)	0.66530 (8)	0.0278 (3)
C21	0.31864 (7)	0.1282 (2)	0.68238 (10)	0.0308 (3)
H21A	0.3294	0.2200	0.7329	0.037*
H21B	0.2877	0.0380	0.7059	0.037*
C22	0.44372 (7)	0.1384 (2)	0.65426 (9)	0.0274 (3)
C23	0.49587 (7)	0.00499 (19)	0.63188 (9)	0.0261 (3)
C24	0.56346 (7)	0.0286 (2)	0.61316 (10)	0.0314 (3)
H24	0.5846	0.1434	0.6157	0.038*
C25	0.59925 (7)	−0.1239 (2)	0.59037 (11)	0.0347 (3)
H25	0.6459	−0.1129	0.5773	0.042*
C26	0.56792 (8)	−0.2915 (2)	0.58645 (11)	0.0336 (3)
H26	0.5934	−0.3927	0.5701	0.040*
C27	0.49967 (8)	−0.3138 (2)	0.60609 (10)	0.0305 (3)
H27	0.4782	−0.4282	0.6038	0.037*
C28	0.46492 (7)	−0.16269 (19)	0.62892 (9)	0.0255 (3)
C29	0.39265 (7)	−0.14212 (19)	0.65286 (10)	0.0266 (3)
O1	0.44822 (6)	0.29938 (14)	0.66130 (7)	0.0349 (3)
O2	0.34920 (5)	−0.25493 (15)	0.66160 (8)	0.0352 (3)
C31	0.18076 (8)	−0.0095 (2)	0.54301 (11)	0.0333 (3)
H31A	0.2102	−0.0952	0.5844	0.040*
H31B	0.1682	−0.0659	0.4794	0.040*
C32	0.11410 (9)	0.0258 (3)	0.58610 (14)	0.0481 (4)

H32A	0.1261	0.0807	0.6494	0.072*
H32B	0.0896	−0.0873	0.5924	0.072*
H32C	0.0838	0.1068	0.5442	0.072*
C41	0.15170 (8)	0.2780 (2)	0.37443 (11)	0.0352 (3)
H41A	0.1266	0.3922	0.3680	0.053*
H41B	0.1191	0.1820	0.3846	0.053*
H41C	0.1720	0.2541	0.3159	0.053*
C51	0.27361 (7)	0.5849 (2)	0.43034 (10)	0.0274 (3)
C52	0.22978 (7)	0.7991 (2)	0.31376 (10)	0.0289 (3)
H52A	0.2669	0.7876	0.2726	0.035*
H52B	0.2435	0.8941	0.3616	0.035*
C53	0.16146 (7)	0.84587 (19)	0.25394 (10)	0.0265 (3)
C54	0.09744 (7)	0.8122 (2)	0.28520 (11)	0.0327 (3)
H54	0.0963	0.7523	0.3443	0.039*
C55	0.03544 (8)	0.8655 (2)	0.23054 (12)	0.0396 (4)
H55	−0.0080	0.8423	0.2523	0.047*
C56	0.03679 (9)	0.9526 (2)	0.14419 (13)	0.0433 (4)
H56	−0.0056	0.9900	0.1069	0.052*
C57	0.09977 (9)	0.9850 (2)	0.11242 (12)	0.0407 (4)
H57	0.1006	1.0440	0.0529	0.049*
C58	0.16192 (8)	0.9320 (2)	0.16687 (11)	0.0318 (3)
H58	0.2051	0.9548	0.1444	0.038*
O3	0.32659 (5)	0.67202 (16)	0.44929 (8)	0.0395 (3)
O4	0.22085 (5)	0.63129 (14)	0.36163 (7)	0.0312 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0231 (6)	0.0301 (6)	0.0275 (6)	0.0005 (5)	0.0049 (5)	0.0009 (5)
C2	0.0278 (7)	0.0286 (7)	0.0284 (7)	0.0044 (6)	0.0094 (5)	0.0017 (6)
C3	0.0277 (7)	0.0272 (7)	0.0299 (7)	0.0033 (6)	0.0078 (5)	−0.0012 (6)
C4	0.0255 (6)	0.0267 (7)	0.0286 (7)	0.0027 (5)	0.0062 (5)	−0.0014 (6)
C5	0.0232 (6)	0.0287 (7)	0.0274 (7)	0.0030 (5)	0.0062 (5)	0.0009 (6)
N2	0.0267 (6)	0.0274 (6)	0.0290 (6)	0.0006 (5)	0.0034 (5)	0.0037 (5)
C21	0.0318 (7)	0.0352 (8)	0.0265 (7)	0.0049 (6)	0.0081 (6)	0.0032 (6)
C22	0.0318 (7)	0.0287 (7)	0.0205 (6)	−0.0024 (6)	0.0003 (5)	0.0046 (5)
C23	0.0267 (7)	0.0283 (7)	0.0221 (6)	−0.0020 (5)	−0.0001 (5)	0.0036 (5)
C24	0.0292 (7)	0.0352 (8)	0.0289 (7)	−0.0073 (6)	0.0010 (6)	0.0044 (6)
C25	0.0240 (7)	0.0480 (9)	0.0320 (7)	−0.0011 (6)	0.0039 (6)	0.0046 (7)
C26	0.0324 (7)	0.0374 (9)	0.0310 (7)	0.0076 (6)	0.0048 (6)	0.0028 (6)
C27	0.0339 (7)	0.0282 (7)	0.0295 (7)	−0.0005 (6)	0.0047 (6)	0.0023 (6)
C28	0.0258 (6)	0.0272 (7)	0.0231 (6)	−0.0022 (5)	0.0018 (5)	0.0053 (5)
C29	0.0274 (7)	0.0287 (7)	0.0236 (6)	−0.0009 (6)	0.0029 (5)	0.0034 (5)
O1	0.0457 (6)	0.0233 (5)	0.0349 (6)	−0.0034 (4)	0.0031 (5)	0.0017 (4)
O2	0.0331 (5)	0.0338 (6)	0.0406 (6)	−0.0086 (5)	0.0116 (5)	0.0004 (5)
C31	0.0373 (8)	0.0264 (8)	0.0362 (8)	0.0001 (6)	0.0056 (6)	0.0016 (6)
C32	0.0444 (10)	0.0386 (10)	0.0652 (12)	−0.0061 (8)	0.0209 (9)	0.0044 (9)
C41	0.0363 (8)	0.0313 (8)	0.0355 (8)	−0.0032 (6)	−0.0030 (6)	0.0001 (6)

C51	0.0251 (6)	0.0312 (8)	0.0267 (7)	0.0016 (6)	0.0069 (5)	−0.0002 (6)
C52	0.0281 (7)	0.0280 (7)	0.0314 (7)	−0.0037 (6)	0.0072 (6)	0.0039 (6)
C53	0.0294 (7)	0.0219 (7)	0.0292 (7)	−0.0010 (5)	0.0074 (5)	−0.0012 (5)
C54	0.0312 (7)	0.0357 (8)	0.0324 (7)	0.0006 (6)	0.0089 (6)	0.0035 (6)
C55	0.0278 (7)	0.0466 (10)	0.0450 (9)	0.0006 (7)	0.0077 (6)	−0.0003 (8)
C56	0.0367 (8)	0.0424 (10)	0.0479 (9)	0.0064 (7)	−0.0035 (7)	0.0073 (8)
C57	0.0473 (9)	0.0357 (9)	0.0378 (8)	−0.0018 (7)	0.0020 (7)	0.0125 (7)
C58	0.0347 (7)	0.0286 (8)	0.0331 (7)	−0.0038 (6)	0.0088 (6)	0.0035 (6)
O3	0.0293 (5)	0.0459 (7)	0.0421 (6)	−0.0093 (5)	0.0011 (5)	0.0114 (5)
O4	0.0287 (5)	0.0280 (5)	0.0355 (5)	−0.0026 (4)	−0.0002 (4)	0.0060 (4)

Geometric parameters (Å, °)

N1—C2	1.3599 (19)	C29—O2	1.2093 (17)
N1—C5	1.3781 (18)	C31—C32	1.524 (2)
N1—H1	0.851 (18)	C31—H31A	0.9900
C2—C3	1.391 (2)	C31—H31B	0.9900
C2—C21	1.498 (2)	C32—H32A	0.9800
C3—C4	1.422 (2)	C32—H32B	0.9800
C3—C31	1.502 (2)	C32—H32C	0.9800
C4—C5	1.391 (2)	C41—H41A	0.9800
C4—C41	1.501 (2)	C41—H41B	0.9800
C5—C51	1.453 (2)	C41—H41C	0.9800
N2—C22	1.3942 (18)	C51—O3	1.2107 (17)
N2—C29	1.401 (2)	C51—O4	1.3471 (17)
N2—C21	1.4643 (18)	C52—O4	1.4475 (18)
C21—H21A	0.9900	C52—C53	1.502 (2)
C21—H21B	0.9900	C52—H52A	0.9900
C22—O1	1.2106 (19)	C52—H52B	0.9900
C22—C23	1.484 (2)	C53—C58	1.388 (2)
C23—C24	1.380 (2)	C53—C54	1.395 (2)
C23—C28	1.388 (2)	C54—C55	1.387 (2)
C24—C25	1.395 (2)	C54—H54	0.9500
C24—H24	0.9500	C55—C56	1.385 (2)
C25—C26	1.390 (2)	C55—H55	0.9500
C25—H25	0.9500	C56—C57	1.377 (2)
C26—C27	1.396 (2)	C56—H56	0.9500
C26—H26	0.9500	C57—C58	1.387 (2)
C27—C28	1.376 (2)	C57—H57	0.9500
C27—H27	0.9500	C58—H58	0.9500
C28—C29	1.4910 (19)		
C2—N1—C5	109.57 (12)	N2—C29—C28	105.44 (11)
C2—N1—H1	127.9 (12)	C3—C31—C32	113.44 (13)
C5—N1—H1	122.4 (13)	C3—C31—H31A	108.9
N1—C2—C3	108.45 (12)	C32—C31—H31A	108.9
N1—C2—C21	121.55 (13)	C3—C31—H31B	108.9
C3—C2—C21	129.98 (14)	C32—C31—H31B	108.9
C2—C3—C4	107.04 (13)	H31A—C31—H31B	107.7
C2—C3—C31	126.27 (13)	C31—C32—H32A	109.5

C4—C3—C31	126.64 (13)	C31—C32—H32B	109.5
C5—C4—C3	107.04 (13)	H32A—C32—H32B	109.5
C5—C4—C41	127.23 (13)	C31—C32—H32C	109.5
C3—C4—C41	125.72 (13)	H32A—C32—H32C	109.5
N1—C5—C4	107.91 (13)	H32B—C32—H32C	109.5
N1—C5—C51	118.59 (12)	C4—C41—H41A	109.5
C4—C5—C51	133.50 (13)	C4—C41—H41B	109.5
C22—N2—C29	112.07 (12)	H41A—C41—H41B	109.5
C22—N2—C21	122.48 (13)	C4—C41—H41C	109.5
C29—N2—C21	125.36 (12)	H41A—C41—H41C	109.5
N2—C21—C2	112.37 (11)	H41B—C41—H41C	109.5
N2—C21—H21A	109.1	O3—C51—O4	123.25 (13)
C2—C21—H21A	109.1	O3—C51—C5	124.48 (13)
N2—C21—H21B	109.1	O4—C51—C5	112.26 (12)
C2—C21—H21B	109.1	O4—C52—C53	108.05 (11)
H21A—C21—H21B	107.9	O4—C52—H52A	110.1
O1—C22—N2	123.91 (14)	C53—C52—H52A	110.1
O1—C22—C23	130.06 (14)	O4—C52—H52B	110.1
N2—C22—C23	106.02 (12)	C53—C52—H52B	110.1
C24—C23—C28	121.69 (14)	H52A—C52—H52B	108.4
C24—C23—C22	130.13 (14)	C58—C53—C54	118.85 (13)
C28—C23—C22	108.15 (12)	C58—C53—C52	119.22 (13)
C23—C24—C25	116.95 (14)	C54—C53—C52	121.87 (13)
C23—C24—H24	121.5	C55—C54—C53	120.45 (14)
C25—C24—H24	121.5	C55—C54—H54	119.8
C26—C25—C24	121.29 (14)	C53—C54—H54	119.8
C26—C25—H25	119.4	C56—C55—C54	120.01 (15)
C24—C25—H25	119.4	C56—C55—H55	120.0
C25—C26—C27	121.21 (15)	C54—C55—H55	120.0
C25—C26—H26	119.4	C57—C56—C55	119.88 (15)
C27—C26—H26	119.4	C57—C56—H56	120.1
C28—C27—C26	117.06 (14)	C55—C56—H56	120.1
C28—C27—H27	121.5	C56—C57—C58	120.30 (15)
C26—C27—H27	121.5	C56—C57—H57	119.9
C27—C28—C23	121.79 (13)	C58—C57—H57	119.9
C27—C28—C29	129.94 (13)	C57—C58—C53	120.50 (14)
C23—C28—C29	108.27 (12)	C57—C58—H58	119.8
O2—C29—N2	124.94 (13)	C53—C58—H58	119.8
O2—C29—C28	129.62 (14)	C51—O4—C52	115.49 (11)
C5—N1—C2—C3	0.47 (15)	C26—C27—C28—C23	0.4 (2)
C5—N1—C2—C21	179.14 (12)	C26—C27—C28—C29	179.78 (13)
N1—C2—C3—C4	−0.34 (15)	C24—C23—C28—C27	−0.8 (2)
C21—C2—C3—C4	−178.86 (13)	C22—C23—C28—C27	177.52 (12)
N1—C2—C3—C31	−178.12 (13)	C24—C23—C28—C29	179.70 (12)
C21—C2—C3—C31	3.4 (2)	C22—C23—C28—C29	−2.01 (14)
C2—C3—C4—C5	0.08 (15)	C22—N2—C29—O2	177.65 (13)
C31—C3—C4—C5	177.86 (13)	C21—N2—C29—O2	−5.7 (2)
C2—C3—C4—C41	178.76 (13)	C22—N2—C29—C28	−1.69 (15)
C31—C3—C4—C41	−3.5 (2)	C21—N2—C29—C28	174.93 (11)

C2—N1—C5—C4	−0.42 (15)	C27—C28—C29—O2	3.5 (2)
C2—N1—C5—C51	−179.78 (12)	C23—C28—C29—O2	−177.01 (14)
C3—C4—C5—N1	0.20 (15)	C27—C28—C29—N2	−177.20 (14)
C41—C4—C5—N1	−178.45 (13)	C23—C28—C29—N2	2.28 (15)
C3—C4—C5—C51	179.43 (14)	C2—C3—C31—C32	98.71 (18)
C41—C4—C5—C51	0.8 (3)	C4—C3—C31—C32	−78.65 (19)
C22—N2—C21—C2	74.63 (17)	N1—C5—C51—O3	11.4 (2)
C29—N2—C21—C2	−101.66 (16)	C4—C5—C51—O3	−167.77 (15)
N1—C2—C21—N2	−76.22 (17)	N1—C5—C51—O4	−168.68 (12)
C3—C2—C21—N2	102.13 (17)	C4—C5—C51—O4	12.2 (2)
C29—N2—C22—O1	179.62 (13)	O4—C52—C53—C58	−145.08 (13)
C21—N2—C22—O1	2.9 (2)	O4—C52—C53—C54	37.72 (18)
C29—N2—C22—C23	0.50 (15)	C58—C53—C54—C55	−0.6 (2)
C21—N2—C22—C23	−176.23 (11)	C52—C53—C54—C55	176.57 (15)
O1—C22—C23—C24	0.0 (2)	C53—C54—C55—C56	0.1 (3)
N2—C22—C23—C24	179.09 (13)	C54—C55—C56—C57	0.5 (3)
O1—C22—C23—C28	−178.05 (14)	C55—C56—C57—C58	−0.5 (3)
N2—C22—C23—C28	0.99 (14)	C56—C57—C58—C53	−0.1 (3)
C28—C23—C24—C25	0.5 (2)	C54—C53—C58—C57	0.6 (2)
C22—C23—C24—C25	−177.42 (13)	C52—C53—C58—C57	−176.68 (14)
C23—C24—C25—C26	0.2 (2)	O3—C51—O4—C52	−2.8 (2)
C24—C25—C26—C27	−0.6 (2)	C5—C51—O4—C52	177.22 (11)
C25—C26—C27—C28	0.3 (2)	C53—C52—O4—C51	−169.44 (11)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.851 (18)	2.506 (17)	3.0130 (18)	119.1 (15)
N1—H1···O2^{i}	0.851 (18)	2.520 (19)	3.201 (2)	137.8 (15)
C24—H24···O3^{ii}	0.95	2.48	3.293 (2)	144
C27—H27···O1^{iii}	0.95	2.30	3.193 (2)	157
C41—H41A···O4	0.98	2.56	2.979 (2)	106
C52—H52A···O2^{iv}	0.99	2.40	3.3857 (19)	175

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

Fig. 1

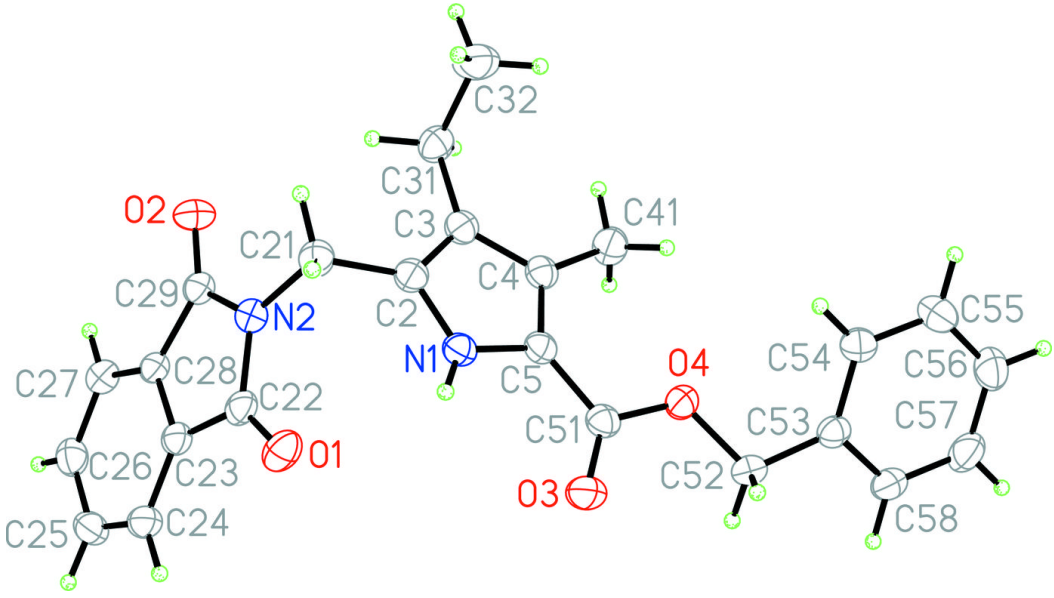
C32
C31
O2
C3
C41
C21
C4
C29
N2
C2
C55
C54
C56
C27
C28
N1
C5
O4
C22
C51
C53
C57
O1
C26
C23
O3
C52
C25
C24
C58

Fig. 2