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(*R**)-1-Benzyl-3-(2-hydroxyphenyl)indoline-2-one

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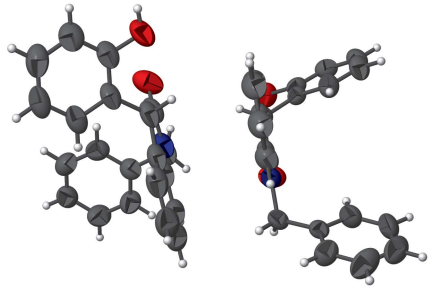
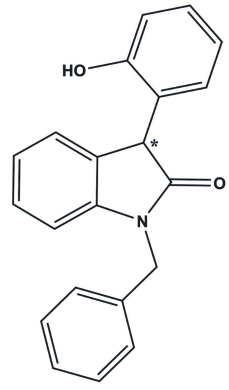
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{21}H_{17}NO_2$, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. The indoline ring system is almost planar in both molecules (r.m.s. deviations = 0.020 and 0.024 Å for molecules *A* and *B*, respectively). The benzyl and phenol rings are inclined to the indole ring system by 80.39 (12) and 68.39 (12)° in molecule *A*, and by 79.90 (13) and 74.88 (10)° in molecule *B*. The aryl rings are inclined to one another by 33.30 (14) and 30.62 (14)° in molecules *A* and *B*, respectively. In the crystal, *A* molecules are linked by pairs of O—H···O hydrogen bonds, forming inversion dimers. The same situation is observed for the *B* molecules and both sets of inversion dimers enclose $R_2^2(14)$ ring motifs. These dimers stack along the *a*-axis direction and are linked by offset π–π interactions [intercentroid distance = 3.6802 (13) Å] involving *A* and *B* indole ring systems, forming layers parallel to the *ab* plane.

3D view



Chemical scheme



Structure description

Isatin is a starting material for the synthesis of a number of organic compounds (Hajare & Chavan, 2014). Isatin and its metabolites are constituents of many natural substances (Medvedev *et al.*, 2007). It is found in humans and acts as a metabolic derivative of adrenaline (Sonawane & Tripathi, 2013). It exhibits endogamous activity in mammals (Chaudhary *et al.*, 2013) and has shown cardioinhibitory effects on a frog's heart, and hypotensive, respiratory depression and antidiuretic effects (Pandeya *et al.*, 2005). Isatin also possess anticancer (Khan *et al.*, 2015), antioxidant (Sammaiah & Pragathi, 2014), antiviral (Gomathi *et al.*, 2013), antimicrobial (Saxena *et al.*, 2015), analgesic (Pal *et al.*, 201), anti-inflammatory (Hajare & Chinchole, 2013), antitubercular (Aboul-fadl & Bin-Jubair, 2010), anticonvulsant (Raj, 2012) and antianxiety (Grewal, 2014) activities.

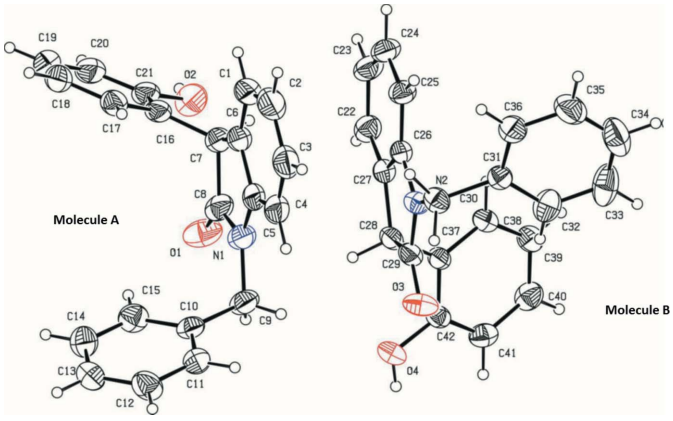


Figure 1
The molecular structure of the two independent molecules (*A* and *B*) of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

The title compound, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit (Fig. 1). The indoline ring system is nearly planar in both molecules, the largest deviation from the mean plane being 0.042 (2) Å for atom C7 in molecule *A* and 0.080 (2) Å for atom O3 in molecule *B*. The dihedral angle between the isatin group and the phenol and benzyl rings are, respectively, 68.39 (12) and 80.39 (12)° for molecule *A* and 74.88 (10) and 79.90 (13)° for molecule *B*. The dihedral angle between the aryl rings is 33.30 (14)° for molecule *A* and 30.62 (14)° for molecule *B*.

In the crystal, the *A* molecules are linked by pairs of O—H···O hydrogen bonds, forming *A*–*A* inversion dimers. Likewise, the *B* molecules are also linked by a pair of O—H···O hydrogen bonds, forming *B*–*B* inversion dimers (see Table 1 and Fig. 2). Both dimers enclose $R_2^2(14)$ ring motifs. These dimers stack along the *a*-axis direction and are linked by offset π–π interactions, involving *A* and *B* indole ring systems (Fig. 3), forming layers parallel to the *ab* plane [$Cg1\cdots Cg2^{i}$ = 3.743 (1) Å, interplanar distance = 3.557 (1) Å, *Cg*1 and *Cg*2 are the centroids of the indole rings N1/C5–C8 and N2/C26–C29, respectively; symmetry code: (i) *x*, *y*, *z*].

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.82	1.93	2.721 (3)	160
O4—H4···O3^{ii}	0.82	1.95	2.735 (3)	160

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{17}NO_2$
M_r	315.36
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, *b*, *c* (Å)	11.1344 (6), 12.0889 (5), 12.4679 (6)
α, β, γ (°)	89.171 (3), 79.125 (3), 84.202 (3)
V (Å^3)	1639.62 (14)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.08
Crystal size (mm)	0.35 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.972, 0.984
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26691, 5763, 3525
R_{int}	0.035
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.053, 0.197, 1.02
No. of reflections	5763
No. of parameters	433
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.39, −0.20

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *SHELXL2016* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

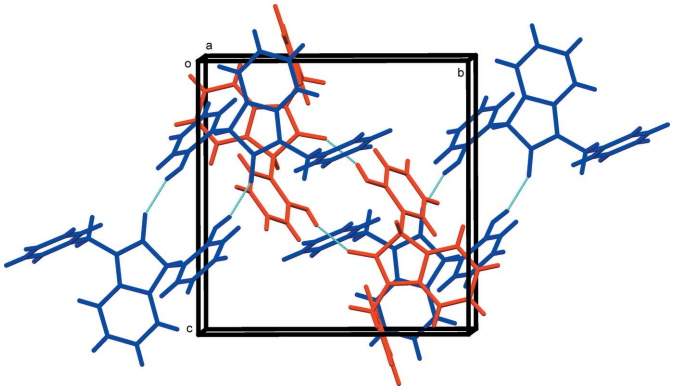


Figure 2
A partial view along the *a* axis of the crystal packing of the title compound, showing the formation of the O—H···O hydrogen-bonded *A*–*A* (blue) and *B*–*B* (red) inversion dimers (see Table 1; hydrogen bonds are shown as dashed lines).

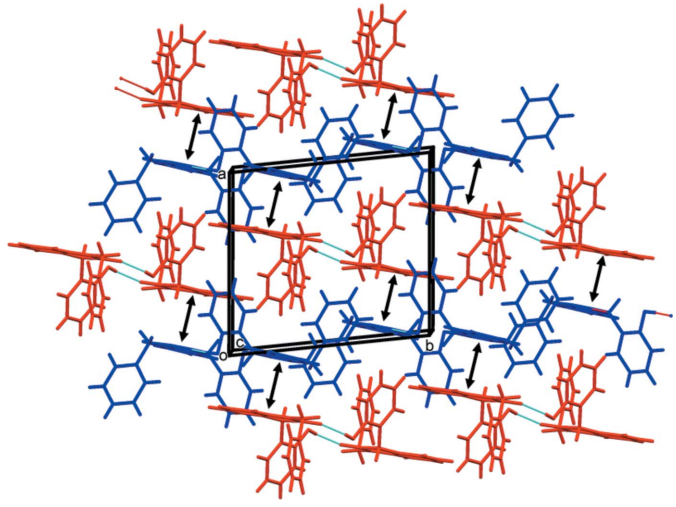


Figure 3
A view along the *c* axis of the crystal packing of the title compound. The π–π interactions are shown as double black arrows and the hydrogen bonds as dashed lines (see Table 1; colour code: *A* molecules blue, *B* molecule red).

Synthesis and crystallization

An isatin-based MBH of adduct 1-benzyl-3-hydroxy-3-(6-oxocyclohex-1-en-1-yl)indolin-2-one (200 mg, 0.5 mmol, 1.0 equiv.) in 15 ml of dry dichloromethane was deposited dropwise in a flame-dried round-bottom flask equipped with a magnetic stirring bar and the solution was stirred vigorously to obtain a homogenous mixture. The resulting solution was purged with nitrogen gas for 15 min. Trifluoroacetic anhydride (0.06 ml, 0.12 mmol, and 1.5 equiv) was added dropwise to the reaction mixture and then dimethylaminopyridine (20 mg, 30 mol %) was added dropwise at 273 K. The reaction mixture was gradually brought to room temperature and stirred for a further 5 h. After completion of the reaction (monitored by TLC), the mixture was diluted with CH_2Cl_2 and the organic layer was washed sequentially with 2 *N* HCl solution, H_2O, and brine, then dried over Na_2SO_4, filtered and concentrated under reduced pressure. It was then purified by silica gel column chromatography using hexane: EtOAc (8:2) as eluent and afforded the title compound. Colourless block-like crystals were obtained by slow evaporation of a solution in CH_2Cl_2:acetonitrile (1:1, *v*/*v*).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

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Crystal data

$C_{21}H_{17}NO_2$
M_r = 315.36
Triclinic, $P\overline{1}$
a = 11.1344 (6) Å
b = 12.0889 (5) Å
c = 12.4679 (6) Å
α = 89.171 (3)°
β = 79.125 (3)°
γ = 84.202 (3)°
V = 1639.62 (14) Å^3
Z = 4
$F(000)$ = 664
D_x = 1.278 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8113 reflections
θ = 2.4–25.7°
μ = 0.08 mm^{-1}
T = 296 K
Block, colourless
0.35 × 0.25 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: sealed tube
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.972, T_{max} = 0.984
26691 measured reflections
5763 independent reflections
3525 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −13→13
k = −14→14
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.197
S = 1.02
5763 reflections
433 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1204P)^2 + 0.1554P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O4	0.46387 (17)	0.61250 (15)	0.44690 (15)	0.0685 (5)
H4	0.492150	0.577156	0.390610	0.103*
N2	0.38028 (18)	0.69335 (16)	0.82332 (15)	0.0503 (5)
O3	0.43219 (19)	0.54674 (15)	0.70547 (15)	0.0718 (6)
C26	0.3491 (2)	0.80907 (19)	0.8179 (2)	0.0484 (6)
C37	0.5165 (2)	0.74505 (18)	0.56209 (18)	0.0456 (6)
C28	0.3937 (2)	0.73869 (19)	0.63812 (19)	0.0494 (6)
H28	0.330556	0.724990	0.596145	0.059*
C27	0.3521 (2)	0.8390 (2)	0.7102 (2)	0.0501 (6)
C42	0.5483 (2)	0.67851 (19)	0.46908 (19)	0.0489 (6)
C29	0.4045 (2)	0.6465 (2)	0.7224 (2)	0.0522 (6)
C31	0.4977 (2)	0.65051 (19)	0.97035 (19)	0.0486 (6)
C41	0.6625 (3)	0.6816 (2)	0.4024 (2)	0.0590 (7)
H41	0.684161	0.636726	0.340486	0.071*
C5	0.0533 (2)	0.7082 (2)	0.8208 (3)	0.0636 (7)
O1	0.0392 (2)	0.80217 (16)	0.5609 (2)	0.0898 (7)
O2	−0.00597 (18)	1.06347 (16)	0.61019 (19)	0.0867 (7)
H2	−0.016343	1.115971	0.569435	0.130*
C30	0.3871 (2)	0.6317 (2)	0.9235 (2)	0.0550 (6)
H30A	0.388706	0.552929	0.908650	0.066*
H30B	0.313738	0.653266	0.977235	0.066*
C10	−0.0150 (2)	0.5262 (2)	0.6615 (2)	0.0570 (7)
C16	−0.1160 (2)	0.9517 (2)	0.7407 (2)	0.0609 (7)
N1	0.0688 (2)	0.69565 (18)	0.7074 (2)	0.0666 (6)
C25	0.3207 (2)	0.8848 (2)	0.9022 (2)	0.0591 (7)
H25	0.319239	0.862822	0.974243	0.071*
C21	−0.1169 (3)	1.0392 (2)	0.6678 (2)	0.0667 (8)
C38	0.6004 (2)	0.8135 (2)	0.5845 (2)	0.0580 (7)
H38	0.579726	0.858638	0.646359	0.070*
C8	0.0386 (2)	0.7933 (2)	0.6585 (3)	0.0689 (8)
C40	0.7439 (3)	0.7510 (2)	0.4276 (2)	0.0677 (8)
H40	0.820268	0.752820	0.382363	0.081*
C7	0.0038 (2)	0.8830 (2)	0.7478 (2)	0.0648 (7)
H7	0.068746	0.933263	0.737248	0.078*
C22	0.3256 (2)	0.9492 (2)	0.6852 (2)	0.0632 (7)
H22	0.327328	0.971179	0.613131	0.076*
C24	0.2945 (3)	0.9949 (2)	0.8759 (3)	0.0694 (8)
H24	0.275422	1.048307	0.931109	0.083*
C11	−0.0165 (3)	0.4223 (2)	0.7062 (2)	0.0683 (8)
H11	0.051960	0.390760	0.732365	0.082*
C17	−0.2264 (3)	0.9277 (2)	0.8038 (2)	0.0690 (8)
H17	−0.227202	0.869856	0.853875	0.083*
C6	0.0122 (2)	0.8185 (2)	0.8486 (3)	0.0643 (7)
C39	0.7136 (3)	0.8171 (2)	0.5184 (2)	0.0672 (8)
H39	0.768729	0.864014	0.535308	0.081*

C13	−0.2193 (3)	0.4095 (3)	0.6766 (2)	0.0700 (8)
H13	−0.287695	0.370238	0.681014	0.084*
C18	−0.3357 (3)	0.9886 (3)	0.7934 (3)	0.0802 (9)
H18	−0.409399	0.972573	0.836734	0.096*
C1	−0.0093 (3)	0.8493 (3)	0.9580 (3)	0.0779 (9)
H1	−0.038062	0.922200	0.978999	0.093*
C36	0.4861 (3)	0.6869 (2)	1.0755 (2)	0.0718 (8)
H36	0.408038	0.702398	1.117624	0.086*
C2	0.0125 (3)	0.7706 (3)	1.0350 (3)	0.0879 (10)
H2A	−0.001137	0.790974	1.108236	0.106*
C20	−0.2257 (3)	1.0979 (2)	0.6558 (3)	0.0780 (9)
H20	−0.225973	1.154959	0.605021	0.094*
C23	0.2962 (3)	1.0267 (2)	0.7696 (3)	0.0726 (8)
H23	0.277373	1.101192	0.753898	0.087*
C4	0.0742 (3)	0.6298 (3)	0.8971 (3)	0.0727 (8)
H4A	0.101207	0.556516	0.876558	0.087*
C9	0.0963 (3)	0.5902 (2)	0.6491 (3)	0.0709 (8)
H9A	0.161286	0.545878	0.676735	0.085*
H9B	0.125575	0.603928	0.572233	0.085*
C3	0.0542 (3)	0.6621 (3)	1.0051 (3)	0.0835 (9)
H3	0.068983	0.610288	1.058122	0.100*
C19	−0.3343 (3)	1.0721 (3)	0.7191 (3)	0.0841 (10)
H19	−0.407784	1.112389	0.710997	0.101*
C32	0.6145 (3)	0.6286 (3)	0.9098 (3)	0.0751 (8)
H32	0.625252	0.603469	0.838144	0.090*
C15	−0.1186 (3)	0.5711 (2)	0.6259 (2)	0.0710 (8)
H15	−0.120036	0.642028	0.595998	0.085*
C12	−0.1174 (3)	0.3632 (2)	0.7134 (3)	0.0777 (9)
H12	−0.116115	0.292220	0.743091	0.093*
C14	−0.2197 (3)	0.5139 (3)	0.6335 (2)	0.0761 (8)
H14	−0.289045	0.546281	0.609107	0.091*
C35	0.5864 (4)	0.7011 (3)	1.1198 (3)	0.0973 (12)
H35	0.575943	0.725624	1.191677	0.117*
C33	0.7156 (3)	0.6440 (3)	0.9551 (4)	0.0982 (12)
H33	0.794259	0.629754	0.913735	0.118*
C34	0.7003 (4)	0.6798 (3)	1.0604 (5)	0.1030 (14)
H34	0.768506	0.689614	1.091063	0.124*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O4	0.0774 (13)	0.0655 (12)	0.0685 (12)	−0.0134 (10)	−0.0242 (10)	−0.0221 (9)
N2	0.0550 (12)	0.0461 (12)	0.0513 (12)	−0.0111 (9)	−0.0102 (10)	−0.0048 (9)
O3	0.1073 (16)	0.0436 (11)	0.0650 (12)	−0.0164 (10)	−0.0124 (10)	−0.0084 (8)
C26	0.0399 (13)	0.0483 (14)	0.0569 (15)	−0.0079 (10)	−0.0066 (11)	−0.0065 (11)
C37	0.0500 (14)	0.0419 (13)	0.0478 (13)	−0.0053 (10)	−0.0160 (11)	−0.0022 (10)
C28	0.0519 (14)	0.0496 (14)	0.0507 (14)	−0.0110 (11)	−0.0163 (11)	−0.0057 (11)
C27	0.0426 (13)	0.0500 (14)	0.0578 (15)	−0.0070 (10)	−0.0085 (11)	−0.0049 (11)

C42	0.0603 (16)	0.0421 (13)	0.0485 (14)	−0.0038 (11)	−0.0213 (12)	−0.0005 (11)
C29	0.0508 (15)	0.0493 (16)	0.0590 (15)	−0.0145 (11)	−0.0112 (12)	−0.0076 (12)
C31	0.0512 (15)	0.0418 (13)	0.0524 (14)	−0.0096 (10)	−0.0069 (12)	0.0047 (11)
C41	0.0724 (19)	0.0532 (15)	0.0485 (14)	0.0038 (13)	−0.0090 (13)	−0.0042 (11)
C5	0.0380 (14)	0.0608 (18)	0.092 (2)	−0.0133 (12)	−0.0069 (14)	−0.0085 (16)
O1	0.1099 (18)	0.0655 (13)	0.0787 (15)	−0.0053 (12)	0.0197 (13)	−0.0025 (11)
O2	0.0701 (14)	0.0613 (12)	0.1211 (18)	−0.0184 (10)	0.0067 (12)	0.0114 (12)
C30	0.0575 (15)	0.0558 (15)	0.0528 (14)	−0.0174 (12)	−0.0069 (12)	0.0029 (12)
C10	0.0591 (17)	0.0497 (15)	0.0562 (15)	0.0016 (12)	0.0018 (12)	−0.0111 (12)
C16	0.0520 (16)	0.0478 (15)	0.0802 (18)	−0.0153 (12)	0.0007 (13)	−0.0177 (13)
N1	0.0558 (14)	0.0536 (14)	0.0845 (17)	−0.0089 (10)	0.0041 (12)	−0.0108 (12)
C25	0.0572 (16)	0.0581 (16)	0.0578 (15)	−0.0057 (12)	0.0004 (12)	−0.0115 (12)
C21	0.0587 (18)	0.0454 (15)	0.092 (2)	−0.0123 (13)	0.0007 (15)	−0.0161 (14)
C38	0.0582 (16)	0.0567 (15)	0.0610 (16)	−0.0092 (12)	−0.0134 (13)	−0.0141 (12)
C8	0.0509 (17)	0.0581 (18)	0.088 (2)	−0.0095 (13)	0.0134 (15)	−0.0064 (16)
C40	0.0599 (17)	0.0609 (17)	0.0768 (19)	−0.0066 (14)	0.0011 (14)	0.0045 (15)
C7	0.0474 (15)	0.0502 (15)	0.093 (2)	−0.0155 (12)	0.0027 (14)	−0.0117 (15)
C22	0.0614 (17)	0.0571 (17)	0.0697 (17)	−0.0020 (13)	−0.0109 (14)	0.0022 (14)
C24	0.0649 (18)	0.0572 (17)	0.079 (2)	0.0022 (13)	0.0011 (15)	−0.0188 (15)
C11	0.0670 (18)	0.0516 (16)	0.088 (2)	0.0033 (13)	−0.0225 (16)	−0.0061 (14)
C17	0.0569 (18)	0.0725 (19)	0.0762 (19)	−0.0184 (15)	−0.0010 (15)	−0.0185 (15)
C6	0.0453 (15)	0.0583 (17)	0.088 (2)	−0.0143 (12)	−0.0031 (14)	−0.0142 (15)
C39	0.0580 (17)	0.0588 (17)	0.086 (2)	−0.0161 (13)	−0.0110 (15)	−0.0076 (15)
C13	0.073 (2)	0.075 (2)	0.0657 (17)	−0.0189 (16)	−0.0169 (15)	−0.0033 (15)
C18	0.0542 (19)	0.091 (2)	0.092 (2)	−0.0155 (17)	0.0013 (16)	−0.031 (2)
C1	0.0603 (19)	0.071 (2)	0.103 (3)	−0.0149 (15)	−0.0110 (17)	−0.0228 (19)
C36	0.073 (2)	0.079 (2)	0.0649 (18)	0.0019 (15)	−0.0204 (15)	−0.0119 (15)
C2	0.074 (2)	0.106 (3)	0.089 (2)	−0.0201 (19)	−0.0206 (18)	−0.012 (2)
C20	0.077 (2)	0.0543 (17)	0.102 (2)	−0.0088 (15)	−0.0115 (18)	−0.0159 (16)
C23	0.0681 (19)	0.0467 (16)	0.097 (2)	0.0043 (13)	−0.0051 (16)	−0.0072 (16)
C4	0.0515 (17)	0.0682 (19)	0.099 (2)	−0.0089 (14)	−0.0147 (16)	−0.0056 (18)
C9	0.0577 (17)	0.0554 (16)	0.090 (2)	−0.0020 (13)	0.0099 (15)	−0.0146 (15)
C3	0.063 (2)	0.091 (3)	0.101 (3)	−0.0152 (17)	−0.0232 (18)	0.001 (2)
C19	0.061 (2)	0.080 (2)	0.111 (3)	0.0014 (16)	−0.0157 (19)	−0.033 (2)
C32	0.0594 (19)	0.088 (2)	0.0713 (19)	−0.0060 (15)	0.0015 (15)	0.0098 (16)
C15	0.081 (2)	0.0563 (16)	0.0761 (19)	−0.0048 (15)	−0.0175 (16)	0.0079 (14)
C12	0.093 (2)	0.0561 (17)	0.092 (2)	−0.0187 (16)	−0.0321 (19)	0.0075 (16)
C14	0.074 (2)	0.082 (2)	0.0760 (19)	−0.0005 (16)	−0.0275 (16)	0.0025 (16)
C35	0.118 (3)	0.083 (2)	0.106 (3)	−0.001 (2)	−0.063 (3)	−0.015 (2)
C33	0.050 (2)	0.110 (3)	0.132 (3)	−0.0178 (18)	−0.008 (2)	0.042 (3)
C34	0.095 (3)	0.076 (2)	0.160 (4)	−0.031 (2)	−0.070 (3)	0.031 (3)

Geometric parameters (Å, º)

O4—C42	1.361 (3)	C40—H40	0.9300
O4—H4	0.8200	C7—C6	1.483 (4)
N2—C29	1.355 (3)	C7—H7	0.9800
N2—C26	1.411 (3)	C22—C23	1.390 (4)

N2—C30	1.456 (3)	C22—H22	0.9300
O3—C29	1.226 (3)	C24—C23	1.371 (4)
C26—C25	1.374 (3)	C24—H24	0.9300
C26—C27	1.382 (3)	C11—C12	1.379 (4)
C37—C38	1.377 (3)	C11—H11	0.9300
C37—C42	1.390 (3)	C17—C18	1.385 (4)
C37—C28	1.518 (3)	C17—H17	0.9300
C28—C27	1.502 (3)	C6—C1	1.389 (4)
C28—C29	1.532 (3)	C39—H39	0.9300
C28—H28	0.9800	C13—C14	1.364 (4)
C27—C22	1.379 (3)	C13—C12	1.368 (4)
C42—C41	1.385 (4)	C13—H13	0.9300
C31—C36	1.367 (4)	C18—C19	1.359 (5)
C31—C32	1.377 (4)	C18—H18	0.9300
C31—C30	1.497 (3)	C1—C2	1.379 (5)
C41—C40	1.375 (4)	C1—H1	0.9300
C41—H41	0.9300	C36—C35	1.362 (5)
C5—C4	1.366 (4)	C36—H36	0.9300
C5—C6	1.392 (4)	C2—C3	1.379 (5)
C5—N1	1.401 (4)	C2—H2A	0.9300
O1—C8	1.220 (4)	C20—C19	1.375 (4)
O2—C21	1.364 (3)	C20—H20	0.9300
O2—H2	0.8200	C23—H23	0.9300
C30—H30A	0.9700	C4—C3	1.378 (5)
C30—H30B	0.9700	C4—H4A	0.9300
C10—C11	1.367 (4)	C9—H9A	0.9700
C10—C15	1.372 (4)	C9—H9B	0.9700
C10—C9	1.508 (4)	C3—H3	0.9300
C16—C17	1.384 (4)	C19—H19	0.9300
C16—C21	1.386 (4)	C32—C33	1.381 (5)
C16—C7	1.514 (4)	C32—H32	0.9300
N1—C8	1.362 (4)	C15—C14	1.368 (4)
N1—C9	1.452 (4)	C15—H15	0.9300
C25—C24	1.382 (4)	C12—H12	0.9300
C25—H25	0.9300	C14—H14	0.9300
C21—C20	1.373 (4)	C35—C34	1.346 (6)
C38—C39	1.374 (4)	C35—H35	0.9300
C38—H38	0.9300	C33—C34	1.363 (6)
C8—C7	1.533 (4)	C33—H33	0.9300
C40—C39	1.365 (4)	C34—H34	0.9300

C42—O4—H4	109.5	C23—C22—H22	120.6
C29—N2—C26	111.12 (19)	C23—C24—C25	121.0 (3)
C29—N2—C30	124.0 (2)	C23—C24—H24	119.5
C26—N2—C30	124.8 (2)	C25—C24—H24	119.5
C25—C26—C27	122.7 (2)	C10—C11—C12	121.5 (3)
C25—C26—N2	128.2 (2)	C10—C11—H11	119.3
C27—C26—N2	109.1 (2)	C12—C11—H11	119.3

C38—C37—C42	118.4 (2)	C18—C17—C16	120.9 (3)
C38—C37—C28	121.5 (2)	C18—C17—H17	119.6
C42—C37—C28	120.2 (2)	C16—C17—H17	119.6
C27—C28—C37	114.06 (18)	C1—C6—C5	118.6 (3)
C27—C28—C29	101.62 (19)	C1—C6—C7	132.1 (3)
C37—C28—C29	110.23 (19)	C5—C6—C7	109.3 (3)
C27—C28—H28	110.2	C40—C39—C38	119.0 (2)
C37—C28—H28	110.2	C40—C39—H39	120.5
C29—C28—H28	110.2	C38—C39—H39	120.5
C22—C27—C26	119.3 (2)	C14—C13—C12	119.4 (3)
C22—C27—C28	131.1 (2)	C14—C13—H13	120.3
C26—C27—C28	109.5 (2)	C12—C13—H13	120.3
O4—C42—C41	122.4 (2)	C19—C18—C17	119.4 (3)
O4—C42—C37	117.8 (2)	C19—C18—H18	120.3
C41—C42—C37	119.8 (2)	C17—C18—H18	120.3
O3—C29—N2	123.7 (2)	C2—C1—C6	119.1 (3)
O3—C29—C28	127.8 (2)	C2—C1—H1	120.4
N2—C29—C28	108.5 (2)	C6—C1—H1	120.4
C36—C31—C32	117.9 (3)	C35—C36—C31	121.5 (3)
C36—C31—C30	121.1 (2)	C35—C36—H36	119.2
C32—C31—C30	120.9 (2)	C31—C36—H36	119.2
C40—C41—C42	120.2 (3)	C3—C2—C1	121.1 (3)
C40—C41—H41	119.9	C3—C2—H2A	119.5
C42—C41—H41	119.9	C1—C2—H2A	119.5
C4—C5—C6	122.4 (3)	C21—C20—C19	119.9 (3)
C4—C5—N1	128.6 (3)	C21—C20—H20	120.1
C6—C5—N1	109.0 (3)	C19—C20—H20	120.1
C21—O2—H2	109.5	C24—C23—C22	120.9 (3)
N2—C30—C31	113.23 (18)	C24—C23—H23	119.5
N2—C30—H30A	108.9	C22—C23—H23	119.5
C31—C30—H30A	108.9	C5—C4—C3	118.4 (3)
N2—C30—H30B	108.9	C5—C4—H4A	120.8
C31—C30—H30B	108.9	C3—C4—H4A	120.8
H30A—C30—H30B	107.7	N1—C9—C10	111.9 (2)
C11—C10—C15	117.7 (3)	N1—C9—H9A	109.2
C11—C10—C9	122.2 (3)	C10—C9—H9A	109.2
C15—C10—C9	120.1 (3)	N1—C9—H9B	109.2
C17—C16—C21	118.5 (3)	C10—C9—H9B	109.2
C17—C16—C7	121.6 (3)	H9A—C9—H9B	107.9
C21—C16—C7	119.9 (2)	C4—C3—C2	120.5 (3)
C8—N1—C5	111.4 (2)	C4—C3—H3	119.8
C8—N1—C9	122.9 (3)	C2—C3—H3	119.8
C5—N1—C9	125.1 (2)	C18—C19—C20	120.8 (3)
C26—C25—C24	117.4 (2)	C18—C19—H19	119.6
C26—C25—H25	121.3	C20—C19—H19	119.6
C24—C25—H25	121.3	C31—C32—C33	120.2 (3)
O2—C21—C20	122.5 (3)	C31—C32—H32	119.9
O2—C21—C16	117.0 (3)	C33—C32—H32	119.9

C20—C21—C16	120.5 (3)	C14—C15—C10	121.5 (3)
C39—C38—C37	122.0 (2)	C14—C15—H15	119.3
C39—C38—H38	119.0	C10—C15—H15	119.3
C37—C38—H38	119.0	C13—C12—C11	119.7 (3)
O1—C8—N1	123.5 (3)	C13—C12—H12	120.1
O1—C8—C7	128.8 (3)	C11—C12—H12	120.1
N1—C8—C7	107.6 (3)	C13—C14—C15	120.2 (3)
C39—C40—C41	120.6 (3)	C13—C14—H14	119.9
C39—C40—H40	119.7	C15—C14—H14	119.9
C41—C40—H40	119.7	C34—C35—C36	120.4 (4)
C6—C7—C16	118.5 (2)	C34—C35—H35	119.8
C6—C7—C8	102.5 (2)	C36—C35—H35	119.8
C16—C7—C8	112.2 (2)	C34—C33—C32	120.2 (3)
C6—C7—H7	107.7	C34—C33—H33	119.9
C16—C7—H7	107.7	C32—C33—H33	119.9
C8—C7—H7	107.7	C35—C34—C33	119.8 (3)
C27—C22—C23	118.7 (3)	C35—C34—H34	120.1
C27—C22—H22	120.6	C33—C34—H34	120.1

C29—N2—C26—C25	−178.9 (2)	C21—C16—C7—C8	−82.0 (3)
C30—N2—C26—C25	0.5 (4)	O1—C8—C7—C6	175.7 (3)
C29—N2—C26—C27	0.5 (3)	N1—C8—C7—C6	−3.4 (3)
C30—N2—C26—C27	179.8 (2)	O1—C8—C7—C16	47.4 (4)
C38—C37—C28—C27	22.5 (3)	N1—C8—C7—C16	−131.7 (2)
C42—C37—C28—C27	−159.4 (2)	C26—C27—C22—C23	−0.3 (4)
C38—C37—C28—C29	−91.0 (3)	C28—C27—C22—C23	−175.8 (2)
C42—C37—C28—C29	87.0 (2)	C26—C25—C24—C23	0.4 (4)
C25—C26—C27—C22	0.0 (4)	C15—C10—C11—C12	1.4 (4)
N2—C26—C27—C22	−179.4 (2)	C9—C10—C11—C12	−177.7 (3)
C25—C26—C27—C28	176.4 (2)	C21—C16—C17—C18	0.9 (4)
N2—C26—C27—C28	−3.0 (3)	C7—C16—C17—C18	−177.5 (3)
C37—C28—C27—C22	61.3 (3)	C4—C5—C6—C1	−0.6 (4)
C29—C28—C27—C22	179.9 (2)	N1—C5—C6—C1	180.0 (2)
C37—C28—C27—C26	−114.6 (2)	C4—C5—C6—C7	177.6 (2)
C29—C28—C27—C26	4.0 (2)	N1—C5—C6—C7	−1.8 (3)
C38—C37—C42—O4	−179.0 (2)	C16—C7—C6—C1	−54.8 (4)
C28—C37—C42—O4	2.9 (3)	C8—C7—C6—C1	−179.0 (3)
C38—C37—C42—C41	0.6 (3)	C16—C7—C6—C5	127.3 (2)
C28—C37—C42—C41	−177.5 (2)	C8—C7—C6—C5	3.1 (3)
C26—N2—C29—O3	−179.0 (2)	C41—C40—C39—C38	0.0 (4)
C30—N2—C29—O3	1.6 (4)	C37—C38—C39—C40	0.1 (4)
C26—N2—C29—C28	2.1 (2)	C16—C17—C18—C19	0.8 (4)
C30—N2—C29—C28	−177.21 (19)	C5—C6—C1—C2	1.0 (4)
C27—C28—C29—O3	177.6 (2)	C7—C6—C1—C2	−176.7 (3)
C37—C28—C29—O3	−61.2 (3)	C32—C31—C36—C35	−0.2 (4)
C27—C28—C29—N2	−3.7 (2)	C30—C31—C36—C35	178.0 (3)
C37—C28—C29—N2	117.6 (2)	C6—C1—C2—C3	−0.5 (5)
O4—C42—C41—C40	179.1 (2)	O2—C21—C20—C19	−177.6 (3)

C37—C42—C41—C40	−0.5 (3)	C16—C21—C20—C19	2.1 (4)
C29—N2—C30—C31	105.8 (3)	C25—C24—C23—C22	−0.7 (4)
C26—N2—C30—C31	−73.5 (3)	C27—C22—C23—C24	0.6 (4)
C36—C31—C30—N2	124.5 (3)	C6—C5—C4—C3	−0.4 (4)
C32—C31—C30—N2	−57.3 (3)	N1—C5—C4—C3	178.9 (3)
C4—C5—N1—C8	−179.9 (2)	C8—N1—C9—C10	−95.5 (3)
C6—C5—N1—C8	−0.5 (3)	C5—N1—C9—C10	75.2 (3)
C4—C5—N1—C9	8.5 (4)	C11—C10—C9—N1	−120.7 (3)
C6—C5—N1—C9	−172.2 (2)	C15—C10—C9—N1	60.2 (4)
C27—C26—C25—C24	0.0 (4)	C5—C4—C3—C2	0.9 (4)
N2—C26—C25—C24	179.2 (2)	C1—C2—C3—C4	−0.5 (5)
C17—C16—C21—O2	177.4 (2)	C17—C18—C19—C20	−1.1 (5)
C7—C16—C21—O2	−4.2 (4)	C21—C20—C19—C18	−0.3 (5)
C17—C16—C21—C20	−2.3 (4)	C36—C31—C32—C33	−0.3 (4)
C7—C16—C21—C20	176.1 (3)	C30—C31—C32—C33	−178.5 (2)
C42—C37—C38—C39	−0.4 (4)	C11—C10—C15—C14	−0.8 (4)
C28—C37—C38—C39	177.7 (2)	C9—C10—C15—C14	178.3 (3)
C5—N1—C8—O1	−176.6 (3)	C14—C13—C12—C11	−0.1 (5)
C9—N1—C8—O1	−4.7 (4)	C10—C11—C12—C13	−1.0 (5)
C5—N1—C8—C7	2.6 (3)	C12—C13—C14—C15	0.8 (5)
C9—N1—C8—C7	174.4 (2)	C10—C15—C14—C13	−0.3 (5)
C42—C41—C40—C39	0.2 (4)	C31—C36—C35—C34	0.3 (5)
C17—C16—C7—C6	−22.9 (4)	C31—C32—C33—C34	0.6 (5)
C21—C16—C7—C6	158.8 (2)	C36—C35—C34—C33	0.0 (5)
C17—C16—C7—C8	96.4 (3)	C32—C33—C34—C35	−0.5 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.82	1.93	2.721 (3)	160
O4—H4···O3^{ii}	0.82	1.95	2.735 (3)	160

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