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Crystal structure and Hirshfeld surface analysis of 4-benzyl-2*H*-benzo[*b*][1,4]oxazin-3(4*H*)-one

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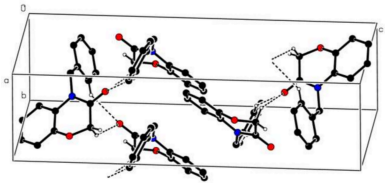
The molecule of the title compound, $C_{15}H_{13}NO_2$, comprises a non-planar oxazine ring (twisted–boat conformation) fused to a benzene ring, and a benzyl moiety. In the crystal, C—H···O hydrogen bonds link the molecules into [010] supramolecular chains, enclosing $R_2^2(9)$ ring motifs. C—H···π interactions and very weak π–π stacking between the benzene rings of adjacent molecules help to consolidate the packing. A Hirshfeld surface analysis revealed that the most important contributions to the crystal packing are from H···H (48.8%), H···C/C···H (29.3%) and H···O/O···H (18.9%) interactions.

1. Chemical context

1,4-Benzoxazine and its derivatives are heterocycles, resulting from the fusion of a benzene ring with an oxazine ring, containing O and N heteroatoms in positions 1 and 4, respectively. These structural elements give these compounds high chemical reactivity and are of particular interest for the development of bioactive molecules. Among them, 1,4-benzoxazin-3-ones constitute a subclass with a wide range of pharmacological properties, including antitumor, antibacterial, antifungal, anticancer, antiviral and antidepressant activities (Hlimi *et al.*, 2018; Oksuzoglu *et al.*, 2023; Tang *et al.*, 2023; Fringuelli *et al.*, 2002; Benarjee & Saritha, 2022; Rao *et al.*, 2022; Zhou *et al.*, 2006). As part of our research on benzoxazines (Sebbar *et al.*, 2025), we developed a selective alkylation strategy aimed at introducing a benzyl group, **2**, onto the 1,4-benzoxazin-3-one nucleus, **1**. This transformation was carried out in a polar aprotic solvent (dimethylformamide, DMF), in the presence of potassium carbonate (K_2CO_3) as a base, allowing for an efficient reaction with a halogenated derivative (Fig. 1). This methodology enables the targeted production of new functionalized derivatives for future structural and biological evaluations and led to the synthesis



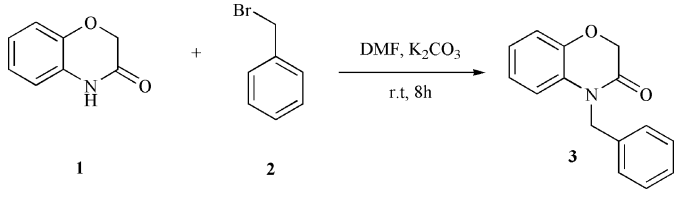
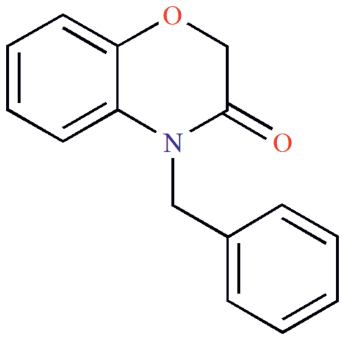


Figure 1
Reaction scheme for obtaining the title compound, **3**.

of 4-benzyl-2*H*-benzo[*b*][1,4]oxazin-3(4*H*)-one ($C_{15}H_{13}NO_2$), **3**, in 90% yield. We report here on the molecular and crystal structures of this compound and also present the results of its Hirshfeld surface analysis.



2. Structural commentary

Compound **3** contains a non-planar oxazine ring fused to a benzene ring, and a benzyl moiety (Fig. 2). The oxazine ring *A* (O1/N1/C1–C4) has a twisted-boat conformation (Fig. 3) with puckering parameters (Cremer & Pople, 1975) Q_T = 0.4286 (10) Å, θ = 112.77 (13)° and φ = 213.01 (15)°. The benzene rings *B* (C3–C8) and *C* (C10–C15) are oriented at a dihedral angle of 87.27 (3)°, and atom C9 is displaced by −0.1060 (11) Å from the mean plane of ring *C*. Bond lengths and angles appear to be in normal ranges.

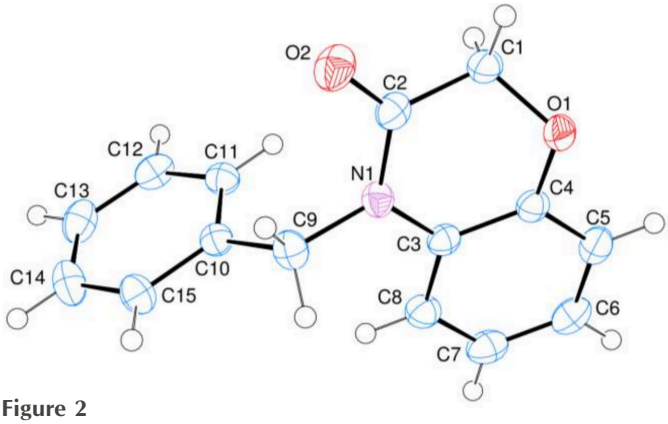


Figure 2
The molecular structure of **3** showing displacement ellipsoids at the 50% probability level.

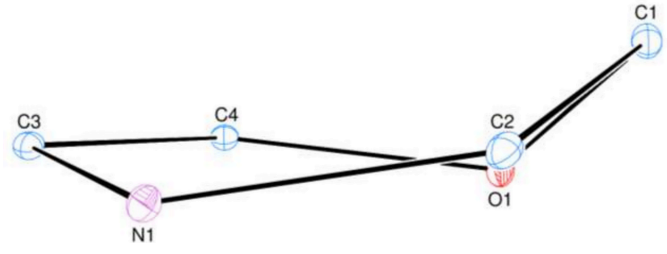


Figure 3
Conformation of the oxazine ring atoms.

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

*Cg*3 is the centroid of the C10–C15 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···O2^{i}	0.99	2.50	3.2592 (12)	133
C11—H11···O2^{i}	0.95	2.56	3.3765 (13)	146
C1—H1*B*···*Cg*3^{i}	0.99	2.78	3.5952 (10)	143

Symmetry code: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

3. Supramolecular features

In the crystal of **3**, C1—H1*A*···O2^{i} and C11—H11···O2^{i} hydrogen bonds (Table 1) link adjacent molecules into [010] supramolecular chains, enclosing $R_2^2(9)$ ring motifs (Etter *et al.*, 1990), Fig. 4. An additional C—H···π(ring) interaction (Table 1) and a very weak π–π stacking interaction between the *B* rings of adjacent molecules with a centroid-to-centroid distance of 4.0255 (6) Å, a dihedral angle α of 0.02 (5)° and a slippage of 2.291 Å help to consolidate the packing within the crystal.

4. Hirshfeld surface analysis

To quantify and visualize the intermolecular interactions in the crystal of **3**, a Hirshfeld surface (HS) analysis was carried

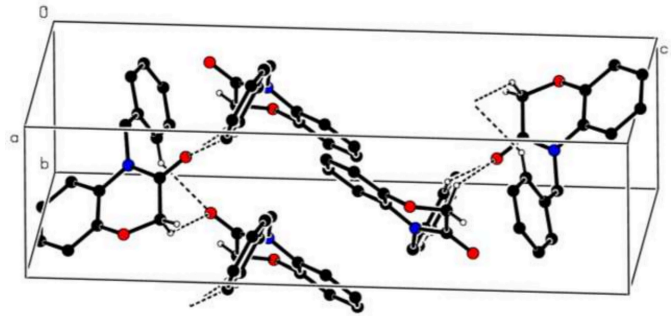


Figure 4
Partial packing diagram of **3** with intermolecular C—H···O hydrogen bonds shown as dashed lines; only those hydrogen atoms involved in these interactions are shown.

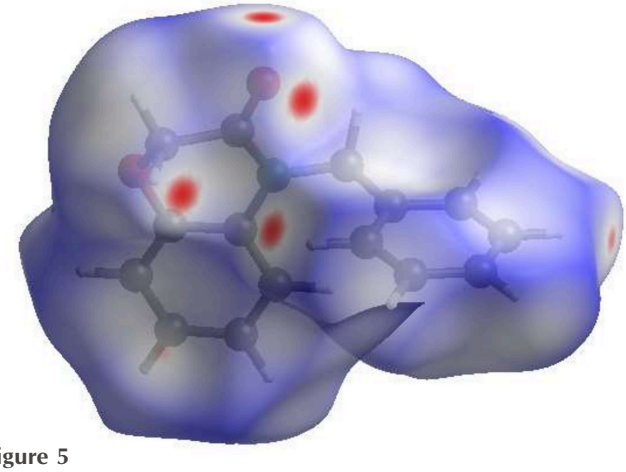


Figure 5
View of the three-dimensional HS of **3** plotted over d_{norm}.

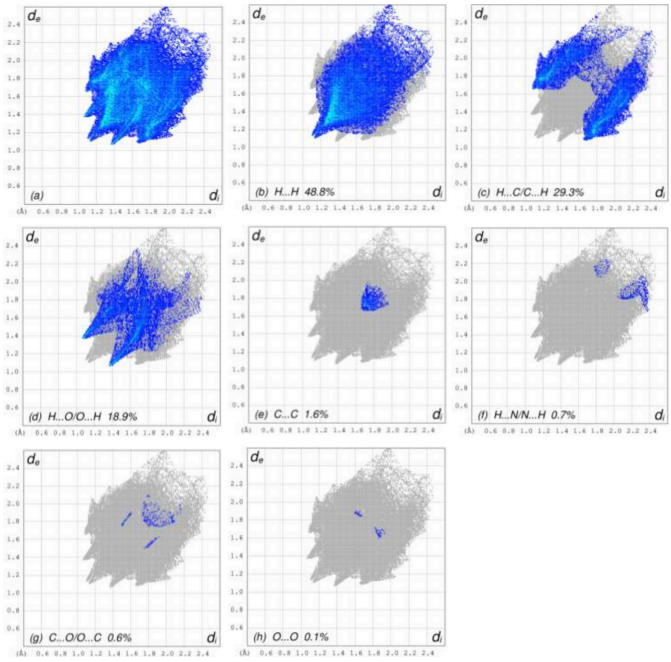


Figure 6
The two-dimensional fingerprint plots of **3**, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) H···C/C···H, (*d*) H···O/O···H, (*e*) C···C, (*f*) H···N/N···H, (*g*) C···O/O···C and (*h*) O···O interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

out with *CrystalExplorer* (Spackman *et al.*, 2021). Fig. 5 shows the contact distances on the HS where the bright-red spots correspond to the respective donors and/or acceptor sites noted above. According to the two-dimensional fingerprint plots (McKinnon *et al.*, 2007), H···H, H···C/C···H and H···O/O···H contacts make the most significant contributions to the HS, at 48.8%, 29.3% and 18.9%, respectively (Fig. 6).

5. Database survey

A search of the Cambridge Structural Database (CSD, updated July 2025; Groom *et al.*, 2016) for compounds with the benzo[b][1,4]oxazin-3(4H)-one moiety substituted in the 2-, 4-, 5-, or 7-positions revealed numerous entries. The compounds most closely related to **3** are schematically displayed in Fig. 7 and include: Structures **I** (CSD refcode DAMYOJ; Shaikh *et al.*, 2021); **II** (BUHROO, with $\boldsymbol{R_1}$ = 4-(3-(2,4-dimethylphenylamino)propan-2-olyl), $\boldsymbol{R_2}$ to $\boldsymbol{R_5}$ = H; Rao *et al.*, 2020); **III** (DUFKEX; Yang *et al.*, 2019); **IV** (HAHCEC, with $\boldsymbol{R}_1$ = CH_3, $\boldsymbol{R_2}$ = 2-(2-methylprop-1-enyl), $\boldsymbol{R}_3$ = 2-(4- methylbenzyl), $\boldsymbol{R_4}$ = $\boldsymbol{R_5}$ = H; Mohanta *et al.*, 2023); **V** (INICIU; Nie *et al.*, 2021) and **VI** (KOQSES; Winter *et al.*, 2024). In comparison, the title compound **3** is N-benzylated and unsubstituted on the ring ($\boldsymbol{R_2}$ – $\boldsymbol{R_5}$ = H) and thus is distinguished by a moderate bulky group at the nitrogen atom and greater rotational freedom of the –CH_2–Ph arm, conditions favorable to (weak) π–π stacking and C—H···O contacts. Conversely, **II** and **VI** carry polar functions (*e.g.*, alcohol/amine or hydroxyl groups) to establish O—H···O / N—H···O networks influencing the local conformation. **III** introduces a strongly electron-withdrawing group (trifluoromethyl sulfonyl), which strengthens the C—H···O contacts and modifies the electron density of oxazinone. **I**, **IV**, and **V** present bulky/aromatic substituents (N-alkyls, aryls), inducing more pronounced shifts (slippage) in the π stacks and higher N—C torsion angles, which result in distinct packing modes. The conformation of the oxazine ring in these structures is similar to that observed in the title compound.

6. Synthesis and crystallization

A dry mixture was prepared by combining 100 mg (0.6 mmol) of 2*H*-benzo[*b*][1,4]oxazin-3(4*H*)-one (previously dried under vacuum in a desiccator) with 92.1 mg (0.66 mmol) of potassium carbonate (K_2CO_3) in 15 ml of anhydrous DMF. To this mixture, 0.66 mmol of benzyl bromide were added. The reaction mixture was stirred at room temperature, and the reaction progress was monitored using thin-layer chromatography (TLC). Once the reaction was complete, the mixture was filtered to remove inorganic salts, and the solvent was evaporated under reduced pressure. The crude product was then purified using silica gel column chromatography,

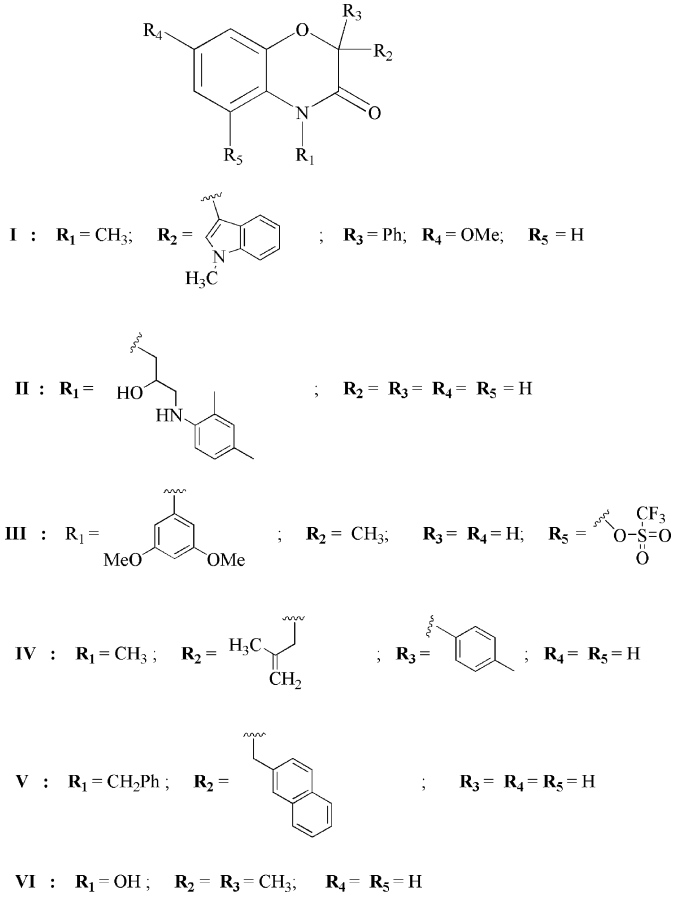


Figure 7
Results of the database search with the closest structures identified.

employing a mixture of hexane and ethyl acetate as the eluent. The target compound **3** was obtained as colorless crystals with an overall yield of 90%.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound hydrogen atoms were calculated geometrically at CH = 0.95 Å and CH_2 = 0.99 Å and refined using a riding model with $U_{iso}(H) = 1.2U_{eq}(C)$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{13}NO_2$
M_r	239.26
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	160
a, b, c (Å)	9.49281 (8), 5.79368 (5), 21.45658 (18)
β (°)	91.3621 (8)
V (Å^3)	1179.74 (2)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.73
Crystal size (mm)	0.30 × 0.13 × 0.11
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Analytical (*CrysAlis PRO*; Rigaku OD, 2024)
T_{min}, T_{max}	0.859, 0.929
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15357, 2477, 2412
R_{int}	0.013
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.633
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.089, 1.04
No. of reflections	2477
No. of parameters	163
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.19

Computer programs: *CrysAlis PRO* (Rigaku OD, 2024), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

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Computing details

4-Benzyl-2*H*-benzo[*b*][1,4]oxazin-3(4*H*)-one

Crystal data

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Monoclinic, $P2_1/n$
$a = 9.49281$ (8) Å
$b = 5.79368$ (5) Å
$c = 21.45658$ (18) Å
$\beta = 91.3621$ (8)°
$V = 1179.74$ (2) Å^3
$Z = 4$
$F(000) = 504$
$D_x = 1.347$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 12385 reflections
$\theta = 4.1$–$79.3°$
$\mu = 0.73$ mm^{-1}
$T = 160$ K
Block, colourless
0.30 × 0.13 × 0.11 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: analytical (CrysAlisPro; Rigaku OD, 2024)
$T_{min} = 0.859$, $T_{max} = 0.929$
15357 measured reflections
2477 independent reflections
2412 reflections with $I > 2\sigma(I)$
$R_{int} = 0.013$
$\theta_{max} = 77.3°$, $\theta_{min} = 4.1°$
$h = -11 \rightarrow 11$
$k = -6 \rightarrow 7$
$l = -27 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.089$
$S = 1.04$
2477 reflections
163 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 0.3423P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ 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}
O1	−0.00508 (7)	0.54481 (13)	0.36181 (3)	0.02998 (18)
O2	0.15569 (8)	0.13347 (15)	0.26572 (4)	0.0379 (2)
N1	0.22040 (8)	0.24375 (14)	0.36413 (4)	0.02528 (19)
C1	0.05704 (10)	0.48342 (19)	0.30398 (4)	0.0284 (2)
H1A	0.115402	0.613732	0.289607	0.034*
H1B	−0.018786	0.457366	0.272281	0.034*
C2	0.14752 (10)	0.26962 (18)	0.30884 (5)	0.0268 (2)
C3	0.20721 (10)	0.40933 (17)	0.41222 (4)	0.0242 (2)
C4	0.09204 (10)	0.55889 (17)	0.41010 (4)	0.0251 (2)
C5	0.06932 (11)	0.71387 (19)	0.45779 (5)	0.0319 (2)
H5	−0.010120	0.813576	0.455994	0.038*
C6	0.16316 (12)	0.7230 (2)	0.50828 (5)	0.0357 (3)
H6	0.147692	0.828356	0.541354	0.043*
C7	0.27928 (12)	0.5787 (2)	0.51046 (5)	0.0356 (3)
H7	0.344034	0.586946	0.544835	0.043*
C8	0.30189 (11)	0.42197 (19)	0.46287 (5)	0.0308 (2)
H8	0.381803	0.323285	0.464743	0.037*
C9	0.30952 (10)	0.04000 (17)	0.37316 (5)	0.0289 (2)
H9A	0.272671	−0.084600	0.345729	0.035*
H9B	0.300835	−0.012997	0.416763	0.035*
C10	0.46435 (10)	0.07306 (16)	0.36029 (4)	0.0239 (2)
C11	0.51780 (10)	0.26787 (17)	0.33164 (4)	0.0264 (2)
H11	0.457398	0.393858	0.321551	0.032*
C12	0.66043 (11)	0.2784 (2)	0.31765 (5)	0.0323 (2)
H12	0.697103	0.412364	0.298315	0.039*
C13	0.74884 (11)	0.0947 (2)	0.33182 (5)	0.0359 (3)
H13	0.845560	0.101544	0.321565	0.043*
C14	0.69600 (12)	−0.0988 (2)	0.36092 (6)	0.0370 (3)
H14	0.756507	−0.224714	0.370939	0.044*
C15	0.55472 (11)	−0.10865 (18)	0.37543 (5)	0.0317 (2)
H15	0.519116	−0.240940	0.395942	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0217 (3)	0.0411 (4)	0.0271 (4)	0.0047 (3)	0.0009 (3)	−0.0012 (3)
O2	0.0347 (4)	0.0444 (5)	0.0346 (4)	−0.0014 (3)	−0.0012 (3)	−0.0142 (3)
N1	0.0218 (4)	0.0267 (4)	0.0274 (4)	0.0008 (3)	0.0003 (3)	−0.0016 (3)
C1	0.0239 (5)	0.0378 (6)	0.0236 (5)	0.0006 (4)	−0.0001 (3)	0.0005 (4)

C2	0.0206 (4)	0.0331 (5)	0.0269 (5)	−0.0043 (4)	0.0019 (3)	−0.0028 (4)
C3	0.0231 (4)	0.0266 (5)	0.0232 (4)	−0.0032 (4)	0.0031 (3)	0.0015 (4)
C4	0.0226 (4)	0.0286 (5)	0.0242 (5)	−0.0026 (4)	0.0031 (3)	0.0025 (4)
C5	0.0322 (5)	0.0316 (5)	0.0324 (5)	0.0007 (4)	0.0081 (4)	−0.0013 (4)
C6	0.0433 (6)	0.0366 (6)	0.0276 (5)	−0.0062 (5)	0.0075 (4)	−0.0061 (4)
C7	0.0365 (5)	0.0453 (6)	0.0249 (5)	−0.0078 (5)	−0.0019 (4)	−0.0005 (4)
C8	0.0269 (5)	0.0377 (6)	0.0276 (5)	−0.0009 (4)	−0.0013 (4)	0.0020 (4)
C9	0.0266 (5)	0.0234 (5)	0.0366 (5)	−0.0011 (4)	0.0024 (4)	0.0018 (4)
C10	0.0247 (5)	0.0236 (4)	0.0235 (4)	−0.0007 (4)	−0.0009 (3)	−0.0025 (3)
C11	0.0287 (5)	0.0256 (5)	0.0248 (4)	−0.0015 (4)	−0.0014 (4)	−0.0005 (4)
C12	0.0330 (5)	0.0356 (6)	0.0283 (5)	−0.0093 (4)	0.0034 (4)	−0.0024 (4)
C13	0.0239 (5)	0.0450 (6)	0.0389 (6)	−0.0031 (4)	0.0028 (4)	−0.0126 (5)
C14	0.0290 (5)	0.0333 (6)	0.0483 (6)	0.0067 (4)	−0.0043 (4)	−0.0074 (5)
C15	0.0314 (5)	0.0244 (5)	0.0391 (6)	0.0012 (4)	−0.0011 (4)	0.0008 (4)

Geometric parameters (Å, º)

O1—C1	1.4313 (12)	C7—C8	1.3869 (16)
O1—C4	1.3729 (12)	C8—H8	0.9500
O2—C2	1.2197 (13)	C9—H9A	0.9900
N1—C2	1.3671 (13)	C9—H9B	0.9900
N1—C3	1.4167 (12)	C9—C10	1.5140 (13)
N1—C9	1.4626 (12)	C10—C11	1.3871 (14)
C1—H1A	0.9900	C10—C15	1.3916 (14)
C1—H1B	0.9900	C11—H11	0.9500
C1—C2	1.5096 (14)	C11—C12	1.3951 (14)
C3—C4	1.3949 (14)	C12—H12	0.9500
C3—C8	1.3957 (14)	C12—C13	1.3847 (16)
C4—C5	1.3822 (14)	C13—H13	0.9500
C5—H5	0.9500	C13—C14	1.3831 (17)
C5—C6	1.3872 (16)	C14—H14	0.9500
C6—H6	0.9500	C14—C15	1.3852 (15)
C6—C7	1.3836 (17)	C15—H15	0.9500
C7—H7	0.9500		

C4—O1—C1	112.70 (7)	C3—C8—H8	120.0
C2—N1—C3	120.41 (8)	C7—C8—C3	119.97 (10)
C2—N1—C9	118.86 (8)	C7—C8—H8	120.0
C3—N1—C9	120.72 (8)	N1—C9—H9A	108.3
O1—C1—H1A	109.0	N1—C9—H9B	108.3
O1—C1—H1B	109.0	N1—C9—C10	115.77 (8)
O1—C1—C2	112.92 (8)	H9A—C9—H9B	107.4
H1A—C1—H1B	107.8	C10—C9—H9A	108.3
C2—C1—H1A	109.0	C10—C9—H9B	108.3
C2—C1—H1B	109.0	C11—C10—C9	123.41 (9)
O2—C2—N1	123.18 (10)	C11—C10—C15	119.28 (9)
O2—C2—C1	121.64 (9)	C15—C10—C9	117.22 (9)
N1—C2—C1	115.17 (8)	C10—C11—H11	120.1

C4—C3—N1	118.66 (9)	C10—C11—C12	119.87 (9)
C4—C3—C8	118.86 (9)	C12—C11—H11	120.1
C8—C3—N1	122.43 (9)	C11—C12—H12	119.8
O1—C4—C3	119.97 (9)	C13—C12—C11	120.36 (10)
O1—C4—C5	118.92 (9)	C13—C12—H12	119.8
C5—C4—C3	121.02 (9)	C12—C13—H13	120.1
C4—C5—H5	120.2	C14—C13—C12	119.84 (10)
C4—C5—C6	119.63 (10)	C14—C13—H13	120.1
C6—C5—H5	120.2	C13—C14—H14	120.1
C5—C6—H6	120.0	C13—C14—C15	119.89 (10)
C7—C6—C5	119.97 (10)	C15—C14—H14	120.1
C7—C6—H6	120.0	C10—C15—H15	119.6
C6—C7—H7	119.7	C14—C15—C10	120.74 (10)
C6—C7—C8	120.52 (10)	C14—C15—H15	119.6
C8—C7—H7	119.7		

O1—C1—C2—O2	145.86 (9)	C4—C3—C8—C7	1.08 (15)
O1—C1—C2—N1	−35.32 (12)	C4—C5—C6—C7	0.48 (16)
O1—C4—C5—C6	177.15 (9)	C5—C6—C7—C8	−0.89 (17)
N1—C3—C4—O1	−0.48 (13)	C6—C7—C8—C3	0.10 (16)
N1—C3—C4—C5	175.91 (9)	C8—C3—C4—O1	−177.89 (8)
N1—C3—C8—C7	−176.23 (9)	C8—C3—C4—C5	−1.50 (14)
N1—C9—C10—C11	−10.84 (14)	C9—N1—C2—O2	−1.88 (14)
N1—C9—C10—C15	172.60 (9)	C9—N1—C2—C1	179.31 (8)
C1—O1—C4—C3	−34.64 (12)	C9—N1—C3—C4	−160.52 (9)
C1—O1—C4—C5	148.89 (9)	C9—N1—C3—C8	16.79 (13)
C2—N1—C3—C4	18.13 (13)	C9—C10—C11—C12	−175.70 (9)
C2—N1—C3—C8	−164.55 (9)	C9—C10—C15—C14	175.23 (10)
C2—N1—C9—C10	96.66 (11)	C10—C11—C12—C13	0.47 (15)
C3—N1—C2—O2	179.44 (9)	C11—C10—C15—C14	−1.48 (15)
C3—N1—C2—C1	0.63 (13)	C11—C12—C13—C14	−1.08 (16)
C3—N1—C9—C10	−84.67 (11)	C12—C13—C14—C15	0.41 (16)
C3—C4—C5—C6	0.72 (15)	C13—C14—C15—C10	0.88 (17)
C4—O1—C1—C2	51.88 (11)	C15—C10—C11—C12	0.80 (14)

Hydrogen-bond geometry (Å, º)

*Cg*3 is the centroid of the C10–C15 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···O2^{i}	0.99	2.50	3.2592 (12)	133
C11—H11···O2^{i}	0.95	2.56	3.3765 (13)	146
C1—H1*B*···*Cg*3^{i}	0.99	2.78	3.5952 (10)	143

Symmetry code: (i) −*x*+1/2, *y*+1/2, −*z*+1/2.