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Synthesis and structure of (*Z*)-2-(ethoxymethylidene)-8-methyl-2,3,4,9-tetrahydro-1*H*-carbazol-1-one

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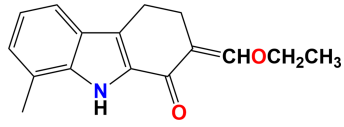
In the title compound, $C_{16}H_{17}NO_2$, the cyclohexene ring adopts an envelope conformation and the side chain is extended. In the extended structure, N—H···O hydrogen bonds connect the molecules into [100] chains and weak C—H···O interactions and pairwise C—H···π interactions consolidate the packing. A Hirshfeld surface analysis indicates that the most important contributions to the crystal packing are from H···H (57.6%), C···H/H···C (24.2%), and H···O/ O···H (13.8%) contacts. Evaluation of the electrostatic, dispersion and total energy frameworks indicates that the cohesion of the crystal largely depends on dispersion energy contributions.

1. Chemical context

Carbazole derivatives represent a class of heteroaromatic compounds that continue to inspire extensive investigation in both organic synthesis and medicinal chemistry (Knölker & Reddy, 2002). Substitution at different positions of the carbazole ring system has yielded derivatives with enhanced reactivity and diverse biological properties, underscoring the versatility of this structural motif.

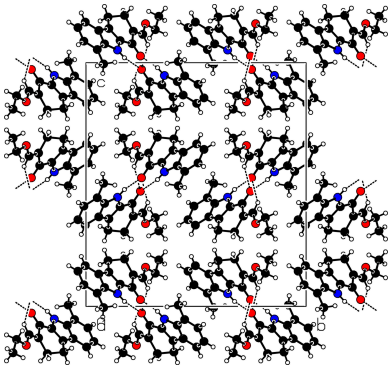
Within this context, 2,3,4,9-tetrahydrocarbazol-1-ones have proven to be valuable precursors, offering a convenient entry point to more elaborate heterocycles. Of particular interest is 2-(ethoxymethylene)-2,3,4,9-tetrahydrocarbazol-1-one, which has been reported as a versatile intermediate in heterocyclic synthesis (Sridharan & Thiruvalluar, 2026). The ethoxymethylene substituent (Dasgupta & Ghatak, 1985) at the 2-position introduces an electrophilic site amenable to condensation and cyclization, while the carbonyl group at the 1-position enhances synthetic flexibility. This dual functionality renders the compound an effective building block for the construction of complex heterocycles with potential pharmaceutical relevance.



As part of our studies in this area, we now describe the synthesis and structure of the title compound, $C_{16}H_{17}NO_2$ (**I**).

2. Structural commentary

As shown in Fig. 1, compound (**I**), which crystallizes in the orthorhombic space group *Pbca* with one molecule in the



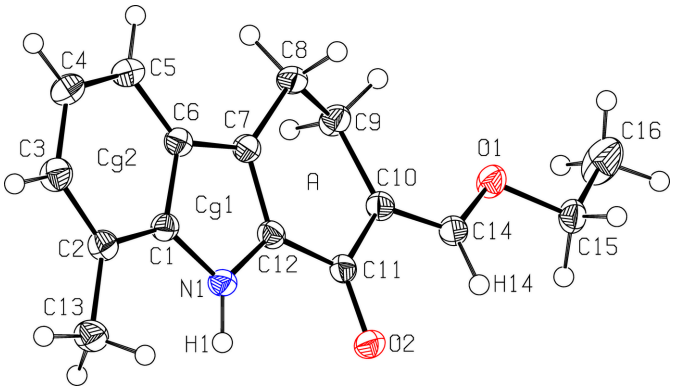


Figure 1
The molecular structure of (**I**), showing displacement ellipsoids drawn at the 50% probability level.

asymmetric unit, consists of indole and cyclohexene units fused *via* the C7—C12 bond. As expected, the pyrrole (N1/C1/C6/C7/C12) and benzene (C1–C6) rings are nearly co-planar, subtending a dihedral angle of 1.38 (6)°. A puckering analysis (Cremer & Pople, 1975) of the C7–C12 ring gave the parameters: q_2 = 0.3271 (13) Å, q_3 = −0.1784 (13) Å, Q_T = 0.3726 (13) Å, θ = 118.6 (2)° and φ = 280.9 (2)°, which corresponds to an envelope conformation, where atom C9 is at the flap position and displaced by −0.497 (2) Å from the best plane of the remaining tricyclic carbazole non-H atoms. The C7—C8—C9—C10 torsion angle is −42.40 (15)°. The ethoxymethylene side chain adopts an extended conformation, as indicated by the C10—C14—O1—C15 and C14—O1—C15—C16 torsion angles of 176.41 (11) and 174.05 (13)°, respectively.

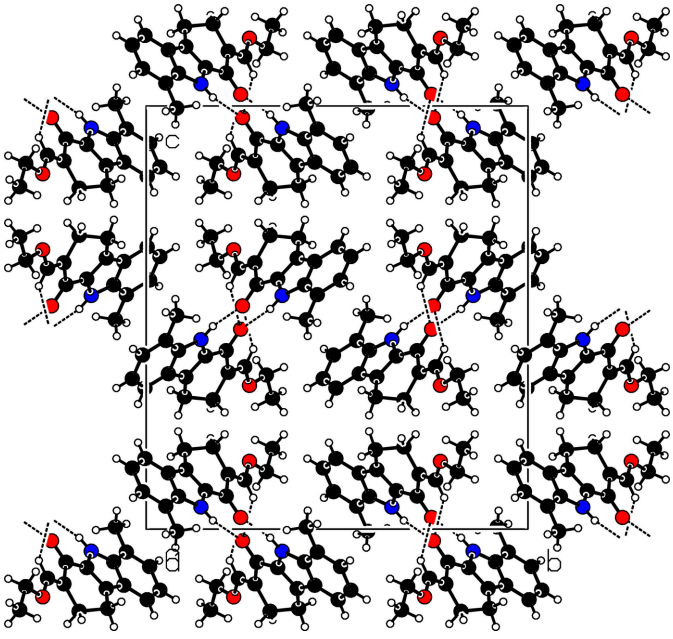


Figure 2
Partial packing view of (**I**), viewed down the *a*-axis direction, showing the hydrogen bonds. Black dashed lines represent C—H···O and N—H···O hydrogen bonds.

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

*Cg*2 is the centroid of the benzene (C1–C6) ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.919 (17)	2.034 (17)	2.9235 (14)	162.2 (15)
C14—H14···O2^{ii}	0.95	2.52	3.2396 (15)	133
C13—H13*B*···*Cg*2^{iii}	0.98	2.76	3.5669 (15)	140

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

3. Supramolecular features

In the extended structure, strong N1—H1···O2 hydrogen bonds (Table 1) form *C*(7) chains of molecules propagating parallel to the *a*-axis direction as shown in Fig. 2. Weak C14—H14···O2 links generate double chains. The molecules are further linked by pairwise C13—H13*B*···*Cg*2 (where *Cg*2 is the centroid of the C1–C6 benzene ring) interactions that connect parallel chains with each other (Fig. 3). No significant π–π stacking interactions are observed in this structure.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 6.01, updated to February 2026; Groom *et al.*, 2016) using the core structure of (**I**) gave zero hits.

5. Hirshfeld surface

A Hirshfeld surface (HS) analysis was carried out using *CrystalExplorer* version 21.5 (Spackman *et al.*, 2021) to further quantify the intermolecular interactions in the crystal of (**I**).

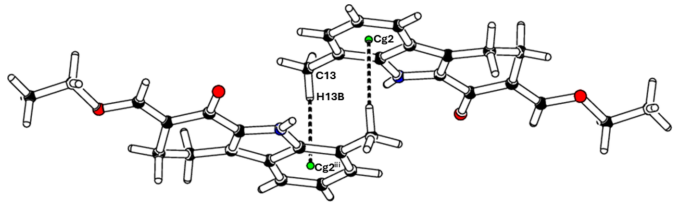


Figure 3
Straw-style packing view of (**I**), showing the C—H···π contacts. Centroids are shown as green spheres and black dashed lines are H···π contacts.

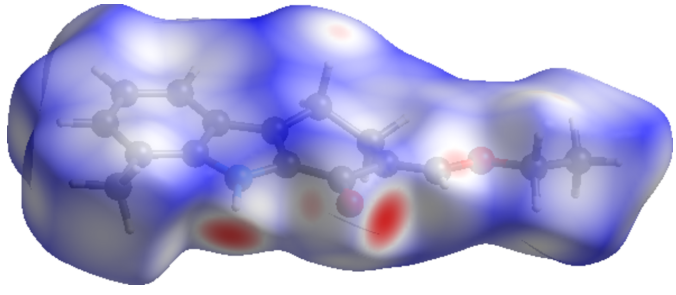


Figure 4
View of the three-dimensional Hirshfeld surface of (**I**), plotted over d_{norm} in the range from −0.51 to 1.22 a.u. with a neighbouring molecule.

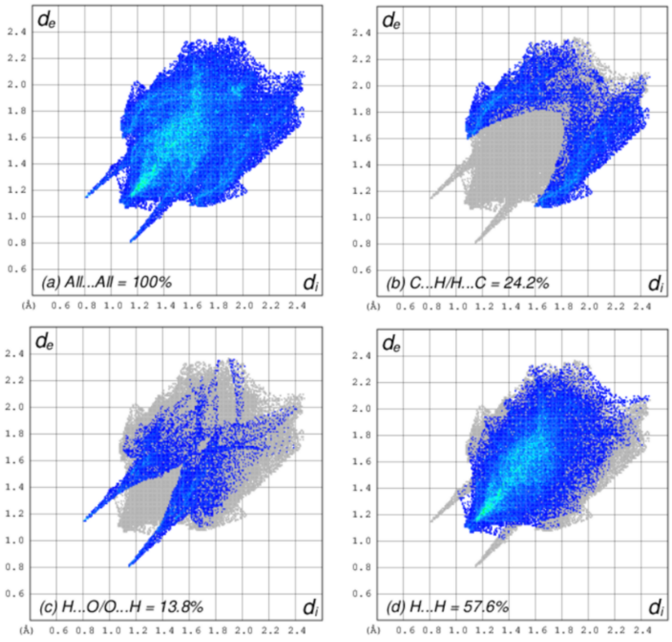


Figure 5
Two-dimensional fingerprint plots for (**I**), showing (*a*) all interactions, and those showing (*b*) C···H/H···C, (*c*) H···O/O···H, and (*d*) H···H interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

The HS plotted over d_{norm} is shown in Fig. 4, where the bright-red spots correspond to donor and/or acceptor sites. According to the two-dimensional fingerprint plots (Fig. 5), C···H/H···C, H···O/O···H and H···H contacts make the most important contributions to the HS, with values of 24.2%, 13.8%, and 57.6% respectively. All other contact types, including C···N/N···C, C···O/O···C, H···N/N···H, N···O/O···N, and C···C contribute less than 2.0% each to the total.

6. Interaction energy calculations and energy frameworks

The CE-B3LYP/6-31G(d,p) energy model available in *CrystalExplorer* was used to calculate the intermolecular interaction energies. Hydrogen-bonding interaction energies (in kJ mol^{-1}) were calculated to be −41.4 (E_{ele}), −13.9 (E_{pol}), −23.1 (E_{dis}), 45.3 (E_{rep}) and −46.3 (E_{tot}) for the collective hydrogen bonds N1—H1···O2 and C14—H14···O2. Values of −9.4 (E_{ele}), −1.8 (E_{pol}), −38.8 (E_{dis}), 21.6 (E_{rep}) and −31.7 (E_{tot}) arose for the C13—H13*B*···π interaction. Energy frameworks (Turner *et al.*, 2015) were constructed for E_{ele} (red cylinders), E_{dis} (green cylinders) and E_{tot} (blue cylinders) [Fig. 6(*a*)–(*c*)], and their evaluation indicates that crystal cohesion largely depends on dispersion energy contributions in the crystal structure of (**I**).

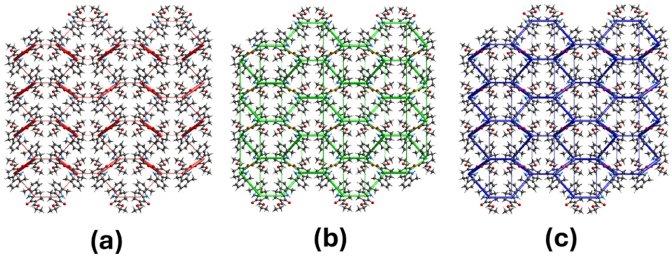


Figure 6
The energy frameworks for a cluster of molecules of (**I**) viewed down the *a*-axis direction, showing (*a*) electrostatic energy E_{ele}, (*b*) dispersion energy E_{dis} and (*c*) total energy E_{tot} diagrams. The cylindrical radius is proportional to the relative strength of the corresponding energies and they were adjusted to the same scale factor of 80 with a cut-off value of 5 kJ mol^{-1} within 2 × 2 × 2 unit cells.

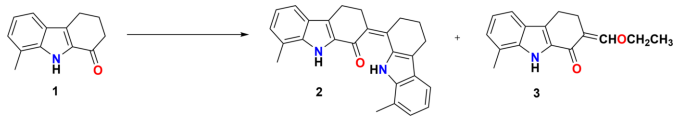


Figure 7
The synthesis scheme for (**I**).

7. Synthesis and crystallization

8-Methyl-2,3,4,9-tetrahydrocarbazol-1-one (**1**) (1.00 g, 0.005 mol) in dichloromethane (15 ml) was added to an ice-cooled solution of diethoxycarbenium fluoroborate [prepared *in situ* from 1.65 ml of $BF_3{\cdot}Et_2O$ (0.01 mol) and 1.25 ml of $HC(OEt_3)$ (0.01 mol)]. The reaction mixture (Fig. 7) was kept at 258 to 263 K. To this mixture, triethylamine (0.01 mol) was added dropwise and the stirring was continued over a period of five h. The reaction was monitored by TLC. After the completion of reaction, the excess solvent was removed and extracted using ethyl acetate dried over anhydrous sodium sulfate. The brown solid separated out was then separated by column chromatography over silica gel using petroleum ether: ethyl acetate as eluants (99:1) and (95:5) to yield (*Z*)-8-methyl-2,3,4,9-tetrahydro-2 (8′-methyl-2′,3′,4′,9′-tetrahydrocarbazol-1-ylidene)-carbazol 1-one (**2**) and (*Z*)-2-(ethoxymethylene)-8-methyl-2,3,4,9 tetrahydro-1*H*-carbazol-1-one (**3**), respectively. The chemical structure of the final products was confirmed by NMR spectroscopy and elementary analysis data. Compound (**3**) was recrystallized from ethanol solution as yellow prisms (0.842 g, 66%), m.p. 377–379 K. The reaction scheme is shown in Fig. 7.

8. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The N-bound H atom was located in a difference-Fourier map and its position was freely refined with U_{iso}(H) = 1.2U_{eq}(N). All the other H atoms were placed in calculated positions and refined as riding atoms with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The methyl group was allowed to rotate, but not to tip, to best fit the experimental electron density.

Acknowledgements

Authors contributions are as follows: conceptualization, synthesis, methodology and writing original draft, MS; crys-

tallographic analysis, Hirshfeld surface analysis, software, validation, review and editing, AAT. AAT acknowledge the Cambridge Crystallographic Data Centre (CCDC) for providing access to the Cambridge Structural Database (CSD, version 6.01). Database searches were performed using CONQUEST, and structural analyses were carried out using Mercury. MS thanks academic and administrative authorities of RV College of Engineering for their support and encouragement. The authors thank Dr Matthias Zeller for the X-ray data collection. The X-ray diffractometer was funded by NSF Grant CHE 0087210, Ohio Board of Regents Grant CAP-491, and by Youngstown State University.

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{17}NO_2$
M_r	255.30
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	100
a, *b*, *c* (Å)	6.9872 (5), 18.3913 (13), 20.3450 (15)
V (Å^3)	2614.4 (3)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.68 × 0.46 × 0.43
Data collection	
Diffractometer	Bruker AXS SMART APEX CCD
Absorption correction	Multi-scan (*SADABS2004*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.885, 0.964
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18986, 3238, 2854
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.124, 1.04
No. of reflections	3238
No. of parameters	177
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.31

Computer programs: *SMART* (Bruker, 2002), *SAINT-Plus* (Bruker, 2003), *SHELXS* (Sheldrick, 2008), *SHELXL2025/1* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

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Computing details

(*Z*)-2-(Ethoxymethylidene)-8-methyl-2,3,4,9-tetrahydro-1*H*-carbazol-1-one

Crystal data

$C_{16}H_{17}NO_2$
$M_r = 255.30$
Orthorhombic, *Pbca*
$a = 6.9872$ (5) Å
$b = 18.3913$ (13) Å
$c = 20.3450$ (15) Å
$V = 2614.4$ (3) Å^3
$Z = 8$
$F(000) = 1088$
$D_x = 1.297$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6074 reflections
$\theta = 2.4$–30.4°
$\mu = 0.09$ mm^{-1}
$T = 100$ K
Block, yellow
0.68 × 0.46 × 0.43 mm

Data collection

Bruker AXS SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS2004*; Krause *et al.*, 2015)
$T_{min} = 0.885$, $T_{max} = 0.964$
18986 measured reflections
3238 independent reflections
2854 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.2°$
$h = -9 \rightarrow 9$
$k = -23 \rightarrow 24$
$l = -23 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.124$
$S = 1.04$
3238 reflections
177 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0659P)^2 + 1.1726P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ 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}
C1	0.98167 (17)	0.08476 (6)	0.42264 (6)	0.0194 (2)
C2	1.14974 (18)	0.05163 (7)	0.44576 (6)	0.0225 (3)
C3	1.20971 (19)	−0.00928 (7)	0.41145 (7)	0.0264 (3)
H3	1.321352	−0.034028	0.425941	0.032*
C4	1.11146 (19)	−0.03616 (7)	0.35569 (6)	0.0264 (3)
H4	1.159354	−0.077761	0.333422	0.032*
C5	0.94764 (18)	−0.00293 (6)	0.33325 (6)	0.0229 (3)
H5	0.882376	−0.020940	0.295664	0.027*
C6	0.87898 (17)	0.05835 (6)	0.36728 (6)	0.0198 (2)
C7	0.71601 (17)	0.10427 (6)	0.35948 (6)	0.0197 (2)
C8	0.55199 (18)	0.10052 (7)	0.31249 (6)	0.0235 (3)
H8A	0.457131	0.064632	0.328424	0.028*
H8B	0.598480	0.084221	0.268949	0.028*
C9	0.45628 (18)	0.17532 (7)	0.30579 (6)	0.0258 (3)
H9A	0.534229	0.205797	0.275922	0.031*
H9B	0.328899	0.168899	0.285286	0.031*
C10	0.43179 (17)	0.21508 (7)	0.37046 (6)	0.0215 (3)
C11	0.57990 (17)	0.20979 (7)	0.42188 (6)	0.0201 (2)
C12	0.72546 (16)	0.15533 (6)	0.40907 (6)	0.0198 (2)
C13	1.2535 (2)	0.08035 (7)	0.50504 (7)	0.0276 (3)
H13A	1.369795	0.051699	0.512380	0.041*
H13B	1.170246	0.076726	0.543665	0.041*
H13C	1.288073	0.131352	0.497714	0.041*
C14	0.28156 (17)	0.25820 (7)	0.38372 (6)	0.0222 (3)
H14	0.273853	0.280696	0.425672	0.027*
C15	−0.01415 (17)	0.31500 (7)	0.36423 (7)	0.0251 (3)
H15A	0.036691	0.360927	0.382643	0.030*
H15B	−0.082869	0.288797	0.399579	0.030*
C16	−0.1470 (3)	0.33099 (11)	0.30927 (8)	0.0480 (5)
H16A	−0.081211	0.360702	0.276282	0.072*
H16B	−0.258376	0.357541	0.326052	0.072*
H16C	−0.189264	0.285313	0.289162	0.072*
N1	0.88530 (14)	0.14364 (6)	0.44784 (5)	0.0202 (2)
O1	0.14156 (13)	0.27071 (5)	0.33973 (4)	0.0259 (2)
O2	0.58335 (13)	0.24760 (5)	0.47242 (4)	0.0253 (2)
H1	0.929 (2)	0.1750 (9)	0.4797 (8)	0.030*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0206 (5)	0.0199 (5)	0.0178 (5)	−0.0011 (4)	0.0012 (4)	0.0003 (4)
C2	0.0223 (6)	0.0235 (6)	0.0216 (6)	0.0001 (4)	−0.0012 (5)	0.0012 (5)
C3	0.0254 (6)	0.0258 (6)	0.0278 (6)	0.0049 (5)	−0.0019 (5)	−0.0001 (5)
C4	0.0314 (7)	0.0223 (6)	0.0254 (6)	0.0038 (5)	0.0011 (5)	−0.0024 (5)
C5	0.0289 (6)	0.0201 (6)	0.0196 (6)	−0.0011 (5)	−0.0001 (5)	−0.0008 (4)
C6	0.0207 (5)	0.0204 (5)	0.0181 (5)	−0.0021 (4)	0.0004 (4)	0.0017 (4)
C7	0.0200 (5)	0.0214 (5)	0.0178 (5)	−0.0016 (4)	0.0004 (4)	0.0004 (4)
C8	0.0221 (6)	0.0281 (6)	0.0202 (6)	0.0002 (5)	−0.0034 (5)	−0.0041 (5)
C9	0.0241 (6)	0.0340 (7)	0.0192 (6)	0.0062 (5)	−0.0035 (5)	−0.0039 (5)
C10	0.0194 (5)	0.0267 (6)	0.0184 (5)	−0.0006 (4)	−0.0009 (4)	−0.0007 (4)
C11	0.0179 (5)	0.0231 (6)	0.0192 (5)	−0.0020 (4)	0.0013 (4)	−0.0006 (4)
C12	0.0182 (5)	0.0229 (6)	0.0184 (5)	−0.0014 (4)	−0.0012 (4)	0.0003 (4)
C13	0.0254 (6)	0.0305 (6)	0.0269 (6)	0.0028 (5)	−0.0066 (5)	−0.0022 (5)
C14	0.0201 (6)	0.0280 (6)	0.0185 (5)	−0.0006 (5)	−0.0004 (4)	−0.0006 (4)
C15	0.0196 (6)	0.0263 (6)	0.0293 (7)	0.0030 (5)	0.0029 (5)	−0.0009 (5)
C16	0.0433 (9)	0.0655 (11)	0.0353 (8)	0.0311 (8)	−0.0068 (7)	−0.0040 (8)
N1	0.0193 (5)	0.0219 (5)	0.0195 (5)	0.0009 (4)	−0.0025 (4)	−0.0026 (4)
O1	0.0207 (4)	0.0350 (5)	0.0221 (4)	0.0076 (4)	−0.0023 (3)	−0.0034 (4)
O2	0.0229 (4)	0.0302 (5)	0.0227 (4)	0.0031 (4)	−0.0023 (3)	−0.0075 (4)

Geometric parameters (Å, º)

C1—N1	1.3744 (15)	C9—H9B	0.9900
C1—C2	1.4041 (17)	C10—C14	1.3430 (17)
C1—C6	1.4211 (16)	C10—C11	1.4747 (17)
C2—C3	1.3848 (18)	C11—O2	1.2416 (15)
C2—C13	1.5030 (17)	C11—C12	1.4510 (16)
C3—C4	1.4152 (18)	C12—N1	1.3841 (15)
C3—H3	0.9500	C13—H13A	0.9800
C4—C5	1.3755 (18)	C13—H13B	0.9800
C4—H4	0.9500	C13—H13C	0.9800
C5—C6	1.4069 (17)	C14—O1	1.3457 (15)
C5—H5	0.9500	C14—H14	0.9500
C6—C7	1.4266 (16)	C15—O1	1.4476 (15)
C7—C12	1.3799 (16)	C15—C16	1.483 (2)
C7—C8	1.4940 (16)	C15—H15A	0.9900
C8—C9	1.5356 (18)	C15—H15B	0.9900
C8—H8A	0.9900	C16—H16A	0.9800
C8—H8B	0.9900	C16—H16B	0.9800
C9—C10	1.5150 (17)	C16—H16C	0.9800
C9—H9A	0.9900	N1—H1	0.919 (17)
N1—C1—C2	128.81 (11)	C14—C10—C9	123.21 (11)
N1—C1—C6	108.52 (10)	C11—C10—C9	120.33 (11)
C2—C1—C6	122.65 (11)	O2—C11—C12	121.45 (11)

C3—C2—C1	115.81 (11)	O2—C11—C10	124.35 (11)
C3—C2—C13	122.87 (11)	C12—C11—C10	114.20 (10)
C1—C2—C13	121.31 (11)	C7—C12—N1	110.46 (10)
C2—C3—C4	122.67 (12)	C7—C12—C11	124.58 (11)
C2—C3—H3	118.7	N1—C12—C11	124.78 (11)
C4—C3—H3	118.7	C2—C13—H13A	109.5
C5—C4—C3	120.96 (12)	C2—C13—H13B	109.5
C5—C4—H4	119.5	H13A—C13—H13B	109.5
C3—C4—H4	119.5	C2—C13—H13C	109.5
C4—C5—C6	118.45 (12)	H13A—C13—H13C	109.5
C4—C5—H5	120.8	H13B—C13—H13C	109.5
C6—C5—H5	120.8	C10—C14—O1	122.38 (11)
C5—C6—C1	119.45 (11)	C10—C14—H14	118.8
C5—C6—C7	133.76 (11)	O1—C14—H14	118.8
C1—C6—C7	106.79 (10)	O1—C15—C16	108.82 (11)
C12—C7—C6	106.46 (10)	O1—C15—H15A	109.9
C12—C7—C8	122.41 (11)	C16—C15—H15A	109.9
C6—C7—C8	131.01 (11)	O1—C15—H15B	109.9
C7—C8—C9	110.46 (10)	C16—C15—H15B	109.9
C7—C8—H8A	109.6	H15A—C15—H15B	108.3
C9—C8—H8A	109.6	C15—C16—H16A	109.5
C7—C8—H8B	109.6	C15—C16—H16B	109.5
C9—C8—H8B	109.6	H16A—C16—H16B	109.5
H8A—C8—H8B	108.1	C15—C16—H16C	109.5
C10—C9—C8	113.86 (10)	H16A—C16—H16C	109.5
C10—C9—H9A	108.8	H16B—C16—H16C	109.5
C8—C9—H9A	108.8	C1—N1—C12	107.77 (10)
C10—C9—H9B	108.8	C1—N1—H1	126.4 (10)
C8—C9—H9B	108.8	C12—N1—H1	124.9 (10)
H9A—C9—H9B	107.7	C14—O1—C15	114.43 (10)
C14—C10—C11	116.42 (11)		

N1—C1—C2—C3	177.44 (12)	C8—C9—C10—C11	36.83 (16)
C6—C1—C2—C3	−0.47 (18)	C14—C10—C11—O2	−7.56 (19)
N1—C1—C2—C13	−1.2 (2)	C9—C10—C11—O2	170.33 (12)
C6—C1—C2—C13	−179.16 (11)	C14—C10—C11—C12	172.13 (11)
C1—C2—C3—C4	1.28 (19)	C9—C10—C11—C12	−9.99 (16)
C13—C2—C3—C4	179.95 (13)	C6—C7—C12—N1	−0.32 (13)
C2—C3—C4—C5	−0.9 (2)	C8—C7—C12—N1	176.05 (11)
C3—C4—C5—C6	−0.35 (19)	C6—C7—C12—C11	−175.65 (11)
C4—C5—C6—C1	1.11 (17)	C8—C7—C12—C11	0.72 (19)
C4—C5—C6—C7	−178.20 (13)	O2—C11—C12—C7	169.91 (12)
N1—C1—C6—C5	−179.00 (10)	C10—C11—C12—C7	−9.78 (17)
C2—C1—C6—C5	−0.72 (18)	O2—C11—C12—N1	−4.76 (19)
N1—C1—C6—C7	0.48 (13)	C10—C11—C12—N1	175.55 (11)
C2—C1—C6—C7	178.76 (11)	C11—C10—C14—O1	176.51 (11)
C5—C6—C7—C12	179.28 (13)	C9—C10—C14—O1	−1.3 (2)
C1—C6—C7—C12	−0.09 (13)	C2—C1—N1—C12	−178.82 (12)

C5—C6—C7—C8	3.3 (2)	C6—C1—N1—C12	−0.68 (13)
C1—C6—C7—C8	−176.04 (12)	C7—C12—N1—C1	0.63 (13)
C12—C7—C8—C9	25.96 (16)	C11—C12—N1—C1	175.94 (11)
C6—C7—C8—C9	−158.65 (12)	C10—C14—O1—C15	176.41 (11)
C7—C8—C9—C10	−42.40 (15)	C16—C15—O1—C14	174.05 (13)
C8—C9—C10—C14	−145.43 (12)		

Hydrogen-bond geometry (Å, º)

*Cg*2 is the centroid of the benzene (C1–C6) ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.919 (17)	2.034 (17)	2.9235 (14)	162.2 (15)
C14—H14···O2^{ii}	0.95	2.52	3.2396 (15)	133
C13—H13*B*···*Cg*2^{iii}	0.98	2.76	3.5669 (15)	140

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