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Crystal structure and Hirshfeld surface analyses, interaction energy calculations and energy frameworks of methyl 2-[(4-cyanophenyl)methoxy]quinoline-4-carboxylate

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The title compound, $C_{19}H_{14}N_2O_3$, features competition and interplay of a range of weak interactions, which actualize under the absence of conventional hydrogen-bond donors. Two kinds of stacking interactions, namely slipped antiparallel interactions of cyanophenyl groups as well as quinoline and carboxy groups, are primarily important. In combination with relatively short tetrel $OCH_3 \cdots N \equiv C$ bonds $[C \cdots N = 3.146 (3) \text{ Å}]$ they are responsible for the generation of the layers, while the interlayer bonding occurs via $C-H \cdots O$ and C-H···N weak hydrogen bonds. These findings are consistent with the results of Hirshfeld surface analysis and calculated interaction energies. Contributions of the $C \cdots C$, $C \cdots N/N \cdots C$ and $C \cdots O/O \cdots C$ contacts originating in the stacking interactions account for 17.0% to the surface area. The largest interactions energies are associated with the two kinds of stacks $(-45.8 \text{ and } -24.3 \text{ kJ mol}^{-1})$ and they are superior to the energies of weak hydrogen bond and tetrel interactions $(-12.4 \text{ to } -22.4 \text{ kJ mol}^{-1})$. Evaluation of the electrostatic, dispersion and total energy frameworks indicate that the consolidation is dominated via the dispersion energy contributions.

1. Chemical context

Heterocyclic compounds, especially nitrogen-containing systems such as quinoline derivatives, play a pivotal role in medicinal chemistry due to their broad spectrum of biological activities (Filali Baba et al., 2019, 2020; Hayani et al., 2021a; El-Mrabet et al., 2023, 2025; Bouzian et al., 2018, 2021). These compounds exhibit antimicrobial (Salam et al., 2023), antifungal (Chen et al., 2021), anti-Alzheimer's (Chen et al., 2023), anti-infective (Muruganantham et al., 2004), antileishmanial (Chanquia et al., 2019), anti-HIV (Strekowski et al., 1991), anti-inflammatory (Ghanim et al., 2022), antiviral (Kaur & Kumar, 2021), and corrosion inhibitive activities (Mahamoud et al., 2006; Filali Baba et al., 2016a,b). Their structural flexibility and ability to interact with diverse biological targets make quinolines attractive frameworks for drug development, especially in addressing significant therapeutic challenges. In this context, we report herein the synthesis and comprehensive structural characterization of a novel quinoline-based compound, methyl 2-(4-cyanobenzyloxy)quinoline-4carboxylate (I). The target molecule was obtained via an Oalkylation reaction of methyl 2-oxo-1,2-dihydroquinoline-4carboxylate with 4-(bromomethyl)benzonitrile under phasetransfer catalysis (PTC). The synthesized compound was analyzed using ¹H and ¹³C NMR, FT-IR spectroscopy, singlecrystal X-ray diffraction, and Hirshfeld surface analysis to elucidate its molecular and crystal structure.



2. Structural commentary

The title compound, (I), contains the almost planar quinoline and cyanophenyl moieties (Fig. 1), where the planar *A* (C1– C6), *B* (N1/C1/C6–C9) and *C* (C13–C18) rings are oriented at dihedral angles of A/B = 0.56 (5)°, A/C = 14.47 (6)° and B/C =15.02 (6)°. The exocyclic atoms O1, O2, O3, C10, C11 and C12 are also nearly coplanar with the quinoline framework and lie 0.005 (2), -0.030 (2), 0.016 (1), -0.015 (2), -0.067 (3) and -0.037 (2) Å, respectively, away from its mean plane.

In the ester group, the O1–C10 and O2–C10 bond lengths are 1.177 (2) Å and 1.308 (2) Å, respectively. This strict differentiation of the C–O bonds indicates mainly the localized single and double bounds rather than delocalized bonding arrangement. The O1–C10–O2 bond angle of 121.6 (2)° agrees well with the parameters for comparable methyl 2-phenyl quinoline-4-carboxylate [122.42 (14)°; Mague *et al.*, 2016], and methyl 2-oxo-1-(propyn-2-yl)-1,2-di hydroquinoline-4-carboxylate [122.55 (12)°; El-Mrabet *et al.*, 2023]. The planes of the carbomethoxy group [defined by the atoms C7, C10, O1 and O2] and ring *B* are related by 0.96 (17)°

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

$D - H \cdot \cdot \cdot A$	$D-\mathrm{H}$	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$C3-H3\cdots O3^{i}$	0.93	2.75	3.651 (2)	163
$C5-H5\cdots O1$	0.93	2.25	2.883 (2)	125
$C15-H15\cdots O1^{ii}$	0.93	2.48	3.337 (2)	154
$C18-H18\cdots N2^{iii}$	0.93	2.68	3.558 (3)	158

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

indicating a coplanar arrangement. The latter is partly caused by the weak intramolecular C5–H5···O1 hydrogen bond (Table 1), similarly to in methyl 6-chloro-1-methyl-2-oxo-1,2dihydroquinoline-4-carboxylate with a corresponding dihedral angle of 4.08 (8)° (Filali Baba *et al.*, 2022). As evidenced by the C11–O2–C10–C7 [178.98 (18)°] torsion angle, the ester group attached to the quinoline moiety is in a *syn* peripheral conformation. The corresponding torsion angles for the related derivatives of benzyl [176.06 (11)°; Bouzian *et al.*, 2018] and ethyl [–176.71 (15)°; Sunitha *et al.*, 2015] quinoline-4-carboxylates represent *syn*- and *anti*-peripheral conformations, respectively.

3. Supramolecular features

In the crystal, intermolecular C15-H15···O1ⁱⁱ hydrogen bonds [symmetry code (ii): x + 1, $y + \frac{1}{2}$, $z + \frac{3}{2}$; Table 1] link the molecules into the infinite chains along the *b*-axis direction (Fig. 2). However, the entire non-covalent framework in the structure may be best described as consisting of corrugated layers, which propagate parallel to the *ac* plane and are linked in the third dimension by a set of very weak hydrogen bonds. The layers themselves are sustained by two kinds of stacking interactions. First, two inversion-related cyanophenyl moieties [symmetry code: (v) -x + 1, -y + 1, -z + 1] afford antiparallel



Figure 1

The molecular structure of the title compound, with the atom and ring labelling schemes and displacement ellipsoids drawn at the 50% probability level. The dotted line indicates a possible weak hydrogen bond.



Figure 2

Fragment of the crystal structure showing hydrogen-bonded chains along the *b*-axis direction and stacking interactions between the adjacent chains. [Symmetry code (ii): x + 1, $y + \frac{1}{2}$, $z + \frac{3}{2}$.]

stacks with interplanar distances of 3.660 (2) Å, in which the centroids of C19–N2 groups [*Cg*2] are situated almost exactly above the centroids of the corresponding aromatic rings (*Cg*1) at 3.735 (2) Å (Figs. 2, 3). The second kind of stacking interaction is identified between nearly parallel ester groups and heterocyclic rings *B* [symmetry code: (vi) $x + \frac{1}{2}$, $y, -z + \frac{3}{2}$; interplanar angle is 3.98 (11)°], with separation $Cg3 \cdots C10^{vi} = 3.817$ (2) Å (*Cg3* is the ring *B* centroid). These layers are further consolidated by relatively short tetrel bonding (Varadwaj *et al.*, 2023) of the type OCH₃···N=C [C11···N2^{iv} = 3.146 (3) Å, symmetry code (iv): $-x + \frac{1}{2}, -y + 1, x + \frac{1}{2}$], which is well compatible to both stacking patterns (Fig. 3).



Figure 3

(a) Projection of the structure nearly on the *ac*-plane showing assembly of the layers by means of stacking interactions (indicated in blue) and tetrel bonds of the type OCH₃···N=C (indicated with dotted red lines). (b) Packing of successive corrugated layers viewed in a projection on the *bc*-plane, with dotted lines representing interlayer weak hydrogen bonding. The individual layers are identified with blue and red colors. *Cg*1, *Cg*2 and *Cg*3 are centroids of the groups C13–C18, N2/C19 and N1/C1/C6–C9, respectively. [Symmetry codes: (iii) $-x + \frac{1}{2}$, $y - \frac{1}{2}$, z; (v) -x + 1, -y + 1, -z + 1; (vi) $x + \frac{1}{2}$, $y - z + \frac{3}{2}$.]

The resulting corrugated layers are separated by 7.849 Å, which is a half of the unit cell parameter b (Fig. 3). In addition to the above most prominent C15-H15...O1ⁱⁱ hydrogen bonds, the suite of interlayer interactions also comprises weaker C3-H3···O3ⁱ and C18-H18···N2ⁱⁱⁱ bonds [symmetry codes (i): $x + \frac{3}{2}$, $y - \frac{1}{2}$, z; (iii) $x + \frac{1}{2}$, $y - \frac{1}{2}$, z; Table 1]. These interactions are also directional, with corresponding angles at the H atoms of 163 and 158°, respectively. No C-H···(ring) or π (ring)-(ring) interactions are observed. The title compound highlights rather the interplay of different kinds of stacking interactions, weak hydrogen and tetrel bonding for consolidating the 3D architecture. The combination of Hirshfeld surface analysis and energy framework calculations reveals dispersion energy as the dominant contributor, offering new insights into the packing features of quinoline-based systems and their potential in crystal engineering.

4. Hirshfeld surface analysis

For visualizing the intermolecular interactions in the crystal of the title compound, a Hirshfeld surface (HS) analysis (Hirshfeld, 1977; Spackman & Jayatilaka, 2009) was carried out using *Crystal Explorer 17.5* (Spackman *et al.*, 2021). In the HS plotted over d_{norm} (Fig. 4), the contact distances equal, shorter and longer than the sum of van der Waals radii are shown in white, red and blue, respectively (Venkatesan *et al.*, 2016). The brightest red spots correspond to the donor and acceptor sites of the C15–H15···O1ⁱⁱ bonds, whereas the positions of the tetrel OCH₃···N=C bonds are also clearly visible as a pair of more diffuse red spots.

The overall two-dimensional fingerprint plots and those delineated into the contributions of the individual types of the contacts (McKinnon *et al.*, 2007) are shown in Fig. 5. Beyond the expected far dominant significance of $H \cdots H$ contacts (43.8%), the main contributors to the Hirshfeld surface are also associated with the H atoms: $C \cdots H/H \cdots C = 14.3\%$, $N \cdots H/H \cdots N = 14.1\%$ and $O \cdots H/H \cdots O = 9.9\%$. However, only the latter ones appear in the plots in the form of two



Figure 4 The Hirshfeld surface of the title compound mapped over d_{norm} .



Figure 5

Two-dimensional fingerprint plots for the title compound: (a) all interactions and delineated into the principal contributions of (b) $H \cdots H$, (c) $C \cdots H$ / $H \cdots C$, (d) $O \cdots H/H \cdots O$, (e) $N \cdots H/H \cdots N$, (f) $C \cdots C$, (g) $C \cdots N/N \cdots C$ and (h) $C \cdots O/O \cdots C$ contacts. Other minor contributors are $O \cdots O$ (0.5%) and $N \cdots O/O \cdots N$ (0.4%) contacts.

relatively sharp spikes pointing to the lower left, thus indicating the hydrogen-bond interactions (shortest $H \cdots O = 2.35$ Å). In the case of $N \cdots H/H \cdots N$ contacts, these spikes are much shorter and diffuse, since most points originate rather in the tetrel interactions of methyl and cyano groups. In addition, the light-blue area centered at *ca* 3.80 Å in the plot for $C \cdots C$ contacts indicates the above stacking interactions. In total, the corresponding contacts, *i.e.* $C \cdots C$, $C \cdots N/N \cdots C$ and $C \cdots O/O \cdots C$, deliver as much as 17.0% to the surface area.

The nearest coordination environment of a molecule can be determined from the color patches on the HS based on how close to other molecules they are. The Hirshfeld surface representations of contact patches plotted onto the surface are shown for the $H \cdots H$, $H \cdots C/C \cdots H$, $H \cdots N/N \cdots H$, $C \cdots C$ and $H \cdots O/O \cdots H$ interactions in Fig. S2*a*–*e*, respectively, in the supporting information. The Hirshfeld surface analysis confirms the importance of H-atom contacts in establishing the packing. The large number of $H \cdots H$, $H \cdots C/C \cdots H$, $H \cdots N/N \cdots H$, $C \cdots C$ and $H \cdots O/O \cdots H$ interactions suggest that van der Waals interactions and hydrogen bonding play the major roles in the crystal packing (Hathwar *et al.*, 2015).

5. Interaction energy calculations and energy frameworks

The intermolecular interaction energies were calculated using the CE–B3LYP/6–31G(d,p) energy model available in *Crystal Explorer 17.5* (Spackman *et al.*, 2021), where a cluster of molecules is generated by applying crystallographic symmetry operations with respect to a selected central molecule within the radius of 3.8 Å by default (Turner *et al.*, 2014). The total intermolecular energy (E_{tot}) is the sum of electrostatic (E_{ele}), polarization (E_{pol}), dispersion (E_{dis}) and exchange-repulsion (E_{rep}) energies (Turner *et al.*, 2015). With a cut-off of $|E_{tot}| > 12.0 \text{ kJ mol}^{-1}$, seven symmetryindependent paths were identified for the closest environment of the title molecules (Table 2). The highest energy $E_{tot} = -45.8 \text{ kJ mol}^{-1}$ corresponds to the pairing pattern involving stacking of quinoline and carboxy groups (path $A \cdots B$, Fig. 6).



Figure 6

The principal pathways of intermolecular interactions, identified with a cut-off limit of 12 kJ mol⁻¹, which involve (*a*) stacking and tetrel interactions and (*a*) weak hydrogen bonding. The interaction energies are given in kJ mol⁻¹.

Table 2

Calculated interaction energies (kJ mol^{-1}).

Interaction energies were calculated employing the CE-B3LYP/6–31G(d,p) functional/basis set combination. The scale factors used to determine E_{tot} are $k_{ele} = 1.057$, $k_{pol} = 0.740$, $k_{dis} = 0.871$, and $k_{rep} = 0.618$ (Mackenzie *et al.*, 2017). *R* is the distance between the centroids of the interacting molecules.

Path	Symmetry code	Type ^a	<i>R</i> (Å)	E_{ele}	$E_{\rm pol}$	$E_{\rm dis}$	$E_{\rm rep}$	$E_{\rm tot}$
$A \cdots B$	$x + \frac{1}{2}, y, -z + \frac{3}{2}$	stacking	5.77	-5.3	-2.1	-66.2	30.8	-45.8
$A \cdots C$	-x + 1, -y + 1, -z + 1	stacking	12.05	-6.1	-2.4	-25.1	9.3	-24.3
$B \cdots C$	$-x + \frac{1}{2}, -y + 1, z + \frac{1}{2}$	tetrel	15.89	-10.5	-2.7	-5.0	8.2	-12.4
$A \cdots D$	$x + 1, y + \frac{1}{2}, z + \frac{3}{2}$	$C-H \cdots O$, dispersion	8.93	-10.3	-2.0	-25.3	19.5	-22.4
$A \cdots E$	$-x + \frac{1}{2}, y + \frac{1}{2}, z$	C−H···N	8.73	-10.1	-2.7	-11.7	8.2	-17.8
$A \cdot \cdot \cdot F$	$x + \frac{3}{2}, y - \frac{1}{2}, z$	$C-H\cdots O$	8.79	-4.2	-0.5	-20.4	10.8	-15.8
$A \cdots G$	$x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$	dispersion	9.56	-4.3	-1.6	-16.0	7.4	-15.1

Note: (a) For details of the interaction modes see Fig. 6. Weak dispersion interaction $A \cdots G$ is not shown in the Figure.

The primary contributor here is London dispersion (E_{dis} = -66.2 kJ mol⁻¹), due to the very large interaction area. Stacking of cyanophenyl moieties is perceptibly weaker with $E_{\rm tot} = -24.3 \text{ kJ mol}^{-1}$. This value approaches the parameter calculated for the slipped antiparallel dimer of nitrobenzene molecules (-28.2 kJ mol⁻¹; Tsuzuki et al., 2006). This stacking is also clearly distinguishable in the present energy landscape and it is even superior to the energies of the intermolecular interactions, which correspond to weak hydrogen bonding $(-15.8 \text{ and } -17.8 \text{ kJ mol}^{-1}; \text{ Table 2})$. In the case of the $A \cdots D$ pair (Fig. 6), slightly higher total energy of $-22.4 \text{ kJ mol}^{-1}$ is due to a combination of weak hydrogen bond C15-H15...O1ⁱⁱ and dispersion forces, with the corresponding principal contributors $E_{ele} = -10.3$ and $E_{dis} =$ -25.3 kJ mol⁻¹. This is in line with larger interaction area and generation of additional vdW contacts, e.g. O2···C3ⁱⁱ = 3.534 (2) Å. Finally, the tetrel bonds $OCH_3 \cdots N \equiv C$ (pair $B \cdots C$, Fig. 6) are very similar in energy to the weak hydrogen bonds ($E_{\text{tot}} = -12.4 \text{ kJ mol}^{-1}$) and therefore their significance to the crystal packing may be regarded as comparable.

The evaluation of the electrostatic, dispersion and total energy frameworks indicate that the consolidation is dominated *via* the dispersion energy contributions (Fig. S2 in the supporting information).

6. Database survey

A search of the Cambridge Structural Database (CSD; updated 16 May 2025; Groom et al., 2016) reveals 18 relevant hits, which include the 2-oxo-1,2-dihydroquinoline-4carboxylate core. Two of these entries, namely PEDKAO (Filali Baba et al., 2022) and ROKCIG (Filali Baba et al., 2019), involve additional Cl-atoms installed on the aromatic rings. Oxygen-derivatization of the selected core is a particularly rare feature. Among 13 alkyl-substituted structures retrieved, including AROPAB (Bouzian et al., 2020) and SECCAH (Hayani et al., 2021b), most were identified as N-alkylated derivatives. The only structural precedent for the O-alkylation of the above core is provided by 2-ethoxy-2-2-(2-ethoxy-2-oxoethoxy)quinoline-4-carboxylate oxoethyl (refcode LIRKIJ; Bouzian et al., 2018). This highlights the need for detailed structural validation when classifying substitution patterns on such frameworks. From a supramolecular perspective, the crystal packing of ROKCIG reveals no π - π stacking interactions or C-H···Cl hydrogen bonds, but it differs markedly from that of the title compound. It forms an inversion dimer through C-H···O hydrogen bonds, lacking the chain-like hydrogen-bonded pattern seen in the title structure. In contrast, its halogen-free analog (ROKCOM; Filali Baba *et al.*, 2019) forms molecular bands *via* C-H···O hydrogen bonding, further stabilized by weak π - π contacts.

7. Synthesis and crystallization

The procedure for synthesizing the methyl 2-[(4-cyanobenzyl)oxy]quinoline-4-carboxylate derivative is as follows. To a solution of methyl 2-oxo-1,2-dihydroquinoline-4-carboxylate (0.60 g, 2.20 mmol) in 15 ml of dimethylformamide (DMF), 4-(bromomethyl)benzonitrile (0.21 ml, 2.41 mmol), K₂CO₃ (0.85 g, 6.10 mmol) and tetra-n-butylammonium bromide (TBAB; 0.05 g, 0.18 mmol) were added and the reaction mixture was agitated at ambient temperature for a period of 12 h. Following completion of the reaction, the precipitated inorganic salts were removed through filtration and the solvent was evaporated under reduced pressure. The resultant residue was dissolved in dichloromethane. This solution was subsequently dried using anhydrous sodium sulfate and then concentrated under reduced pressure. The compound was purified through column chromatography, employing a hexane/ethyl acetate eluent (4:1 v/v). The target product was obtained in a yield of 45%. It was further recrystallized from a mixture of dichloromethane and hexane (1:4 v/v) giving transparent colorless crystals, m.p. = 394 K. ¹H NMR $(300 \text{ MHz}, \text{ CDCl}_3), \delta$, ppm: 8.61 (dd, J = 8.6, 1.4 Hz, 1H,CH_{Ar}), 7.90–7.86 (*m*, 1H, CH_{Ar}), 7.70–7.60 (*m*, 5H, CH_{Ar}), 7.53-7.47 (m, 2H, CH_{Ar}), 5.63 (s, 2H, CH₂), 4.03 (s, 3H, CH₃). ¹³C NMR (75 MHz, CDCl₃), δ, ppm: 166.21, 160.57, 147.34, 142.64, 138.51, 132.40, 130.25, 128.35, 127.85, 125.77, 125.74, 122.1, 118.87, 115.18, 111.74, 66.82, 52.87. FT-IR (cm⁻¹): 2858 $(C-H_{sp}^{3})$, 1727 (C=O), 2226 (C=N), 1575-1607 (C=C, aromatic stretching); 1238 (C-O-C, ether bond).

8. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. H atoms were positioned geometrically and refined as riding, with C-H = 0.95 Å (aromatic

 Table 3

 Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{14}N_2O_3$
$M_{\rm r}$	318.32
Crystal system, space group	Orthorhombic, Pbca
Temperature (K)	299
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.7810 (6), 15.6978 (11), 25.966 (2)
$V(Å^3)$	3171.6 (4)
Ζ	8
Radiation type	Μο Κα
$\mu (\mathrm{mm}^{-1})$	0.09
Crystal size (mm)	$0.26 \times 0.22 \times 0.19$
•	
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON
	3 CPAD
Absorption correction	Multi-scan (SADABS; Krause et
-	al., 2015)
T_{\min}, T_{\max}	0.719, 0.745
No. of measured, independent and	78015, 3234, 2897
observed $[I > 2\sigma(I)]$ reflections	
R _{int}	0.041
$(\sin \theta / \lambda)_{max} (\text{\AA}^{-1})$	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.049, 0.136, 1.05
No. of reflections	3234
No. of parameters	218
H-atom treatment	H-atom parameters constrained
$\Delta \rho_{\text{max}} \Delta \rho_{\text{max}} (e \text{\AA}^{-3})$	0.25 - 0.21

Computer programs: APEX4 (Bruker, 2019), SAINT (Bruker, 2016), SHELXT2018/2 (Sheldrick, 2015a), SHELXL2019/1 (Sheldrick, 2015b), DIAMOND (Brandenburg, 1999) and WinGX (Farrugia, 2012).

CH), 0.97 Å (CH₂) and 0.98 Å (CH₃) and with $U_{iso}(H) = 1.2U_{eq}$ or $1.5U_{eq}$ of the carrier C-atom for CH and CH₂ or CH₃ groups, respectively. Four outliers (108, 204, 222 and 232) were omitted in the last cycles of refinement.

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Crystal structure and Hirshfeld surface analyses, interaction energy calculations and energy frameworks of methyl 2-[(4-cyanophenyl)methoxy]quinoline-4carboxylate

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Computing details

Methyl 2-[(4-cyanophenyl)methoxy]quinoline-4-carboxylate

Crystal data

 $C_{19}H_{14}N_2O_3$ $M_r = 318.32$ Orthorhombic, *Pbca* a = 7.7810 (6) Å b = 15.6978 (11) Å c = 25.966 (2) Å V = 3171.6 (4) Å³ Z = 8F(000) = 1328

Data collection

Bruker D8 VENTURE PHOTON 3 CPAD diffractometer Radiation source: microfocus sealed X-ray tube φ and ω scans Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015) $T_{\min} = 0.719$, $T_{\max} = 0.745$ 78015 measured reflections

Refinement

Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.049$ $wR(F^2) = 0.136$ S = 1.053234 reflections 218 parameters 0 restraints Primary atom site location: structure-invariant direct methods $D_x = 1.333 \text{ Mg m}^{-3}$ Mo K α radiation, $\lambda = 0.71073 \text{ Å}$ Cell parameters from 9947 reflections $\theta = 3.0-26.1^{\circ}$ $\mu = 0.09 \text{ mm}^{-1}$ T = 299 KPrism, colourless $0.26 \times 0.22 \times 0.19 \text{ mm}$

3234 independent reflections 2897 reflections with $I > 2\sigma(I)$ $R_{int} = 0.041$ $\theta_{max} = 26.4^{\circ}, \ \theta_{min} = 2.6^{\circ}$ $h = -9 \rightarrow 9$ $k = -19 \rightarrow 17$ $l = -32 \rightarrow 32$

Secondary atom site location: difference Fourier map Hydrogen site location: inferred from neighbouring sites H-atom parameters constrained $w = 1/[\sigma^2(F_o^2) + (0.0634P)^2 + 1.2076P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{max} < 0.001$ $\Delta\rho_{max} = 0.25$ e Å⁻³ $\Delta\rho_{min} = -0.21$ 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.

	x	у	Ζ	$U_{ m iso}$ */ $U_{ m eq}$
01	0.6069 (3)	0.13417 (10)	0.85140 (5)	0.1081 (8)
O2	0.4881 (2)	0.25179 (9)	0.82571 (5)	0.0777 (5)
O3	0.46253 (17)	0.26146 (7)	0.64306 (4)	0.0539 (3)
N1	0.58631 (19)	0.12898 (8)	0.65387 (5)	0.0472 (3)
N2	0.1671 (3)	0.61040 (12)	0.47079 (7)	0.0908 (7)
C1	0.6466 (2)	0.06874 (9)	0.68811 (6)	0.0434 (4)
C2	0.7132 (3)	-0.00718 (11)	0.66761 (7)	0.0587 (5)
H2	0.7149	-0.0151	0.6321	0.070*
C3	0.7751 (3)	-0.06941 (11)	0.69907 (8)	0.0626 (5)
Н3	0.8188	-0.1193	0.6849	0.075*
C4	0.7735 (3)	-0.05892 (11)	0.75228 (8)	0.0573 (4)
H4	0.8159	-0.1018	0.7734	0.069*
C5	0.7101 (2)	0.01379 (10)	0.77346 (6)	0.0490 (4)
Н5	0.7105	0.0202	0.8091	0.059*
C6	0.64375 (19)	0.07983 (9)	0.74226 (6)	0.0394 (3)
C7	0.57211 (19)	0.15814 (9)	0.76106 (5)	0.0379 (3)
C8	0.5129 (2)	0.21656 (9)	0.72667 (5)	0.0407 (3)
H8	0.4662	0.2678	0.7380	0.049*
C9	0.5236 (2)	0.19824 (9)	0.67342 (6)	0.0420 (4)
C10	0.5590 (2)	0.17753 (10)	0.81731 (6)	0.0459 (4)
C11	0.4652 (3)	0.27757 (17)	0.87850 (7)	0.0821 (7)
H11A	0.4454	0.3379	0.8799	0.123*
H11B	0.5666	0.2638	0.8979	0.123*
H11C	0.3683	0.2482	0.8929	0.123*
C12	0.4609 (3)	0.24802 (11)	0.58871 (6)	0.0529 (4)
H12A	0.3873	0.2002	0.5802	0.063*
H12B	0.5761	0.2357	0.5765	0.063*
C13	0.3942 (2)	0.32785 (10)	0.56377 (6)	0.0455 (4)
C14	0.3756 (3)	0.40331 (11)	0.59018 (6)	0.0630 (5)
H14	0.4035	0.4054	0.6250	0.076*
C15	0.3163 (3)	0.47576 (11)	0.56604 (7)	0.0668 (6)
H15	0.3036	0.5261	0.5845	0.080*
C16	0.2760 (3)	0.47327 (10)	0.51442 (6)	0.0531 (4)
C17	0.2941 (3)	0.39821 (11)	0.48727 (7)	0.0680 (6)
H17	0.2664	0.3962	0.4525	0.082*
C18	0.3534 (3)	0.32634 (11)	0.51194 (6)	0.0630 (5)
H18	0.3663	0.2760	0.4935	0.076*
C19	0.2146 (3)	0.54952 (12)	0.48955 (7)	0.0663 (6)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\hat{A}^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
01	0.207 (2)	0.0747 (10)	0.0423 (7)	0.0505 (12)	-0.0176 (10)	0.0059 (7)
O2	0.1235 (13)	0.0744 (9)	0.0352 (6)	0.0408 (9)	0.0013 (7)	-0.0046 (6)
03	0.0886 (9)	0.0396 (6)	0.0336 (6)	0.0134 (6)	-0.0052 (6)	0.0023 (4)
N1	0.0644 (8)	0.0390 (7)	0.0384 (7)	0.0040 (6)	-0.0002 (6)	0.0014 (5)
N2	0.148 (2)	0.0554 (10)	0.0691 (11)	0.0207 (11)	-0.0237 (12)	0.0127 (9)
C1	0.0493 (8)	0.0364 (7)	0.0445 (8)	0.0001 (6)	0.0009 (7)	0.0025 (6)
C2	0.0774 (12)	0.0459 (9)	0.0529 (10)	0.0109 (9)	0.0050 (9)	-0.0033 (7)
C3	0.0752 (13)	0.0415 (9)	0.0710 (12)	0.0152 (9)	0.0028 (10)	-0.0019 (8)
C4	0.0602 (10)	0.0420 (9)	0.0697 (11)	0.0072 (8)	-0.0049 (9)	0.0116 (8)
C5	0.0531 (9)	0.0437 (8)	0.0501 (9)	-0.0003 (7)	-0.0043 (7)	0.0093 (7)
C6	0.0395 (8)	0.0354 (7)	0.0433 (8)	-0.0045 (6)	-0.0002 (6)	0.0042 (6)
C7	0.0398 (7)	0.0367 (7)	0.0373 (7)	-0.0051 (6)	-0.0001 (6)	0.0037 (6)
C8	0.0505 (9)	0.0338 (7)	0.0376 (8)	0.0005 (6)	0.0011 (6)	0.0007 (6)
C9	0.0530 (9)	0.0353 (7)	0.0376 (8)	0.0009 (6)	-0.0015 (6)	0.0042 (6)
C10	0.0553 (9)	0.0444 (8)	0.0380 (8)	-0.0031 (7)	-0.0015 (7)	0.0048 (6)
C11	0.1124 (18)	0.0963 (16)	0.0377 (10)	0.0283 (14)	0.0028 (11)	-0.0135 (10)
C12	0.0792 (12)	0.0454 (8)	0.0341 (8)	0.0106 (8)	-0.0042 (8)	-0.0011 (6)
C13	0.0622 (10)	0.0387 (8)	0.0357 (7)	0.0012 (7)	-0.0037 (7)	0.0008 (6)
C14	0.1068 (16)	0.0476 (9)	0.0347 (8)	0.0127 (10)	-0.0189 (9)	-0.0046 (7)
C15	0.1149 (17)	0.0423 (9)	0.0432 (9)	0.0134 (10)	-0.0172 (10)	-0.0075 (7)
C16	0.0788 (12)	0.0389 (8)	0.0416 (8)	0.0011 (8)	-0.0119 (8)	0.0033 (6)
C17	0.1211 (18)	0.0473 (9)	0.0356 (8)	0.0025 (10)	-0.0210 (10)	0.0000 (7)
C18	0.1131 (16)	0.0393 (8)	0.0366 (8)	0.0046 (9)	-0.0112 (9)	-0.0049 (7)
C19	0.1043 (16)	0.0469 (10)	0.0476 (9)	0.0043 (10)	-0.0163 (10)	0.0023 (8)

Atomic displacement parameters $(Å^2)$

Geometric parameters (Å, °)

01—C10	1.177 (2)	C7—C10	1.496 (2)
O2—C10	1.308 (2)	C8—C9	1.415 (2)
O2—C11	1.440 (2)	С8—Н8	0.9300
O3—C9	1.3535 (18)	C11—H11A	0.9600
O3—C12	1.4269 (18)	C11—H11B	0.9600
N1—C9	1.296 (2)	C11—H11C	0.9600
N1—C1	1.380 (2)	C12—C13	1.503 (2)
N2—C19	1.135 (2)	C12—H12A	0.9700
C1—C2	1.404 (2)	C12—H12B	0.9700
C1—C6	1.417 (2)	C13—C14	1.376 (2)
C2—C3	1.362 (2)	C13—C18	1.383 (2)
С2—Н2	0.9300	C14—C15	1.378 (2)
C3—C4	1.391 (3)	C14—H14	0.9300
С3—Н3	0.9300	C15—C16	1.377 (2)
C4—C5	1.360 (2)	C15—H15	0.9300
C4—H4	0.9300	C16—C17	1.380 (2)
C5—C6	1.413 (2)	C16—C19	1.442 (2)
С5—Н5	0.9300	C17—C18	1.377 (2)

C6—C7	1.435 (2)	C17—H17	0.9300
C7—C8	1.360 (2)	C18—H18	0.9300
C10—O2—C11	117.47 (15)	O2—C10—C7	111.91 (13)
C9—O3—C12	118.09 (12)	O2—C11—H11A	109.5
C9—N1—C1	116.79 (13)	O2—C11—H11B	109.5
N1—C1—C2	117.56 (14)	H11A—C11—H11B	109.5
N1—C1—C6	123.34 (14)	O2—C11—H11C	109.5
C2—C1—C6	119.09 (14)	H11A—C11—H11C	109.5
C3—C2—C1	120.79 (16)	H11B—C11—H11C	109.5
C3—C2—H2	119.6	O3—C12—C13	107.82 (13)
С1—С2—Н2	119.6	O3—C12—H12A	110.1
C2—C3—C4	120.51 (16)	C13—C12—H12A	110.1
C2—C3—H3	119.7	03—C12—H12B	110.1
С4—С3—Н3	119.7	C13—C12—H12B	110.1
C5—C4—C3	120.29 (16)	H12A—C12—H12B	108.5
C5—C4—H4	119.9	C14—C13—C18	118.39 (15)
C3—C4—H4	119.9	C14-C13-C12	122.62 (14)
C4—C5—C6	121.09 (16)	C18—C13—C12	118.97 (14)
C4—C5—H5	119.5	C13—C14—C15	121.25 (15)
C6—C5—H5	119.5	C13—C14—H14	119.4
C5—C6—C1	118.22 (14)	C15—C14—H14	119.4
C5—C6—C7	125.11 (14)	C16—C15—C14	119.71 (16)
C1—C6—C7	116.66 (13)	C16—C15—H15	120.1
C8—C7—C6	119.06 (13)	C14—C15—H15	120.1
C8—C7—C10	118.73 (13)	C15—C16—C17	119.87 (15)
C6—C7—C10	122.21 (13)	C15—C16—C19	119.21 (15)
C7—C8—C9	118.99 (14)	C17—C16—C19	120.92 (14)
С7—С8—Н8	120.5	C18—C17—C16	119.73 (15)
С9—С8—Н8	120.5	С18—С17—Н17	120.1
N1-C9-O3	121.28 (14)	С16—С17—Н17	120.1
N1-C9-C8	125.15 (14)	C17—C18—C13	121.04 (15)
03-09-08	113.57 (13)	С17—С18—Н18	119.5
01-01-02	121.57 (16)	C13—C18—H18	119.5
01	126.52 (16)	N2-C19-C16	178.7 (2)
	120102 (10)		(-)
C9—N1—C1—C2	179.24 (16)	C12—O3—C9—C8	-177.52 (15)
C9—N1—C1—C6	-0.5(2)	C7—C8—C9—N1	0.0 (3)
N1—C1—C2—C3	179.93 (18)	C7—C8—C9—O3	-179.29 (14)
C6-C1-C2-C3	-0.3(3)	C11—O2—C10—O1	-2.1(3)
C1—C2—C3—C4	0.1 (3)	C11—O2—C10—C7	178.98 (18)
C2-C3-C4-C5	-0.1(3)	C8-C7-C10-O1	-178.7(2)
C3—C4—C5—C6	0.4 (3)	C6-C7-C10-O1	1.8 (3)
C4—C5—C6—C1	-0.7 (2)	C8—C7—C10—O2	0.2 (2)
C4—C5—C6—C7	179.06 (16)	C6—C7—C10—O2	-179.31 (15)
N1-C1-C6-C5	-179.64 (15)	C9—O3—C12—C13	-177.94(14)
C2-C1-C6-C5	0.6 (2)	O3-C12-C13-C14	12.1 (3)
N1 - C1 - C6 - C7	0.6(2)	03-C12-C13-C18	-169.42(18)
	(-)		

C2—C1—C6—C7	-179.15 (15)	C18—C13—C14—C15	0.6 (3)
C5—C6—C7—C8	179.86 (15)	C12—C13—C14—C15	179.1 (2)
C1—C6—C7—C8	-0.4 (2)	C13—C14—C15—C16	-0.5 (4)
C5—C6—C7—C10	-0.6 (2)	C14—C15—C16—C17	0.4 (4)
C1—C6—C7—C10	179.15 (14)	C14—C15—C16—C19	-179.9 (2)
C6—C7—C8—C9	0.1 (2)	C15—C16—C17—C18	-0.4 (4)
C10—C7—C8—C9	-179.43 (14)	C19—C16—C17—C18	179.9 (2)
C1—N1—C9—O3	179.42 (14)	C16—C17—C18—C13	0.5 (4)
C1—N1—C9—C8	0.2 (2)	C14—C13—C18—C17	-0.6 (3)
C12—O3—C9—N1	3.2 (2)	C12-C13-C18-C17	-179.1 (2)

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	H···A	D····A	<i>D</i> —H··· <i>A</i>
C3—H3…O3 ⁱ	0.93	2.75	3.651 (2)	163
С5—Н5…О1	0.93	2.25	2.883 (2)	125
C15—H15…O1 ⁱⁱ	0.93	2.48	3.337 (2)	154
C18—H18…N2 ⁱⁱⁱ	0.93	2.68	3.558 (3)	158

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