

Crystal structure, Hirshfeld surface analysis and density functional theory study of 1-nonyl-3-phenylquinoxalin-2-one

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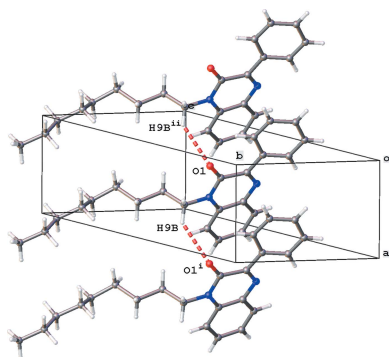
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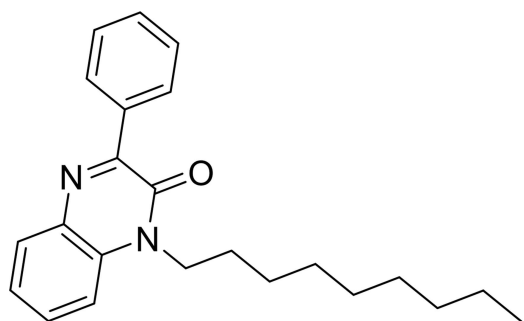
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In the title molecule, C₂₃H₂₈N₂O, the phenyl ring is inclined to the quinoxaline ring system at a dihedral angle of 20.40 (9)°. In the crystal, C—H···O interactions between neighbouring molecules form chains along the *a*-axis direction. Hirshfeld surface analysis indicates that the most important contributions to the crystal packing are from H···H (70.6%), H···C/C···H (15.5%) and H···O/O···H (4.6%) interactions. The optimized structure calculated using density functional theory at the B3LYP/6–311 G(d,p) level is compared with the experimentally determined structure in the solid state. The calculated highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy gap is 3.8904 eV. Part of the *n*-nonyl chain attached to one of the nitrogen atoms of the quinoxaline ring system shows disorder and was refined with a double conformation with occupancies of 0.604 (11) and 0.396 (11).

1. Chemical context

Nitrogen-based structures have attracted increased attention in structural and inorganic chemistry in recent years because of their interesting properties (Chkirate *et al.*, 2019, 2020*a,b*, 2021, 2022; Bouzian *et al.*, 2021). The family of quinoxalines, particularly those containing the quinoxalin-2-one moiety, is important in medicinal chemistry because of their wide range of pharmacological applications, including their use as anti-tumor active agents (Galal *et al.*, 2014), and their antimicrobial (Carta *et al.*, 2003) and biological (Carta *et al.*, 2002) activity. In particular, 3-phenylquinoxaline derivatives are used as anti-cancer drugs (Abad, Sallam *et al.*, 2021). They also have anti-folate activities (Corona *et al.*, 2008). Given the wide range of therapeutic applications for such compounds, and in a continuation of the work already carried out on the synthesis of compounds resulting from quinoxalin-2-one (Al Ati *et al.*, 2021), a similar approach gave the title compound, 1-nonyl-3-phenylquinoxalin-2-one C₂₃H₂₈N₂O, (I). Besides the synthesis, we also report the molecular and crystal structures along with a Hirshfeld surface analysis and a density functional theory computational calculation carried out at the B3LYP/6–311G(d,p) level.





2. Structural commentary

The title compound crystallizes in the triclinic space group $P\bar{1}$ with one molecule in the asymmetric unit (Fig. 1). The molecule is not planar, as indicated by the torsion angles C1–C2–C18–C23 [$-18.6(3)^\circ$] and N2–C2–C18–C19 [$-17.3(3)^\circ$]. The best plane of the phenyl ring C18–C23 (r.m.s. deviation = 0.006 \AA) makes a dihedral angle of $20.40(9)^\circ$ with the best plane of the quinoxaline ring system N1/C1/C2/N2/C3–C8 (r.m.s. deviation = 0.029 \AA). This allows two intramolecular interactions C23–H23 \cdots O1 and C19–H19 \cdots N2 (Table 1). The *n*-nonyl chain attached to one of the nitrogen atoms of the quinoxaline ring system shows disorder and was refined with a double conformation for atoms C13 to C16 with occupancies of 0.604 (11) for C12A–C16A and 0.396 (11) for C12B–C16B. The *n*-nonyl chain of set *A* (starting from C9) has a *ap, ap, ap, +sc, ap, ap, ap* conformation, while for set *B* the conformation can be describes as *ap, ap, ap, -sc, ap, -sc, ap*.

3. Supramolecular features and Hirshfeld surface analysis

The crystal packing is characterized by C9–H9B \cdots O1 interactions [Fig. 2; H9B \cdots O1ⁱ = 2.772 \AA ; symmetry code: (i) $1 + x, y, z$] resulting in ribbon formation in the *a*-axis direction.

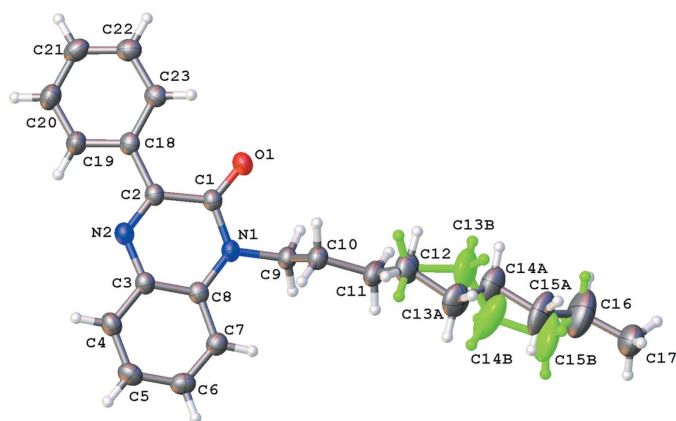


Figure 1
Molecular structure of the title compound with the atom-labelling scheme and ellipsoids drawn at the 50% probability level. The disordered component of the *n*-nonyl chain with occupancy 0.396 (11) is shown in green.

Table 1
Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

| <i>D</i> –H \cdots <i>A</i> | <i>D</i> –H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> –H \cdots <i>A</i> |
|-------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| C19–H19 \cdots N2 | 0.93 | 2.44 | 2.758 (3) | 100 |
| C23–H23 \cdots O1 | 0.93 | 2.21 | 2.832 (3) | 123 |

Parallel ribbons show short C9–H9A \cdots O1 contacts [Fig. 3; H9A \cdots O1ⁱⁱ = 2.899 \AA ; symmetry code: (ii) $1 - x, 1 - y, 1 - z$]. The crystal packing shows layers of *n*-nonyl chains parallel to the (110) plane with layers of rings in between. Despite the presence of aromatic rings, the packing shows no C–H \cdots π or π – π interactions [the shortest centroid–centroid distance is $3.8945(15) \text{ \AA}$ for rings N1/N2/C1–C3/C8 and C18–C23]. The unit cell contains no residual solvent-accessible voids.

The *CrystalExplorer* program (Turner *et al.*, 2017) was used to further investigate and visualize the intermolecular interactions of (I). The Hirshfeld surfaces for the major and minor occupancy components plotted over d_{norm} are shown in Fig. 4. The Hirshfeld surface of the major component (Fig. 4a) is dominated by white regions representing contacts equal to the van der Waals separation and shows only one red spot (close contacts with a negative d_{norm} value) indicative of a H16B \cdots H16Bⁱⁱⁱ contact [1.995 \AA ; symmetry code: (iii) $2 - x, 2 - y, 2 - z$]. A similar observation is made for the minor component (Fig. 4b) where the tiny red spot represents a H15B \cdots H13Bⁱ contact (2.316 \AA).

The overall two-dimensional fingerprint plots (McKinnon *et al.*, 2007) for the two components are shown in Fig. 5a and b, while those delineated into H \cdots H and H \cdots C/C \cdots H contacts are illustrated in Fig. 5c–f, respectively, together with their

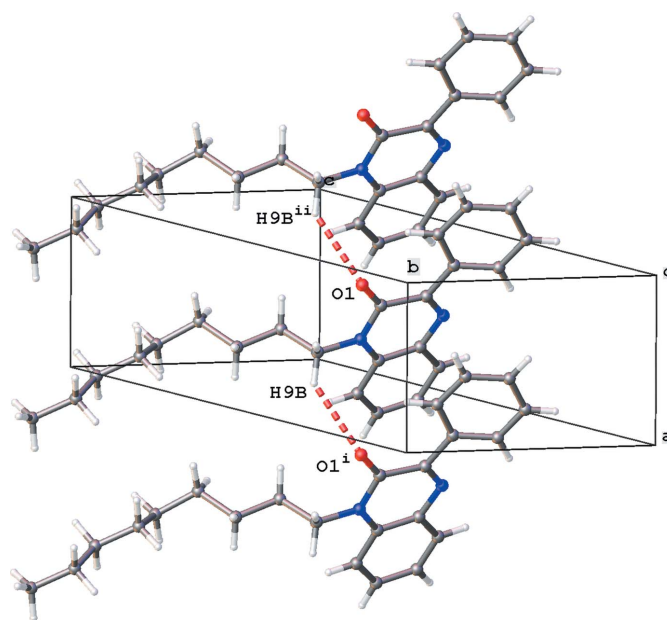
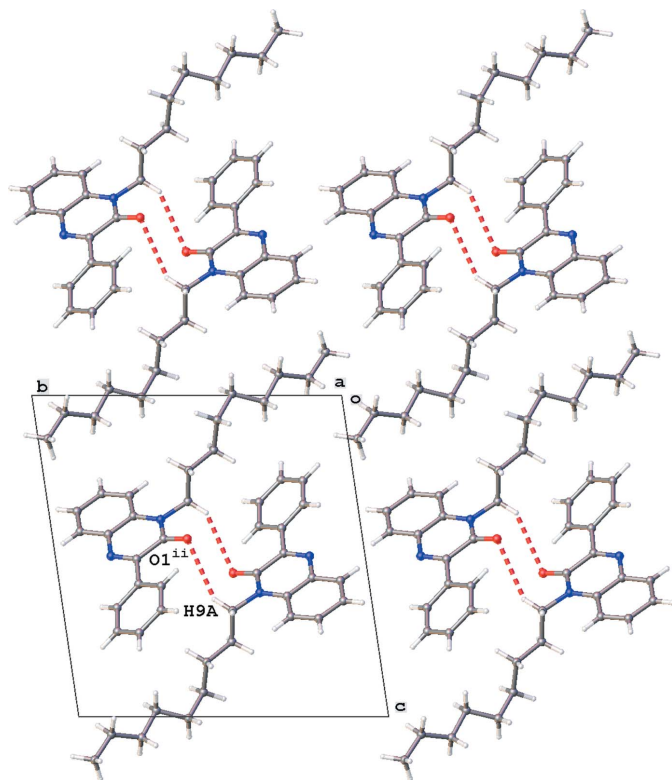
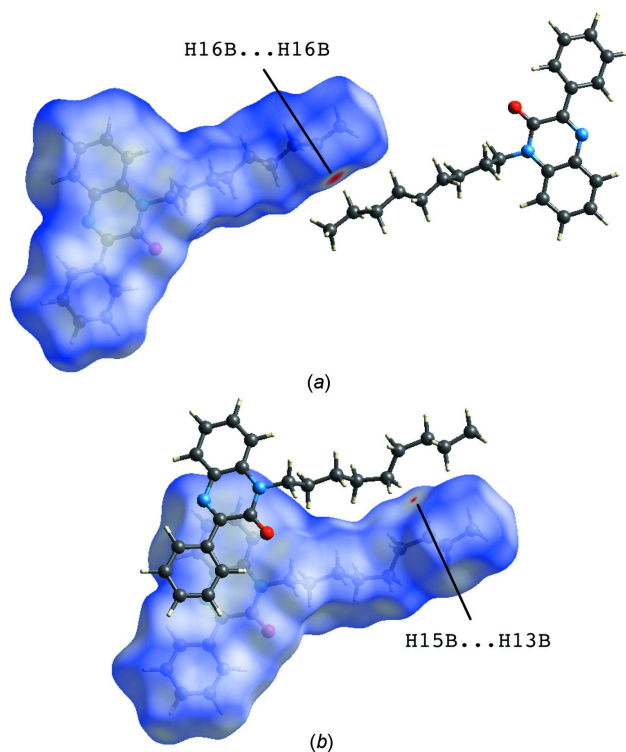


Figure 2
Partial view of the crystal packing of the title compound showing the C–H \cdots O interaction (red dashed lines) and chain formation in the *a*-axis direction. Only the major component of the *n*-nonyl chain is shown. Symmetry codes: (i) $1 + x, y, z$; (ii) $-1 + x, y, z$.

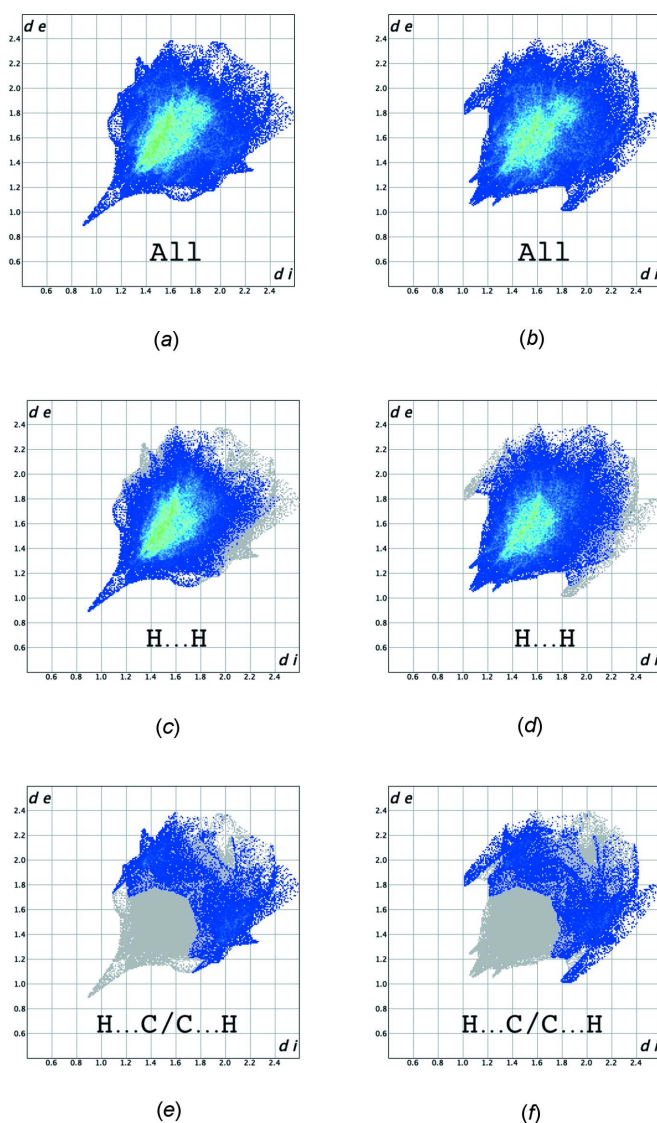

Figure 3

A view down the a axis of the crystal packing of the title compound showing the alternating layers of n -octyl chains and aromatic rings. Only the major disorder component of the n -nonyl chain is shown.


Figure 4

View of the three-dimensional Hirshfeld surface plotted over d_{norm} for (a) the major component (range -0.3582 to 1.3718 a.u.) and (b) the minor component (range -0.0395 to 1.5398 a.u.) of the title compound.

relative contributions to the Hirshfeld surface. The most important interaction is $\text{H}\cdots\text{H}$, contributing 70.6% (major component) or 70.5% (minor component) to the overall crystal packing, which is reflected in Fig. 5c and d as widely scattered points of high density due to the large hydrogen content of the molecule, with a sharp tip at $d_e = d_i = 0.87$ Å in the case of the major component. The second most important are $\text{C}\cdots\text{H}$ interactions, contributing 15.5% (major component) or 15.6% (minor component), for which the fingerprint plot (Fig. 5e and f) shows characteristic wings with tips at $d_e + d_i \simeq 2.80$ Å. Other contacts contribute only 4.6% ($\text{H}\cdots\text{O}/\text{O}\cdots\text{H}$), 4.3% ($\text{C}\cdots\text{C}$), 2.4% ($\text{H}\cdots\text{N}/\text{N}\cdots\text{H}$), 2.2% ($\text{N}\cdots\text{C}/\text{C}\cdots\text{N}$), 0.3% ($\text{O}\cdots\text{O}$) and 0.1% ($\text{O}\cdots\text{C}/\text{C}\cdots\text{O}$) to the Hirshfeld surface.


Figure 5

The full two-dimensional fingerprint plots showing (a,b) all interactions, and delineated into (c,d) $\text{H}\cdots\text{H}$ and (e,f) $\text{H}\cdots\text{C}/\text{C}\cdots\text{H}$ interactions for the major (left) and minor (right) component of the title compound. The d_i and d_e values are the closest internal and external distances (in Å) from points on the Hirshfeld surface.

Table 2

Comparison (X-ray and density functional theory) of selected bond lengths and angles (Å, °).

| | X-ray | B3LYP/6-311G(d,p) |
|-----------|-------------|-------------------|
| O1—C1 | 1.221 (3) | 1.2236 |
| N1—C1 | 1.379 (3) | 1.3975 |
| N1—C8 | 1.387 (3) | 1.3892 |
| N1—C9 | 1.474 (3) | 1.4735 |
| N2—C2 | 1.296 (3) | 1.299 |
| N2—C3 | 1.384 (3) | 1.3723 |
| C2—C18 | 1.481 (3) | 1.4862 |
| C1—N1—C8 | 122.74 (19) | 122.5778 |
| C1—N1—C9 | 116.64 (19) | 116.1328 |
| C8—N1—C9 | 120.60 (19) | 121.2682 |
| O1—C1—N1 | 120.6 (2) | 120.2255 |
| O1—C1—C2 | 124.1 (2) | 124.5602 |
| N1—C1—C2 | 115.22 (19) | 115.2104 |
| C2—N2—C3 | 120.3 (2) | 120.949 |
| N2—C2—C1 | 122.0 (2) | 121.844 |
| N2—C2—C18 | 117.6 (2) | 117.4937 |
| N2—C3—C4 | 118.7 (2) | 118.5343 |
| N2—C3—C8 | 121.6 (2) | 121.9008 |
| N1—C8—C3 | 117.6 (2) | 117.4153 |
| N1—C8—C7 | 123.5 (2) | 123.4308 |
| N1—C9—C10 | 112.61 (19) | 112.9655 |

4. Density functional theory calculations

The structure in the gas phase of the title compound was optimized by means of density functional theory. The density functional theory calculation was performed by the hybrid B3LYP method and the 6-311 G(d,p) basis-set, which is based on Becke's model (Becke, 1993) and considers a mixture of the exact (Hartree-Fock) and density functional theory exchange utilizing the B3 functional, together with the LYP correlation functional (Lee *et al.*, 1988). After obtaining the converged geometry, the harmonic vibrational frequencies were calculated at the same theoretical level to confirm that the number of imaginary frequencies is zero for the stationary point. Both the geometry optimization and harmonic vibrational frequency analysis of the title compound were performed with the *GAUSSIAN 09* program (Frisch *et al.*, 2009). Theoretical and experimental results related to bond lengths and angles, which are in good agreement, are summarized in Table 2. Calculated numerical values for the title compound, including electronegativity (χ), hardness (η), ionization potential (I), dipole moment (μ), electron affinity (A), electrophilicity (ω) and softness (σ), are collated in Table 3. The electron transition from the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO) energy level is shown in Fig. 6. The HOMO and LUMO are localized in the plane extending over the whole 1-nonyl-3-phenylquinoxalin-2-one system. The energy band gap [$\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}}$] of the molecule is 3.8904 eV, and the frontier molecular orbital energies, E_{HOMO} and E_{LUMO} , are -6.1155 and -2.2251 eV, respectively.

5. Database survey

A search of the Cambridge Structural Database (CSD version 5.42, updated May 2021; Groom *et al.*, 2016) for the quinox-

Table 3

Calculated energies.

| Molecular Energy | Compound (I) |
|--|--------------|
| Total Energy, TE (eV) | -29343.5617 |
| E_{HOMO} (eV) | -6.1155 |
| E_{LUMO} (eV) | -2.2251 |
| Gap, ΔE (eV) | 3.8904 |
| Dipole moment, μ (Debye) | 3.0783 |
| Ionization potential, I (eV) | 6.1155 |
| Electron affinity, A | 2.2251 |
| Electronegativity, χ | 4.1703 |
| Hardness, η | 1.9452 |
| Electrophilicity index, ω | 4.4703 |
| Softness, σ | 0.5141 |
| Fraction of electron transferred, ΔN | 0.7274 |

alin-2(1*H*)-one fragment yielded multiple matches (180 hits). Of these, three compounds had an alkyl substituent on N1 and a phenyl ring on C2 comparable to (I) and are shown in Fig. 7. The first two compounds carry an ethyl [(II), refcode MAGBIJ; Al Ati *et al.*, 2021] or methyl [(III), refcode BUDMAP; Benzeid *et al.*, 2009] on N1. The third one [(IV), refcode ASAZEC; Abad, Ferfra *et al.*, 2021] has an *n*-octyl chain on N1 instead of a *n*-nonyl chain. The phenyl ring in MAGBIJ is inclined to the quinoxaline ring system by

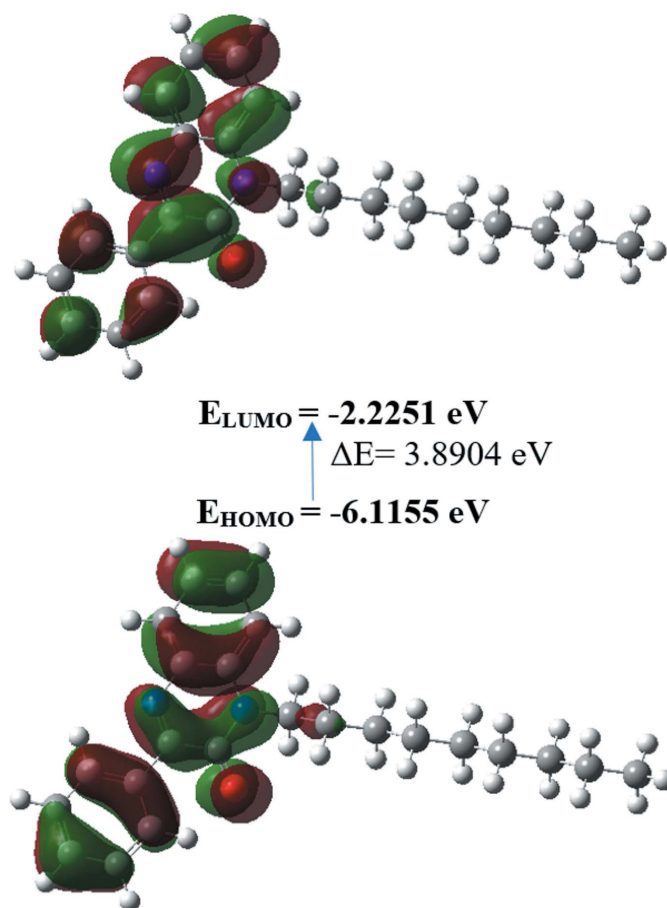


Figure 6
HOMO-LUMO and the energy band gap of the title compound.

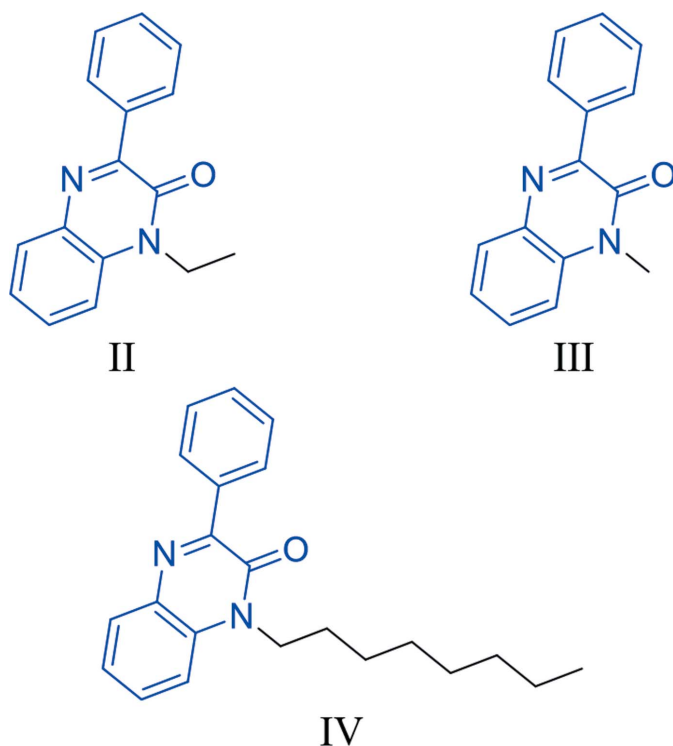


Figure 7
Structures similar to (I): (II) (CSD refcode MAGBIJ), (III) (CSD refcode BUDMAP) and (IV) (CSD refcode ASAZEC) obtained during the database search. The search fragment is indicated in blue.

25.81 (12)°. For BUDMAP, the dihedral angles are 19.3 (1) and 30.4 (1)° for the two molecules present in the asymmetric unit. For ASAZEC, the dihedral angle is 12.90 (4)° and no disorder is observed in the *n*-octyl chain, which could be the consequence of the data collection being undertaken at 150 (2) K. Despite the similarity to the title compound, ASAZEC crystallizes in space group *C2/c* and the molecules are linked by C—H... π interactions and form stacks in the *b*-axis direction.

6. Synthesis and crystallization

To a solution of 3-phenylquinoxalin-2(1*H*)-one (0.5 g, 2.25 mmol) in dichloromethane (20 ml) were added 1-chlorononane (0.2 ml, 2.25 mmol), sodium hydroxide (0.1 g, 2.25 mmol) and a catalytic quantity of tetra-*n*-butylammonium bromide. The reaction mixture was stirred at room temperature for 24 h. The solution was filtered and the solvent removed under reduced pressure. The residue thus obtained was chromatographed on a silica gel column using a hexane/ethyl acetate 9:1 mixture as eluent. The solid obtained was recrystallized from ethanol to afford colourless crystals (yield: 70%). ¹H NMR (300 MHz, CDCl₃) δ ppm: 0.89 (*t*, 3H, CH₃, *J* = 6 Hz); 1.19–1.42 (*m*, 12H, CH₂); 1.65–1.76 (*quin*, 2H, N—CH₂—CH₂); 4.20 (*t*, 2H, N—CH₂, *J* = 6 Hz); 7.22–8.24 (*m*, 9H, CH_{arom}); ¹³C NMR (75 MHz, CDCl₃) δ ppm: 14.12 (CH₃); 22.67, 27.11, 27.32, 29.24, 29.36, 29.51, 31.85 (CH₂); 42.68 (N—CH₂); 113.59, 123.49, 128.05, 129.63, 130.22, 130.28, 130.72 (CH_{arom}); 132.61, 133.42, 136.14, 154.11 (C_q); 154.40 (C=O).

Table 4
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | C ₂₃ H ₂₈ N ₂ O |
| <i>M_r</i> | 348.47 |
| Crystal system, space group | Triclinic, <i>P</i> $\bar{1}$ |
| Temperature (K) | 293 |
| <i>a</i> , <i>b</i> , <i>c</i> (Å) | 5.2353 (2), 13.5065 (5), 14.3158 (5) |
| α , β , γ (°) | 98.045 (3), 98.327 (3), 91.255 (3) |
| <i>V</i> (Å ³) | 990.83 (6) |
| <i>Z</i> | 2 |
| Radiation type | Mo <i>K</i> α |
| μ (mm ⁻¹) | 0.07 |
| Crystal size (mm) | 0.45 × 0.3 × 0.15 |
| Data collection | |
| Diffractometer | SuperNova, Single source at offset/far, Eos |
| Absorption correction | Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2018) |
| <i>T_{min}</i> , <i>T_{max}</i> | 0.686, 1.000 |
| No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections | 20242, 4058, 2864 |
| <i>R_{int}</i> | 0.022 |
| (<i>sin</i> θ / λ) _{max} (Å ⁻¹) | 0.625 |
| Refinement | |
| <i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i> | 0.070, 0.240, 1.05 |
| No. of reflections | 4058 |
| No. of parameters | 264 |
| No. of restraints | 70 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³) | 0.37, -0.45 |

Computer programs: *CrysAlis PRO* (Rigaku OD, 2018), *SHELXT2014/5* (Sheldrick, 2015a), *SHELXL2016/4* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

7. Refinement

Crystal data, data collection and structure refinement details are given in Table 4. C-bound H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and included as riding contributions with isotropic displacement parameters fixed at 1.2 times *U*_{eq} of the parent atoms (1.5 for methyl groups). During the refinement, the difference-Fourier map revealed disorder for atoms C13, C14 and C15 of the nonyl chain and two conformations were refined with distance restraints (1.512 Å) for the C—C bonds involved and RIGU restraints for the nonyl chain C11–C17. At the end of the refinement, the occupancy factors of the two components converged to 0.604 (11) and 0.396 (11) and the final difference-Fourier map showed no residual peaks of chemical significance.

Acknowledgements

Authors' contributions are as follows. Conceptualization, NA; methodology, NA and YR; investigation, KC and NA; theoretical calculations, KC; writing (original draft), KC and LVM; writing (review and editing of the manuscript), FHAO; formal analysis, SL and SF; supervision, EME; crystal-structure determination and validation, LVM.

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Crystal structure, Hirshfeld surface analysis and density functional theory study of 1-nonyl-3-phenylquinoxalin-2-one

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2018); cell refinement: *CrysAlis PRO* (Rigaku OD, 2018); data reduction: *CrysAlis PRO* (Rigaku OD, 2018); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2016/4* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

1-Nonyl-3-phenylquinoxalin-2-one

Crystal data

$C_{23}H_{28}N_2O$

$M_r = 348.47$

Triclinic, $P\bar{1}$

$a = 5.2353$ (2) Å

$b = 13.5065$ (5) Å

$c = 14.3158$ (5) Å

$\alpha = 98.045$ (3)°

$\beta = 98.327$ (3)°

$\gamma = 91.255$ (3)°

$V = 990.83$ (6) Å³

$Z = 2$

$F(000) = 376$

$D_x = 1.168$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 6605 reflections

$\theta = 3.0$ – 26.4 °

$\mu = 0.07$ mm⁻¹

$T = 293$ K

Block, colourless

$0.45 \times 0.3 \times 0.15$ mm

Data collection

SuperNova, Single source at offset/far, Eos diffractometer

Radiation source: micro-focus sealed X-ray tube, SuperNova (Mo) X-ray Source

Mirror monochromator

Detector resolution: 15.9631 pixels mm⁻¹

ω scans

Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2018)

$T_{\min} = 0.686$, $T_{\max} = 1.000$

20242 measured reflections

4058 independent reflections

2864 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$

$\theta_{\max} = 26.4$ °, $\theta_{\min} = 2.9$ °

$h = -6 \rightarrow 6$

$k = -16 \rightarrow 16$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.070$

$wR(F^2) = 0.240$

$S = 1.05$

4058 reflections

264 parameters

70 restraints

Primary atom site location: dual

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.1119P)^2 + 0.4832P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 0.37 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.45 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|------|------------|--------------|--------------|----------------------------------|------------|
| O1 | 0.3177 (4) | 0.43358 (13) | 0.55347 (14) | 0.0685 (5) | |
| N1 | 0.6712 (4) | 0.35716 (13) | 0.61382 (14) | 0.0498 (5) | |
| C1 | 0.4408 (5) | 0.35784 (17) | 0.55355 (17) | 0.0510 (5) | |
| N2 | 0.4810 (4) | 0.17973 (14) | 0.50005 (14) | 0.0527 (5) | |
| C2 | 0.3592 (4) | 0.26106 (16) | 0.49062 (16) | 0.0489 (5) | |
| C3 | 0.6998 (5) | 0.18102 (17) | 0.56737 (17) | 0.0516 (6) | |
| C4 | 0.8245 (5) | 0.09152 (19) | 0.5763 (2) | 0.0625 (7) | |
| H4 | 0.755288 | 0.032153 | 0.539594 | 0.075* | |
| C5 | 1.0489 (6) | 0.0911 (2) | 0.6392 (2) | 0.0698 (7) | |
| H5 | 1.131744 | 0.031553 | 0.644889 | 0.084* | |
| C6 | 1.1516 (5) | 0.1794 (2) | 0.6940 (2) | 0.0672 (7) | |
| H6 | 1.305232 | 0.178777 | 0.735651 | 0.081* | |
| C7 | 1.0310 (5) | 0.2677 (2) | 0.68807 (18) | 0.0594 (6) | |
| H7 | 1.100928 | 0.326025 | 0.726530 | 0.071* | |
| C8 | 0.8032 (4) | 0.27050 (17) | 0.62436 (16) | 0.0497 (5) | |
| C9 | 0.7704 (5) | 0.45374 (17) | 0.66992 (17) | 0.0547 (6) | |
| H9A | 0.711702 | 0.507452 | 0.634775 | 0.066* | |
| H9B | 0.957721 | 0.455955 | 0.678226 | 0.066* | |
| C10 | 0.6832 (5) | 0.47073 (19) | 0.76690 (18) | 0.0606 (6) | |
| H10A | 0.498084 | 0.479028 | 0.758694 | 0.073* | |
| H10B | 0.717777 | 0.412121 | 0.798120 | 0.073* | |
| C11 | 0.8169 (6) | 0.5614 (2) | 0.8298 (2) | 0.0745 (8) | |
| H11A | 0.798334 | 0.618437 | 0.795459 | 0.089* | |
| H11B | 0.999863 | 0.549819 | 0.843410 | 0.089* | |
| C12 | 0.7119 (8) | 0.5865 (3) | 0.9237 (2) | 0.0978 (11) | |
| H12C | 0.774577 | 0.539337 | 0.966060 | 0.117* | 0.396 (11) |
| H12D | 0.524815 | 0.579172 | 0.911703 | 0.117* | 0.396 (11) |
| H12A | 0.555095 | 0.622546 | 0.911469 | 0.117* | 0.604 (11) |
| H12B | 0.663609 | 0.524143 | 0.944183 | 0.117* | 0.604 (11) |
| C13B | 0.791 (3) | 0.6928 (9) | 0.9730 (12) | 0.143 (6) | 0.396 (11) |
| H13A | 0.733512 | 0.738151 | 0.928155 | 0.172* | 0.396 (11) |
| H13B | 0.694988 | 0.706615 | 1.026028 | 0.172* | 0.396 (11) |
| C14B | 1.067 (3) | 0.7193 (11) | 1.0101 (13) | 0.178 (8) | 0.396 (11) |
| H14A | 1.144535 | 0.724151 | 0.953271 | 0.214* | 0.396 (11) |
| H14B | 1.131999 | 0.659083 | 1.033095 | 0.214* | 0.396 (11) |
| C15B | 1.203 (5) | 0.8041 (10) | 1.0834 (14) | 0.213 (9) | 0.396 (11) |

| | | | | | |
|------|-------------|--------------|--------------|-------------|------------|
| H15A | 1.115971 | 0.809553 | 1.139137 | 0.255* | 0.396 (11) |
| H15B | 1.377951 | 0.784635 | 1.103084 | 0.255* | 0.396 (11) |
| C13A | 0.8860 (18) | 0.6470 (6) | 1.0052 (4) | 0.108 (3) | 0.604 (11) |
| H13C | 0.803887 | 0.653364 | 1.062129 | 0.129* | 0.604 (11) |
| H13D | 1.046676 | 0.613550 | 1.018024 | 0.129* | 0.604 (11) |
| C14A | 0.9394 (19) | 0.7469 (5) | 0.9806 (5) | 0.109 (3) | 0.604 (11) |
| H14C | 0.778583 | 0.778877 | 0.963392 | 0.130* | 0.604 (11) |
| H14D | 1.033828 | 0.741313 | 0.926736 | 0.130* | 0.604 (11) |
| C15A | 1.095 (3) | 0.8071 (7) | 1.0650 (5) | 0.151 (4) | 0.604 (11) |
| H15C | 0.983493 | 0.820608 | 1.113487 | 0.182* | 0.604 (11) |
| H15D | 1.229528 | 0.765333 | 1.089666 | 0.182* | 0.604 (11) |
| C16 | 1.2192 (15) | 0.9031 (5) | 1.0549 (5) | 0.208 (3) | |
| H16C | 1.047455 | 0.927886 | 1.040740 | 0.250* | 0.396 (11) |
| H16D | 1.302078 | 0.900230 | 0.998269 | 0.250* | 0.396 (11) |
| H16A | 1.331550 | 0.888114 | 1.006973 | 0.250* | 0.604 (11) |
| H16B | 1.083193 | 0.942764 | 1.027665 | 0.250* | 0.604 (11) |
| C17 | 1.3710 (9) | 0.9691 (3) | 1.1345 (4) | 0.1294 (16) | |
| H17A | 1.353016 | 1.037431 | 1.124155 | 0.194* | |
| H17B | 1.549689 | 0.953042 | 1.138569 | 0.194* | |
| H17C | 1.309895 | 0.959940 | 1.192911 | 0.194* | |
| C18 | 0.1379 (5) | 0.25620 (17) | 0.41263 (17) | 0.0517 (6) | |
| C19 | 0.1175 (6) | 0.1751 (2) | 0.33936 (19) | 0.0663 (7) | |
| H19 | 0.242243 | 0.127165 | 0.340750 | 0.080* | |
| C20 | -0.0844 (6) | 0.1652 (2) | 0.2653 (2) | 0.0780 (8) | |
| H20 | -0.094842 | 0.110612 | 0.217213 | 0.094* | |
| C21 | -0.2709 (6) | 0.2351 (2) | 0.2615 (2) | 0.0749 (8) | |
| H21 | -0.408785 | 0.227544 | 0.211843 | 0.090* | |
| C22 | -0.2513 (5) | 0.3164 (2) | 0.3319 (2) | 0.0680 (7) | |
| H22 | -0.375143 | 0.364646 | 0.328908 | 0.082* | |
| C23 | -0.0503 (5) | 0.32754 (19) | 0.40714 (19) | 0.0574 (6) | |
| H23 | -0.040380 | 0.382880 | 0.454350 | 0.069* | |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|-------------|-------------|
| O1 | 0.0726 (11) | 0.0453 (9) | 0.0818 (13) | 0.0079 (8) | 0.0004 (9) | -0.0005 (8) |
| N1 | 0.0560 (11) | 0.0410 (10) | 0.0511 (11) | -0.0013 (8) | 0.0092 (9) | 0.0018 (8) |
| C1 | 0.0567 (13) | 0.0449 (12) | 0.0511 (13) | 0.0017 (10) | 0.0094 (10) | 0.0046 (10) |
| N2 | 0.0590 (11) | 0.0431 (10) | 0.0556 (11) | 0.0006 (8) | 0.0100 (9) | 0.0046 (8) |
| C2 | 0.0544 (12) | 0.0427 (11) | 0.0506 (12) | -0.0014 (9) | 0.0124 (10) | 0.0058 (9) |
| C3 | 0.0596 (13) | 0.0458 (12) | 0.0503 (13) | 0.0015 (10) | 0.0110 (10) | 0.0071 (10) |
| C4 | 0.0740 (16) | 0.0466 (13) | 0.0672 (16) | 0.0068 (12) | 0.0115 (13) | 0.0079 (11) |
| C5 | 0.0749 (17) | 0.0602 (16) | 0.0772 (18) | 0.0160 (13) | 0.0096 (14) | 0.0203 (14) |
| C6 | 0.0635 (15) | 0.0762 (18) | 0.0627 (16) | 0.0087 (13) | 0.0034 (12) | 0.0179 (13) |
| C7 | 0.0627 (14) | 0.0593 (15) | 0.0545 (14) | 0.0002 (11) | 0.0060 (11) | 0.0058 (11) |
| C8 | 0.0567 (13) | 0.0466 (12) | 0.0480 (12) | 0.0014 (10) | 0.0143 (10) | 0.0083 (9) |
| C9 | 0.0591 (13) | 0.0446 (12) | 0.0574 (14) | -0.0047 (10) | 0.0057 (11) | 0.0014 (10) |
| C10 | 0.0643 (15) | 0.0564 (14) | 0.0583 (15) | -0.0017 (11) | 0.0083 (12) | 0.0000 (11) |

| | | | | | | |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| C11 | 0.0707 (17) | 0.0774 (18) | 0.0667 (16) | -0.0048 (14) | 0.0051 (13) | -0.0135 (14) |
| C12 | 0.110 (3) | 0.101 (2) | 0.075 (2) | 0.001 (2) | 0.0198 (18) | -0.0184 (18) |
| C13B | 0.185 (12) | 0.124 (9) | 0.100 (11) | -0.017 (9) | 0.017 (8) | -0.049 (8) |
| C14B | 0.234 (15) | 0.157 (11) | 0.116 (11) | -0.097 (12) | -0.048 (11) | 0.019 (9) |
| C15B | 0.204 (19) | 0.152 (8) | 0.249 (18) | -0.094 (11) | 0.037 (13) | -0.073 (8) |
| C13A | 0.143 (6) | 0.120 (5) | 0.054 (3) | -0.002 (4) | 0.009 (3) | -0.004 (3) |
| C14A | 0.128 (7) | 0.119 (5) | 0.067 (4) | -0.024 (4) | 0.009 (4) | -0.015 (3) |
| C15A | 0.192 (11) | 0.174 (7) | 0.070 (4) | -0.062 (6) | 0.028 (5) | -0.047 (4) |
| C16 | 0.213 (7) | 0.174 (5) | 0.206 (7) | -0.081 (5) | 0.012 (5) | -0.051 (5) |
| C17 | 0.123 (3) | 0.099 (3) | 0.146 (4) | -0.008 (2) | -0.013 (3) | -0.015 (3) |
| C18 | 0.0560 (13) | 0.0455 (12) | 0.0544 (13) | -0.0054 (10) | 0.0102 (10) | 0.0089 (10) |
| C19 | 0.0733 (17) | 0.0538 (14) | 0.0655 (16) | 0.0023 (12) | -0.0016 (13) | -0.0008 (12) |
| C20 | 0.086 (2) | 0.0679 (18) | 0.0694 (18) | -0.0039 (15) | -0.0073 (15) | -0.0054 (14) |
| C21 | 0.0684 (17) | 0.081 (2) | 0.0702 (18) | -0.0068 (15) | -0.0100 (14) | 0.0153 (15) |
| C22 | 0.0617 (15) | 0.0711 (17) | 0.0718 (17) | 0.0044 (13) | 0.0051 (13) | 0.0174 (14) |
| C23 | 0.0570 (13) | 0.0554 (13) | 0.0616 (14) | -0.0001 (11) | 0.0122 (11) | 0.0114 (11) |

Geometric parameters (Å, °)

| | | | |
|------------|------------|----------|-----------|
| O1—C1 | 1.221 (3) | C7—C8 | 1.397 (3) |
| C13Bb—H13A | 0.9700 | C9—H9A | 0.9700 |
| C13Bb—H13B | 0.9700 | C9—H9B | 0.9700 |
| C13Bb—C14B | 1.482 (10) | C9—C10 | 1.512 (3) |
| C14Bb—H14A | 0.9700 | C10—H10A | 0.9700 |
| C14Bb—H14B | 0.9700 | C10—H10B | 0.9700 |
| C14Bb—C15B | 1.527 (9) | C10—C11 | 1.507 (4) |
| C15Bb—H15A | 0.9700 | C11—H11A | 0.9700 |
| C15Bb—H15B | 0.9700 | C11—H11B | 0.9700 |
| C13Aa—H13C | 0.9700 | C11—C12 | 1.523 (4) |
| C13Aa—H13D | 0.9700 | C12—H12C | 0.9700 |
| C13Aa—C14A | 1.472 (8) | C12—H12D | 0.9700 |
| C14Aa—H14C | 0.9700 | C12—H12A | 0.9700 |
| C14Aa—H14D | 0.9700 | C12—H12B | 0.9700 |
| C14Aa—C15A | 1.481 (7) | C12—C13B | 1.528 (9) |
| C15Aa—H15C | 0.9700 | C12—C13A | 1.500 (6) |
| C15Aa—H15D | 0.9700 | C16—H16C | 0.9700 |
| C15Bb—C16 | 1.456 (10) | C16—H16D | 0.9700 |
| C15Aa—C16 | 1.473 (5) | C16—H16A | 0.9700 |
| N1—C1 | 1.379 (3) | C16—H16B | 0.9700 |
| N1—C8 | 1.387 (3) | C16—C17 | 1.466 (7) |
| N1—C9 | 1.474 (3) | C17—H17A | 0.9600 |
| C1—C2 | 1.496 (3) | C17—H17B | 0.9600 |
| N2—C2 | 1.296 (3) | C17—H17C | 0.9600 |
| N2—C3 | 1.384 (3) | C18—C19 | 1.397 (3) |
| C2—C18 | 1.481 (3) | C18—C23 | 1.395 (3) |
| C3—C4 | 1.399 (3) | C19—H19 | 0.9300 |
| C3—C8 | 1.410 (3) | C19—C20 | 1.375 (4) |
| C4—H4 | 0.9300 | C20—H20 | 0.9300 |

| | | | |
|------------------|-------------|----------------|-------------|
| C4—C5 | 1.373 (4) | C20—C21 | 1.374 (4) |
| C5—H5 | 0.9300 | C21—H21 | 0.9300 |
| C5—C6 | 1.385 (4) | C21—C22 | 1.374 (4) |
| C6—H6 | 0.9300 | C22—H22 | 0.9300 |
| C6—C7 | 1.369 (4) | C22—C23 | 1.382 (4) |
| C7—H7 | 0.9300 | C23—H23 | 0.9300 |
| C1—N1—C8 | 122.74 (19) | C15Bb—C16—C17 | 107.4 (8) |
| C14Aa—C13Aa—C12 | 109.4 (6) | N1—C8—C7 | 123.5 (2) |
| C14Bb—C13Bb—C12 | 119.6 (10) | C7—C8—C3 | 118.9 (2) |
| C14Bb—C13Bb—H13A | 107.4 | N1—C9—H9A | 109.1 |
| H13Ab—C13Bb—H13B | 106.9 | N1—C9—H9B | 109.1 |
| C14Bb—C13Bb—H13B | 107.4 | N1—C9—C10 | 112.61 (19) |
| C13Bb—C14Bb—H14A | 104.0 | H9A—C9—H9B | 107.8 |
| C1—N1—C9 | 116.64 (19) | C10—C9—H9A | 109.1 |
| C8—N1—C9 | 120.60 (19) | C10—C9—H9B | 109.1 |
| O1—C1—N1 | 120.6 (2) | C9—C10—H10A | 109.1 |
| O1—C1—C2 | 124.1 (2) | C9—C10—H10B | 109.1 |
| C15Bb—C14Bb—H14A | 104.0 | H10A—C10—H10B | 107.8 |
| H14Ab—C14Bb—H14B | 105.4 | C11—C10—C9 | 112.5 (2) |
| C13Bb—C14Bb—H14B | 104.0 | C11—C10—H10A | 109.1 |
| C15Bb—C14Bb—H14B | 104.0 | C11—C10—H10B | 109.1 |
| C13Bb—C14Bb—C15B | 133.0 (17) | C10—C11—H11A | 108.9 |
| C14Bb—C15Bb—H15A | 107.9 | C10—C11—H11B | 108.9 |
| C14Bb—C15Bb—H15B | 107.9 | C10—C11—C12 | 113.5 (3) |
| H15Ab—C15Bb—H15B | 107.2 | H11A—C11—H11B | 107.7 |
| N1—C1—C2 | 115.22 (19) | C12—C11—H11A | 108.9 |
| C2—N2—C3 | 120.3 (2) | C12—C11—H11B | 108.9 |
| N2—C2—C1 | 122.0 (2) | C11—C12—H12C | 109.1 |
| N2—C2—C18 | 117.6 (2) | C11—C12—H12D | 109.1 |
| C18—C2—C1 | 120.4 (2) | C11—C12—H12A | 107.9 |
| N2—C3—C4 | 118.7 (2) | C11—C12—H12B | 107.9 |
| N2—C3—C8 | 121.6 (2) | C11—C12—C13B | 112.6 (8) |
| C4—C3—C8 | 119.7 (2) | C17—C16—C15A | 123.6 (7) |
| C3—C4—H4 | 119.9 | C17—C16—H16C | 110.2 |
| C5—C4—C3 | 120.2 (2) | C12—C13Bb—H13A | 107.4 |
| C5—C4—H4 | 119.9 | C12—C13Bb—H13B | 107.4 |
| C14Aa—C13Aa—H13C | 109.8 | C12—C13Aa—H13C | 109.8 |
| C14Aa—C13Aa—H13D | 109.8 | C12—C13Aa—H13D | 109.8 |
| H13Ca—C13Aa—H13D | 108.2 | C16—C15Bb—C14B | 117.8 (12) |
| C13Aa—C14Aa—H14C | 110.1 | C17—C16—H16D | 110.2 |
| C15Aa—C14Aa—H14C | 110.1 | C17—C16—H16A | 106.4 |
| C15Aa—C14Aa—H14D | 110.1 | C17—C16—H16B | 106.4 |
| H14Ca—C14Aa—H14D | 108.4 | C16—C17—H17A | 109.5 |
| C13Aa—C14Aa—H14D | 110.1 | C16—C17—H17B | 109.5 |
| C13Aa—C14Aa—C15A | 108.0 (6) | C16—C17—H17C | 109.5 |
| C14Aa—C15Aa—H15C | 107.4 | H17A—C17—H17B | 109.5 |
| C14Aa—C15Aa—H15D | 107.4 | H17A—C17—H17C | 109.5 |

| | | | |
|-----------------------|--------------|-----------------------|-------------|
| C4—C5—H5 | 120.1 | H17B—C17—H17C | 109.5 |
| C4—C5—C6 | 119.9 (2) | C19—C18—C2 | 117.8 (2) |
| C6—C5—H5 | 120.1 | C23—C18—C2 | 124.4 (2) |
| C5—C6—H6 | 119.4 | C23—C18—C19 | 117.9 (2) |
| C7—C6—C5 | 121.2 (3) | C18—C19—H19 | 119.5 |
| C7—C6—H6 | 119.4 | C20—C19—C18 | 120.9 (3) |
| C6—C7—H7 | 119.9 | C20—C19—H19 | 119.5 |
| C6—C7—C8 | 120.2 (2) | C19—C20—H20 | 119.7 |
| C8—C7—H7 | 119.9 | C21—C20—C19 | 120.6 (3) |
| N1—C8—C3 | 117.6 (2) | C21—C20—H20 | 119.7 |
| H15Ca—C15Aa—H15D | 107.0 | C20—C21—H21 | 120.4 |
| C13Aa—C12—C11 | 117.4 (5) | C22—C21—C20 | 119.3 (3) |
| C13Bb—C12—H12C | 109.1 | C22—C21—H21 | 120.4 |
| H12Cb—C12—H12D | 107.8 | C21—C22—H22 | 119.5 |
| C13Bb—C12—H12D | 109.1 | C21—C22—C23 | 121.0 (3) |
| C13Aa—C12—H12A | 107.9 | C23—C22—H22 | 119.5 |
| C13Aa—C12—H12B | 107.9 | C18—C23—H23 | 119.8 |
| H12Aa—C12—H12B | 107.2 | C22—C23—C18 | 120.3 (3) |
| C15Bb—C16—H16C | 110.2 | C22—C23—H23 | 119.8 |
| C15Bb—C16—H16D | 110.2 | C16—C15Bb—H15A | 107.9 |
| H16Cb—C16—H16D | 108.5 | C16—C15Bb—H15B | 107.9 |
| C15Aa—C16—H16A | 106.4 | C16—C15Aa—C14A | 119.5 (7) |
| H16Aa—C16—H16B | 106.5 | C16—C15Aa—H15C | 107.4 |
| C15Aa—C16—H16B | 106.4 | C16—C15Aa—H15D | 107.4 |
| | | | |
| C13Aa—C14Aa—C15Aa—C16 | 168.0 (12) | C4—C3—C8—C7 | 0.7 (4) |
| C13Bb—C14Bb—C15Bb—C16 | -76 (3) | C4—C5—C6—C7 | 1.1 (4) |
| C14Bb—C15Bb—C16—C17 | -176.5 (18) | C5—C6—C7—C8 | -1.4 (4) |
| C14Aa—C15Aa—C16—C17 | 178.4 (9) | C6—C7—C8—N1 | -179.5 (2) |
| O1—C1—C2—N2 | -172.5 (2) | C6—C7—C8—C3 | 0.5 (4) |
| O1—C1—C2—C18 | 9.4 (4) | C8—N1—C1—O1 | 172.5 (2) |
| N1—C1—C2—N2 | 7.6 (3) | C8—N1—C1—C2 | -7.6 (3) |
| N1—C1—C2—C18 | -170.52 (19) | C8—N1—C9—C10 | -86.1 (3) |
| N1—C9—C10—C11 | 171.1 (2) | C8—C3—C4—C5 | -1.1 (4) |
| C1—N1—C8—C3 | 2.8 (3) | C9—N1—C1—O1 | -5.8 (3) |
| C1—N1—C8—C7 | -177.2 (2) | C9—N1—C1—C2 | 174.13 (19) |
| C1—N1—C9—C10 | 92.3 (3) | C9—N1—C8—C3 | -179.0 (2) |
| C1—C2—C18—C19 | 160.9 (2) | C9—N1—C8—C7 | 1.0 (3) |
| C1—C2—C18—C23 | -18.6 (3) | C9—C10—C11—C12 | 173.8 (3) |
| N2—C2—C18—C19 | -17.3 (3) | C10—C11—C12—C13Aa | 157.2 (5) |
| N2—C2—C18—C23 | 163.2 (2) | C10—C11—C12—C13Bb | -163.5 (7) |
| N2—C3—C4—C5 | 176.9 (2) | C11—C12—C13Bb—C14Bb | -66.5 (19) |
| N2—C3—C8—N1 | 2.9 (3) | C11—C12—C13Aa—C14Aa | 64.2 (9) |
| N2—C3—C8—C7 | -177.2 (2) | C12—C13Aa—C14Aa—C15Aa | 175.8 (8) |
| C2—N2—C3—C4 | 179.2 (2) | C12—C13Bb—C14Bb—C15Bb | -160.7 (14) |
| C2—N2—C3—C8 | -2.8 (3) | C18—C19—C20—C21 | 0.1 (5) |
| C2—C18—C19—C20 | 179.3 (3) | C19—C18—C23—C22 | 1.0 (4) |
| C2—C18—C23—C22 | -179.5 (2) | C19—C20—C21—C22 | 1.1 (5) |

| | | | |
|--------------|-------------|-----------------|----------|
| C3—N2—C2—C1 | −2.5 (3) | C20—C21—C22—C23 | −1.3 (5) |
| C3—N2—C2—C18 | 175.63 (19) | C21—C22—C23—C18 | 0.3 (4) |
| C3—C4—C5—C6 | 0.2 (4) | C23—C18—C19—C20 | −1.2 (4) |
| C4—C3—C8—N1 | −179.3 (2) | | |

Hydrogen-bond geometry (Å, °)

| <i>D—H⋯A</i> | <i>D—H</i> | <i>H⋯A</i> | <i>D⋯A</i> | <i>D—H⋯A</i> |
|--------------|------------|------------|------------|--------------|
| C19—H19⋯N2 | 0.93 | 2.44 | 2.758 (3) | 100 |
| C23—H23⋯O1 | 0.93 | 2.21 | 2.832 (3) | 123 |