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# 3-Isobutyl-5,5-diphenylimidazolidine-2,4-dione

Walid Guerrab,[a] Abderrazzak El Moutaouakil Ala Allah,[a] Abdulsalam Alsubari,[b]* Joel T. Mague[c] and Youssef Ramli[a]‡

[a]Laboratory of Medicinal Chemistry, Drug Sciences Research Center, Faculty of Medicine and Pharmacy, Mohammed V University in Rabat, Morocco, [b]Laboratory of Medicinal Chemistry, Faculty of Clinical Pharmacy, 21 September University, Yemen, and [c]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA. *Correspondence e-mail: alsubaripharmaco@21umas.edu.ye

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‡ Additional correspondence author, e-mail: y.ramli@um5r.ac.ma.

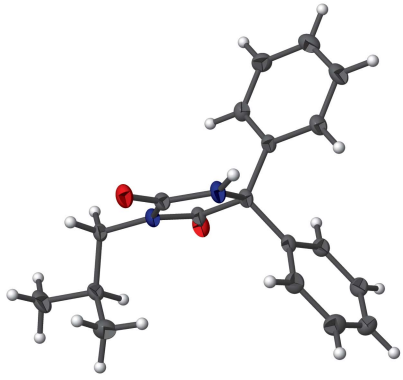
**Keywords:** crystal structure; imidazolidine-dione; hydrogen bond; C—H···$\pi$(ring) interaction.

**CCDC reference**: 2176804

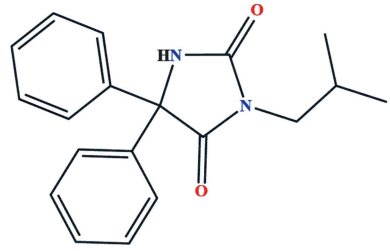
**Structural data**: full structural data are available from iucrdata.iucr.org

The imidazolidine ring in the title molecule, $C_{19}H_{20}N_2O_2$, is slightly 'ruffled'. In the crystal, a layer structure is generated by N—H···O and C—H···O hydrogen bonds plus C—H···$\pi$(ring) interactions.

**3D view**



**Chemical scheme**




## Structure description

Imidazolidin-2,4-dione, also known as hydantoin, is an important nucleus found in numerous natural products and in several clinically important medicines. One of the best known examples of such a derivative is phenytoine, 5,5-diphenylimidazolidine-2,4-dione, a drug widely prescribed as an anticonvulsant agent and for the treatment of many other diseases including HIV (Weichet, 1974; Havera & Strycker, 1976; Khodair *et al.*, 1997; Thenmozhiyal *et al.*, 2004).

Given the wide range of therapeutic applications for such compounds, and in a continuation of our work in this area (Ramli *et al.*, 2017*a*,*b*; Akrad *et al.* 2017; Guerrab *et al.* 2019, 2020*a*,*b*, 2021, 2022), the title compound (Fig. 1) was prepared and its crystal structure is reported here.

The two phenyl rings (C4–C9 and C10–C15) are disposed on either side of the five-membered ring and make dihedral angles of 68.42 (3) and 73.04 (3)°, respectively, with the mean plane of the latter ring. The five-membered ring is slightly 'ruffled' with deviations from the mean plane ranging from 0.206 (5) Å (N2) to −0.218 (5) Å (C3) (r.m.s. deviation = 0.0155 Å). The isobutyl group is rotated well out of the mean plane of the five-membered ring, as indicated by the C2—N1—C16—C17 torsion angle of 72.64 (10)°. In the crystal, inversion dimers are formed by pairs of N2—H2···O2 hydrogen bonds (Table 1) with the dimers connected by C8—H8···O1 hydrogen bonds, forming chains of molecules extending parallel to $(10\bar{1})$ (Fig. 2 and Table 2). The chains

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

*Cg*1 is the centroid of the five-membered ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2···O2$^{i}$ | 0.91 (1) | 1.95 (1) | 2.8512 (9) | 174 (1) |
| C7—H7···*Cg*1$^{ii}$ | 0.95 | 2.99 | 3.9308 (13) | 170 |
| C8—H8···O1$^{iii}$ | 0.95 | 2.46 | 3.4069 (13) | 172 |

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

are connected into layers parallel to the *ac* plane by C7—H7···*Cg*1 interactions (Table 1 and Fig. 3).

## Synthesis and crystallization

To a solution of 5,5-diphenylimidazolidine-2,4-dione (500 mg, 1.98 mmol), one equivalent of isobutyl bromide (246.88 mL, 1.98 mmol) in absolute dimethylformamide (DMF, 15 ml) was added and the resulting solution heated under reflux for 3 h in the presence of 1.1 equivalents of $K_2CO_3$ (301.31 mg, 2.18 mmol). The reaction mixture was filtered while hot, and the solvent evaporated under reduced pressure. The residue obtained was dried and recrystallized from an ethanol solution to yield colourless prism-like crystals (Guerrab *et al.*, 2018)

## Refinement

Crystal data, data collection and structure refinement details are presented in Table 2. A small amount of residual density, well removed from the main molecule and which could not be satisfactorily modelled by a plausible solvent molecule disordered across a centre of symmetry was removed with *PLATON* SQUEEZE (Spek, 2015). Three reflections affected by the beamstop were omitted from the final refinement.

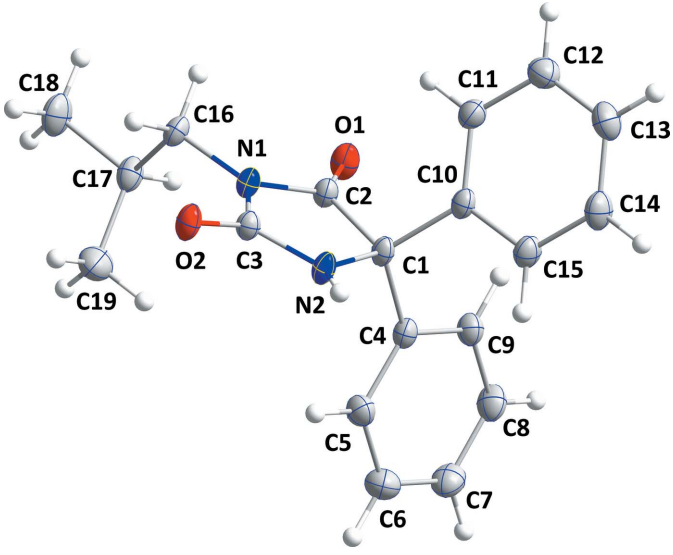



**Figure 1**
The title molecule with the labelling scheme and 50% probability ellipsoids.

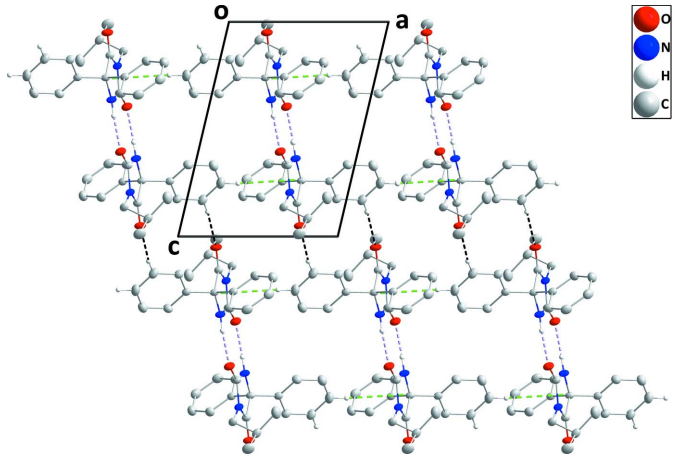



**Figure 2**
A portion of one layer viewed along the *b*-axis direction with N—H···O and C—H···O hydrogen bonds depicted, respectively, by violet and black dashed lines. C—H···$\pi$(ring) interactions are depicted by green dashed lines and non-interacting hydrogen atoms are omitted for clarity.

## Acknowledgements

JTM thanks Tulane University for support of the Tulane Crystallography Laboratory. Author contributions are as follows. Conceptualization, YR; methodology, WG and AS; investigation, WG, AEMAA; writing (original draft), JMT and YR; writing (review and editing of the manuscript), YR; formal analysis, AS and YR; supervision, YR; crystal-structure determination and validation, JTM.

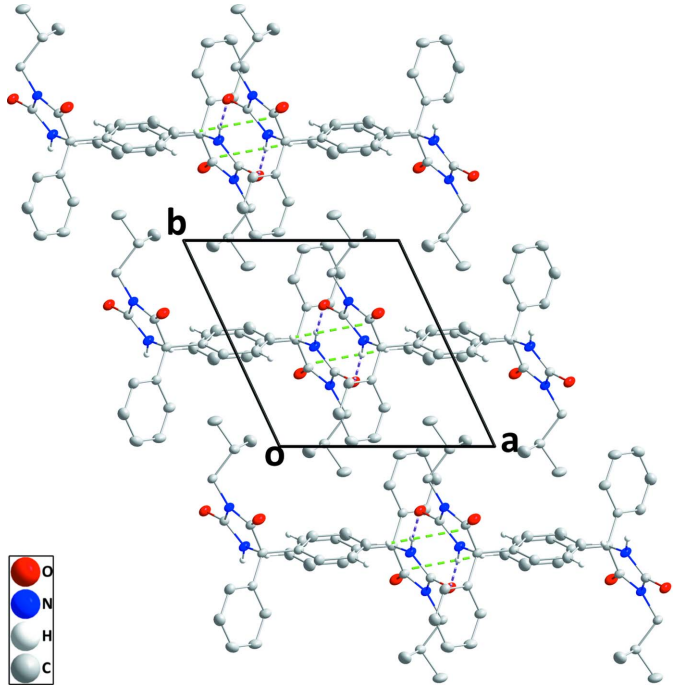



**Figure 3**
Packing viewed along the *c*-axis direction with intermolecular interactions depicted as in Fig. 2 and non-interacting hydrogen atoms omitted for clarity.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{19}H_{20}N_2O_2$ |
| $M_r$ | 308.37 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 150 |
| $a, b, c$ (Å) | 8.9747 (7), 9.7306 (7), 11.8780 (8) |
| $\alpha, \beta, \gamma$ (°) | 104.676 (3), 96.334 (3), 112.243 (3) |
| $V$ (Å$^3$) | 903.81 (12) |
| $Z$ | 2 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.07 |
| Crystal size (mm) | 0.46 × 0.41 × 0.13 |
| | |
| Data collection | |
| Diffractometer | Bruker D8 QUEST PHOTON 3 diffractometer |
| Absorption correction | Numerical (*SADABS*; Krause *et al.*, 2015) |
| $T_{min}$, $T_{max}$ | 0.93, 0.99 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 42215, 6214, 5222 |
| $R_{int}$ | 0.040 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.755 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.044, 0.128, 1.05 |
| No. of reflections | 6214 |
| No. of parameters | 213 |
| No. of restraints | 1 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.41, −0.19 |

Computer programs: *APEX4* and *SAINT* (Bruker, 2021), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/1* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

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# full crystallographic data

*IUCrData* (2022). **7**, x220598 [https://doi.org/10.1107/S2414314622005983]

## 3-Isobutyl-5,5-diphenylimidazolidine-2,4-dione

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### 3-Isobutyl-5,5-diphenylimidazolidine-2,4-dione

*Crystal data*

$C_{19}H_{20}N_2O_2$
$M_r$ = 308.37
Triclinic, $P\overline{1}$
$a$ = 8.9747 (7) Å
$b$ = 9.7306 (7) Å
$c$ = 11.8780 (8) Å
$\alpha$ = 104.676 (3)°
$\beta$ = 96.334 (3)°
$\gamma$ = 112.243 (3)°
$V$ = 903.81 (12) Å$^3$
$Z$ = 2
$F(000)$ = 328
$D_x$ = 1.133 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9909 reflections
$\theta$ = 2.5–31.9°
$\mu$ = 0.07 mm$^{-1}$
$T$ = 150 K
Thick plate, colourless
0.46 × 0.41 × 0.13 mm

*Data collection*

Bruker D8 QUEST PHOTON 3 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.3910 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: numerical (*SADABS*; Krause *et al.*, 2015)
$T_{min}$ = 0.93, $T_{max}$ = 0.99
42215 measured reflections
6214 independent reflections
5222 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.040
$\theta_{max}$ = 32.5°, $\theta_{min}$ = 2.5°
$h$ = −13→13
$k$ = −14→14
$l$ = −17→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.128
$S$ = 1.05
6214 reflections
213 parameters
1 restraint
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0689P)^2 + 0.1685P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

*Special details*

**Experimental**. The diffraction data were obtained from 9 sets of frames, each of width 0.5° in $\omega$ or $\varphi$, collected with scan parameters determined by the "strategy" routine in *APEX3*. The scan time was 5 sec/frame.

**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.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on $F^2$, conventional R-factors R are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 1.00 Å) and were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms. That attached to nitrogen was placed in a location derived from a difference map and refined with a DFIX 0.91 0.01 instruction. A small amount of residual density, well-removed from the main molecule and which could not be satisfactorily modeled by a plausible solvent molecule disordered across a center of symmetry was removed with *PLATON SQUEEZE* (Spek, 2015). Three reflections affected by the beamstop were omitted from the final refinement.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.74629 (9) | 0.64608 (8) | 0.94977 (5) | 0.02535 (14) |
| O2 | 0.51349 (8) | 0.68712 (7) | 0.60449 (5) | 0.02359 (14) |
| N1 | 0.63385 (9) | 0.70411 (8) | 0.79418 (6) | 0.01786 (13) |
| N2 | 0.62040 (9) | 0.51465 (8) | 0.63706 (6) | 0.01972 (14) |
| H2 | 0.5822 (15) | 0.4472 (13) | 0.5613 (8) | 0.030* |
| C1 | 0.68961 (10) | 0.48254 (9) | 0.73985 (7) | 0.01730 (14) |
| C2 | 0.69602 (10) | 0.61866 (9) | 0.84376 (7) | 0.01818 (15) |
| C3 | 0.58232 (10) | 0.63811 (9) | 0.66914 (7) | 0.01764 (15) |
| C4 | 0.86580 (10) | 0.49751 (9) | 0.74187 (7) | 0.01831 (15) |
| C5 | 0.95614 (12) | 0.56243 (11) | 0.66554 (8) | 0.02490 (17) |
| H5 | 0.908433 | 0.598669 | 0.610614 | 0.030* |
| C6 | 1.11659 (13) | 0.57417 (12) | 0.66981 (9) | 0.0306 (2) |
| H6 | 1.177780 | 0.617680 | 0.617333 | 0.037* |
| C7 | 1.18692 (12) | 0.52243 (12) | 0.75054 (10) | 0.0305 (2) |
| H7 | 1.295578 | 0.529077 | 0.752362 | 0.037* |
| C8 | 1.09899 (11) | 0.46090 (11) | 0.82877 (9) | 0.02727 (18) |
| H8 | 1.148247 | 0.427406 | 0.885034 | 0.033* |
| C9 | 0.93872 (11) | 0.44843 (10) | 0.82459 (8) | 0.02205 (16) |
| H9 | 0.878635 | 0.406433 | 0.878110 | 0.026* |
| C10 | 0.57204 (10) | 0.32284 (9) | 0.74399 (7) | 0.01842 (15) |
| C11 | 0.45908 (11) | 0.30670 (10) | 0.81674 (8) | 0.02336 (17) |
| H11 | 0.459215 | 0.397322 | 0.870843 | 0.028* |
| C12 | 0.34570 (12) | 0.15808 (12) | 0.81053 (9) | 0.02819 (19) |
| H12 | 0.268623 | 0.147944 | 0.860092 | 0.034* |
| C13 | 0.34519 (12) | 0.02510 (11) | 0.73224 (9) | 0.02882 (19) |
| H13 | 0.267373 | −0.075954 | 0.727691 | 0.035* |
| C14 | 0.45904 (13) | 0.04021 (11) | 0.66037 (9) | 0.02807 (19) |
| H14 | 0.459695 | −0.050708 | 0.607264 | 0.034* |

| | | | | |
|---|---|---|---|---|
| C15 | 0.57189 (11) | 0.18826 (10) | 0.66618 (8) | 0.02336 (17) |
| H15 | 0.649371 | 0.197963 | 0.616936 | 0.028* |
| C16 | 0.61826 (10) | 0.84333 (9) | 0.86303 (7) | 0.01963 (15) |
| H16A | 0.564388 | 0.820207 | 0.928583 | 0.024* |
| H16B | 0.545921 | 0.868521 | 0.810459 | 0.024* |
| C17 | 0.78453 (11) | 0.98600 (10) | 0.91629 (8) | 0.02349 (17) |
| H17 | 0.854577 | 0.961276 | 0.972365 | 0.028* |
| C18 | 0.75511 (15) | 1.12407 (11) | 0.98774 (10) | 0.0339 (2) |
| H18A | 0.689042 | 1.151726 | 0.933699 | 0.051* |
| H18B | 0.861657 | 1.214255 | 1.026831 | 0.051* |
| H18C | 0.695748 | 1.094763 | 1.048519 | 0.051* |
| C19 | 0.87543 (13) | 1.02639 (13) | 0.81979 (11) | 0.0353 (2) |
| H19A | 0.899177 | 0.938670 | 0.778900 | 0.053* |
| H19B | 0.979417 | 1.120428 | 0.856671 | 0.053* |
| H19C | 0.806095 | 1.046019 | 0.761788 | 0.053* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0371 (4) | 0.0246 (3) | 0.0156 (3) | 0.0173 (3) | 0.0006 (2) | 0.0042 (2) |
| O2 | 0.0304 (3) | 0.0223 (3) | 0.0201 (3) | 0.0158 (2) | −0.0010 (2) | 0.0056 (2) |
| N1 | 0.0219 (3) | 0.0160 (3) | 0.0157 (3) | 0.0104 (2) | 0.0007 (2) | 0.0029 (2) |
| N2 | 0.0279 (3) | 0.0191 (3) | 0.0142 (3) | 0.0143 (3) | 0.0004 (2) | 0.0036 (2) |
| C1 | 0.0225 (3) | 0.0167 (3) | 0.0143 (3) | 0.0110 (3) | 0.0017 (3) | 0.0046 (2) |
| C2 | 0.0218 (3) | 0.0165 (3) | 0.0170 (3) | 0.0099 (3) | 0.0027 (3) | 0.0046 (3) |
| C3 | 0.0195 (3) | 0.0165 (3) | 0.0165 (3) | 0.0083 (3) | 0.0016 (3) | 0.0045 (3) |
| C4 | 0.0213 (3) | 0.0159 (3) | 0.0178 (3) | 0.0095 (3) | 0.0019 (3) | 0.0041 (3) |
| C5 | 0.0286 (4) | 0.0262 (4) | 0.0242 (4) | 0.0135 (3) | 0.0073 (3) | 0.0115 (3) |
| C6 | 0.0283 (4) | 0.0324 (5) | 0.0332 (5) | 0.0124 (4) | 0.0119 (4) | 0.0128 (4) |
| C7 | 0.0218 (4) | 0.0295 (4) | 0.0395 (5) | 0.0114 (3) | 0.0058 (4) | 0.0097 (4) |
| C8 | 0.0235 (4) | 0.0257 (4) | 0.0329 (4) | 0.0117 (3) | 0.0001 (3) | 0.0106 (3) |
| C9 | 0.0231 (4) | 0.0214 (4) | 0.0227 (4) | 0.0102 (3) | 0.0022 (3) | 0.0087 (3) |
| C10 | 0.0213 (3) | 0.0174 (3) | 0.0176 (3) | 0.0104 (3) | 0.0015 (3) | 0.0050 (3) |
| C11 | 0.0256 (4) | 0.0228 (4) | 0.0246 (4) | 0.0133 (3) | 0.0069 (3) | 0.0071 (3) |
| C12 | 0.0261 (4) | 0.0289 (4) | 0.0311 (4) | 0.0109 (3) | 0.0088 (3) | 0.0122 (4) |
| C13 | 0.0293 (4) | 0.0214 (4) | 0.0303 (4) | 0.0058 (3) | 0.0018 (3) | 0.0094 (3) |
| C14 | 0.0344 (5) | 0.0177 (4) | 0.0270 (4) | 0.0099 (3) | 0.0018 (3) | 0.0029 (3) |
| C15 | 0.0287 (4) | 0.0190 (4) | 0.0212 (4) | 0.0112 (3) | 0.0048 (3) | 0.0030 (3) |
| C16 | 0.0211 (3) | 0.0162 (3) | 0.0212 (3) | 0.0103 (3) | 0.0024 (3) | 0.0025 (3) |
| C17 | 0.0223 (4) | 0.0167 (3) | 0.0269 (4) | 0.0078 (3) | −0.0009 (3) | 0.0030 (3) |
| C18 | 0.0423 (5) | 0.0190 (4) | 0.0335 (5) | 0.0128 (4) | 0.0026 (4) | −0.0001 (3) |
| C19 | 0.0294 (5) | 0.0288 (5) | 0.0462 (6) | 0.0090 (4) | 0.0126 (4) | 0.0132 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C2 | 1.2139 (10) | C10—C15 | 1.3980 (11) |
| O2—C3 | 1.2259 (9) | C11—C12 | 1.3956 (13) |
| N1—C2 | 1.3698 (10) | C11—H11 | 0.9500 |

| | | | |
|---|---|---|---|
| N1—C3 | 1.4045 (10) | C12—C13 | 1.3870 (14) |
| N1—C16 | 1.4598 (10) | C12—H12 | 0.9500 |
| N2—C3 | 1.3465 (10) | C13—C14 | 1.3916 (15) |
| N2—C1 | 1.4652 (10) | C13—H13 | 0.9500 |
| N2—H2 | 0.906 (8) | C14—C15 | 1.3913 (13) |
| C1—C4 | 1.5289 (11) | C14—H14 | 0.9500 |
| C1—C10 | 1.5295 (11) | C15—H15 | 0.9500 |
| C1—C2 | 1.5425 (11) | C16—C17 | 1.5273 (12) |
| C4—C5 | 1.3939 (12) | C16—H16A | 0.9900 |
| C4—C9 | 1.3979 (11) | C16—H16B | 0.9900 |
| C5—C6 | 1.3948 (13) | C17—C19 | 1.5250 (14) |
| C5—H5 | 0.9500 | C17—C18 | 1.5282 (13) |
| C6—C7 | 1.3868 (14) | C17—H17 | 1.0000 |
| C6—H6 | 0.9500 | C18—H18A | 0.9800 |
| C7—C8 | 1.3895 (15) | C18—H18B | 0.9800 |
| C7—H7 | 0.9500 | C18—H18C | 0.9800 |
| C8—C9 | 1.3911 (12) | C19—H19A | 0.9800 |
| C8—H8 | 0.9500 | C19—H19B | 0.9800 |
| C9—H9 | 0.9500 | C19—H19C | 0.9800 |
| C10—C11 | 1.3930 (12) | | |

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| C2—N1—C3 | 111.47 (6) | C10—C11—C12 | 120.34 (8) |
| C2—N1—C16 | 124.21 (7) | C10—C11—H11 | 119.8 |
| C3—N1—C16 | 124.29 (6) | C12—C11—H11 | 119.8 |
| C3—N2—C1 | 112.87 (6) | C13—C12—C11 | 120.22 (9) |
| C3—N2—H2 | 120.9 (8) | C13—C12—H12 | 119.9 |
| C1—N2—H2 | 124.6 (8) | C11—C12—H12 | 119.9 |
| N2—C1—C4 | 112.60 (7) | C12—C13—C14 | 119.79 (9) |
| N2—C1—C10 | 109.66 (6) | C12—C13—H13 | 120.1 |
| C4—C1—C10 | 112.73 (6) | C14—C13—H13 | 120.1 |
| N2—C1—C2 | 100.71 (6) | C15—C14—C13 | 120.09 (9) |
| C4—C1—C2 | 108.58 (6) | C15—C14—H14 | 120.0 |
| C10—C1—C2 | 111.97 (6) | C13—C14—H14 | 120.0 |
| O1—C2—N1 | 125.93 (7) | C14—C15—C10 | 120.44 (8) |
| O1—C2—C1 | 126.97 (7) | C14—C15—H15 | 119.8 |
| N1—C2—C1 | 107.10 (6) | C10—C15—H15 | 119.8 |
| O2—C3—N2 | 128.11 (7) | N1—C16—C17 | 112.91 (7) |
| O2—C3—N1 | 124.19 (7) | N1—C16—H16A | 109.0 |
| N2—C3—N1 | 107.69 (6) | C17—C16—H16A | 109.0 |
| C5—C4—C9 | 119.56 (8) | N1—C16—H16B | 109.0 |
| C5—C4—C1 | 121.55 (7) | C17—C16—H16B | 109.0 |
| C9—C4—C1 | 118.87 (7) | H16A—C16—H16B | 107.8 |
| C4—C5—C6 | 119.99 (8) | C19—C17—C16 | 111.65 (8) |
| C4—C5—H5 | 120.0 | C19—C17—C18 | 111.13 (8) |
| C6—C5—H5 | 120.0 | C16—C17—C18 | 108.81 (8) |
| C7—C6—C5 | 120.10 (9) | C19—C17—H17 | 108.4 |
| C7—C6—H6 | 120.0 | C16—C17—H17 | 108.4 |
| C5—C6—H6 | 120.0 | C18—C17—H17 | 108.4 |

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| C6—C7—C8 | 120.22 (9) | C17—C18—H18A | 109.5 |
| C6—C7—H7 | 119.9 | C17—C18—H18B | 109.5 |
| C8—C7—H7 | 119.9 | H18A—C18—H18B | 109.5 |
| C7—C8—C9 | 119.90 (8) | C17—C18—H18C | 109.5 |
| C7—C8—H8 | 120.1 | H18A—C18—H18C | 109.5 |
| C9—C8—H8 | 120.1 | H18B—C18—H18C | 109.5 |
| C8—C9—C4 | 120.21 (8) | C17—C19—H19A | 109.5 |
| C8—C9—H9 | 119.9 | C17—C19—H19B | 109.5 |
| C4—C9—H9 | 119.9 | H19A—C19—H19B | 109.5 |
| C11—C10—C15 | 119.12 (8) | C17—C19—H19C | 109.5 |
| C11—C10—C1 | 122.52 (7) | H19A—C19—H19C | 109.5 |
| C15—C10—C1 | 118.25 (7) | H19B—C19—H19C | 109.5 |

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| C3—N2—C1—C4 | −118.52 (8) | C1—C4—C5—C6 | −179.97 (8) |
| C3—N2—C1—C10 | 115.10 (8) | C4—C5—C6—C7 | −0.49 (15) |
| C3—N2—C1—C2 | −3.05 (9) | C5—C6—C7—C8 | −0.99 (15) |
| C3—N1—C2—O1 | −178.32 (8) | C6—C7—C8—C9 | 1.21 (15) |
| C16—N1—C2—O1 | −0.15 (14) | C7—C8—C9—C4 | 0.04 (14) |
| C3—N1—C2—C1 | 1.65 (9) | C5—C4—C9—C8 | −1.51 (13) |
| C16—N1—C2—C1 | 179.81 (7) | C1—C4—C9—C8 | −179.85 (8) |
| N2—C1—C2—O1 | −179.29 (9) | N2—C1—C10—C11 | −97.67 (9) |
| C4—C1—C2—O1 | −60.86 (11) | C4—C1—C10—C11 | 136.02 (8) |
| C10—C1—C2—O1 | 64.25 (11) | C2—C1—C10—C11 | 13.23 (10) |
| N2—C1—C2—N1 | 0.74 (8) | N2—C1—C10—C15 | 78.35 (9) |
| C4—C1—C2—N1 | 119.18 (7) | C4—C1—C10—C15 | −47.96 (9) |
| C10—C1—C2—N1 | −115.71 (7) | C2—C1—C10—C15 | −170.75 (7) |
| C1—N2—C3—O2 | −174.97 (8) | C15—C10—C11—C12 | −0.97 (13) |
| C1—N2—C3—N1 | 4.19 (9) | C1—C10—C11—C12 | 175.01 (8) |
| C2—N1—C3—O2 | 175.58 (8) | C10—C11—C12—C13 | 0.34 (14) |
| C16—N1—C3—O2 | −2.58 (13) | C11—C12—C13—C14 | 0.48 (15) |
| C2—N1—C3—N2 | −3.61 (9) | C12—C13—C14—C15 | −0.65 (15) |
| C16—N1—C3—N2 | 178.23 (7) | C13—C14—C15—C10 | 0.00 (14) |
| N2—C1—C4—C5 | 10.83 (11) | C11—C10—C15—C14 | 0.81 (13) |
| C10—C1—C4—C5 | 135.55 (8) | C1—C10—C15—C14 | −175.35 (8) |
| C2—C1—C4—C5 | −99.79 (9) | C2—N1—C16—C17 | 72.64 (10) |
| N2—C1—C4—C9 | −170.85 (7) | C3—N1—C16—C17 | −109.43 (9) |
| C10—C1—C4—C9 | −46.14 (10) | N1—C16—C17—C19 | 57.80 (10) |
| C2—C1—C4—C9 | 78.52 (9) | N1—C16—C17—C18 | −179.18 (7) |
| C9—C4—C5—C6 | 1.73 (13) | | |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the five-membered ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2···O2$^{i}$ | 0.91 (1) | 1.95 (1) | 2.8512 (9) | 174 (1) |

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|---|---|---|---|---|
| C7—H7···*Cg*1[ii] | 0.95 | 2.99 | 3.9308 (13) | 170 |
| C8—H8···O1[iii] | 0.95 | 2.46 | 3.4069 (13) | 172 |

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