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1-Decyl-6-nitro-1*H*-benzimidazol-2(3*H*)-one

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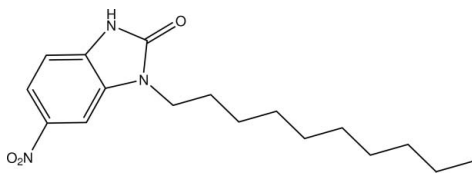
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 Key indicators: single-crystal X-ray study; $T = 206$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.041; wR factor = 0.126; data-to-parameter ratio = 19.9.

The title molecule, $\text{C}_{17}\text{H}_{25}\text{N}_3\text{O}_3$, is built up from fused six- and five-membered rings linked to a $-\text{C}_{10}\text{H}_{21}$ chain. The fused-ring system is essentially planar, the largest deviation from the mean plane being 0.009 (2) Å. The chain is roughly perpendicular to this plane, making a dihedral angle of 79.5 (2)°. In the crystal, $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds build infinite chains along [010]. There are channels in the structure containing disordered hexane. The contribution of this solvent to the scattering power was suppressed using the SQUEEZE option in PLATON [Spek (2009)]. *Acta Cryst.* **D65**, 148–155].

Related literature

For the pharmacological and biochemical properties of related compounds, see: Gravatt *et al.* (1994); Horton *et al.* (2003); Kim *et al.* (1996); Roth *et al.* (1997). For related structures, see Ouzidan *et al.* (2011a,b).



Experimental

Crystal data

$\text{C}_{17}\text{H}_{25}\text{N}_3\text{O}_3$
 $M_r = 319.40$
 Monoclinic, $C2/c$
 $a = 32.9827$ (6) Å
 $b = 4.55881$ (9) Å
 $c = 29.3435$ (5) Å
 $\beta = 109.481$ (2)°
 $V = 4159.56$ (13) Å³
 $Z = 8$
 Cu $K\alpha$ radiation
 $\mu = 0.57$ mm⁻¹
 $T = 206$ K
 $0.15 \times 0.11 \times 0.05$ mm

Data collection

Agilent SuperNova Dual (Cu at zero) Atlas diffractometer
 Absorption correction: analytical [CrysAlis PRO (Agilent, 2011) based on expressions derived by Clark & Reid (1995)]
 $T_{\min} = 0.952$, $T_{\max} = 0.985$
 20838 measured reflections
 4129 independent reflections
 3475 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.126$
 $S = 1.09$
 4129 reflections
 208 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.16$ e Å⁻³
 $\Delta\rho_{\min} = -0.17$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{N1}-\text{H1}\cdots\text{O1}^i$ | 0.86 | 1.88 | 2.743 (1) | 178 |

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2324).

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supporting information

Acta Cryst. (2011). E67, o2937 [doi:10.1107/S1600536811041389]

1-Decyl-6-nitro-1*H*-benzimidazol-2(3*H*)-one

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S1. Comment

Benzimidazoles are very useful intermediates/subunits for the development of molecules of pharmaceutical or biological interest. Benzimidazole derivatives have found applications in diverse therapeutic areas including anti-ulcers, anti-hypertensives, anti-virals, anti-fungals and anti-cancers (Gravatt *et al.* 1994; Horton *et al.* 2003; Kim *et al.* 1996; Roth *et al.* 1997).

As a continuation of our research work devoted to the development of substituted benzimidazol-2-one derivatives (Ouzidan *et al.*, 2011*a*, 2011*b*), we report in this paper the synthesis of a new benzimidazol-2-one derivative by action of 1-bromodecane with 5-nitro-1,3-dihydro-benzimidazol-2-one in the presence of a catalytic quantity of tetra-*n*-butylammonium bromide under mild conditions to furnish the title compound (Scheme 1).

The molecular structure of 1-decyl-6-nitro-1,3-dihydro-benzimidazol-2-one is built up from two fused six- and five-membered rings linked to a C₁₀H₂₁ chain as shown in Fig.1. The fused rings are essentially planar, with maximum deviations of 0.008 (2) Å and -0.004 (2) Å for C2 and N1, respectively. The dihedral angle between them does not exceed 0.68 (7)°. The torsional angles C7–N2–C11–C12 and C17–C18–C19–C20 are -98.4 (2) ° and 176.7 (2)°, respectively. N1—H···O1 hydrogen bonds build up infinite one-dimensional chains along the [0 1 0] direction as shown in Fig.2 and Table 1.

S2. Experimental

To 5-nitro-1,3-dihydro-benzimidazol-2-one (0.2 g, 1.1 mmol), potassium carbonate (0.30 g, 2.2 mmol) and tetra-*n*-butylammonium bromide (0.07 g, 0.2 mmol) in DMF (15 ml) was added 1-bromodecane (0.34 ml, 1.65 mmol). Stirring was continued at room temperature for 6 h. The precipitated salt was removed by filtration and the filtrate was concentrated under reduced pressure. The residue was separated by chromatography on a column of silica gel with ethyl acetate/hexane (1/2) as eluent. Colorless crystals were isolated when the solvent was allowed to evaporate (yield: 27%).

S3. Refinement

There are channels in the structure containing disordered hexane. The contribution of this solvent to the scattering power was suppressed using the SQUEEZE option in PLATON (Spek, 2009) and the reflections were merged.

H atoms were located in a difference map and treated as riding with C—H = 0.93 Å for all H atoms with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{aromatic, methine})$ and $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{methyl})$.

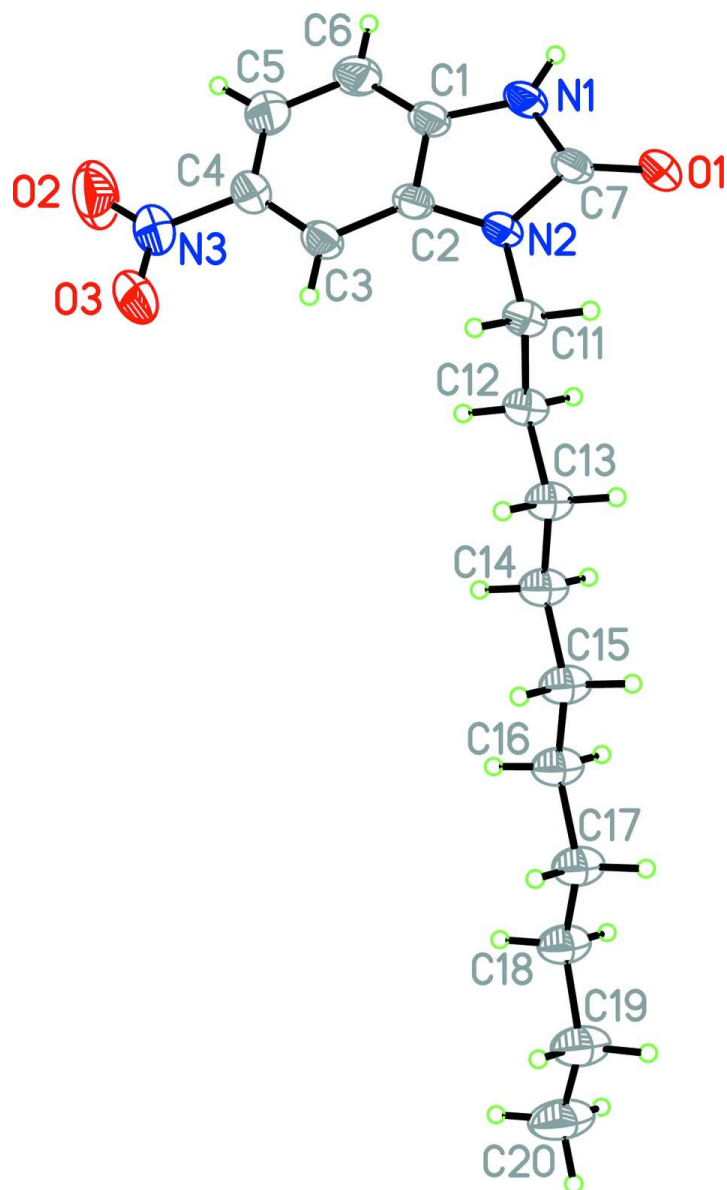


Figure 1

Molecular structure of the title compound with displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small circles.

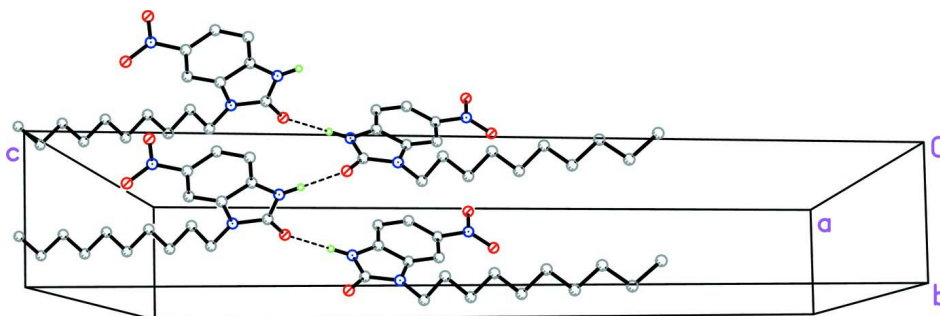


Figure 2
Packing diagram.

1-Decyl-6-nitro-1H-benzimidazol-2(3H)-one

Crystal data

$C_{17}H_{25}N_3O_3$
 $M_r = 319.40$
 Monoclinic, $C2/c$
 Hall symbol: $-C 2yc$
 $a = 32.9827 (6) \text{ \AA}$
 $b = 4.55881 (9) \text{ \AA}$
 $c = 29.3435 (5) \text{ \AA}$
 $\beta = 109.481 (2)^\circ$
 $V = 4159.56 (13) \text{ \AA}^3$
 $Z = 8$

$F(000) = 1376$
 $D_x = 1.020 \text{ Mg m}^{-3}$
 Cu $K\alpha$ radiation, $\lambda = 1.54184 \text{ \AA}$
 Cell parameters from 8979 reflections
 $\theta = 2.8\text{--}73.1^\circ$
 $\mu = 0.57 \text{ mm}^{-1}$
 $T = 206 \text{ K}$
 Block, colourless
 $0.15 \times 0.11 \times 0.05 \text{ mm}$

Data collection

Agilent SuperNova Dual (Cu at zero) Atlas diffractometer
 Radiation source: fine-focus sealed tube
 Mirror monochromator
 Detector resolution: $0.4051 \text{ pixels mm}^{-1}$
 ω scans
 Absorption correction: analytical
 [CrysAlis PRO (Agilent, 2011) based on expressions derived by Clark & Reid (1995)]

$T_{\min} = 0.952$, $T_{\max} = 0.985$
 20838 measured reflections
 4129 independent reflections
 3475 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$
 $\theta_{\max} = 73.3^\circ$, $\theta_{\min} = 2.8^\circ$
 $h = -40 \rightarrow 40$
 $k = -4 \rightarrow 5$
 $l = -36 \rightarrow 36$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.126$
 $S = 1.09$
 4129 reflections
 208 parameters
 0 restraints
 Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
 Hydrogen site location: difference Fourier map
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0706P)^2 + 0.8537P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.16 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.17 \text{ e \AA}^{-3}$

Special details

Experimental. CrysAlisPro, Agilent Technologies, Version 1.171.35.11 (release 16-05-2011 CrysAlis171 .NET) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid. Clark & Reid (1995).

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s 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 $F^2 > \sigma(F^2)$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|-------------|------------|-------------|----------------------------------|
| N1 | 0.76316 (3) | 0.5176 (2) | 0.70158 (3) | 0.0389 (3) |
| H1 | 0.7727 | 0.4612 | 0.7312 | 0.047* |
| N2 | 0.72508 (3) | 0.7438 (2) | 0.63471 (3) | 0.0319 (2) |
| N3 | 0.80707 (4) | 0.2956 (3) | 0.53894 (4) | 0.0493 (3) |
| O1 | 0.70806 (3) | 0.8310 (2) | 0.70415 (3) | 0.0459 (3) |
| O2 | 0.83330 (4) | 0.1068 (3) | 0.53903 (4) | 0.0817 (4) |
| O3 | 0.78870 (3) | 0.4442 (2) | 0.50339 (3) | 0.0571 (3) |
| C1 | 0.77940 (3) | 0.4278 (3) | 0.66624 (4) | 0.0337 (3) |
| C2 | 0.75516 (3) | 0.5736 (3) | 0.62357 (4) | 0.0304 (3) |
| C3 | 0.76366 (3) | 0.5367 (3) | 0.58100 (4) | 0.0341 (3) |
| H3 | 0.7482 | 0.6341 | 0.5527 | 0.041* |
| C4 | 0.79688 (4) | 0.3445 (3) | 0.58314 (4) | 0.0384 (3) |
| C5 | 0.82078 (4) | 0.1954 (3) | 0.62471 (5) | 0.0451 (3) |
| H5 | 0.8425 | 0.0676 | 0.6240 | 0.054* |
| C6 | 0.81208 (4) | 0.2379 (3) | 0.66730 (4) | 0.0433 (3) |
| H6 | 0.8278 | 0.1413 | 0.6956 | 0.052* |
| C7 | 0.72984 (3) | 0.7087 (3) | 0.68291 (4) | 0.0350 (3) |
| C11 | 0.69093 (3) | 0.9198 (3) | 0.60136 (4) | 0.0325 (3) |
| H11A | 0.7026 | 1.0276 | 0.5800 | 0.039* |
| H11B | 0.6806 | 1.0613 | 0.6197 | 0.039* |
| C12 | 0.65344 (3) | 0.7327 (3) | 0.57121 (4) | 0.0342 (3) |
| H12A | 0.6418 | 0.6247 | 0.5925 | 0.041* |
| H12B | 0.6637 | 0.5915 | 0.5529 | 0.041* |
| C13 | 0.61786 (4) | 0.9169 (3) | 0.53654 (4) | 0.0355 (3) |
| H13A | 0.6063 | 1.0490 | 0.5551 | 0.043* |
| H13B | 0.6300 | 1.0352 | 0.5168 | 0.043* |
| C14 | 0.58145 (4) | 0.7315 (3) | 0.50369 (4) | 0.0380 (3) |
| H14A | 0.5691 | 0.6155 | 0.5235 | 0.046* |
| H14B | 0.5931 | 0.5970 | 0.4856 | 0.046* |
| C15 | 0.54594 (4) | 0.9122 (3) | 0.46821 (4) | 0.0403 (3) |
| H15A | 0.5584 | 1.0310 | 0.4488 | 0.048* |
| H15B | 0.5339 | 1.0442 | 0.4863 | 0.048* |
| C16 | 0.50987 (4) | 0.7262 (3) | 0.43470 (5) | 0.0409 (3) |

| | | | | |
|------|-------------|------------|-------------|------------|
| H16A | 0.5220 | 0.5927 | 0.4170 | 0.049* |
| H16B | 0.4973 | 0.6089 | 0.4541 | 0.049* |
| C17 | 0.47449 (4) | 0.9044 (3) | 0.39880 (5) | 0.0417 (3) |
| H17A | 0.4611 | 1.0287 | 0.4165 | 0.050* |
| H17B | 0.4873 | 1.0311 | 0.3808 | 0.050* |
| C18 | 0.43994 (4) | 0.7188 (3) | 0.36328 (5) | 0.0444 (3) |
| H18A | 0.4535 | 0.5884 | 0.3466 | 0.053* |
| H18B | 0.4263 | 0.5982 | 0.3812 | 0.053* |
| C19 | 0.40558 (4) | 0.8947 (3) | 0.32606 (5) | 0.0530 (4) |
| H19A | 0.3908 | 1.0171 | 0.3426 | 0.064* |
| H19B | 0.4193 | 1.0233 | 0.3092 | 0.064* |
| C20 | 0.37271 (5) | 0.7073 (4) | 0.28924 (6) | 0.0673 (5) |
| H20A | 0.3528 | 0.8315 | 0.2659 | 0.101* |
| H20B | 0.3575 | 0.5894 | 0.3053 | 0.101* |
| H20C | 0.3871 | 0.5820 | 0.2732 | 0.101* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|-------------|------------|-------------|-------------|-------------|
| N1 | 0.0368 (5) | 0.0594 (7) | 0.0176 (4) | -0.0018 (5) | 0.0051 (3) | 0.0043 (4) |
| N2 | 0.0304 (4) | 0.0432 (6) | 0.0192 (4) | -0.0013 (4) | 0.0046 (3) | -0.0007 (4) |
| N3 | 0.0505 (6) | 0.0633 (8) | 0.0392 (6) | 0.0032 (6) | 0.0218 (5) | -0.0011 (5) |
| O1 | 0.0411 (4) | 0.0714 (7) | 0.0241 (4) | -0.0004 (4) | 0.0095 (3) | -0.0087 (4) |
| O2 | 0.0945 (9) | 0.1005 (10) | 0.0648 (7) | 0.0446 (8) | 0.0461 (7) | 0.0090 (7) |
| O3 | 0.0644 (6) | 0.0789 (8) | 0.0333 (5) | 0.0066 (5) | 0.0236 (4) | 0.0067 (5) |
| C1 | 0.0310 (5) | 0.0458 (7) | 0.0217 (5) | -0.0058 (5) | 0.0051 (4) | 0.0020 (4) |
| C2 | 0.0287 (5) | 0.0372 (6) | 0.0228 (5) | -0.0059 (4) | 0.0054 (4) | -0.0003 (4) |
| C3 | 0.0357 (5) | 0.0422 (7) | 0.0227 (5) | -0.0028 (5) | 0.0075 (4) | 0.0027 (4) |
| C4 | 0.0390 (6) | 0.0479 (7) | 0.0299 (6) | -0.0012 (5) | 0.0137 (5) | -0.0006 (5) |
| C5 | 0.0398 (6) | 0.0542 (8) | 0.0399 (6) | 0.0078 (6) | 0.0115 (5) | 0.0037 (6) |
| C6 | 0.0393 (6) | 0.0544 (8) | 0.0312 (6) | 0.0046 (6) | 0.0050 (5) | 0.0098 (5) |
| C7 | 0.0316 (5) | 0.0510 (7) | 0.0199 (5) | -0.0082 (5) | 0.0052 (4) | -0.0048 (5) |
| C11 | 0.0329 (5) | 0.0361 (6) | 0.0251 (5) | -0.0005 (5) | 0.0050 (4) | -0.0008 (4) |
| C12 | 0.0330 (6) | 0.0345 (6) | 0.0299 (5) | -0.0011 (5) | 0.0037 (4) | -0.0006 (5) |
| C13 | 0.0330 (5) | 0.0337 (7) | 0.0341 (6) | 0.0002 (5) | 0.0037 (4) | -0.0001 (5) |
| C14 | 0.0349 (6) | 0.0345 (7) | 0.0366 (6) | 0.0005 (5) | 0.0013 (5) | -0.0007 (5) |
| C15 | 0.0350 (6) | 0.0365 (7) | 0.0403 (6) | 0.0008 (5) | 0.0003 (5) | -0.0010 (5) |
| C16 | 0.0367 (6) | 0.0362 (7) | 0.0403 (6) | 0.0005 (5) | 0.0000 (5) | -0.0011 (5) |
| C17 | 0.0366 (6) | 0.0381 (7) | 0.0413 (6) | 0.0013 (5) | 0.0006 (5) | -0.0014 (5) |
| C18 | 0.0372 (6) | 0.0414 (7) | 0.0436 (7) | 0.0011 (5) | -0.0011 (5) | -0.0024 (5) |
| C19 | 0.0447 (7) | 0.0489 (9) | 0.0499 (7) | 0.0060 (6) | -0.0050 (6) | -0.0026 (6) |
| C20 | 0.0483 (8) | 0.0687 (11) | 0.0608 (9) | 0.0079 (7) | -0.0140 (7) | -0.0078 (8) |

Geometric parameters (Å, °)

| | | | |
|-------|-------------|----------|-------------|
| N1—C7 | 1.3659 (16) | C13—C14 | 1.5208 (15) |
| N1—C1 | 1.3785 (15) | C13—H13A | 0.9700 |
| N1—H1 | 0.8600 | C13—H13B | 0.9700 |

| | | | |
|-----------|-------------|---------------|-------------|
| N2—C7 | 1.3793 (13) | C14—C15 | 1.5235 (15) |
| N2—C2 | 1.3819 (15) | C14—H14A | 0.9700 |
| N2—C11 | 1.4612 (14) | C14—H14B | 0.9700 |
| N3—O2 | 1.2198 (16) | C15—C16 | 1.5235 (16) |
| N3—O3 | 1.2218 (15) | C15—H15A | 0.9700 |
| N3—C4 | 1.4612 (15) | C15—H15B | 0.9700 |
| O1—C7 | 1.2304 (14) | C16—C17 | 1.5201 (16) |
| C1—C6 | 1.3745 (18) | C16—H16A | 0.9700 |
| C1—C2 | 1.4077 (15) | C16—H16B | 0.9700 |
| C2—C3 | 1.3789 (14) | C17—C18 | 1.5194 (16) |
| C3—C4 | 1.3879 (17) | C17—H17A | 0.9700 |
| C3—H3 | 0.9300 | C17—H17B | 0.9700 |
| C4—C5 | 1.3890 (17) | C18—C19 | 1.5148 (17) |
| C5—C6 | 1.3862 (18) | C18—H18A | 0.9700 |
| C5—H5 | 0.9300 | C18—H18B | 0.9700 |
| C6—H6 | 0.9300 | C19—C20 | 1.5138 (19) |
| C11—C12 | 1.5197 (15) | C19—H19A | 0.9700 |
| C11—H11A | 0.9700 | C19—H19B | 0.9700 |
| C11—H11B | 0.9700 | C20—H20A | 0.9600 |
| C12—C13 | 1.5234 (15) | C20—H20B | 0.9600 |
| C12—H12A | 0.9700 | C20—H20C | 0.9600 |
| C12—H12B | 0.9700 | | |
| | | | |
| C7—N1—C1 | 110.52 (9) | C14—C13—H13B | 109.0 |
| C7—N1—H1 | 124.7 | C12—C13—H13B | 109.0 |
| C1—N1—H1 | 124.7 | H13A—C13—H13B | 107.8 |
| C7—N2—C2 | 109.41 (9) | C13—C14—C15 | 113.41 (10) |
| C7—N2—C11 | 123.32 (9) | C13—C14—H14A | 108.9 |
| C2—N2—C11 | 127.13 (8) | C15—C14—H14A | 108.9 |
| O2—N3—O3 | 122.85 (11) | C13—C14—H14B | 108.9 |
| O2—N3—C4 | 118.60 (11) | C15—C14—H14B | 108.9 |
| O3—N3—C4 | 118.55 (11) | H14A—C14—H14B | 107.7 |
| C6—C1—N1 | 131.94 (10) | C14—C15—C16 | 113.39 (10) |
| C6—C1—C2 | 121.76 (10) | C14—C15—H15A | 108.9 |
| N1—C1—C2 | 106.31 (10) | C16—C15—H15A | 108.9 |
| C3—C2—N2 | 131.46 (10) | C14—C15—H15B | 108.9 |
| C3—C2—C1 | 121.41 (10) | C16—C15—H15B | 108.9 |
| N2—C2—C1 | 107.12 (9) | H15A—C15—H15B | 107.7 |
| C2—C3—C4 | 115.61 (10) | C17—C16—C15 | 113.80 (10) |
| C2—C3—H3 | 122.2 | C17—C16—H16A | 108.8 |
| C4—C3—H3 | 122.2 | C15—C16—H16A | 108.8 |
| C3—C4—C5 | 123.84 (11) | C17—C16—H16B | 108.8 |
| C3—C4—N3 | 117.89 (10) | C15—C16—H16B | 108.8 |
| C5—C4—N3 | 118.28 (12) | H16A—C16—H16B | 107.7 |
| C6—C5—C4 | 119.74 (12) | C18—C17—C16 | 113.88 (10) |
| C6—C5—H5 | 120.1 | C18—C17—H17A | 108.8 |
| C4—C5—H5 | 120.1 | C16—C17—H17A | 108.8 |
| C1—C6—C5 | 117.64 (11) | C18—C17—H17B | 108.8 |

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|---------------|-------------|---------------|-------------|
| C1—C6—H6 | 121.2 | C16—C17—H17B | 108.8 |
| C5—C6—H6 | 121.2 | H17A—C17—H17B | 107.7 |
| O1—C7—N1 | 127.86 (10) | C19—C18—C17 | 114.19 (11) |
| O1—C7—N2 | 125.50 (11) | C19—C18—H18A | 108.7 |
| N1—C7—N2 | 106.64 (9) | C17—C18—H18A | 108.7 |
| N2—C11—C12 | 112.17 (10) | C19—C18—H18B | 108.7 |
| N2—C11—H11A | 109.2 | C17—C18—H18B | 108.7 |
| C12—C11—H11A | 109.2 | H18A—C18—H18B | 107.6 |
| N2—C11—H11B | 109.2 | C20—C19—C18 | 113.67 (12) |
| C12—C11—H11B | 109.2 | C20—C19—H19A | 108.8 |
| H11A—C11—H11B | 107.9 | C18—C19—H19A | 108.8 |
| C11—C12—C13 | 112.06 (10) | C20—C19—H19B | 108.8 |
| C11—C12—H12A | 109.2 | C18—C19—H19B | 108.8 |
| C13—C12—H12A | 109.2 | H19A—C19—H19B | 107.7 |
| C11—C12—H12B | 109.2 | C19—C20—H20A | 109.5 |
| C13—C12—H12B | 109.2 | C19—C20—H20B | 109.5 |
| H12A—C12—H12B | 107.9 | H20A—C20—H20B | 109.5 |
| C14—C13—C12 | 112.76 (10) | C19—C20—H20C | 109.5 |
| C14—C13—H13A | 109.0 | H20A—C20—H20C | 109.5 |
| C12—C13—H13A | 109.0 | H20B—C20—H20C | 109.5 |

Hydrogen-bond geometry (Å, °)

| <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> |
|--------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| N1—H1 \cdots O1 ⁱ | 0.86 | 1.88 | 2.743 (1) | 178 |

Symmetry code: (i) $-x+3/2, y-1/2, -z+3/2$.