Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 1-(1-Adamantylmethyl)-1*H*-benzimidazole

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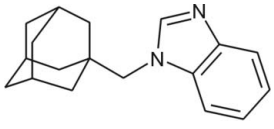
Received 26 September 2011; accepted 5 October 2011

Key indicators: single-crystal X-ray study; $T$ = 120 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.030; $wR$ factor = 0.064; data-to-parameter ratio = 13.6.

The asymmetric unit of the title compound, $C_{18}H_{22}N_2$, contains two independent molecules which differ slightly with respect to the torsion angles involving the atoms joining the adamantyl and benzimidazole groups. The bond angles in the adamantane cage vary within the range 108.27 (9)–110.55 (10)°. The benzimidazole ring system in both molecules is essentially planar, the maximum deviations from the best planes being 0.0134 (15) and 0.0229 (14) Å. In the crystal, weak C—H$\cdots\pi$ interactions link the molecules.

## Related literature

For the synthesis, spectroscopic characterization and biological activity of the title compound, see: Hille *et al.* (2011). For background to C($sp^2$)—H$\cdots\pi$ interactions, see: Takahashi *et al.* (2010). For two polymorphs of a related structure, see: Lei & Zhou (2009); Zhang *et al.* (2010).



## Experimental

### Crystal data

$C_{18}H_{22}N_2$
$M_r$ = 266.38
Monoclinic, $P2_1/n$
$a$ = 22.0249 (9) Å
$b$ = 6.4628 (1) Å
$c$ = 22.2739 (8) Å
$\beta$ = 118.694 (5)°
$V$ = 2781.2 (2) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 120 K
0.30 × 0.20 × 0.20 mm

### Data collection

Oxford Diffraction Xcalibur Sapphire2 diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
$T_{min}$ = 0.928, $T_{max}$ = 1.000
32353 measured reflections
4899 independent reflections
3314 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.064
$S$ = 0.83
4899 reflections
361 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

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

*Cg*1 is the centroid of the C2–C7 ring.

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C1—H1$\cdots$*Cg*1$^{i}$ | 0.95 | 3.07 | 3.9197 (16) | 150 |

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97*.

The financial support of this work by the Czech Ministry of Education (project No. MSM 7088352101), the Internal Funding Agency of Tomas Bata University in Zlin, project No. IGA/6/FT/11/D and the Operational Program Research and Development for Innovations co-funded by the European Regional Development Fund (ERDF) and the national budget of the Czech Republic, within the framework of project Centre of Polymer Systems (reg. number: CZ.1.05/2.1.00/03.0111) is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5341).

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# supporting information

*Acta Cryst.* (2011). E**67**, o2906 [doi:10.1107/S1600536811041018]

## 1-(1-Adamantylmethyl)-1*H*-benzimidazole

**Jarmila Černochová, Marek Nečas, Ivo Kuřitka and Robert Vícha**

### S1. Comment

Title compound has been prepared as a suitable building block for benzimidazolium-based carbene ligands synthesis and recently, the biological activity related to treatment of cortisole-dependent diseases has been studied (Hille *et al.*, 2011). Two polymorphs of a related structure have already been published (Lei & Zhou, 2009; Zhang *et al.*, 2010).

Both crystallographically independent molecules in the asymmetric unit (Fig. 1) contain essentially planar 1*H*-benzo[*d*]imidazole heterocycle with a maximum deviations from the best plane being 0.0134 (15) Å for C2 and 0.0229 (14) Å for C21, respectively. The torsion angles C7—N1—C8—C9 and N1—C8—C9—C16 describing the mutual orientation of benzimidazole and adamantane groups are 95.31 (15)° and -179.38 (10)°, respectively. The corresponding angles in the other molecule are -92.89 (15)° and -177.52 (10)°, respectively. The crystal packing is stabilized *via* weak C—H···$\pi$ interactions (Fig. 2, Table 1).

### S2. Experimental

Benzimidazole (0.40 g, 3.39 mmol) was dissolved in 40 $cm^3$ of dry DMF and sodium hydride (0.2 g, 8.46 mmol) was added portionwise at room temperature. Into this mixture, 1-adamantylbromomethane (1.16 g, 5.09 mmol) was added and the mixture was stirred under argon for 5 days at 373 K. The reaction mixture was poured onto 100 g of crushed ice, extracted with 4 × 25 $cm^3$ of dichloromethane and the collected organic portions were washed several times with distilled water, brine and dried over $Na_2SO_4$. The solvent was distilled off under reduced pressure and residual DMF was removed *via* azeotropic distillation with trichloromethane. The crude material was purified by crystallization (petroleum ether:ethyl acetate, 1:1, v:v) to yield 850 mg (94%) of colorless powder with mp=483–488 K. The crystal used for data collection was grown by spontaneous evaporation of a trichloromethane:methanol solution of the title compound at room temperature.

### S3. Refinement

All carbon bound H atoms were placed at calculated positions and were refined as riding with their $U_{iso}$ set to 1.2$U_{eq}$ of the respective carrier atoms.

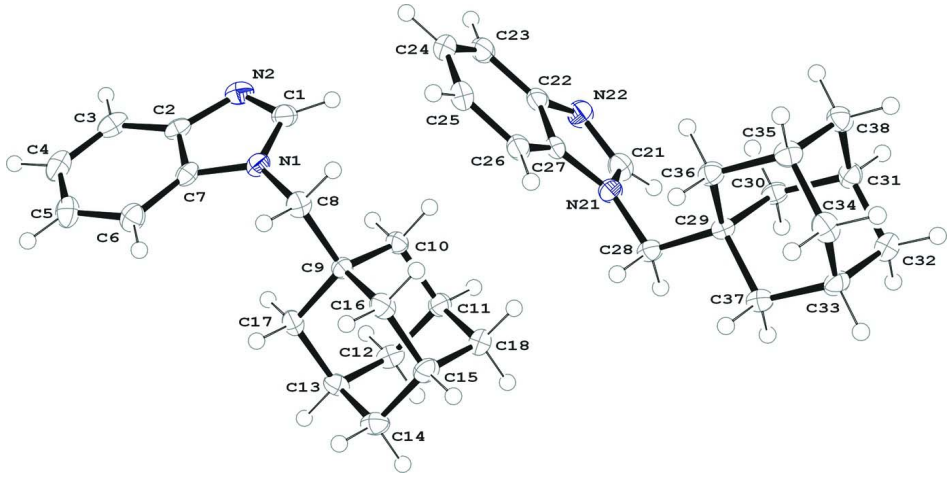


**Figure 1**

The asymmetric unit with 50% probability ellipsoids for non hydrogen atoms. H-atoms are shown as spheres at arbitrary radii.

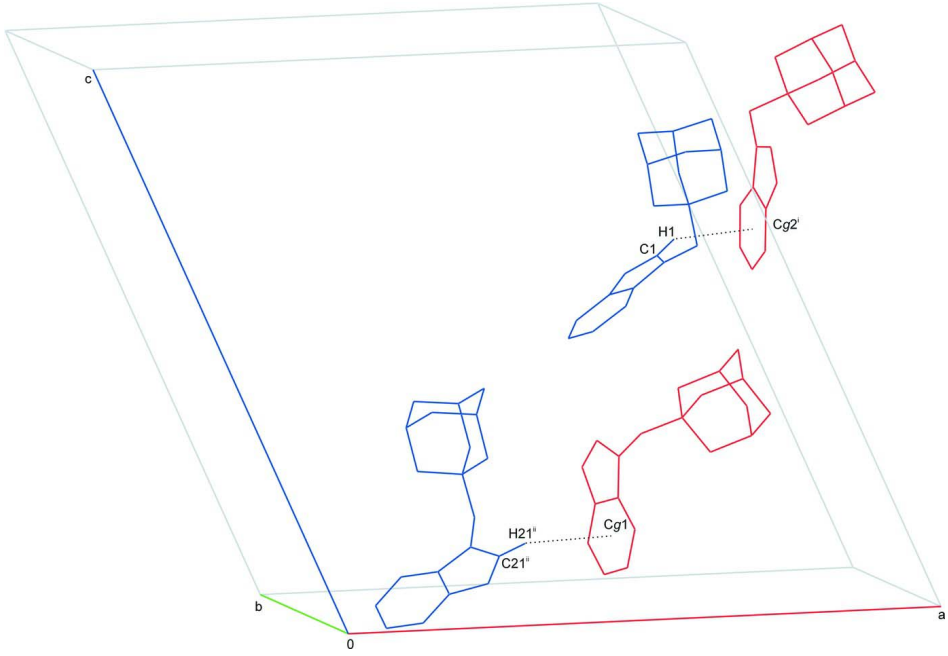


**Figure 2**

Two pairs of molecules linked *via* weak C—H···$\pi$ interactions (dotted lines) are colored by symmetry equivalence. H-atoms are omitted except for those participating in H-bonds. *Cg*1 is centre of gravity of C2–C7, Symmetry codes: (i) $x$ + 1/2, -$y$ + 1/2, $z$ + 1/2; (ii) $x$ - 1/2, -$y$ + 1/2, $y$ - 1/2.

### 1-(1-Adamantylmethyl)-1*H*-benzimidazole

*Crystal data*

$C_{18}H_{22}N_2$
$M_r$ = 266.38
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn

$a$ = 22.0249 (9) Å
$b$ = 6.4628 (1) Å
$c$ = 22.2739 (8) Å
$\beta$ = 118.694 (5)°

$V$ = 2781.2 (2) Å$^3$
$Z$ = 8
$F$(000) = 1152
$D_x$ = 1.272 Mg m$^{-3}$
Melting point: 486 K
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å

Cell parameters from 9351 reflections
$\theta$ = 2.8–27.3°
$\mu$ = 0.08 mm$^{-1}$
$T$ = 120 K
Block, colourless
0.30 × 0.20 × 0.20 mm

*Data collection*

Oxford Diffraction Xcalibur Sapphire2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.4353 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
$T_{min}$ = 0.928, $T_{max}$ = 1.000

32353 measured reflections
4899 independent reflections
3314 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 3.2°
$h$ = −26→17
$k$ = −7→7
$l$ = −26→26

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.064
$S$ = 0.83
4899 reflections
361 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

*Special details*

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.58857 (5) | 0.07364 (14) | 0.28113 (5) | 0.0206 (2) |
| N2 | 0.55730 (5) | 0.39787 (15) | 0.24104 (5) | 0.0258 (3) |
| C1 | 0.58788 (6) | 0.27873 (18) | 0.29503 (6) | 0.0238 (3) |
| H1 | 0.6080 | 0.3312 | 0.3404 | 0.029* |
| C2 | 0.53553 (6) | 0.26067 (18) | 0.18631 (6) | 0.0212 (3) |
| C3 | 0.49849 (6) | 0.2979 (2) | 0.11594 (6) | 0.0272 (3) |
| H3 | 0.4847 | 0.4340 | 0.0986 | 0.033* |
| C4 | 0.48257 (7) | 0.1313 (2) | 0.07262 (6) | 0.0297 (3) |
| H4 | 0.4574 | 0.1531 | 0.0246 | 0.036* |
| C5 | 0.50261 (6) | −0.0698 (2) | 0.09772 (6) | 0.0290 (3) |

| | | | | |
|---|---|---|---|---|
| H5 | 0.4909 | −0.1811 | 0.0662 | 0.035* |
| C6 | 0.53897 (6) | −0.11098 (19) | 0.16698 (6) | 0.0249 (3) |
| H6 | 0.5526 | −0.2474 | 0.1840 | 0.030* |
| C7 | 0.55451 (6) | 0.05820 (18) | 0.21038 (6) | 0.0201 (3) |
| C8 | 0.62286 (6) | −0.09207 (18) | 0.33114 (6) | 0.0221 (3) |
| H8A | 0.6009 | −0.2255 | 0.3100 | 0.026* |
| H8B | 0.6150 | −0.0687 | 0.3708 | 0.026* |
| C9 | 0.70077 (6) | −0.10925 (17) | 0.35702 (5) | 0.0170 (3) |
| C10 | 0.73908 (6) | 0.08829 (17) | 0.39375 (6) | 0.0204 (3) |
| H10A | 0.7223 | 0.2061 | 0.3614 | 0.025* |
| H10B | 0.7293 | 0.1191 | 0.4318 | 0.025* |
| C11 | 0.81690 (6) | 0.06242 (18) | 0.42177 (6) | 0.0227 (3) |
| H11 | 0.8412 | 0.1921 | 0.4458 | 0.027* |
| C12 | 0.83131 (7) | 0.01928 (18) | 0.36233 (6) | 0.0248 (3) |
| H12A | 0.8817 | 0.0039 | 0.3798 | 0.030* |
| H12B | 0.8148 | 0.1368 | 0.3298 | 0.030* |
| C13 | 0.79412 (6) | −0.17918 (18) | 0.32558 (6) | 0.0222 (3) |
| H13 | 0.8035 | −0.2068 | 0.2866 | 0.027* |
| C14 | 0.82057 (7) | −0.36073 (18) | 0.37585 (6) | 0.0255 (3) |
| H14A | 0.8709 | −0.3786 | 0.3934 | 0.031* |
| H14B | 0.7970 | −0.4899 | 0.3522 | 0.031* |
| C15 | 0.80601 (7) | −0.31763 (18) | 0.43533 (6) | 0.0239 (3) |
| H15 | 0.8231 | −0.4360 | 0.4683 | 0.029* |
| C16 | 0.72824 (7) | −0.29034 (18) | 0.40795 (6) | 0.0229 (3) |
| H16A | 0.7189 | −0.2635 | 0.4465 | 0.027* |
| H16B | 0.7039 | −0.4192 | 0.3849 | 0.027* |
| C17 | 0.71637 (6) | −0.15487 (18) | 0.29825 (6) | 0.0210 (3) |
| H17A | 0.6924 | −0.2835 | 0.2746 | 0.025* |
| H17B | 0.6988 | −0.0403 | 0.2647 | 0.025* |
| C18 | 0.84322 (7) | −0.11922 (18) | 0.47179 (6) | 0.0276 (3) |
| H18A | 0.8347 | −0.0918 | 0.5108 | 0.033* |
| H18B | 0.8937 | −0.1356 | 0.4899 | 0.033* |
| N21 | 0.81236 (5) | 0.11037 (14) | 0.61146 (5) | 0.0206 (2) |
| N22 | 0.77666 (6) | 0.43222 (15) | 0.57082 (5) | 0.0266 (3) |
| C21 | 0.82934 (7) | 0.31252 (19) | 0.60867 (6) | 0.0247 (3) |
| H21 | 0.8756 | 0.3621 | 0.6323 | 0.030* |
| C22 | 0.71997 (7) | 0.29919 (18) | 0.54557 (6) | 0.0221 (3) |
| C23 | 0.65052 (7) | 0.3378 (2) | 0.50043 (6) | 0.0276 (3) |
| H23 | 0.6351 | 0.4728 | 0.4828 | 0.033* |
| C24 | 0.60493 (7) | 0.1751 (2) | 0.48206 (6) | 0.0297 (3) |
| H24 | 0.5572 | 0.1988 | 0.4516 | 0.036* |
| C25 | 0.62717 (7) | −0.0254 (2) | 0.50718 (6) | 0.0279 (3) |
| H25 | 0.5942 | −0.1344 | 0.4931 | 0.033* |
| C26 | 0.69569 (7) | −0.06793 (19) | 0.55175 (6) | 0.0231 (3) |
| H26 | 0.7109 | −0.2035 | 0.5689 | 0.028* |
| C27 | 0.74142 (7) | 0.09792 (18) | 0.57037 (6) | 0.0202 (3) |
| C28 | 0.86030 (6) | −0.05658 (18) | 0.65027 (6) | 0.0211 (3) |
| H28A | 0.9047 | −0.0329 | 0.6503 | 0.025* |

| | | | | |
|---|---|---|---|---|
| H28B | 0.8411 | −0.1891 | 0.6264 | 0.025* |
| C29 | 0.87474 (6) | −0.07727 (17) | 0.72453 (6) | 0.0170 (3) |
| C30 | 0.90524 (6) | 0.12265 (17) | 0.76505 (6) | 0.0196 (3) |
| H30A | 0.9475 | 0.1611 | 0.7625 | 0.023* |
| H30B | 0.8713 | 0.2365 | 0.7447 | 0.023* |
| C31 | 0.92319 (6) | 0.09273 (18) | 0.83991 (6) | 0.0214 (3) |
| H31 | 0.9433 | 0.2237 | 0.8658 | 0.026* |
| C32 | 0.97601 (6) | −0.08287 (18) | 0.87178 (6) | 0.0252 (3) |
| H32A | 1.0189 | −0.0479 | 0.8700 | 0.030* |
| H32B | 0.9879 | −0.1014 | 0.9203 | 0.030* |
| C33 | 0.94509 (7) | −0.28301 (18) | 0.83216 (6) | 0.0227 (3) |
| H33 | 0.9794 | −0.3980 | 0.8528 | 0.027* |
| C34 | 0.87901 (7) | −0.33678 (18) | 0.83533 (6) | 0.0254 (3) |
| H34A | 0.8592 | −0.4672 | 0.8102 | 0.031* |
| H34B | 0.8900 | −0.3571 | 0.8835 | 0.031* |
| C35 | 0.82659 (6) | −0.16154 (18) | 0.80349 (6) | 0.0223 (3) |
| H35 | 0.7834 | −0.1967 | 0.8056 | 0.027* |
| C36 | 0.80937 (6) | −0.13371 (18) | 0.72869 (6) | 0.0208 (3) |
| H36A | 0.7895 | −0.2636 | 0.7032 | 0.025* |
| H36B | 0.7744 | −0.0228 | 0.7074 | 0.025* |
| C37 | 0.92803 (6) | −0.25205 (17) | 0.75754 (6) | 0.0210 (3) |
| H37A | 0.9092 | −0.3821 | 0.7317 | 0.025* |
| H37B | 0.9708 | −0.2171 | 0.7556 | 0.025* |
| C38 | 0.85747 (7) | 0.03925 (18) | 0.84316 (6) | 0.0239 (3) |
| H38A | 0.8235 | 0.1531 | 0.8230 | 0.029* |
| H38B | 0.8683 | 0.0217 | 0.8915 | 0.029* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0174 (6) | 0.0193 (6) | 0.0220 (5) | 0.0012 (5) | 0.0070 (5) | 0.0012 (4) |
| N2 | 0.0240 (7) | 0.0219 (6) | 0.0326 (6) | 0.0042 (5) | 0.0145 (5) | 0.0022 (5) |
| C1 | 0.0203 (8) | 0.0231 (7) | 0.0282 (7) | 0.0005 (6) | 0.0118 (6) | −0.0036 (6) |
| C2 | 0.0135 (8) | 0.0227 (7) | 0.0282 (7) | 0.0014 (6) | 0.0104 (6) | 0.0035 (5) |
| C3 | 0.0192 (8) | 0.0300 (7) | 0.0336 (7) | 0.0041 (6) | 0.0136 (6) | 0.0109 (6) |
| C4 | 0.0196 (8) | 0.0416 (9) | 0.0237 (7) | −0.0017 (7) | 0.0070 (6) | 0.0063 (6) |
| C5 | 0.0239 (9) | 0.0330 (8) | 0.0249 (7) | −0.0076 (7) | 0.0077 (6) | −0.0033 (6) |
| C6 | 0.0218 (8) | 0.0231 (7) | 0.0263 (7) | −0.0038 (6) | 0.0087 (6) | 0.0005 (6) |
| C7 | 0.0124 (8) | 0.0242 (7) | 0.0221 (7) | −0.0016 (6) | 0.0071 (6) | 0.0025 (5) |
| C8 | 0.0247 (8) | 0.0200 (7) | 0.0218 (7) | −0.0003 (6) | 0.0113 (6) | 0.0023 (5) |
| C9 | 0.0177 (8) | 0.0164 (6) | 0.0163 (6) | 0.0014 (5) | 0.0076 (6) | 0.0010 (5) |
| C10 | 0.0235 (8) | 0.0178 (6) | 0.0190 (6) | 0.0025 (6) | 0.0094 (6) | −0.0011 (5) |
| C11 | 0.0193 (8) | 0.0190 (7) | 0.0244 (7) | −0.0009 (6) | 0.0063 (6) | −0.0052 (5) |
| C12 | 0.0216 (8) | 0.0223 (7) | 0.0315 (7) | 0.0026 (6) | 0.0134 (7) | 0.0043 (6) |
| C13 | 0.0258 (9) | 0.0226 (7) | 0.0232 (6) | 0.0017 (6) | 0.0156 (6) | −0.0014 (5) |
| C14 | 0.0254 (8) | 0.0194 (7) | 0.0329 (7) | 0.0030 (6) | 0.0149 (7) | −0.0008 (6) |
| C15 | 0.0253 (9) | 0.0221 (7) | 0.0221 (7) | 0.0077 (6) | 0.0097 (6) | 0.0075 (5) |
| C16 | 0.0303 (9) | 0.0203 (7) | 0.0207 (6) | 0.0020 (6) | 0.0143 (6) | 0.0025 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C17 | 0.0262 (8) | 0.0186 (6) | 0.0171 (6) | −0.0011 (6) | 0.0095 (6) | −0.0013 (5) |
| C18 | 0.0235 (8) | 0.0330 (8) | 0.0199 (7) | 0.0052 (6) | 0.0053 (6) | −0.0007 (6) |
| N21 | 0.0234 (7) | 0.0184 (6) | 0.0190 (5) | 0.0037 (5) | 0.0094 (5) | 0.0028 (4) |
| N22 | 0.0324 (7) | 0.0223 (6) | 0.0233 (6) | 0.0043 (6) | 0.0119 (5) | 0.0039 (5) |
| C21 | 0.0309 (9) | 0.0223 (7) | 0.0222 (7) | −0.0010 (6) | 0.0138 (6) | 0.0012 (6) |
| C22 | 0.0292 (9) | 0.0221 (7) | 0.0160 (6) | 0.0058 (6) | 0.0116 (6) | 0.0011 (5) |
| C23 | 0.0354 (9) | 0.0260 (7) | 0.0185 (7) | 0.0111 (7) | 0.0108 (7) | 0.0020 (6) |
| C24 | 0.0256 (9) | 0.0367 (8) | 0.0196 (7) | 0.0097 (7) | 0.0051 (6) | −0.0019 (6) |
| C25 | 0.0279 (9) | 0.0321 (8) | 0.0200 (7) | −0.0007 (7) | 0.0085 (7) | −0.0054 (6) |
| C26 | 0.0280 (9) | 0.0216 (7) | 0.0176 (6) | 0.0041 (6) | 0.0093 (6) | −0.0005 (5) |
| C27 | 0.0224 (8) | 0.0246 (7) | 0.0131 (6) | 0.0036 (6) | 0.0083 (6) | −0.0016 (5) |
| C28 | 0.0205 (8) | 0.0196 (6) | 0.0229 (7) | 0.0045 (6) | 0.0102 (6) | 0.0017 (5) |
| C29 | 0.0155 (7) | 0.0163 (6) | 0.0196 (6) | 0.0009 (5) | 0.0087 (6) | 0.0015 (5) |
| C30 | 0.0160 (8) | 0.0179 (6) | 0.0258 (7) | 0.0003 (5) | 0.0108 (6) | 0.0018 (5) |
| C31 | 0.0214 (8) | 0.0181 (6) | 0.0210 (6) | −0.0016 (6) | 0.0074 (6) | −0.0019 (5) |
| C32 | 0.0221 (8) | 0.0274 (7) | 0.0221 (7) | 0.0012 (6) | 0.0073 (6) | 0.0026 (6) |
| C33 | 0.0224 (8) | 0.0193 (6) | 0.0230 (7) | 0.0060 (6) | 0.0084 (6) | 0.0053 (5) |
| C34 | 0.0348 (9) | 0.0197 (7) | 0.0235 (7) | −0.0012 (6) | 0.0154 (6) | 0.0027 (5) |
| C35 | 0.0206 (8) | 0.0233 (7) | 0.0264 (7) | −0.0019 (6) | 0.0140 (6) | 0.0014 (5) |
| C36 | 0.0183 (8) | 0.0193 (6) | 0.0238 (6) | −0.0002 (6) | 0.0094 (6) | −0.0006 (5) |
| C37 | 0.0199 (8) | 0.0184 (6) | 0.0256 (7) | 0.0014 (6) | 0.0117 (6) | 0.0003 (5) |
| C38 | 0.0284 (9) | 0.0237 (7) | 0.0220 (7) | 0.0033 (6) | 0.0141 (6) | 0.0019 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C1 | 1.3629 (14) | N21—C21 | 1.3685 (14) |
| N1—C7 | 1.3860 (14) | N21—C27 | 1.3829 (15) |
| N1—C8 | 1.4664 (13) | N21—C28 | 1.4661 (14) |
| N2—C1 | 1.3096 (14) | N22—C21 | 1.3100 (15) |
| N2—C2 | 1.3931 (15) | N22—C22 | 1.3929 (15) |
| C1—H1 | 0.9500 | C21—H21 | 0.9500 |
| C2—C3 | 1.3972 (16) | C22—C23 | 1.3915 (17) |
| C2—C7 | 1.3997 (16) | C22—C27 | 1.4035 (16) |
| C3—C4 | 1.3744 (17) | C23—C24 | 1.3738 (18) |
| C3—H3 | 0.9500 | C23—H23 | 0.9500 |
| C4—C5 | 1.4000 (17) | C24—C25 | 1.4029 (17) |
| C4—H4 | 0.9500 | C24—H24 | 0.9500 |
| C5—C6 | 1.3805 (16) | C25—C26 | 1.3784 (17) |
| C5—H5 | 0.9500 | C25—H25 | 0.9500 |
| C6—C7 | 1.3889 (16) | C26—C27 | 1.3908 (16) |
| C6—H6 | 0.9500 | C26—H26 | 0.9500 |
| C8—C9 | 1.5294 (16) | C28—C29 | 1.5329 (15) |
| C8—H8A | 0.9900 | C28—H28A | 0.9900 |
| C8—H8B | 0.9900 | C28—H28B | 0.9900 |
| C9—C10 | 1.5324 (15) | C29—C36 | 1.5306 (16) |
| C9—C17 | 1.5331 (15) | C29—C30 | 1.5340 (15) |
| C9—C16 | 1.5374 (15) | C29—C37 | 1.5380 (15) |
| C10—C11 | 1.5257 (16) | C30—C31 | 1.5299 (15) |

| | | | |
|---|---|---|---|
| C10—H10A | 0.9900 | C30—H30A | 0.9900 |
| C10—H10B | 0.9900 | C30—H30B | 0.9900 |
| C11—C12 | 1.5280 (16) | C31—C38 | 1.5234 (17) |
| C11—C18 | 1.5281 (16) | C31—C32 | 1.5337 (15) |
| C11—H11 | 1.0000 | C31—H31 | 1.0000 |
| C12—C13 | 1.5304 (16) | C32—C33 | 1.5292 (16) |
| C12—H12A | 0.9900 | C32—H32A | 0.9900 |
| C12—H12B | 0.9900 | C32—H32B | 0.9900 |
| C13—C17 | 1.5253 (16) | C33—C34 | 1.5305 (17) |
| C13—C14 | 1.5308 (16) | C33—C37 | 1.5310 (15) |
| C13—H13 | 1.0000 | C33—H33 | 1.0000 |
| C14—C15 | 1.5308 (16) | C34—C35 | 1.5273 (16) |
| C14—H14A | 0.9900 | C34—H34A | 0.9900 |
| C14—H14B | 0.9900 | C34—H34B | 0.9900 |
| C15—C16 | 1.5277 (16) | C35—C36 | 1.5314 (16) |
| C15—C18 | 1.5285 (16) | C35—C38 | 1.5331 (16) |
| C15—H15 | 1.0000 | C35—H35 | 1.0000 |
| C16—H16A | 0.9900 | C36—H36A | 0.9900 |
| C16—H16B | 0.9900 | C36—H36B | 0.9900 |
| C17—H17A | 0.9900 | C37—H37A | 0.9900 |
| C17—H17B | 0.9900 | C37—H37B | 0.9900 |
| C18—H18A | 0.9900 | C38—H38A | 0.9900 |
| C18—H18B | 0.9900 | C38—H38B | 0.9900 |

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|---|---|---|---|
| C1—N1—C7 | 105.63 (10) | C21—N21—C27 | 105.78 (10) |
| C1—N1—C8 | 126.55 (10) | C21—N21—C28 | 126.46 (11) |
| C7—N1—C8 | 127.68 (10) | C27—N21—C28 | 127.76 (10) |
| C1—N2—C2 | 103.80 (10) | C21—N22—C22 | 103.92 (10) |
| N2—C1—N1 | 114.83 (11) | N22—C21—N21 | 114.59 (12) |
| N2—C1—H1 | 122.6 | N22—C21—H21 | 122.7 |
| N1—C1—H1 | 122.6 | N21—C21—H21 | 122.7 |
| N2—C2—C3 | 129.95 (11) | C23—C22—N22 | 129.96 (11) |
| N2—C2—C7 | 110.23 (10) | C23—C22—C27 | 119.75 (12) |
| C3—C2—C7 | 119.79 (11) | N22—C22—C27 | 110.24 (11) |
| C4—C3—C2 | 117.86 (12) | C24—C23—C22 | 118.07 (12) |
| C4—C3—H3 | 121.1 | C24—C23—H23 | 121.0 |
| C2—C3—H3 | 121.1 | C22—C23—H23 | 121.0 |
| C3—C4—C5 | 121.46 (12) | C23—C24—C25 | 121.53 (12) |
| C3—C4—H4 | 119.3 | C23—C24—H24 | 119.2 |
| C5—C4—H4 | 119.3 | C25—C24—H24 | 119.2 |
| C6—C5—C4 | 121.84 (12) | C26—C25—C24 | 121.56 (13) |
| C6—C5—H5 | 119.1 | C26—C25—H25 | 119.2 |
| C4—C5—H5 | 119.1 | C24—C25—H25 | 119.2 |
| C5—C6—C7 | 116.30 (12) | C25—C26—C27 | 116.53 (12) |
| C5—C6—H6 | 121.9 | C25—C26—H26 | 121.7 |
| C7—C6—H6 | 121.9 | C27—C26—H26 | 121.7 |
| N1—C7—C6 | 131.75 (11) | N21—C27—C26 | 131.96 (11) |
| N1—C7—C2 | 105.50 (10) | N21—C27—C22 | 105.45 (11) |

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| C6—C7—C2 | 122.74 (11) | C26—C27—C22 | 122.55 (12) |
| N1—C8—C9 | 114.51 (9) | N21—C28—C29 | 114.71 (9) |
| N1—C8—H8A | 108.6 | N21—C28—H28A | 108.6 |
| C9—C8—H8A | 108.6 | C29—C28—H28A | 108.6 |
| N1—C8—H8B | 108.6 | N21—C28—H28B | 108.6 |
| C9—C8—H8B | 108.6 | C29—C28—H28B | 108.6 |
| H8A—C8—H8B | 107.6 | H28A—C28—H28B | 107.6 |
| C8—C9—C10 | 111.79 (9) | C36—C29—C28 | 111.85 (9) |
| C8—C9—C17 | 111.28 (9) | C36—C29—C30 | 108.90 (9) |
| C10—C9—C17 | 108.93 (9) | C28—C29—C30 | 111.52 (9) |
| C8—C9—C16 | 107.83 (9) | C36—C29—C37 | 108.67 (9) |
| C10—C9—C16 | 108.64 (9) | C28—C29—C37 | 107.17 (9) |
| C17—C9—C16 | 108.27 (9) | C30—C29—C37 | 108.62 (9) |
| C11—C10—C9 | 110.46 (9) | C31—C30—C29 | 110.23 (9) |
| C11—C10—H10A | 109.6 | C31—C30—H30A | 109.6 |
| C9—C10—H10A | 109.6 | C29—C30—H30A | 109.6 |
| C11—C10—H10B | 109.6 | C31—C30—H30B | 109.6 |
| C9—C10—H10B | 109.6 | C29—C30—H30B | 109.6 |
| H10A—C10—H10B | 108.1 | H30A—C30—H30B | 108.1 |
| C10—C11—C12 | 108.99 (10) | C38—C31—C30 | 109.04 (9) |
| C10—C11—C18 | 109.93 (10) | C38—C31—C32 | 109.70 (10) |
| C12—C11—C18 | 109.12 (10) | C30—C31—C32 | 109.85 (10) |
| C10—C11—H11 | 109.6 | C38—C31—H31 | 109.4 |
| C12—C11—H11 | 109.6 | C30—C31—H31 | 109.4 |
| C18—C11—H11 | 109.6 | C32—C31—H31 | 109.4 |
| C11—C12—C13 | 109.63 (10) | C33—C32—C31 | 109.28 (10) |
| C11—C12—H12A | 109.7 | C33—C32—H32A | 109.8 |
| C13—C12—H12A | 109.7 | C31—C32—H32A | 109.8 |
| C11—C12—H12B | 109.7 | C33—C32—H32B | 109.8 |
| C13—C12—H12B | 109.7 | C31—C32—H32B | 109.8 |
| H12A—C12—H12B | 108.2 | H32A—C32—H32B | 108.3 |
| C17—C13—C12 | 109.70 (10) | C32—C33—C34 | 109.59 (10) |
| C17—C13—C14 | 109.32 (10) | C32—C33—C37 | 108.97 (9) |
| C12—C13—C14 | 109.46 (10) | C34—C33—C37 | 109.67 (10) |
| C17—C13—H13 | 109.4 | C32—C33—H33 | 109.5 |
| C12—C13—H13 | 109.4 | C34—C33—H33 | 109.5 |
| C14—C13—H13 | 109.4 | C37—C33—H33 | 109.5 |
| C13—C14—C15 | 109.23 (10) | C35—C34—C33 | 109.50 (10) |
| C13—C14—H14A | 109.8 | C35—C34—H34A | 109.8 |
| C15—C14—H14A | 109.8 | C33—C34—H34A | 109.8 |
| C13—C14—H14B | 109.8 | C35—C34—H34B | 109.8 |
| C15—C14—H14B | 109.8 | C33—C34—H34B | 109.8 |
| H14A—C14—H14B | 108.3 | H34A—C34—H34B | 108.2 |
| C16—C15—C18 | 109.12 (10) | C34—C35—C36 | 109.23 (10) |
| C16—C15—C14 | 109.64 (10) | C34—C35—C38 | 109.44 (10) |
| C18—C15—C14 | 109.32 (10) | C36—C35—C38 | 109.71 (9) |
| C16—C15—H15 | 109.6 | C34—C35—H35 | 109.5 |
| C18—C15—H15 | 109.6 | C36—C35—H35 | 109.5 |

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|---|---|---|---|
| C14—C15—H15 | 109.6 | C38—C35—H35 | 109.5 |
| C15—C16—C9 | 110.55 (10) | C29—C36—C35 | 110.19 (10) |
| C15—C16—H16A | 109.5 | C29—C36—H36A | 109.6 |
| C9—C16—H16A | 109.5 | C35—C36—H36A | 109.6 |
| C15—C16—H16B | 109.5 | C29—C36—H36B | 109.6 |
| C9—C16—H16B | 109.5 | C35—C36—H36B | 109.6 |
| H16A—C16—H16B | 108.1 | H36A—C36—H36B | 108.1 |
| C13—C17—C9 | 110.37 (9) | C33—C37—C29 | 110.37 (9) |
| C13—C17—H17A | 109.6 | C33—C37—H37A | 109.6 |
| C9—C17—H17A | 109.6 | C29—C37—H37A | 109.6 |
| C13—C17—H17B | 109.6 | C33—C37—H37B | 109.6 |
| C9—C17—H17B | 109.6 | C29—C37—H37B | 109.6 |
| H17A—C17—H17B | 108.1 | H37A—C37—H37B | 108.1 |
| C11—C18—C15 | 109.76 (10) | C31—C38—C35 | 109.47 (10) |
| C11—C18—H18A | 109.7 | C31—C38—H38A | 109.8 |
| C15—C18—H18A | 109.7 | C35—C38—H38A | 109.8 |
| C11—C18—H18B | 109.7 | C31—C38—H38B | 109.8 |
| C15—C18—H18B | 109.7 | C35—C38—H38B | 109.8 |
| H18A—C18—H18B | 108.2 | H38A—C38—H38B | 108.2 |

*Hydrogen-bond geometry (Å, º)*

*Cg*1 is the centroid of the C2–C7 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1···*Cg*1$^{i}$ | 0.95 | 3.07 | 3.9197 (16) | 150 |

Symmetry code: (i) *x*+1/2, −*y*+1/2, *z*+1/2.