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# (*E*)-1,2-Bis(1-propyl-5,6-dimethyl-1*H*-benzimidazol-2-yl)ethene

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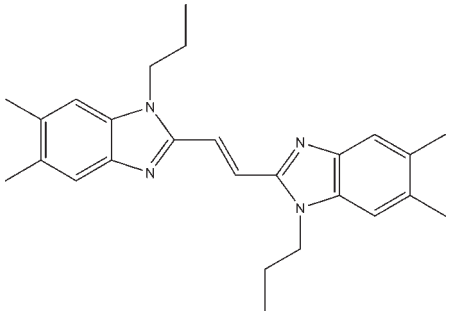
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.057; $wR$ factor = 0.151; data-to-parameter ratio = 15.6.

In the title compound, $C_{26}H_{32}N_4$, the essentially planar (r.m.s. deviations of 0.0053 and 0.0242 Å) benzimidazole fragments are *trans* with respect to a central ethene fragment, and are canted in opposite directions by 2.78 (6) and 5.87 (6)° with respect to the ethene plane, giving the molecule a propeller conformation. The terminal ethyl fragments of the pendant *n*-propyl groups protrude to either side of the benzimidazole planes. Overall, the molecule exhibits a pseudo-center of symmetry at the mid-point of the ethene fragment. Both $\pi$–$\pi$ stacking and typical C—H$\cdots\pi$ interactions are notably absent, as are intermolecular hydrogen bonds. When viewed along the *a* axis, the structure appears as criss-crossed layers of molecules with the planar fragments separated along the *c*-cell direction by the protruding ethyl groups.

## Related literature

For applications of bis(imidazoles), bis(benzimidazoles) and their complexes with metal ions, see: Knapp *et al.* (1990); Stibrany *et al.* (2002, 2003, 2004); Stibrany & Potenza (2008). The title compound was prepared from *rac*-1,2-bis(1*H*-5,6-dimethylbenzimidazol-2-yl)-1-hydroxyethane (Taffs *et al.*, 1961). Alkylation was effected according to a reported method (Stibrany *et al.*, 2004). For related structures see: Stibrany *et al.* (2005); Stibrany & Potenza (2006*a*,*b*, 2009). For a description of the Cambridge Structural Database, see: Allen (2002).



## Experimental

### Crystal data

$C_{26}H_{32}N_4$
$M_r$ = 400.56
Monoclinic, $P2_1/n$
$a$ = 12.7822 (15) Å
$b$ = 10.4802 (12) Å
$c$ = 16.5944 (19) Å
$\beta$ = 100.284 (2)°
$V$ = 2187.3 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 100 K
0.32 × 0.28 × 0.11 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Blessing, 1995)
$T_{min}$ = 0.795, $T_{max}$ = 1.00
20415 measured reflections
4324 independent reflections
3596 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.151
$S$ = 1.00
4324 reflections
277 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-32* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2128).

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# supporting information

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## (*E*)-1,2-Bis(1-propyl-5,6-dimethyl-1*H*-benzimidazol-2-yl)ethene

**Robert T. Stibrany and Joseph A. Potenza**

### S1. Comment

The title compound (I) was prepared as part of our long-term interest in the chemistry of bis(imidazoles), bis-(benzimidazoles), and their complexes with metal ions. These species have demonstrated their usefulness as proton sponges (Stibrany *et al.*, 2002), geometrically constraining ligands (Stibrany *et al.*, 2004), agents to study electron transfer (Knapp *et al.*, 1990), polymerization catalysts (Stibrany *et al.*, 2003), and in the formation of metal-organic copolymers (Stibrany & Potenza, 2008), The present structure (Fig. 1) contains a central, planar *trans* 1,2-disubstituted ethene fragment linked at the 2 positions (C12 and C22) to 1-propyl, 5,6-dimethylbenzimidazole fragments. Excluding alkyl substituents, the structure can be viewed as three essentially planar fragments connected by two hinges, the C1—C12 and C2—C22 bonds. The benzimidazole fragments are canted in opposite directions by 2.78 (6)° (bzim 1) and 5.87 (6)°(bzim2) to give the molecule a slight propeller-like shape, while the ethyl fragments of the pendant *n*-propyl groups, which protrude above and below the planes of the benzimidazole fragments, help to ensure that the molecule has an approximate center of symmetry at the midpoint of the C1—C2 bond.

When viewed approximately along the a cell direction (Fig.2), the structure appears as layers of criss-crossed molecules with the planar fragments separated along the c cell direction by the protruding ethyl groups. A comparative view along the b cell direction (Fig. 3) shows the protruding ethyl groups in a different orientation and indicates clearly the lack of coplanarity of the benzimidazole fragments. These figures are consistent with the absence of $\pi$–$\pi$ stacking and typical C—H···$\pi$ interactions found by *Platon* (Spek, 2009). The absences noted above are consistent with the ethyl group conformations, which appear to prevent effective overlap of the $\pi$ systems. The lack of intermolecular hydrogen bonds is also attributed to the *n*-propyl substituents, which prevent the formation of intermolecular *N*(imine)··· *H*–*N*(amine) hydrogen bonds.

### S2. Experimental

Compound (I) was prepared from *rac*-1,2-bis(1*H*-5,6-dimethylbenzimidazol-2-yl)-1-hydroxyethane (Taffs *et al.*, 1961). Alkylation was effected according to a reported method (Stibrany *et al.*, 2004). Under Ar, NaH (6 molar equivalents) was added to amixture of *rac*-1,2-bis(1*H*-5,6-dimethylbenzimidazol-2-yl)-1-hydroxyethane in dry dimethyl sulfoxide (DMSO). After a reaction time of 10 minutes, *n*-propyl iodide (2 molar equivalents) was added dropwise. After an additional hour, the product was precipitated with water, collected by filtration, and dried in air. Crystals of (I) (m.p. 523 (soften) 538-539 K(melt)) were obtained by slow cooling of a hot DMSO solution of (I). $R_f$ = 0.64 (ethyl acetate/silica). IR (KBr pellet, $cm^{-1}$): 2967 (w), 2785 (w), 2700(w), 1582 (s), 1431 (m), 1367 (m), 1326 (w), 1004 (w), 768 (w), 669 (w), 649(w). Compound (I) is remarkably less soluble in a variety of solvents than analogous bis(benzimidazole)ethene compounds previously reported (Stibrany *et al.*, 2005; Stibrany & Potenza, 2006a,b; Stibrany & Potenza, 2009) which, in contrast to (I), were not substituted at the 5 and 6 positions.

### S3. Refinement

Hydrogen atoms were positioned geometrically using a riding model, with C—H = 0.93 Å and $U_{iso}$(H) = 1.2 $U_{eq}$(C).

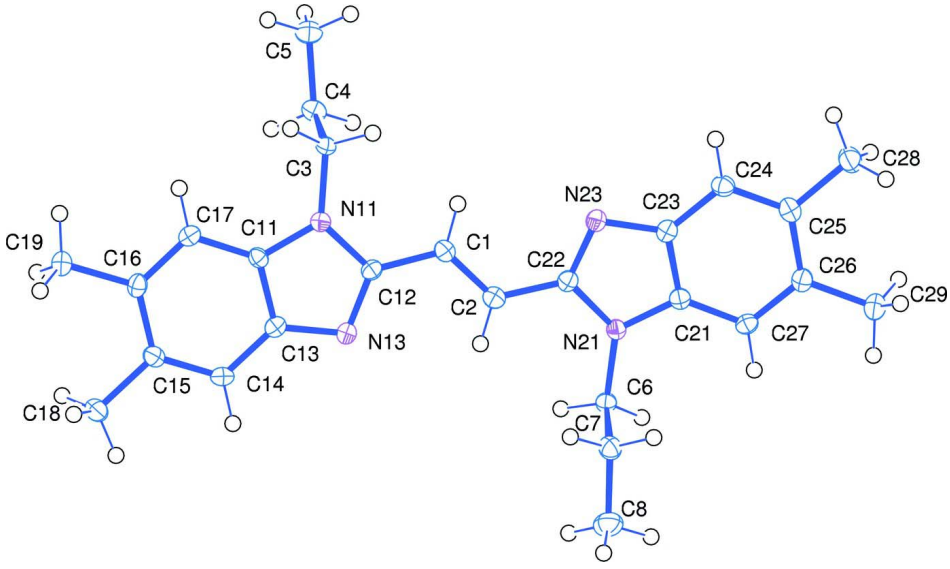


**Figure 1**

The molecular structure of the title compound showing the atom-numbering scheme. Displacement ellipsoids are shown at the 50% probability level. H atoms are shown as spheres of arbitrary radius

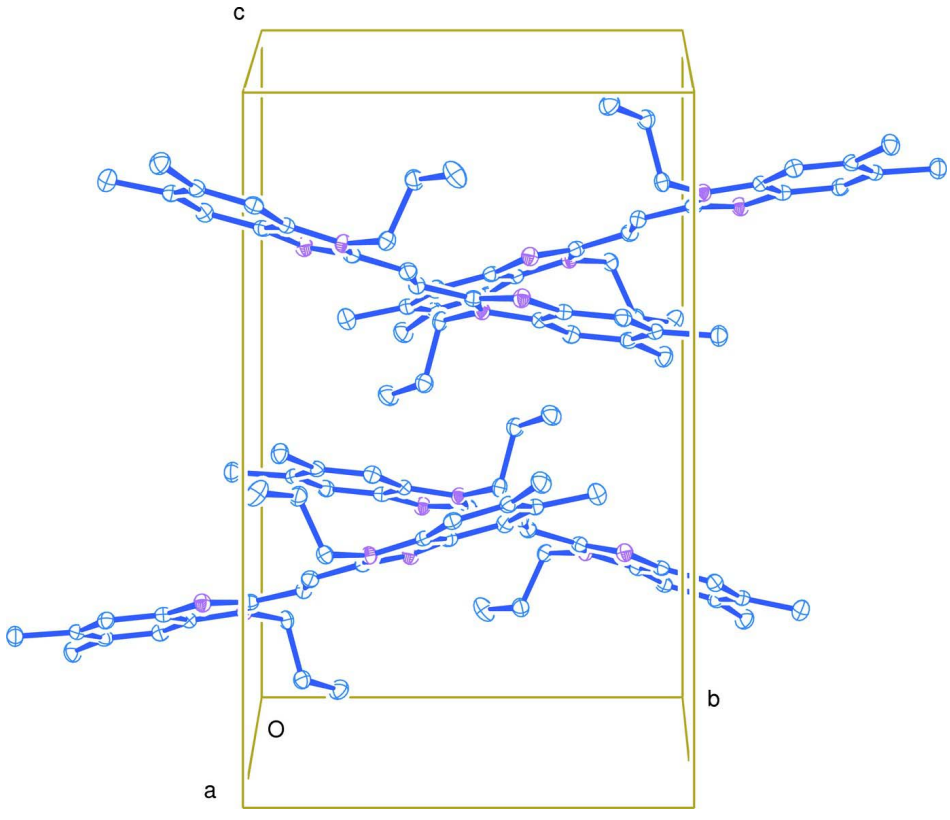

**Figure 2**

The structure viewed approximately along the a cell direction. H atoms have been omitted for clarity.

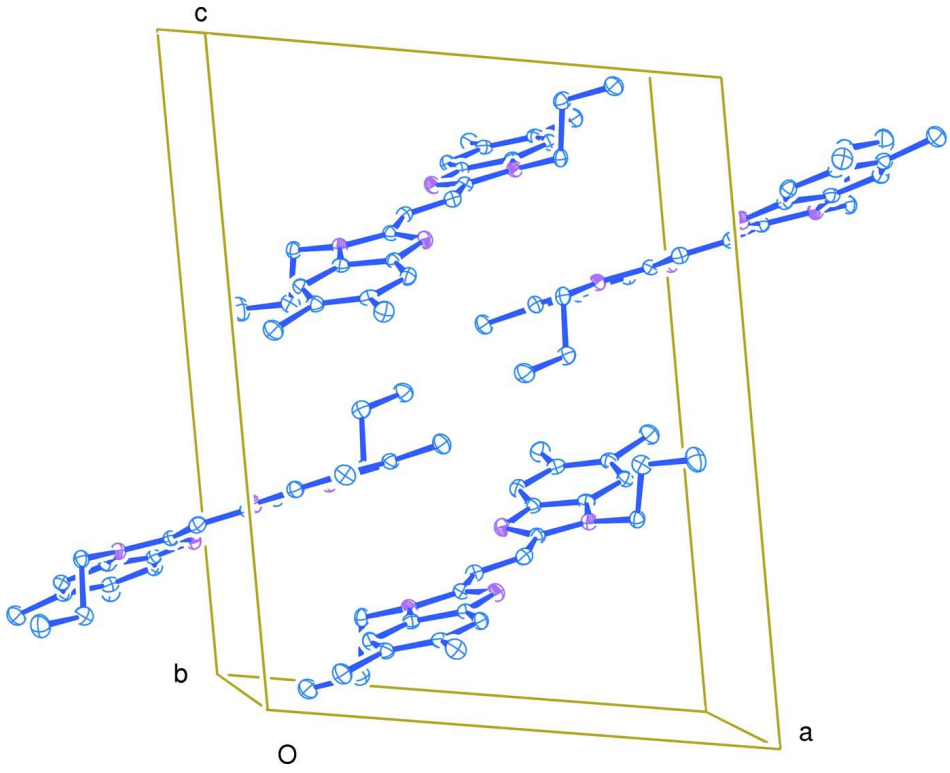


**Figure 3**

The structure viewed approximately along the b cell direction. H atoms have been omitted for clarity.

### (*E*)-1,2-Bis(1-propyl-5,6-dimethyl-1*H*-benzimidazol-2-yl)ethene

*Crystal data*

$C_{26}H_{32}N_4$
$M_r = 400.56$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 12.7822\ (15)$ Å
$b = 10.4802\ (12)$ Å
$c = 16.5944\ (19)$ Å
$\beta = 100.284\ (2)°$
$V = 2187.3\ (4)$ Å$^3$
$Z = 4$
$F(000) = 864$
$D_x = 1.216$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 953 reflections
$\theta = 2.3–25.6°$
$\mu = 0.07$ mm$^{-1}$
$T = 100$ K
Plate, yellow
0.32 × 0.28 × 0.11 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Blessing, 1995)
$T_{min} = 0.795$, $T_{max} = 1.00$
20415 measured reflections
4324 independent reflections
3596 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 26.1°$, $\theta_{min} = 1.9°$
$h = -15\rightarrow15$
$k = -12\rightarrow12$
$l = -20\rightarrow20$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.151$
$S = 1.00$
4324 reflections
277 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
$w = 1/[\sigma^2(F_o^2) + (0.090P)^2 + 1.071P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å$^{-3}$
$\Delta\rho_{min} = -0.18$ e Å$^{-3}$

*Special details*

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

**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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N23 | −0.03575 (12) | 0.86314 (15) | 0.21188 (9) | 0.0185 (4) |
| N13 | 0.04680 (12) | 0.38211 (15) | 0.29290 (9) | 0.0184 (4) |
| C13 | 0.12082 (14) | 0.28848 (18) | 0.32073 (10) | 0.0162 (4) |
| N11 | 0.20831 (12) | 0.47168 (14) | 0.32962 (9) | 0.0164 (3) |
| N21 | −0.19800 (12) | 0.77194 (14) | 0.18947 (9) | 0.0164 (3) |
| C16 | 0.29931 (14) | 0.13963 (18) | 0.38184 (11) | 0.0179 (4) |
| C24 | −0.10049 (14) | 1.08026 (18) | 0.15724 (11) | 0.0188 (4) |
| H24 | −0.0327 | 1.1202 | 0.1677 | 0.023* |
| C11 | 0.22163 (14) | 0.34258 (17) | 0.34411 (10) | 0.0154 (4) |
| C21 | −0.21246 (14) | 0.89625 (18) | 0.16303 (10) | 0.0168 (4) |
| C26 | −0.29142 (15) | 1.08870 (18) | 0.10388 (11) | 0.0187 (4) |
| C17 | 0.31163 (14) | 0.27017 (18) | 0.37496 (11) | 0.0182 (4) |
| H17 | 0.3792 | 0.3093 | 0.3907 | 0.022* |
| C23 | −0.11131 (14) | 0.95179 (18) | 0.17796 (10) | 0.0170 (4) |
| C15 | 0.19728 (14) | 0.08225 (18) | 0.35742 (10) | 0.0175 (4) |
| C14 | 0.10936 (14) | 0.15596 (18) | 0.32759 (11) | 0.0179 (4) |
| H14 | 0.0416 | 0.1172 | 0.3118 | 0.021* |
| C25 | −0.18941 (15) | 1.14824 (18) | 0.12140 (11) | 0.0191 (4) |
| C12 | 0.10150 (14) | 0.49004 (17) | 0.29953 (11) | 0.0164 (4) |
| C22 | −0.09024 (14) | 0.75650 (18) | 0.21683 (11) | 0.0167 (4) |
| C27 | −0.30311 (14) | 0.96279 (18) | 0.12593 (11) | 0.0180 (4) |
| H27 | −0.3709 | 0.9227 | 0.1161 | 0.022* |
| C2 | −0.04547 (15) | 0.63331 (18) | 0.24519 (11) | 0.0186 (4) |
| H2 | −0.0918 | 0.5619 | 0.2418 | 0.022* |
| C1 | 0.05794 (14) | 0.61551 (18) | 0.27588 (11) | 0.0178 (4) |

| | | | | |
|---|---|---|---|---|
| H1 | 0.1042 | 0.6872 | 0.2824 | 0.021* |
| C19 | 0.39431 (15) | 0.05820 (19) | 0.41661 (12) | 0.0221 (4) |
| H19A | 0.4580 | 0.1119 | 0.4284 | 0.033* |
| H19B | 0.4045 | −0.0075 | 0.3767 | 0.033* |
| H19C | 0.3821 | 0.0174 | 0.4673 | 0.033* |
| C18 | 0.18662 (16) | −0.06113 (18) | 0.36216 (12) | 0.0228 (4) |
| H18A | 0.1118 | −0.0852 | 0.3457 | 0.034* |
| H18B | 0.2125 | −0.0895 | 0.4185 | 0.034* |
| H18C | 0.2288 | −0.1016 | 0.3254 | 0.034* |
| C28 | −0.17841 (16) | 1.28882 (19) | 0.10451 (13) | 0.0251 (5) |
| H28A | −0.1030 | 1.3123 | 0.1150 | 0.038* |
| H28B | −0.2161 | 1.3385 | 0.1404 | 0.038* |
| H28C | −0.2090 | 1.3068 | 0.0472 | 0.038* |
| C29 | −0.38687 (16) | 1.1613 (2) | 0.06029 (12) | 0.0250 (5) |
| H29A | −0.4496 | 1.1060 | 0.0533 | 0.037* |
| H29B | −0.3741 | 1.1888 | 0.0065 | 0.037* |
| H29C | −0.3989 | 1.2362 | 0.0928 | 0.037* |
| C6 | −0.28135 (14) | 0.67505 (18) | 0.17675 (11) | 0.0175 (4) |
| H6A | −0.3499 | 0.7144 | 0.1829 | 0.021* |
| H6B | −0.2645 | 0.6078 | 0.2190 | 0.021* |
| C3 | 0.29247 (14) | 0.56624 (17) | 0.35368 (11) | 0.0167 (4) |
| H3A | 0.2768 | 0.6433 | 0.3192 | 0.020* |
| H3B | 0.3611 | 0.5308 | 0.3443 | 0.020* |
| C4 | 0.30192 (15) | 0.60307 (19) | 0.44332 (11) | 0.0210 (4) |
| H4A | 0.2370 | 0.6497 | 0.4509 | 0.025* |
| H4B | 0.3067 | 0.5246 | 0.4770 | 0.025* |
| C5 | 0.39858 (16) | 0.6861 (2) | 0.47298 (12) | 0.0248 (4) |
| H5A | 0.4634 | 0.6375 | 0.4703 | 0.037* |
| H5B | 0.3986 | 0.7124 | 0.5297 | 0.037* |
| H5C | 0.3961 | 0.7618 | 0.4381 | 0.037* |
| C7 | −0.29199 (15) | 0.61516 (19) | 0.09218 (12) | 0.0222 (4) |
| H7A | −0.3002 | 0.6833 | 0.0502 | 0.027* |
| H7B | −0.2265 | 0.5669 | 0.0884 | 0.027* |
| C8 | −0.38697 (17) | 0.5262 (2) | 0.07528 (14) | 0.0312 (5) |
| H8A | −0.3838 | 0.4657 | 0.1207 | 0.047* |
| H8B | −0.3858 | 0.4793 | 0.0244 | 0.047* |
| H8C | −0.4527 | 0.5761 | 0.0699 | 0.047* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N23 | 0.0164 (8) | 0.0184 (8) | 0.0205 (8) | 0.0018 (6) | 0.0026 (6) | 0.0001 (6) |
| N13 | 0.0171 (8) | 0.0177 (8) | 0.0194 (8) | 0.0012 (6) | 0.0008 (6) | 0.0012 (6) |
| C13 | 0.0158 (9) | 0.0196 (10) | 0.0134 (8) | 0.0000 (7) | 0.0030 (7) | −0.0004 (7) |
| N11 | 0.0164 (8) | 0.0155 (8) | 0.0169 (7) | −0.0006 (6) | 0.0017 (6) | −0.0001 (6) |
| N21 | 0.0160 (8) | 0.0153 (8) | 0.0179 (7) | 0.0006 (6) | 0.0028 (6) | 0.0006 (6) |
| C16 | 0.0191 (9) | 0.0193 (10) | 0.0150 (8) | 0.0041 (7) | 0.0023 (7) | 0.0000 (7) |
| C24 | 0.0178 (9) | 0.0186 (10) | 0.0207 (9) | −0.0016 (7) | 0.0053 (7) | −0.0018 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C11 | 0.0188 (9) | 0.0137 (9) | 0.0138 (8) | −0.0003 (7) | 0.0035 (7) | −0.0004 (7) |
| C21 | 0.0200 (9) | 0.0172 (9) | 0.0131 (8) | 0.0006 (7) | 0.0027 (7) | −0.0020 (7) |
| C26 | 0.0204 (10) | 0.0193 (10) | 0.0163 (9) | 0.0032 (8) | 0.0032 (7) | −0.0013 (7) |
| C17 | 0.0153 (9) | 0.0203 (10) | 0.0184 (9) | −0.0006 (7) | 0.0012 (7) | −0.0006 (7) |
| C23 | 0.0175 (9) | 0.0195 (10) | 0.0144 (8) | 0.0020 (7) | 0.0038 (7) | −0.0012 (7) |
| C15 | 0.0226 (10) | 0.0161 (9) | 0.0137 (8) | −0.0021 (7) | 0.0028 (7) | 0.0005 (7) |
| C14 | 0.0171 (9) | 0.0190 (10) | 0.0173 (9) | −0.0043 (7) | 0.0025 (7) | −0.0022 (7) |
| C25 | 0.0247 (10) | 0.0178 (10) | 0.0160 (9) | 0.0014 (8) | 0.0070 (7) | 0.0002 (7) |
| C12 | 0.0160 (9) | 0.0184 (9) | 0.0144 (8) | −0.0002 (7) | 0.0015 (7) | −0.0003 (7) |
| C22 | 0.0169 (9) | 0.0181 (9) | 0.0149 (8) | 0.0013 (7) | 0.0025 (7) | −0.0014 (7) |
| C27 | 0.0173 (9) | 0.0203 (10) | 0.0160 (9) | −0.0011 (7) | 0.0016 (7) | −0.0022 (7) |
| C2 | 0.0196 (10) | 0.0186 (10) | 0.0183 (9) | −0.0011 (7) | 0.0056 (7) | −0.0003 (7) |
| C1 | 0.0200 (10) | 0.0158 (9) | 0.0179 (9) | 0.0002 (7) | 0.0041 (7) | −0.0003 (7) |
| C19 | 0.0214 (10) | 0.0190 (10) | 0.0244 (10) | 0.0032 (8) | 0.0004 (8) | 0.0024 (8) |
| C18 | 0.0263 (10) | 0.0168 (10) | 0.0242 (10) | −0.0014 (8) | 0.0014 (8) | 0.0001 (8) |
| C28 | 0.0267 (11) | 0.0204 (11) | 0.0284 (10) | 0.0008 (8) | 0.0056 (8) | 0.0039 (8) |
| C29 | 0.0247 (11) | 0.0237 (11) | 0.0252 (10) | 0.0037 (8) | 0.0010 (8) | 0.0033 (8) |
| C6 | 0.0154 (9) | 0.0172 (9) | 0.0198 (9) | −0.0013 (7) | 0.0029 (7) | 0.0016 (7) |
| C3 | 0.0144 (9) | 0.0140 (9) | 0.0216 (9) | −0.0023 (7) | 0.0030 (7) | 0.0014 (7) |
| C4 | 0.0226 (10) | 0.0190 (10) | 0.0221 (10) | −0.0033 (8) | 0.0056 (8) | −0.0007 (8) |
| C5 | 0.0255 (10) | 0.0245 (11) | 0.0236 (10) | −0.0039 (9) | 0.0022 (8) | −0.0044 (8) |
| C7 | 0.0245 (10) | 0.0189 (10) | 0.0226 (10) | 0.0014 (8) | 0.0028 (8) | −0.0011 (8) |
| C8 | 0.0253 (11) | 0.0297 (12) | 0.0370 (12) | 0.0001 (9) | 0.0013 (9) | −0.0121 (10) |

*Geometric parameters (Å, º)*

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| N23—C22 | 1.327 (2) | C2—H2 | 0.9500 |
| N23—C23 | 1.385 (2) | C1—H1 | 0.9500 |
| N13—C12 | 1.324 (2) | C19—H19A | 0.9800 |
| N13—C13 | 1.384 (2) | C19—H19B | 0.9800 |
| C13—C11 | 1.398 (2) | C19—H19C | 0.9800 |
| C13—C14 | 1.403 (3) | C18—H18A | 0.9800 |
| N11—C11 | 1.379 (2) | C18—H18B | 0.9800 |
| N11—C12 | 1.381 (2) | C18—H18C | 0.9800 |
| N11—C3 | 1.465 (2) | C28—H28A | 0.9800 |
| N21—C21 | 1.377 (2) | C28—H28B | 0.9800 |
| N21—C22 | 1.381 (2) | C28—H28C | 0.9800 |
| N21—C6 | 1.460 (2) | C29—H29A | 0.9800 |
| C16—C17 | 1.384 (3) | C29—H29B | 0.9800 |
| C16—C15 | 1.428 (3) | C29—H29C | 0.9800 |
| C16—C19 | 1.512 (3) | C6—C7 | 1.521 (3) |
| C24—C25 | 1.383 (3) | C6—H6A | 0.9900 |
| C24—C23 | 1.403 (3) | C6—H6B | 0.9900 |
| C24—H24 | 0.9500 | C3—C4 | 1.521 (3) |
| C11—C17 | 1.397 (3) | C3—H3A | 0.9900 |
| C21—C27 | 1.397 (3) | C3—H3B | 0.9900 |
| C21—C23 | 1.399 (3) | C4—C5 | 1.519 (3) |
| C26—C27 | 1.385 (3) | C4—H4A | 0.9900 |

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| C26—C25 | 1.428 (3) | C4—H4B | 0.9900 |
| C26—C29 | 1.508 (3) | C5—H5A | 0.9800 |
| C17—H17 | 0.9500 | C5—H5B | 0.9800 |
| C15—C14 | 1.381 (3) | C5—H5C | 0.9800 |
| C15—C18 | 1.512 (3) | C7—C8 | 1.517 (3) |
| C14—H14 | 0.9500 | C7—H7A | 0.9900 |
| C25—C28 | 1.511 (3) | C7—H7B | 0.9900 |
| C12—C1 | 1.454 (3) | C8—H8A | 0.9800 |
| C22—C2 | 1.456 (3) | C8—H8B | 0.9800 |
| C27—H27 | 0.9500 | C8—H8C | 0.9800 |
| C2—C1 | 1.342 (3) | | |

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| C22—N23—C23 | 104.73 (15) | H19A—C19—H19B | 109.5 |
| C12—N13—C13 | 104.98 (15) | C16—C19—H19C | 109.5 |
| N13—C13—C11 | 110.28 (16) | H19A—C19—H19C | 109.5 |
| N13—C13—C14 | 130.83 (17) | H19B—C19—H19C | 109.5 |
| C11—C13—C14 | 118.90 (17) | C15—C18—H18A | 109.5 |
| C11—N11—C12 | 106.44 (15) | C15—C18—H18B | 109.5 |
| C11—N11—C3 | 123.67 (15) | H18A—C18—H18B | 109.5 |
| C12—N11—C3 | 129.41 (15) | C15—C18—H18C | 109.5 |
| C21—N21—C22 | 106.56 (15) | H18A—C18—H18C | 109.5 |
| C21—N21—C6 | 124.01 (15) | H18B—C18—H18C | 109.5 |
| C22—N21—C6 | 128.73 (15) | C25—C28—H28A | 109.5 |
| C17—C16—C15 | 120.30 (17) | C25—C28—H28B | 109.5 |
| C17—C16—C19 | 119.60 (17) | H28A—C28—H28B | 109.5 |
| C15—C16—C19 | 120.09 (17) | C25—C28—H28C | 109.5 |
| C25—C24—C23 | 119.38 (17) | H28A—C28—H28C | 109.5 |
| C25—C24—H24 | 120.3 | H28B—C28—H28C | 109.5 |
| C23—C24—H24 | 120.3 | C26—C29—H29A | 109.5 |
| N11—C11—C17 | 131.66 (17) | C26—C29—H29B | 109.5 |
| N11—C11—C13 | 105.69 (16) | H29A—C29—H29B | 109.5 |
| C17—C11—C13 | 122.65 (17) | C26—C29—H29C | 109.5 |
| N21—C21—C27 | 131.78 (17) | H29A—C29—H29C | 109.5 |
| N21—C21—C23 | 105.66 (15) | H29B—C29—H29C | 109.5 |
| C27—C21—C23 | 122.53 (17) | N21—C6—C7 | 111.30 (15) |
| C27—C26—C25 | 120.02 (17) | N21—C6—H6A | 109.4 |
| C27—C26—C29 | 119.42 (17) | C7—C6—H6A | 109.4 |
| C25—C26—C29 | 120.55 (17) | N21—C6—H6B | 109.4 |
| C16—C17—C11 | 117.96 (17) | C7—C6—H6B | 109.4 |
| C16—C17—H17 | 121.0 | H6A—C6—H6B | 108.0 |
| C11—C17—H17 | 121.0 | N11—C3—C4 | 111.38 (14) |
| N23—C23—C21 | 110.38 (16) | N11—C3—H3A | 109.4 |
| N23—C23—C24 | 130.64 (17) | C4—C3—H3A | 109.4 |
| C21—C23—C24 | 118.97 (17) | N11—C3—H3B | 109.4 |
| C14—C15—C16 | 120.66 (17) | C4—C3—H3B | 109.4 |
| C14—C15—C18 | 119.97 (17) | H3A—C3—H3B | 108.0 |
| C16—C15—C18 | 119.34 (17) | C5—C4—C3 | 112.34 (16) |
| C15—C14—C13 | 119.53 (17) | C5—C4—H4A | 109.1 |

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| C15—C14—H14 | 120.2 | C3—C4—H4A | 109.1 |
| C13—C14—H14 | 120.2 | C5—C4—H4B | 109.1 |
| C24—C25—C26 | 120.87 (17) | C3—C4—H4B | 109.1 |
| C24—C25—C28 | 119.06 (17) | H4A—C4—H4B | 107.9 |
| C26—C25—C28 | 120.01 (17) | C4—C5—H5A | 109.5 |
| N13—C12—N11 | 112.60 (16) | C4—C5—H5B | 109.5 |
| N13—C12—C1 | 125.38 (16) | H5A—C5—H5B | 109.5 |
| N11—C12—C1 | 121.99 (16) | C4—C5—H5C | 109.5 |
| N23—C22—N21 | 112.63 (16) | H5A—C5—H5C | 109.5 |
| N23—C22—C2 | 125.90 (16) | H5B—C5—H5C | 109.5 |
| N21—C22—C2 | 121.45 (16) | C8—C7—C6 | 111.16 (16) |
| C26—C27—C21 | 118.16 (17) | C8—C7—H7A | 109.4 |
| C26—C27—H27 | 120.9 | C6—C7—H7A | 109.4 |
| C21—C27—H27 | 120.9 | C8—C7—H7B | 109.4 |
| C1—C2—C22 | 123.34 (18) | C6—C7—H7B | 109.4 |
| C1—C2—H2 | 118.3 | H7A—C7—H7B | 108.0 |
| C22—C2—H2 | 118.3 | C7—C8—H8A | 109.5 |
| C2—C1—C12 | 122.13 (18) | C7—C8—H8B | 109.5 |
| C2—C1—H1 | 118.9 | H8A—C8—H8B | 109.5 |
| C12—C1—H1 | 118.9 | C7—C8—H8C | 109.5 |
| C16—C19—H19A | 109.5 | H8A—C8—H8C | 109.5 |
| C16—C19—H19B | 109.5 | H8B—C8—H8C | 109.5 |

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| C12—N13—C13—C11 | −0.16 (19) | C23—C24—C25—C26 | −1.2 (3) |
| C12—N13—C13—C14 | −179.65 (18) | C23—C24—C25—C28 | 175.89 (17) |
| C12—N11—C11—C17 | −179.41 (18) | C27—C26—C25—C24 | 2.7 (3) |
| C3—N11—C11—C17 | −6.7 (3) | C29—C26—C25—C24 | −176.39 (17) |
| C12—N11—C11—C13 | 0.71 (18) | C27—C26—C25—C28 | −174.33 (17) |
| C3—N11—C11—C13 | 173.39 (15) | C29—C26—C25—C28 | 6.6 (3) |
| N13—C13—C11—N11 | −0.36 (19) | C13—N13—C12—N11 | 0.6 (2) |
| C14—C13—C11—N11 | 179.20 (15) | C13—N13—C12—C1 | 178.64 (17) |
| N13—C13—C11—C17 | 179.75 (16) | C11—N11—C12—N13 | −0.9 (2) |
| C14—C13—C11—C17 | −0.7 (3) | C3—N11—C12—N13 | −172.99 (16) |
| C22—N21—C21—C27 | 176.43 (18) | C11—N11—C12—C1 | −178.96 (16) |
| C6—N21—C21—C27 | 5.3 (3) | C3—N11—C12—C1 | 8.9 (3) |
| C22—N21—C21—C23 | −1.54 (18) | C23—N23—C22—N21 | −1.3 (2) |
| C6—N21—C21—C23 | −172.65 (15) | C23—N23—C22—C2 | 176.97 (16) |
| C15—C16—C17—C11 | 0.4 (3) | C21—N21—C22—N23 | 1.9 (2) |
| C19—C16—C17—C11 | −178.72 (16) | C6—N21—C22—N23 | 172.42 (16) |
| N11—C11—C17—C16 | −179.49 (18) | C21—N21—C22—C2 | −176.52 (16) |
| C13—C11—C17—C16 | 0.4 (3) | C6—N21—C22—C2 | −6.0 (3) |
| C22—N23—C23—C21 | 0.30 (19) | C25—C26—C27—C21 | −1.9 (3) |
| C22—N23—C23—C24 | −178.94 (18) | C29—C26—C27—C21 | 177.25 (16) |
| N21—C21—C23—N23 | 0.80 (19) | N21—C21—C27—C26 | −178.11 (18) |
| C27—C21—C23—N23 | −177.40 (15) | C23—C21—C27—C26 | −0.4 (3) |
| N21—C21—C23—C24 | −179.86 (15) | N23—C22—C2—C1 | 5.1 (3) |
| C27—C21—C23—C24 | 1.9 (3) | N21—C22—C2—C1 | −176.72 (17) |
| C25—C24—C23—N23 | 178.11 (17) | C22—C2—C1—C12 | −176.52 (16) |

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| C25—C24—C23—C21 | −1.1 (3) | N13—C12—C1—C2 | 0.9 (3) |
| C17—C16—C15—C14 | −0.8 (3) | N11—C12—C1—C2 | 178.73 (16) |
| C19—C16—C15—C14 | 178.29 (16) | C21—N21—C6—C7 | 83.2 (2) |
| C17—C16—C15—C18 | 177.44 (17) | C22—N21—C6—C7 | −85.9 (2) |
| C19—C16—C15—C18 | −3.5 (2) | C11—N11—C3—C4 | −81.9 (2) |
| C16—C15—C14—C13 | 0.5 (3) | C12—N11—C3—C4 | 89.0 (2) |
| C18—C15—C14—C13 | −177.76 (16) | N11—C3—C4—C5 | 171.72 (15) |
| N13—C13—C14—C15 | 179.71 (17) | N21—C6—C7—C8 | −173.22 (16) |
| C11—C13—C14—C15 | 0.3 (2) | | |