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# 4-Allyl-2-[1-(5-allyl-2-hydroxy-3-methoxybenzyl)-1*H*-benzimidazol-2-yl]-6-methoxyphenol pyridine solvate

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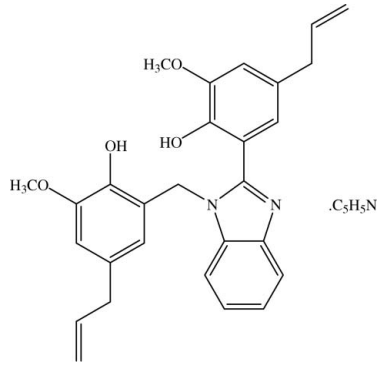
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.052; $wR$ factor = 0.143; data-to-parameter ratio = 21.6.

The title compound, $C_{28}H_{28}N_2O_4\cdot C_5H_5N$, crystallizes with two molecules in the asymmetric unit. In both molecules, the benzimidazole ring system is essentially planar and forms dihedral angles of 85.35 (5) and 50.51 (5)° with the two benzene rings in one molecule, and 82.93 (5) and 51.30 (5)° in the other molecule. The hydroxy groups are coplanar with the attached benzene rings, whereas the methoxy groups are slightly twisted away from the planes of the attached benzene rings. O—H···O intramolecular hydrogen bonds involving the hydroxy and methoxy groups generate $S$(6) ring motifs. In the crystal structure, molecules are linked into chains along the [110] direction by O—H···N and C—H···O hydrogen bonds.

## Related literature

For biological activities of benzimidazoles, see: Barreca *et al.* (2003); Demirayak *et al.* (2002); Minoura *et al.* (2004); Pawar *et al.* (2004); Tomei *et al.* (2003). For related structures, see: Eltayeb *et al.* (2007*a*,*b*). For bond-length data, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).




## Experimental

### Crystal data

$C_{28}H_{28}N_2O_4\cdot C_5H_5N$
$M_r$ = 535.62
Triclinic, $P\overline{1}$
$a$ = 9.5355 (1) Å
$b$ = 17.3405 (3) Å
$c$ = 17.8604 (3) Å
$\alpha$ = 92.840 (1)°
$\beta$ = 105.372 (1)°
$\gamma$ = 102.523 (1)°
$V$ = 2761.80 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 100.0 (1) K
0.40 × 0.27 × 0.23 mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.967, $T_{max}$ = 0.980
44895 measured reflections
16031 independent reflections
11052 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.035

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.143
$S$ = 1.10
16031 reflections
741 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

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

*Cg*1, *Cg*2 and *Cg*3 are centroids of the N1*A*/C13*A*/C8*A*/N2*A*/C14*A*, C8*A*–C13*A* and N3*B*/C29*B*–C33*B* rings.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1*A*—H1*OA*···O2*A* | 0.93 (2) | 2.30 (2) | 2.6977 (14) | 105 (1) |
| O1*A*—H1*OA*···N1*B* | 0.93 (2) | 1.81 (2) | 2.6932 (15) | 157 (2) |
| O3*A*—H3*OA*···O4*A* | 0.93 (2) | 2.25 (2) | 2.6798 (13) | 108 (2) |
| O3*A*—H3*OA*···N3*B*$^{i}$ | 0.93 (2) | 1.90 (2) | 2.7859 (14) | 160 (2) |
| O1*B*—H1*OB*···O2*B* | 0.90 (2) | 2.33 (2) | 2.7197 (14) | 106 (2) |
| O1*B*—H1*OB*···N1*A*$^{ii}$ | 0.90 (2) | 1.87 (2) | 2.7114 (15) | 153 (2) |
| O3*B*—H3*OB*···O4*B* | 0.99 (2) | 2.27 (2) | 2.6789 (13) | 103 (1) |
| O3*B*—H3*OB*···N3*A*$^{iii}$ | 0.99 (2) | 1.68 (2) | 2.6461 (15) | 161 (2) |
| C7*A*—H7*A*···O3*A* | 0.97 | 2.38 | 3.1017 (15) | 131 |
| C7*A*—H7*B*···O1*A* | 0.97 | 2.35 | 2.7525 (16) | 104 |
| C7*B*—H7*C*···O3*B* | 0.97 | 2.30 | 3.0302 (16) | 132 |
| C7*B*—H7*D*···O1*B* | 0.97 | 2.35 | 2.7231 (16) | 102 |
| C11*B*—H11*B*···O2*A*$^{iv}$ | 0.93 | 2.59 | 3.5010 (17) | 165 |
| C31*A*—H31*A*···O1*A* | 0.93 | 2.36 | 3.2382 (18) | 158 |
| C23*A*—H23*A*···*Cg*1$^{v}$ | 0.93 | 2.90 | 3.3950 (17) | 115 |
| C28*B*—H28*C*···*Cg*2$^{vi}$ | 0.93 | 2.99 | 3.4562 (18) | 113 |
| C33*A*—H33*A*···*Cg*3$^{i}$ | 0.93 | 2.74 | 3.4888 (16) | 139 |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2468).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, o4141-o4142 [ **doi:10.1107/S1600536807046065** ]

# 4-Allyl-2-[1-(5-allyl-2-hydroxy-3-methoxybenzyl)-1*H*-benzimidazol-2-yl]-6-methoxyphenol pyridine solvate

**N. E. Eltayeb, S. G. Teoh, S. Chantrapromma and H.-K. Fun**

## Comment

The synthesis of benzimidazoles has received much attention owing to their various biological activities such as antidiabetic (Minoura *et al.*, 2004), antimicrobial, antifungal (Pawar *et al.*, 2004), antiviral (Tomei *et al.*, 2003), anti-HIV (Barreca *et al.*, 2003), and anticancer (Demirayak *et al.*, 2002). Recently, we reported the crystal structures of 2-(benzimidazol-2-yl)-6-methoxyphenol (Eltayeb *et al.*, 2007*a*) and 2-(2-methoxynaphthalen-1-yl)-1-[(2-methoxynaphthalen-1-yl)methyl]-1*H*- benzimidazole (Eltayeb *et al.*, 2007*b*). The title compound was synthesized as an extension of our investigations of benzimidazole derivatives. We report here the crystal structure of the title compound.

The title compound crystalizes with two molecules of the benzimidazole derivative [*A* and *B*] and two molecules of pyridine in the asymmetric unit. In both *A* and *B*, the benzimidazole ring system is essentially planar. The benzimidazole ring system makes dihedral angles of 85.35 (5)° and 50.51 (5)°, respectively, with the C1–C6 and C15—C20 benzene rings in molecule *A*, and 82.93 (5)° and 51.30 (5)°, respectively, in molecule *B*. The hydroxyl groups are coplanar with the attached benzene rings, whereas the methoxy groups are slightly twisted away from the mean plane of the attached benzene rings, as indicated by the C25–O2–C2–C3 [4.29 (18)° in molecule *A* and 2.11 (18)° in molecule *B*] and C24–O4–C17–C18 [6.52 (19)° in molecule *A* and 12.40 (19) ° in molecule *B*] torsion angles. The orientation of the allyl groups with respect to the attached benzene rings can be described by the torsion angle C3–C4–C26–C27 of 104.09 (15)° in molecule *A* [−81.78 (16)° in molecule *B*] and C18–C19–C21–C22 torsion angle of 168.38 (12)° in molecule *A* [171.79 (12)° in molecule *B*]. Bond lengths and angles in both molecules are in normal ranges (Allen *et al.*, 1987) and are comparable to those in related structures (Eltayeb *et al.*, 2007*a*; 2007*b*).

There are two O—H···O intramolecular hydrogen bonds involving the two hydroxyl and the two methoxyl groups [O1A—H1OA···O2A and O3A—H3OA···O4A in molecule *A*, and O1B—H1OB···O2B and O3B—H3OB···O4B in molecule *B*] (Table 1) which generate S(6) ring motifs. In addition, C—H···O intramolecular hydrogen bonds are also observed.

The crystal structure is stabilized by intermolecular O—H···N and C—H···O hydrogen bonds, which link the molecules into chains along the [1 1 0] direction (Fig. 2). The structure is further stabilized by intermolecular C—H···π interactions (Table 1), involving the N1A/C13A/C8A/N2A/C14A (centroid *Cg*1), C8A–C13A (centroid *Cg*2) and N3B/C29B—C33B (centroid *Cg*3) rings.

## Experimental

The title compound was synthesized by adding 5-allyl-2-hydroxy-3-methoxybenzaldehyde (0.216 g, 4 mmol) into a solution of *o*-phenylenediamine (0.216 g, 2 mmol) in ethanol (30 ml). The mixture was refluxed with stirring for 0.5 h. Then zinc chloride (0.272 g, 2 mmol) in ethanol (10 ml) was added, followed by triethylamine (0.5 ml, 3.6 mmol). The mixture was stirred at room temperature for 2 h. The orange precipitate obtained was washed with about 5 ml e thanol, dried, and then

washed with copious amounts of diethyl ether. Pale-yellow single crystals of the title compound suitable for X-ray analysis were obtained by slow evaporation of the pyridine solution at room temperature after four weeks.

### Refinement

Hydroxyl H atoms were located in a difference map and refined isotropically. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with and C—H distances in the range 0.93–0.97 Å. The $U_{iso}$ values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups.

### Figures

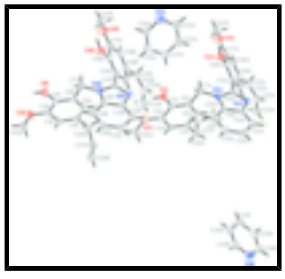

Fig. 1. The asymmetric unit of the title compound, showing 80% probability displacement ellipsoids and the atomic numbering.

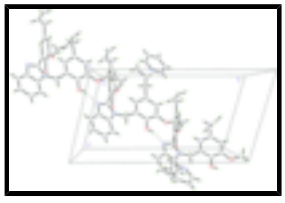

Fig. 2. Part of the crystal packing of the title compound, viewed approximately along the *c* axis. Hydrogen bonds are shown as dashed lines.

### 4-Allyl-2-[1-(5-allyl-2-hydroxy-3-methoxybenzyl)-1*H*-benzimidazol-2-yl]- 6-methoxyphenol pyridine solvate

*Crystal data*

| | |
|---|---|
| $C_{28}H_{28}N_2O_4 \cdot C_5H_5N$ | $Z = 4$ |
| $M_r = 535.62$ | $F_{000} = 1136$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.288$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $a = 9.5355$ (1) Å | Cell parameters from 16031 reflections |
| $b = 17.3405$ (3) Å | $\theta = 1.2$–$30.0^\circ$ |
| $c = 17.8604$ (3) Å | $\mu = 0.09$ mm$^{-1}$ |
| $\alpha = 92.840$ (1)° | $T = 100.0$ (1) K |
| $\beta = 105.372$ (1)° | Block, pale yellow |
| $\gamma = 102.523$ (1)° | 0.40 × 0.27 × 0.23 mm |
| $V = 2761.80$ (8) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII CCD area-detector | 16031 independent reflections |

diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 8.33 pixels $mm^{-1}$

$T$ = 100.0(1) K

ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2005)

$T_{min}$ = 0.967, $T_{max}$ = 0.980

44895 measured reflections

11052 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.035

$\theta_{max}$ = 30.0º

$\theta_{min}$ = 1.2º

$h = -13 \rightarrow 11$

$k = -19 \rightarrow 24$

$l = -25 \rightarrow 25$

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.052

$wR(F^2)$ = 0.143

$S$ = 1.10

16031 reflections

741 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0668P)^2 + 0.0718P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.34 e $Å^{-3}$

$\Delta\rho_{min}$ = −0.29 e $Å^{-3}$

Extinction correction: none

*Special details*

**Experimental**. The low-temparture data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1A | 0.69329 (11) | 0.40199 (6) | 0.28400 (6) | 0.0198 (2) |
| H1OA | 0.746 (2) | 0.4550 (12) | 0.2942 (11) | 0.059 (6)* |
| O2A | 0.61443 (10) | 0.51795 (5) | 0.35805 (5) | 0.0193 (2) |
| O3A | 0.42381 (10) | 0.13523 (6) | 0.09510 (5) | 0.0183 (2) |
| H3OA | 0.423 (2) | 0.1324 (11) | 0.0430 (11) | 0.049 (6)* |
| O4A | 0.19547 (11) | 0.14126 (6) | −0.02821 (5) | 0.0218 (2) |

| | | | | |
|---|---|---|---|---|
| N1A | 0.37505 (12) | 0.04523 (6) | 0.28948 (6) | 0.0144 (2) |
| N2A | 0.50051 (12) | 0.16685 (6) | 0.27712 (6) | 0.0133 (2) |
| C1A | 0.56764 (14) | 0.38543 (7) | 0.30790 (7) | 0.0142 (3) |
| C2A | 0.52048 (14) | 0.44352 (7) | 0.34607 (7) | 0.0154 (3) |
| C3A | 0.38987 (15) | 0.42383 (8) | 0.36832 (7) | 0.0170 (3) |
| H3A | 0.3594 | 0.4628 | 0.3934 | 0.020* |
| C4A | 0.30335 (15) | 0.34527 (8) | 0.35323 (8) | 0.0175 (3) |
| C5A | 0.35165 (15) | 0.28816 (8) | 0.31613 (7) | 0.0167 (3) |
| H5A | 0.2948 | 0.2360 | 0.3060 | 0.020* |
| C6A | 0.48255 (14) | 0.30686 (7) | 0.29373 (7) | 0.0134 (2) |
| C7A | 0.53506 (15) | 0.24556 (7) | 0.25165 (7) | 0.0147 (3) |
| H7A | 0.4881 | 0.2421 | 0.1959 | 0.018* |
| H7B | 0.6425 | 0.2630 | 0.2605 | 0.018* |
| C8A | 0.58195 (14) | 0.14521 (7) | 0.34609 (7) | 0.0138 (3) |
| C9A | 0.71464 (15) | 0.18474 (8) | 0.40171 (8) | 0.0183 (3) |
| H9A | 0.7651 | 0.2359 | 0.3974 | 0.022* |
| C10A | 0.76712 (15) | 0.14376 (8) | 0.46368 (8) | 0.0203 (3) |
| H10A | 0.8553 | 0.1680 | 0.5020 | 0.024* |
| C11A | 0.69072 (15) | 0.06663 (8) | 0.47024 (8) | 0.0205 (3) |
| H11A | 0.7298 | 0.0408 | 0.5125 | 0.025* |
| C12A | 0.55826 (15) | 0.02824 (8) | 0.41505 (7) | 0.0179 (3) |
| H12A | 0.5078 | −0.0228 | 0.4195 | 0.021* |
| C13A | 0.50319 (14) | 0.06894 (7) | 0.35252 (7) | 0.0148 (3) |
| C14A | 0.37763 (14) | 0.10462 (7) | 0.24591 (7) | 0.0132 (2) |
| C15A | 0.25636 (14) | 0.10407 (7) | 0.17408 (7) | 0.0142 (3) |
| C16A | 0.28195 (14) | 0.12015 (7) | 0.10242 (7) | 0.0151 (3) |
| C17A | 0.15828 (15) | 0.12027 (8) | 0.03814 (7) | 0.0169 (3) |
| C18A | 0.01458 (15) | 0.09840 (8) | 0.04422 (8) | 0.0183 (3) |
| H18A | −0.0658 | 0.0972 | 0.0008 | 0.022* |
| C19A | −0.01247 (14) | 0.07781 (8) | 0.11501 (8) | 0.0168 (3) |
| C20A | 0.10845 (14) | 0.08213 (7) | 0.17913 (7) | 0.0159 (3) |
| H20A | 0.0919 | 0.0703 | 0.2267 | 0.019* |
| C21A | −0.17410 (15) | 0.05094 (8) | 0.11641 (8) | 0.0200 (3) |
| H21A | −0.2180 | 0.0966 | 0.1110 | 0.024* |
| H21B | −0.2277 | 0.0127 | 0.0709 | 0.024* |
| C22A | −0.20089 (15) | 0.01432 (8) | 0.18715 (8) | 0.0201 (3) |
| H22A | −0.1487 | −0.0234 | 0.2061 | 0.024* |
| C23A | −0.29377 (16) | 0.03243 (9) | 0.22407 (8) | 0.0247 (3) |
| H23A | −0.3475 | 0.0700 | 0.2065 | 0.030* |
| H23B | −0.3058 | 0.0077 | 0.2677 | 0.030* |
| C24A | 0.07727 (17) | 0.14857 (9) | −0.09374 (8) | 0.0255 (3) |
| H24A | 0.1181 | 0.1666 | −0.1352 | 0.038* |
| H24B | 0.0264 | 0.1862 | −0.0788 | 0.038* |
| H24C | 0.0078 | 0.0978 | −0.1112 | 0.038* |
| C25A | 0.58045 (18) | 0.57919 (8) | 0.40139 (8) | 0.0248 (3) |
| H25A | 0.6582 | 0.6269 | 0.4093 | 0.037* |
| H25B | 0.5735 | 0.5628 | 0.4511 | 0.037* |
| H25C | 0.4867 | 0.5891 | 0.3729 | 0.037* |
| C26A | 0.15495 (15) | 0.32332 (9) | 0.37223 (8) | 0.0220 (3) |

| | | | | |
|---|---|---|---|---|
| H26A | 0.1489 | 0.2751 | 0.3977 | 0.026* |
| H26B | 0.1484 | 0.3655 | 0.4080 | 0.026* |
| C27A | 0.02750 (16) | 0.31078 (9) | 0.29955 (9) | 0.0264 (3) |
| H27A | 0.0083 | 0.3554 | 0.2758 | 0.032* |
| C28A | −0.05956 (17) | 0.24102 (9) | 0.26674 (9) | 0.0303 (4) |
| H28A | −0.0436 | 0.1951 | 0.2889 | 0.036* |
| H28B | −0.1371 | 0.2376 | 0.2214 | 0.036* |
| O1B | 1.19577 (11) | 0.90182 (6) | 0.29353 (6) | 0.0203 (2) |
| H1OB | 1.235 (2) | 0.9548 (13) | 0.2989 (12) | 0.068 (7)* |
| O2B | 1.09294 (10) | 1.01306 (5) | 0.36193 (5) | 0.0193 (2) |
| O3B | 0.96691 (10) | 0.64026 (6) | 0.10956 (5) | 0.0199 (2) |
| H3OB | 0.986 (2) | 0.6472 (12) | 0.0579 (12) | 0.070 (7)* |
| O4B | 0.75469 (11) | 0.64354 (6) | −0.02223 (5) | 0.0232 (2) |
| N1B | 0.88956 (12) | 0.54180 (6) | 0.29220 (6) | 0.0146 (2) |
| N2B | 1.02152 (12) | 0.66375 (6) | 0.28601 (6) | 0.0142 (2) |
| C1B | 1.06728 (14) | 0.88114 (7) | 0.31508 (7) | 0.0147 (3) |
| C2B | 1.00811 (15) | 0.93630 (7) | 0.34968 (7) | 0.0156 (3) |
| C3B | 0.87434 (15) | 0.91182 (8) | 0.36796 (7) | 0.0168 (3) |
| H3B | 0.8367 | 0.9487 | 0.3913 | 0.020* |
| C4B | 0.79479 (14) | 0.83190 (8) | 0.35160 (7) | 0.0162 (3) |
| C5B | 0.85647 (15) | 0.77762 (8) | 0.31965 (7) | 0.0163 (3) |
| H5B | 0.8064 | 0.7242 | 0.3101 | 0.020* |
| C6B | 0.99201 (14) | 0.80129 (7) | 0.30143 (7) | 0.0147 (3) |
| C7B | 1.05948 (15) | 0.74390 (7) | 0.26440 (8) | 0.0166 (3) |
| H7C | 1.0246 | 0.7422 | 0.2080 | 0.020* |
| H7D | 1.1676 | 0.7633 | 0.2801 | 0.020* |
| C8B | 1.09676 (14) | 0.63925 (8) | 0.35443 (7) | 0.0148 (3) |
| C9B | 1.22821 (15) | 0.67600 (8) | 0.41216 (8) | 0.0195 (3) |
| H9B | 1.2819 | 0.7270 | 0.4099 | 0.023* |
| C10B | 1.27469 (16) | 0.63259 (9) | 0.47308 (8) | 0.0227 (3) |
| H10B | 1.3622 | 0.6548 | 0.5126 | 0.027* |
| C11B | 1.19300 (16) | 0.55598 (9) | 0.47661 (8) | 0.0216 (3) |
| H11B | 1.2273 | 0.5286 | 0.5185 | 0.026* |
| C12B | 1.06213 (15) | 0.51991 (8) | 0.41906 (7) | 0.0185 (3) |
| H12B | 1.0086 | 0.4689 | 0.4216 | 0.022* |
| C13B | 1.01378 (14) | 0.56272 (7) | 0.35738 (7) | 0.0147 (3) |
| C14B | 0.89811 (14) | 0.60316 (7) | 0.25106 (7) | 0.0136 (3) |
| C15B | 0.78385 (14) | 0.60625 (7) | 0.17782 (7) | 0.0147 (3) |
| C16B | 0.82149 (14) | 0.62438 (7) | 0.10954 (7) | 0.0154 (3) |
| C17B | 0.70587 (15) | 0.62437 (8) | 0.04144 (7) | 0.0177 (3) |
| C18B | 0.55764 (15) | 0.60432 (8) | 0.04185 (8) | 0.0190 (3) |
| H18B | 0.4825 | 0.6038 | −0.0038 | 0.023* |
| C19B | 0.51918 (15) | 0.58466 (8) | 0.11046 (8) | 0.0179 (3) |
| C20B | 0.63284 (14) | 0.58603 (7) | 0.17762 (7) | 0.0160 (3) |
| H15B | 0.6090 | 0.5733 | 0.2234 | 0.019* |
| C21B | 0.35492 (15) | 0.56373 (9) | 0.10803 (8) | 0.0225 (3) |
| H21C | 0.3162 | 0.6108 | 0.0992 | 0.027* |
| H21D | 0.3009 | 0.5241 | 0.0637 | 0.027* |
| C22B | 0.32253 (15) | 0.53259 (9) | 0.17998 (8) | 0.0237 (3) |

| | | | | |
|---|---|---|---|---|
| H22B | 0.3570 | 0.4883 | 0.1966 | 0.028* |
| C23B | 0.24884 (18) | 0.56352 (11) | 0.22121 (9) | 0.0354 (4) |
| H23C | 0.2128 | 0.6078 | 0.2063 | 0.042* |
| H23D | 0.2326 | 0.5412 | 0.2654 | 0.042* |
| C24B | 0.64838 (17) | 0.65859 (9) | −0.08925 (8) | 0.0263 (3) |
| H24D | 0.6974 | 0.6746 | −0.1284 | 0.039* |
| H24E | 0.6054 | 0.7002 | −0.0748 | 0.039* |
| H24F | 0.5707 | 0.6111 | −0.1097 | 0.039* |
| C25B | 1.03920 (16) | 1.07091 (8) | 0.39887 (8) | 0.0224 (3) |
| H25D | 1.1056 | 1.1223 | 0.4037 | 0.034* |
| H25E | 1.0352 | 1.0573 | 0.4498 | 0.034* |
| H25F | 0.9408 | 1.0720 | 0.3679 | 0.034* |
| C26B | 0.64624 (15) | 0.80558 (8) | 0.36944 (8) | 0.0193 (3) |
| H26C | 0.5897 | 0.8457 | 0.3563 | 0.023* |
| H26D | 0.5897 | 0.7567 | 0.3364 | 0.023* |
| C27B | 0.66083 (15) | 0.79207 (8) | 0.45316 (8) | 0.0202 (3) |
| H27B | 0.7281 | 0.7625 | 0.4759 | 0.024* |
| C28B | 0.58663 (17) | 0.81850 (9) | 0.49721 (9) | 0.0271 (3) |
| H28C | 0.5183 | 0.8483 | 0.4768 | 0.033* |
| H28D | 0.6025 | 0.8073 | 0.5488 | 0.033* |
| N3A | 0.92807 (13) | 0.34672 (7) | 0.01349 (7) | 0.0224 (3) |
| C29A | 0.96230 (16) | 0.41376 (9) | 0.06201 (8) | 0.0238 (3) |
| H29A | 1.0380 | 0.4557 | 0.0576 | 0.029* |
| C30A | 0.89068 (16) | 0.42350 (9) | 0.11814 (8) | 0.0248 (3) |
| H30A | 0.9178 | 0.4709 | 0.1509 | 0.030* |
| C31A | 0.77808 (16) | 0.36174 (9) | 0.12486 (8) | 0.0255 (3) |
| H31A | 0.7272 | 0.3668 | 0.1619 | 0.031* |
| C32A | 0.74217 (16) | 0.29227 (9) | 0.07563 (8) | 0.0251 (3) |
| H32A | 0.6672 | 0.2495 | 0.0792 | 0.030* |
| C33A | 0.81932 (16) | 0.28732 (9) | 0.02099 (8) | 0.0233 (3) |
| H33A | 0.7943 | 0.2403 | −0.0122 | 0.028* |
| N3B | 0.49267 (13) | 0.13148 (7) | 0.95301 (6) | 0.0205 (3) |
| C29B | 0.57110 (15) | 0.08262 (8) | 0.93302 (8) | 0.0215 (3) |
| H29B | 0.5889 | 0.0420 | 0.9636 | 0.026* |
| C30B | 0.62726 (16) | 0.08964 (9) | 0.86879 (8) | 0.0239 (3) |
| H30B | 0.6816 | 0.0546 | 0.8570 | 0.029* |
| C31B | 0.60102 (16) | 0.14943 (9) | 0.82286 (8) | 0.0260 (3) |
| H31B | 0.6380 | 0.1557 | 0.7797 | 0.031* |
| C32B | 0.51883 (17) | 0.19984 (9) | 0.84209 (8) | 0.0259 (3) |
| H32B | 0.4986 | 0.2404 | 0.8119 | 0.031* |
| C33B | 0.46716 (16) | 0.18877 (8) | 0.90711 (8) | 0.0222 (3) |
| H33B | 0.4118 | 0.2229 | 0.9197 | 0.027* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1A | 0.0206 (5) | 0.0133 (5) | 0.0267 (5) | −0.0003 (4) | 0.0126 (4) | −0.0001 (4) |
| O2A | 0.0236 (5) | 0.0117 (5) | 0.0224 (5) | 0.0019 (4) | 0.0085 (4) | −0.0017 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O3A | 0.0159 (5) | 0.0238 (5) | 0.0162 (5) | 0.0035 (4) | 0.0072 (4) | 0.0022 (4) |
| O4A | 0.0209 (5) | 0.0316 (6) | 0.0138 (4) | 0.0071 (4) | 0.0052 (4) | 0.0070 (4) |
| N1A | 0.0151 (6) | 0.0130 (5) | 0.0151 (5) | 0.0028 (4) | 0.0048 (4) | 0.0020 (4) |
| N2A | 0.0133 (5) | 0.0114 (5) | 0.0148 (5) | 0.0017 (4) | 0.0042 (4) | 0.0012 (4) |
| C1A | 0.0152 (6) | 0.0146 (6) | 0.0133 (6) | 0.0041 (5) | 0.0039 (5) | 0.0034 (5) |
| C2A | 0.0184 (7) | 0.0122 (6) | 0.0138 (6) | 0.0027 (5) | 0.0027 (5) | 0.0009 (5) |
| C3A | 0.0213 (7) | 0.0157 (7) | 0.0158 (6) | 0.0079 (5) | 0.0056 (5) | 0.0009 (5) |
| C4A | 0.0175 (7) | 0.0186 (7) | 0.0177 (6) | 0.0057 (5) | 0.0061 (5) | 0.0026 (5) |
| C5A | 0.0171 (7) | 0.0137 (6) | 0.0189 (6) | 0.0027 (5) | 0.0051 (5) | 0.0029 (5) |
| C6A | 0.0145 (6) | 0.0138 (6) | 0.0117 (6) | 0.0041 (5) | 0.0027 (5) | 0.0015 (5) |
| C7A | 0.0175 (7) | 0.0108 (6) | 0.0169 (6) | 0.0024 (5) | 0.0072 (5) | 0.0027 (5) |
| C8A | 0.0141 (6) | 0.0158 (6) | 0.0132 (6) | 0.0046 (5) | 0.0059 (5) | 0.0026 (5) |
| C9A | 0.0166 (7) | 0.0177 (7) | 0.0194 (6) | 0.0019 (5) | 0.0059 (5) | −0.0019 (5) |
| C10A | 0.0148 (7) | 0.0279 (8) | 0.0165 (6) | 0.0060 (5) | 0.0015 (5) | −0.0015 (6) |
| C11A | 0.0223 (7) | 0.0267 (8) | 0.0159 (6) | 0.0121 (6) | 0.0054 (6) | 0.0058 (6) |
| C12A | 0.0206 (7) | 0.0188 (7) | 0.0171 (6) | 0.0070 (5) | 0.0077 (6) | 0.0054 (5) |
| C13A | 0.0156 (7) | 0.0153 (6) | 0.0149 (6) | 0.0043 (5) | 0.0066 (5) | −0.0005 (5) |
| C14A | 0.0133 (6) | 0.0121 (6) | 0.0150 (6) | 0.0026 (5) | 0.0060 (5) | 0.0000 (5) |
| C15A | 0.0148 (6) | 0.0124 (6) | 0.0146 (6) | 0.0032 (5) | 0.0030 (5) | 0.0019 (5) |
| C16A | 0.0152 (7) | 0.0140 (6) | 0.0164 (6) | 0.0032 (5) | 0.0052 (5) | 0.0020 (5) |
| C17A | 0.0202 (7) | 0.0174 (7) | 0.0138 (6) | 0.0058 (5) | 0.0049 (5) | 0.0029 (5) |
| C18A | 0.0167 (7) | 0.0223 (7) | 0.0151 (6) | 0.0054 (5) | 0.0026 (5) | 0.0030 (5) |
| C19A | 0.0148 (7) | 0.0179 (7) | 0.0175 (6) | 0.0050 (5) | 0.0034 (5) | 0.0020 (5) |
| C20A | 0.0177 (7) | 0.0156 (6) | 0.0147 (6) | 0.0042 (5) | 0.0052 (5) | 0.0021 (5) |
| C21A | 0.0144 (7) | 0.0253 (8) | 0.0192 (7) | 0.0044 (5) | 0.0035 (5) | 0.0012 (6) |
| C22A | 0.0148 (7) | 0.0231 (7) | 0.0199 (7) | 0.0025 (5) | 0.0024 (5) | 0.0013 (6) |
| C23A | 0.0203 (8) | 0.0319 (8) | 0.0213 (7) | 0.0042 (6) | 0.0065 (6) | 0.0016 (6) |
| C24A | 0.0269 (8) | 0.0359 (9) | 0.0157 (6) | 0.0121 (6) | 0.0047 (6) | 0.0086 (6) |
| C25A | 0.0363 (9) | 0.0145 (7) | 0.0240 (7) | 0.0068 (6) | 0.0093 (7) | −0.0020 (6) |
| C26A | 0.0210 (7) | 0.0219 (7) | 0.0273 (7) | 0.0063 (5) | 0.0127 (6) | 0.0030 (6) |
| C27A | 0.0203 (8) | 0.0278 (8) | 0.0370 (8) | 0.0111 (6) | 0.0120 (7) | 0.0142 (7) |
| C28A | 0.0236 (8) | 0.0332 (9) | 0.0347 (9) | 0.0090 (6) | 0.0065 (7) | 0.0088 (7) |
| O1B | 0.0199 (5) | 0.0129 (5) | 0.0303 (5) | 0.0007 (4) | 0.0132 (4) | 0.0021 (4) |
| O2B | 0.0225 (5) | 0.0115 (5) | 0.0241 (5) | 0.0028 (4) | 0.0084 (4) | −0.0013 (4) |
| O3B | 0.0178 (5) | 0.0268 (5) | 0.0167 (5) | 0.0053 (4) | 0.0074 (4) | 0.0031 (4) |
| O4B | 0.0240 (6) | 0.0339 (6) | 0.0149 (5) | 0.0106 (4) | 0.0067 (4) | 0.0084 (4) |
| N1B | 0.0154 (6) | 0.0145 (5) | 0.0134 (5) | 0.0028 (4) | 0.0038 (4) | 0.0012 (4) |
| N2B | 0.0153 (6) | 0.0113 (5) | 0.0154 (5) | 0.0024 (4) | 0.0044 (4) | 0.0008 (4) |
| C1B | 0.0153 (6) | 0.0148 (6) | 0.0141 (6) | 0.0033 (5) | 0.0044 (5) | 0.0018 (5) |
| C2B | 0.0185 (7) | 0.0128 (6) | 0.0139 (6) | 0.0029 (5) | 0.0027 (5) | 0.0013 (5) |
| C3B | 0.0204 (7) | 0.0173 (7) | 0.0141 (6) | 0.0072 (5) | 0.0051 (5) | 0.0010 (5) |
| C4B | 0.0156 (7) | 0.0187 (7) | 0.0144 (6) | 0.0041 (5) | 0.0041 (5) | 0.0024 (5) |
| C5B | 0.0180 (7) | 0.0127 (6) | 0.0171 (6) | 0.0008 (5) | 0.0054 (5) | 0.0018 (5) |
| C6B | 0.0164 (7) | 0.0138 (6) | 0.0137 (6) | 0.0034 (5) | 0.0043 (5) | 0.0011 (5) |
| C7B | 0.0190 (7) | 0.0119 (6) | 0.0202 (6) | 0.0025 (5) | 0.0084 (5) | 0.0035 (5) |
| C8B | 0.0156 (7) | 0.0156 (6) | 0.0143 (6) | 0.0036 (5) | 0.0062 (5) | 0.0006 (5) |
| C9B | 0.0178 (7) | 0.0191 (7) | 0.0195 (7) | 0.0014 (5) | 0.0049 (6) | −0.0020 (5) |
| C10B | 0.0183 (7) | 0.0289 (8) | 0.0173 (7) | 0.0046 (6) | 0.0007 (6) | −0.0031 (6) |
| C11B | 0.0233 (8) | 0.0279 (8) | 0.0160 (6) | 0.0117 (6) | 0.0044 (6) | 0.0054 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C12B | 0.0216 (7) | 0.0190 (7) | 0.0171 (6) | 0.0065 (5) | 0.0073 (6) | 0.0055 (5) |
| C13B | 0.0148 (6) | 0.0154 (6) | 0.0147 (6) | 0.0040 (5) | 0.0056 (5) | 0.0000 (5) |
| C14B | 0.0143 (6) | 0.0119 (6) | 0.0152 (6) | 0.0028 (5) | 0.0059 (5) | 0.0002 (5) |
| C15B | 0.0160 (7) | 0.0118 (6) | 0.0156 (6) | 0.0035 (5) | 0.0034 (5) | 0.0004 (5) |
| C16B | 0.0160 (7) | 0.0147 (6) | 0.0166 (6) | 0.0047 (5) | 0.0056 (5) | 0.0019 (5) |
| C17B | 0.0224 (7) | 0.0184 (7) | 0.0139 (6) | 0.0073 (5) | 0.0053 (5) | 0.0035 (5) |
| C18B | 0.0181 (7) | 0.0211 (7) | 0.0169 (6) | 0.0070 (5) | 0.0017 (5) | 0.0025 (5) |
| C19B | 0.0175 (7) | 0.0171 (7) | 0.0185 (6) | 0.0052 (5) | 0.0034 (5) | 0.0013 (5) |
| C20B | 0.0177 (7) | 0.0149 (6) | 0.0163 (6) | 0.0038 (5) | 0.0061 (5) | 0.0026 (5) |
| C21B | 0.0160 (7) | 0.0277 (8) | 0.0218 (7) | 0.0054 (5) | 0.0021 (6) | 0.0017 (6) |
| C22B | 0.0156 (7) | 0.0303 (8) | 0.0238 (7) | 0.0049 (6) | 0.0039 (6) | 0.0017 (6) |
| C23B | 0.0277 (9) | 0.0536 (11) | 0.0290 (8) | 0.0180 (8) | 0.0086 (7) | 0.0032 (8) |
| C24B | 0.0300 (9) | 0.0364 (9) | 0.0156 (7) | 0.0147 (7) | 0.0055 (6) | 0.0087 (6) |
| C25B | 0.0290 (8) | 0.0160 (7) | 0.0219 (7) | 0.0073 (6) | 0.0058 (6) | −0.0027 (6) |
| C26B | 0.0158 (7) | 0.0228 (7) | 0.0186 (6) | 0.0031 (5) | 0.0051 (5) | 0.0009 (5) |
| C27B | 0.0199 (7) | 0.0184 (7) | 0.0218 (7) | 0.0031 (5) | 0.0064 (6) | 0.0020 (6) |
| C28B | 0.0276 (8) | 0.0297 (8) | 0.0247 (7) | 0.0035 (6) | 0.0111 (7) | 0.0023 (6) |
| N3A | 0.0174 (6) | 0.0311 (7) | 0.0174 (6) | 0.0037 (5) | 0.0048 (5) | 0.0013 (5) |
| C29A | 0.0217 (8) | 0.0229 (8) | 0.0230 (7) | −0.0008 (6) | 0.0050 (6) | 0.0029 (6) |
| C30A | 0.0249 (8) | 0.0237 (8) | 0.0230 (7) | 0.0071 (6) | 0.0024 (6) | −0.0040 (6) |
| C31A | 0.0216 (8) | 0.0393 (9) | 0.0178 (7) | 0.0092 (6) | 0.0079 (6) | 0.0012 (6) |
| C32A | 0.0197 (8) | 0.0282 (8) | 0.0245 (7) | −0.0016 (6) | 0.0072 (6) | 0.0036 (6) |
| C33A | 0.0205 (7) | 0.0248 (8) | 0.0212 (7) | 0.0026 (6) | 0.0034 (6) | −0.0015 (6) |
| N3B | 0.0172 (6) | 0.0249 (7) | 0.0176 (6) | 0.0021 (5) | 0.0045 (5) | 0.0004 (5) |
| C29B | 0.0168 (7) | 0.0219 (7) | 0.0213 (7) | 0.0016 (5) | 0.0006 (6) | 0.0012 (6) |
| C30B | 0.0179 (7) | 0.0259 (8) | 0.0254 (7) | 0.0043 (6) | 0.0046 (6) | −0.0074 (6) |
| C31B | 0.0227 (8) | 0.0351 (9) | 0.0180 (7) | −0.0005 (6) | 0.0086 (6) | −0.0017 (6) |
| C32B | 0.0252 (8) | 0.0288 (8) | 0.0228 (7) | 0.0048 (6) | 0.0059 (6) | 0.0065 (6) |
| C33B | 0.0219 (7) | 0.0228 (7) | 0.0226 (7) | 0.0058 (6) | 0.0072 (6) | 0.0009 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1A—C1A | 1.3544 (15) | N2B—C8B | 1.3811 (16) |
| O1A—H1OA | 0.93 (2) | N2B—C7B | 1.4562 (15) |
| O2A—C2A | 1.3724 (15) | C1B—C6B | 1.3909 (17) |
| O2A—C25A | 1.4258 (16) | C1B—C2B | 1.4055 (18) |
| O3A—C16A | 1.3635 (15) | C2B—C3B | 1.3833 (18) |
| O3A—H3OA | 0.929 (19) | C3B—C4B | 1.4029 (18) |
| O4A—C17A | 1.3684 (15) | C3B—H3B | 0.93 |
| O4A—C24A | 1.4260 (16) | C4B—C5B | 1.3864 (18) |
| N1A—C14A | 1.3211 (16) | C4B—C26B | 1.5132 (18) |
| N1A—C13A | 1.3917 (16) | C5B—C6B | 1.3968 (17) |
| N2A—C14A | 1.3761 (15) | C5B—H5B | 0.93 |
| N2A—C8A | 1.3878 (16) | C6B—C7B | 1.5099 (18) |
| N2A—C7A | 1.4575 (15) | C7B—H7C | 0.97 |
| C1A—C6A | 1.3987 (17) | C7B—H7D | 0.97 |
| C1A—C2A | 1.4044 (18) | C8B—C9B | 1.3942 (18) |
| C2A—C3A | 1.3845 (18) | C8B—C13B | 1.4013 (17) |
| C3A—C4A | 1.4026 (18) | C9B—C10B | 1.3846 (19) |

| | | | |
|---|---|---|---|
| C3A—H3A | 0.93 | C9B—H9B | 0.93 |
| C4A—C5A | 1.3880 (18) | C10B—C11B | 1.400 (2) |
| C4A—C26A | 1.5153 (18) | C10B—H10B | 0.93 |
| C5A—C6A | 1.3875 (17) | C11B—C12B | 1.3866 (19) |
| C5A—H5A | 0.93 | C11B—H11B | 0.93 |
| C6A—C7A | 1.5156 (17) | C12B—C13B | 1.3919 (18) |
| C7A—H7A | 0.97 | C12B—H12B | 0.93 |
| C7A—H7B | 0.97 | C14B—C15B | 1.4757 (17) |
| C8A—C9A | 1.3956 (18) | C15B—C16B | 1.3914 (17) |
| C8A—C13A | 1.3988 (17) | C15B—C20B | 1.4052 (18) |
| C9A—C10A | 1.3854 (19) | C16B—C17B | 1.4085 (18) |
| C9A—H9A | 0.93 | C17B—C18B | 1.3826 (19) |
| C10A—C11A | 1.4040 (19) | C18B—C19B | 1.4062 (18) |
| C10A—H10A | 0.93 | C18B—H18B | 0.93 |
| C11A—C12A | 1.3857 (19) | C19B—C20B | 1.3823 (18) |
| C11A—H11A | 0.93 | C19B—C21B | 1.5175 (19) |
| C12A—C13A | 1.3961 (18) | C20B—H15B | 0.93 |
| C12A—H12A | 0.93 | C21B—C22B | 1.4983 (19) |
| C14A—C15A | 1.4802 (17) | C21B—H21C | 0.97 |
| C15A—C16A | 1.3952 (17) | C21B—H21D | 0.97 |
| C15A—C20A | 1.4072 (18) | C22B—C23B | 1.312 (2) |
| C16A—C17A | 1.4114 (18) | C22B—H22B | 0.93 |
| C17A—C18A | 1.3750 (18) | C23B—H23C | 0.93 |
| C18A—C19A | 1.4037 (18) | C23B—H23D | 0.93 |
| C18A—H18A | 0.93 | C24B—H24D | 0.96 |
| C19A—C20A | 1.3785 (18) | C24B—H24E | 0.96 |
| C19A—C21A | 1.5176 (18) | C24B—H24F | 0.96 |
| C20A—H20A | 0.93 | C25B—H25D | 0.96 |
| C21A—C22A | 1.4984 (18) | C25B—H25E | 0.96 |
| C21A—H21A | 0.97 | C25B—H25F | 0.96 |
| C21A—H21B | 0.97 | C26B—C27B | 1.4996 (18) |
| C22A—C23A | 1.3143 (19) | C26B—H26C | 0.97 |
| C22A—H22A | 0.93 | C26B—H26D | 0.97 |
| C23A—H23A | 0.93 | C27B—C28B | 1.3151 (19) |
| C23A—H23B | 0.93 | C27B—H27B | 0.93 |
| C24A—H24A | 0.96 | C28B—H28C | 0.93 |
| C24A—H24B | 0.96 | C28B—H28D | 0.93 |
| C24A—H24C | 0.96 | N3A—C33A | 1.3336 (17) |
| C25A—H25A | 0.96 | N3A—C29A | 1.3397 (18) |
| C25A—H25B | 0.96 | C29A—C30A | 1.377 (2) |
| C25A—H25C | 0.96 | C29A—H29A | 0.93 |
| C26A—C27A | 1.493 (2) | C30A—C31A | 1.377 (2) |
| C26A—H26A | 0.97 | C30A—H30A | 0.93 |
| C26A—H26B | 0.97 | C31A—C32A | 1.378 (2) |
| C27A—C28A | 1.316 (2) | C31A—H31A | 0.93 |
| C27A—H27A | 0.93 | C32A—C33A | 1.3786 (19) |
| C28A—H28A | 0.93 | C32A—H32A | 0.93 |
| C28A—H28B | 0.93 | C33A—H33A | 0.93 |
| O1B—C1B | 1.3606 (15) | N3B—C29B | 1.3383 (18) |

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|---|---|---|---|
| O1B—H1OB | 0.90 (2) | N3B—C33B | 1.3408 (18) |
| O2B—C2B | 1.3727 (15) | C29B—C30B | 1.389 (2) |
| O2B—C25B | 1.4285 (16) | C29B—H29B | 0.93 |
| O3B—C16B | 1.3538 (15) | C30B—C31B | 1.378 (2) |
| O3B—H3OB | 0.99 (2) | C30B—H30B | 0.93 |
| O4B—C17B | 1.3679 (15) | C31B—C32B | 1.381 (2) |
| O4B—C24B | 1.4252 (16) | C31B—H31B | 0.93 |
| N1B—C14B | 1.3229 (16) | C32B—C33B | 1.3830 (19) |
| N1B—C13B | 1.3895 (16) | C32B—H32B | 0.93 |
| N2B—C14B | 1.3740 (15) | C33B—H33B | 0.93 |
| C1A—O1A—H1OA | 114.9 (12) | C4B—C3B—H3B | 119.7 |
| C2A—O2A—C25A | 117.52 (10) | C5B—C4B—C3B | 118.40 (12) |
| C16A—O3A—H3OA | 111.5 (12) | C5B—C4B—C26B | 120.93 (12) |
| C17A—O4A—C24A | 117.37 (10) | C3B—C4B—C26B | 120.67 (12) |
| C14A—N1A—C13A | 105.60 (10) | C4B—C5B—C6B | 121.56 (12) |
| C14A—N2A—C8A | 106.81 (10) | C4B—C5B—H5B | 119.2 |
| C14A—N2A—C7A | 128.94 (11) | C6B—C5B—H5B | 119.2 |
| C8A—N2A—C7A | 123.80 (10) | C1B—C6B—C5B | 119.63 (12) |
| O1A—C1A—C6A | 117.93 (11) | C1B—C6B—C7B | 117.63 (11) |
| O1A—C1A—C2A | 122.79 (11) | C5B—C6B—C7B | 122.70 (11) |
| C6A—C1A—C2A | 119.28 (12) | N2B—C7B—C6B | 112.87 (10) |
| O2A—C2A—C3A | 125.45 (12) | N2B—C7B—H7C | 109.0 |
| O2A—C2A—C1A | 113.95 (11) | C6B—C7B—H7C | 109.0 |
| C3A—C2A—C1A | 120.60 (12) | N2B—C7B—H7D | 109.0 |
| C2A—C3A—C4A | 120.20 (12) | C6B—C7B—H7D | 109.0 |
| C2A—C3A—H3A | 119.9 | H7C—C7B—H7D | 107.8 |
| C4A—C3A—H3A | 119.9 | N2B—C8B—C9B | 131.90 (12) |
| C5A—C4A—C3A | 118.76 (12) | N2B—C8B—C13B | 105.64 (11) |
| C5A—C4A—C26A | 119.99 (12) | C9B—C8B—C13B | 122.45 (12) |
| C3A—C4A—C26A | 121.15 (12) | C10B—C9B—C8B | 116.54 (13) |
| C6A—C5A—C4A | 121.75 (12) | C10B—C9B—H9B | 121.7 |
| C6A—C5A—H5A | 119.1 | C8B—C9B—H9B | 121.7 |
| C4A—C5A—H5A | 119.1 | C9B—C10B—C11B | 121.57 (13) |
| C5A—C6A—C1A | 119.40 (12) | C9B—C10B—H10B | 119.2 |
| C5A—C6A—C7A | 122.38 (11) | C11B—C10B—H10B | 119.2 |
| C1A—C6A—C7A | 118.18 (11) | C12B—C11B—C10B | 121.54 (13) |
| N2A—C7A—C6A | 113.00 (10) | C12B—C11B—H11B | 119.2 |
| N2A—C7A—H7A | 109.0 | C10B—C11B—H11B | 119.2 |
| C6A—C7A—H7A | 109.0 | C11B—C12B—C13B | 117.64 (12) |
| N2A—C7A—H7B | 109.0 | C11B—C12B—H12B | 121.2 |
| C6A—C7A—H7B | 109.0 | C13B—C12B—H12B | 121.2 |
| H7A—C7A—H7B | 107.8 | N1B—C13B—C12B | 130.21 (12) |
| N2A—C8A—C9A | 131.98 (12) | N1B—C13B—C8B | 109.53 (11) |
| N2A—C8A—C13A | 105.56 (11) | C12B—C13B—C8B | 120.25 (12) |
| C9A—C8A—C13A | 122.46 (12) | N1B—C14B—N2B | 112.18 (11) |
| C10A—C9A—C8A | 116.43 (12) | N1B—C14B—C15B | 123.12 (11) |
| C10A—C9A—H9A | 121.8 | N2B—C14B—C15B | 124.66 (11) |
| C8A—C9A—H9A | 121.8 | C16B—C15B—C20B | 120.20 (12) |
| C9A—C10A—C11A | 121.77 (13) | C16B—C15B—C14B | 121.96 (11) |

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| C9A—C10A—H10A | 119.1 | C20B—C15B—C14B | 117.76 (11) |
| C11A—C10A—H10A | 119.1 | O3B—C16B—C15B | 119.68 (11) |
| C12A—C11A—C10A | 121.31 (12) | O3B—C16B—C17B | 121.62 (11) |
| C12A—C11A—H11A | 119.3 | C15B—C16B—C17B | 118.70 (12) |
| C10A—C11A—H11A | 119.3 | O4B—C17B—C18B | 125.26 (12) |
| C11A—C12A—C13A | 117.66 (12) | O4B—C17B—C16B | 114.11 (11) |
| C11A—C12A—H12A | 121.2 | C18B—C17B—C16B | 120.61 (12) |
| C13A—C12A—H12A | 121.2 | C17B—C18B—C19B | 120.78 (12) |
| N1A—C13A—C12A | 129.94 (12) | C17B—C18B—H18B | 119.6 |
| N1A—C13A—C8A | 109.70 (11) | C19B—C18B—H18B | 119.6 |
| C12A—C13A—C8A | 120.35 (12) | C20B—C19B—C18B | 118.57 (12) |
| N1A—C14A—N2A | 112.31 (11) | C20B—C19B—C21B | 122.68 (12) |
| N1A—C14A—C15A | 122.58 (11) | C18B—C19B—C21B | 118.75 (12) |
| N2A—C14A—C15A | 125.03 (11) | C19B—C20B—C15B | 121.11 (12) |
| C16A—C15A—C20A | 119.61 (12) | C19B—C20B—H15B | 119.4 |
| C16A—C15A—C14A | 123.35 (11) | C15B—C20B—H15B | 119.4 |
| C20A—C15A—C14A | 116.96 (11) | C22B—C21B—C19B | 115.21 (11) |
| O3A—C16A—C15A | 120.33 (11) | C22B—C21B—H21C | 108.5 |
| O3A—C16A—C17A | 121.05 (11) | C19B—C21B—H21C | 108.5 |
| C15A—C16A—C17A | 118.62 (12) | C22B—C21B—H21D | 108.5 |
| O4A—C17A—C18A | 125.04 (12) | C19B—C21B—H21D | 108.5 |
| O4A—C17A—C16A | 114.28 (11) | H21C—C21B—H21D | 107.5 |
| C18A—C17A—C16A | 120.65 (12) | C23B—C22B—C21B | 124.46 (15) |
| C17A—C18A—C19A | 120.90 (12) | C23B—C22B—H22B | 117.8 |
| C17A—C18A—H18A | 119.6 | C21B—C22B—H22B | 117.8 |
| C19A—C18A—H18A | 119.6 | C22B—C23B—H23C | 120.0 |
| C20A—C19A—C18A | 118.54 (12) | C22B—C23B—H23D | 120.0 |
| C20A—C19A—C21A | 123.52 (12) | H23C—C23B—H23D | 120.0 |
| C18A—C19A—C21A | 117.93 (11) | O4B—C24B—H24D | 109.5 |
| C19A—C20A—C15A | 121.43 (12) | O4B—C24B—H24E | 109.5 |
| C19A—C20A—H20A | 119.3 | H24D—C24B—H24E | 109.5 |
| C15A—C20A—H20A | 119.3 | O4B—C24B—H24F | 109.5 |
| C22A—C21A—C19A | 116.96 (11) | H24D—C24B—H24F | 109.5 |
| C22A—C21A—H21A | 108.1 | H24E—C24B—H24F | 109.5 |
| C19A—C21A—H21A | 108.1 | O2B—C25B—H25D | 109.5 |
| C22A—C21A—H21B | 108.1 | O2B—C25B—H25E | 109.5 |
| C19A—C21A—H21B | 108.1 | H25D—C25B—H25E | 109.5 |
| H21A—C21A—H21B | 107.3 | O2B—C25B—H25F | 109.5 |
| C23A—C22A—C21A | 123.88 (14) | H25D—C25B—H25F | 109.5 |
| C23A—C22A—H22A | 118.1 | H25E—C25B—H25F | 109.5 |
| C21A—C22A—H22A | 118.1 | C27B—C26B—C4B | 113.79 (11) |
| C22A—C23A—H23A | 120.0 | C27B—C26B—H26C | 108.8 |
| C22A—C23A—H23B | 120.0 | C4B—C26B—H26C | 108.8 |
| H23A—C23A—H23B | 120.0 | C27B—C26B—H26D | 108.8 |
| O4A—C24A—H24A | 109.5 | C4B—C26B—H26D | 108.8 |
| O4A—C24A—H24B | 109.5 | H26C—C26B—H26D | 107.7 |
| H24A—C24A—H24B | 109.5 | C28B—C27B—C26B | 125.58 (14) |
| O4A—C24A—H24C | 109.5 | C28B—C27B—H27B | 117.2 |
| H24A—C24A—H24C | 109.5 | C26B—C27B—H27B | 117.2 |

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| H24B—C24A—H24C | 109.5 | C27B—C28B—H28C | 120.0 |
| O2A—C25A—H25A | 109.5 | C27B—C28B—H28D | 120.0 |
| O2A—C25A—H25B | 109.5 | H28C—C28B—H28D | 120.0 |
| H25A—C25A—H25B | 109.5 | C33A—N3A—C29A | 117.41 (12) |
| O2A—C25A—H25C | 109.5 | N3A—C29A—C30A | 123.10 (13) |
| H25A—C25A—H25C | 109.5 | N3A—C29A—H29A | 118.4 |
| H25B—C25A—H25C | 109.5 | C30A—C29A—H29A | 118.4 |
| C27A—C26A—C4A | 110.61 (11) | C29A—C30A—C31A | 118.78 (13) |
| C27A—C26A—H26A | 109.5 | C29A—C30A—H30A | 120.6 |
| C4A—C26A—H26A | 109.5 | C31A—C30A—H30A | 120.6 |
| C27A—C26A—H26B | 109.5 | C30A—C31A—C32A | 118.77 (13) |
| C4A—C26A—H26B | 109.5 | C30A—C31A—H31A | 120.6 |
| H26A—C26A—H26B | 108.1 | C32A—C31A—H31A | 120.6 |
| C28A—C27A—C26A | 124.60 (14) | C31A—C32A—C33A | 118.84 (13) |
| C28A—C27A—H27A | 117.7 | C31A—C32A—H32A | 120.6 |
| C26A—C27A—H27A | 117.7 | C33A—C32A—H32A | 120.6 |
| C27A—C28A—H28A | 120.0 | N3A—C33A—C32A | 123.10 (13) |
| C27A—C28A—H28B | 120.0 | N3A—C33A—H33A | 118.5 |
| H28A—C28A—H28B | 120.0 | C32A—C33A—H33A | 118.5 |
| C1B—O1B—H1OB | 114.2 (14) | C29B—N3B—C33B | 116.99 (12) |
| C2B—O2B—C25B | 116.37 (10) | N3B—C29B—C30B | 123.19 (14) |
| C16B—O3B—H3OB | 115.7 (12) | N3B—C29B—H29B | 118.4 |
| C17B—O4B—C24B | 117.47 (11) | C30B—C29B—H29B | 118.4 |
| C14B—N1B—C13B | 105.63 (10) | C31B—C30B—C29B | 118.87 (14) |
| C14B—N2B—C8B | 107.01 (10) | C31B—C30B—H30B | 120.6 |
| C14B—N2B—C7B | 128.51 (11) | C29B—C30B—H30B | 120.6 |
| C8B—N2B—C7B | 123.89 (10) | C30B—C31B—C32B | 118.73 (13) |
| O1B—C1B—C6B | 117.52 (11) | C30B—C31B—H31B | 120.6 |
| O1B—C1B—C2B | 123.21 (11) | C32B—C31B—H31B | 120.6 |
| C6B—C1B—C2B | 119.26 (12) | C31B—C32B—C33B | 118.71 (14) |
| O2B—C2B—C3B | 125.24 (12) | C31B—C32B—H32B | 120.6 |
| O2B—C2B—C1B | 114.37 (11) | C33B—C32B—H32B | 120.6 |
| C3B—C2B—C1B | 120.38 (12) | N3B—C33B—C32B | 123.51 (14) |
| C2B—C3B—C4B | 120.69 (12) | N3B—C33B—H33B | 118.2 |
| C2B—C3B—H3B | 119.7 | C32B—C33B—H33B | 118.2 |
| C25A—O2A—C2A—C3A | 4.29 (18) | O2B—C2B—C3B—C4B | 178.77 (12) |
| C25A—O2A—C2A—C1A | −175.63 (11) | C1B—C2B—C3B—C4B | −0.66 (19) |
| O1A—C1A—C2A—O2A | −1.06 (17) | C2B—C3B—C4B—C5B | 2.58 (19) |
| C6A—C1A—C2A—O2A | 178.78 (11) | C2B—C3B—C4B—C26B | −178.20 (12) |
| O1A—C1A—C2A—C3A | 179.02 (12) | C3B—C4B—C5B—C6B | −2.08 (19) |
| C6A—C1A—C2A—C3A | −1.14 (19) | C26B—C4B—C5B—C6B | 178.70 (12) |
| O2A—C2A—C3A—C4A | −179.61 (12) | O1B—C1B—C6B—C5B | −177.44 (11) |
| C1A—C2A—C3A—C4A | 0.30 (19) | C2B—C1B—C6B—C5B | 2.29 (19) |
| C2A—C3A—C4A—C5A | 0.31 (19) | O1B—C1B—C6B—C7B | 0.45 (17) |
| C2A—C3A—C4A—C26A | −175.97 (12) | C2B—C1B—C6B—C7B | −179.81 (11) |
| C3A—C4A—C5A—C6A | −0.06 (19) | C4B—C5B—C6B—C1B | −0.35 (19) |
| C26A—C4A—C5A—C6A | 176.26 (12) | C4B—C5B—C6B—C7B | −178.13 (12) |
| C4A—C5A—C6A—C1A | −0.78 (19) | C14B—N2B—C7B—C6B | 87.21 (15) |
| C4A—C5A—C6A—C7A | −178.67 (12) | C8B—N2B—C7B—C6B | −82.87 (15) |

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|---|---|---|---|
| O1A—C1A—C6A—C5A | −178.78 (11) | C1B—C6B—C7B—N2B | 151.99 (11) |
| C2A—C1A—C6A—C5A | 1.37 (18) | C5B—C6B—C7B—N2B | −30.18 (17) |
| O1A—C1A—C6A—C7A | −0.81 (17) | C14B—N2B—C8B—C9B | 179.48 (14) |
| C2A—C1A—C6A—C7A | 179.34 (11) | C7B—N2B—C8B—C9B | −8.6 (2) |
| C14A—N2A—C7A—C6A | 93.27 (15) | C14B—N2B—C8B—C13B | 0.48 (13) |
| C8A—N2A—C7A—C6A | −78.04 (15) | C7B—N2B—C8B—C13B | 172.37 (11) |
| C5A—C6A—C7A—N2A | −35.08 (17) | N2B—C8B—C9B—C10B | −178.23 (13) |
| C1A—C6A—C7A—N2A | 147.02 (11) | C13B—C8B—C9B—C10B | 0.6 (2) |
| C14A—N2A—C8A—C9A | −179.57 (14) | C8B—C9B—C10B—C11B | −0.4 (2) |
| C7A—N2A—C8A—C9A | −6.6 (2) | C9B—C10B—C11B—C12B | 0.3 (2) |
| C14A—N2A—C8A—C13A | 0.75 (13) | C10B—C11B—C12B—C13B | −0.3 (2) |
| C7A—N2A—C8A—C13A | 173.69 (11) | C14B—N1B—C13B—C12B | −178.45 (13) |
| N2A—C8A—C9A—C10A | −178.39 (13) | C14B—N1B—C13B—C8B | 0.57 (14) |
| C13A—C8A—C9A—C10A | 1.25 (19) | C11B—C12B—C13B—N1B | 179.37 (13) |
| C8A—C9A—C10A—C11A | −0.1 (2) | C11B—C12B—C13B—C8B | 0.44 (19) |
| C9A—C10A—C11A—C12A | −0.5 (2) | N2B—C8B—C13B—N1B | −0.66 (14) |
| C10A—C11A—C12A—C13A | 0.0 (2) | C9B—C8B—C13B—N1B | −179.78 (12) |
| C14A—N1A—C13A—C12A | −177.93 (13) | N2B—C8B—C13B—C12B | 178.48 (11) |
| C14A—N1A—C13A—C8A | 0.91 (14) | C9B—C8B—C13B—C12B | −0.6 (2) |
| C11A—C12A—C13A—N1A | 179.82 (13) | C13B—N1B—C14B—N2B | −0.27 (14) |
| C11A—C12A—C13A—C8A | 1.09 (19) | C13B—N1B—C14B—C15B | −177.99 (11) |
| N2A—C8A—C13A—N1A | −1.03 (14) | C8B—N2B—C14B—N1B | −0.14 (14) |
| C9A—C8A—C13A—N1A | 179.24 (12) | C7B—N2B—C14B—N1B | −171.53 (11) |
| N2A—C8A—C13A—C12A | 177.93 (11) | C8B—N2B—C14B—C15B | 177.54 (11) |
| C9A—C8A—C13A—C12A | −1.79 (19) | C7B—N2B—C14B—C15B | 6.1 (2) |
| C13A—N1A—C14A—N2A | −0.43 (14) | N1B—C14B—C15B—C16B | −128.32 (14) |
| C13A—N1A—C14A—C15A | −177.57 (11) | N2B—C14B—C15B—C16B | 54.24 (18) |
| C8A—N2A—C14A—N1A | −0.21 (14) | N1B—C14B—C15B—C20B | 48.37 (17) |
| C7A—N2A—C14A—N1A | −172.67 (11) | N2B—C14B—C15B—C20B | −129.07 (13) |
| C8A—N2A—C14A—C15A | 176.86 (11) | C20B—C15B—C16B—O3B | −177.02 (11) |
| C7A—N2A—C14A—C15A | 4.4 (2) | C14B—C15B—C16B—O3B | −0.41 (19) |
| N1A—C14A—C15A—C16A | −129.32 (14) | C20B—C15B—C16B—C17B | 1.92 (19) |
| N2A—C14A—C15A—C16A | 53.91 (18) | C14B—C15B—C16B—C17B | 178.53 (12) |
| N1A—C14A—C15A—C20A | 47.43 (17) | C24B—O4B—C17B—C18B | 12.40 (19) |
| N2A—C14A—C15A—C20A | −129.35 (13) | C24B—O4B—C17B—C16B | −169.18 (12) |
| C20A—C15A—C16A—O3A | −174.71 (11) | O3B—C16B—C17B—O4B | −1.57 (18) |
| C14A—C15A—C16A—O3A | 1.95 (19) | C15B—C16B—C17B—O4B | 179.51 (11) |
| C20A—C15A—C16A—C17A | 5.15 (19) | O3B—C16B—C17B—C18B | 176.93 (12) |
| C14A—C15A—C16A—C17A | −178.18 (12) | C15B—C16B—C17B—C18B | −1.99 (19) |
| C24A—O4A—C17A—C18A | 6.52 (19) | O4B—C17B—C18B—C19B | 179.27 (13) |
| C24A—O4A—C17A—C16A | −175.33 (11) | C16B—C17B—C18B—C19B | 0.9 (2) |
| O3A—C16A—C17A—O4A | −3.82 (18) | C17B—C18B—C19B—C20B | 0.2 (2) |
| C15A—C16A—C17A—O4A | 176.31 (11) | C17B—C18B—C19B—C21B | 179.51 (12) |
| O3A—C16A—C17A—C18A | 174.42 (12) | C18B—C19B—C20B—C15B | −0.25 (19) |
| C15A—C16A—C17A—C18A | −5.44 (19) | C21B—C19B—C20B—C15B | −179.54 (12) |
| O4A—C17A—C18A—C19A | 180.00 (12) | C16B—C15B—C20B—C19B | −0.83 (19) |
| C16A—C17A—C18A—C19A | 2.0 (2) | C14B—C15B—C20B—C19B | −177.58 (12) |
| C17A—C18A—C19A—C20A | 1.8 (2) | C20B—C19B—C21B—C22B | −8.9 (2) |
| C17A—C18A—C19A—C21A | −177.46 (12) | C18B—C19B—C21B—C22B | 171.79 (12) |

| | | | |
|---|---|---|---|
| C18A—C19A—C20A—C15A | −2.07 (19) | C19B—C21B—C22B—C23B | 124.11 (16) |
| C21A—C19A—C20A—C15A | 177.17 (12) | C5B—C4B—C26B—C27B | 97.42 (15) |
| C16A—C15A—C20A—C19A | −1.46 (19) | C3B—C4B—C26B—C27B | −81.78 (16) |
| C14A—C15A—C20A—C19A | −178.33 (12) | C4B—C26B—C27B—C28B | 133.17 (15) |
| C20A—C19A—C21A—C22A | −10.9 (2) | C33A—N3A—C29A—C30A | −0.1 (2) |
| C18A—C19A—C21A—C22A | 168.38 (12) | N3A—C29A—C30A—C31A | −0.2 (2) |
| C19A—C21A—C22A—C23A | 134.61 (14) | C29A—C30A—C31A—C32A | 0.6 (2) |
| C5A—C4A—C26A—C27A | −72.15 (16) | C30A—C31A—C32A—C33A | −0.6 (2) |
| C3A—C4A—C26A—C27A | 104.09 (15) | C29A—N3A—C33A—C32A | 0.1 (2) |
| C4A—C26A—C27A—C28A | 107.50 (16) | C31A—C32A—C33A—N3A | 0.2 (2) |
| C25B—O2B—C2B—C3B | 2.11 (18) | C33B—N3B—C29B—C30B | 0.9 (2) |
| C25B—O2B—C2B—C1B | −178.42 (11) | N3B—C29B—C30B—C31B | −0.3 (2) |
| O1B—C1B—C2B—O2B | −1.58 (18) | C29B—C30B—C31B—C32B | −0.5 (2) |
| C6B—C1B—C2B—O2B | 178.70 (11) | C30B—C31B—C32B—C33B | 0.6 (2) |
| O1B—C1B—C2B—C3B | 177.92 (12) | C29B—N3B—C33B—C32B | −0.8 (2) |
| C6B—C1B—C2B—C3B | −1.80 (19) | C31B—C32B—C33B—N3B | 0.1 (2) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1A—H1OA···O2A | 0.93 (2) | 2.30 (2) | 2.6977 (14) | 105 (1) |
| O1A—H1OA···N1B | 0.93 (2) | 1.81 (2) | 2.6932 (15) | 157 (2) |
| O3A—H3OA···O4A | 0.93 (2) | 2.25 (2) | 2.6798 (13) | 108 (2) |
| O3A—H3OA···N3B$^{i}$ | 0.93 (2) | 1.90 (2) | 2.7859 (14) | 160 (2) |
| O1B—H1OB···O2B | 0.90 (2) | 2.33 (2) | 2.7197 (14) | 106 (2) |
| O1B—H1OB···N1A$^{ii}$ | 0.90 (2) | 1.87 (2) | 2.7114 (15) | 153 (2) |
| O3B—H3OB···O4B | 0.99 (2) | 2.27 (2) | 2.6789 (13) | 103 (1) |
| O3B—H3OB···N3A$^{iii}$ | 0.99 (2) | 1.68 (2) | 2.6461 (15) | 161 (2) |
| C7A—H7A···O3A | 0.97 | 2.38 | 3.1017 (15) | 131 |
| C7A—H7B···O1A | 0.97 | 2.35 | 2.7525 (16) | 104 |
| C7B—H7C···O3B | 0.97 | 2.30 | 3.0302 (16) | 132 |
| C7B—H7D···O1B | 0.97 | 2.35 | 2.7231 (16) | 102 |
| C11B—H11B···O2A$^{iv}$ | 0.93 | 2.59 | 3.5010 (17) | 165 |
| C31A—H31A···O1A | 0.93 | 2.36 | 3.2382 (18) | 158 |
| C23A—H23A···Cg1$^{v}$ | 0.93 | 2.90 | 3.3950 (17) | 115 |
| C28B—H28C···Cg2$^{vi}$ | 0.93 | 2.99 | 3.4562 (18) | 113 |
| C33A—H33A···Cg3$^{i}$ | 0.93 | 2.74 | 3.4888 (16) | 139 |

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

**Fig. 1**

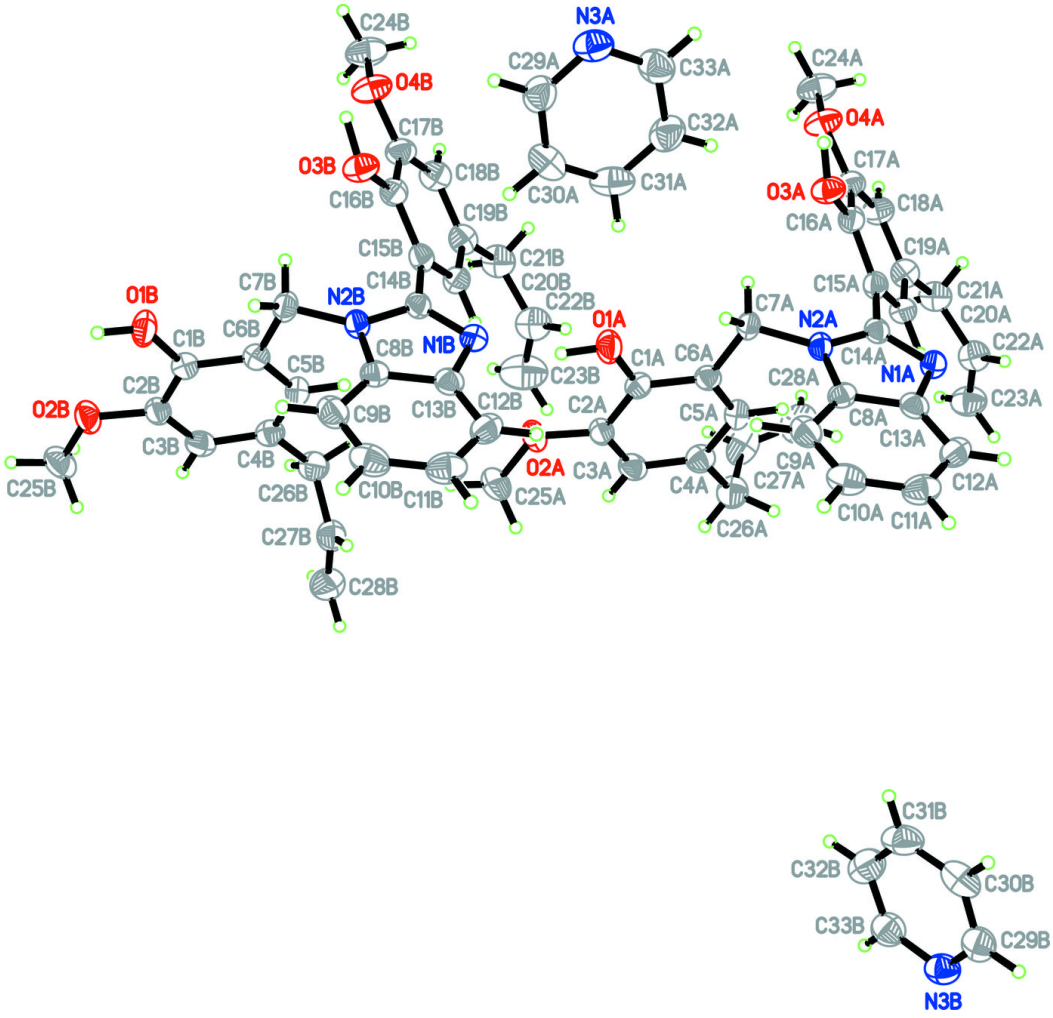
C24B
N3A
C29A
C33A
O4B
C32A
C24A
O4A
C17B
C17A
O3B
C18B
C30A
C31A
O3A
C18A
C16B
C16A
C19B
C19A
C15B
C21B
C15A
C21A
C7B
C14B
C20B
C20A
O1B
N2B
C22B
O1A
C7A
N2A
C22A
C1B
C6B
C8B
N1B
C1A
C6A
C14A
N1A
C5B
C23B
C28A
C23A
C2B
C2A
C5A
C8A
O2B
C9B
C13B
C12B
C13A
C3B
C4B
O2A
C3A
C9A
C12A
C25B
C26B
C10B
C11B
C25A
C4A
C27A
C10A
C11A
C26A
C27B
C28B
C31B
C32B
C30B
C33B
C29B
N3B

**Fig. 2**