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

# 2-Amino-*N*-(2-benzyloxy-3-methoxybenzylidene)aniline

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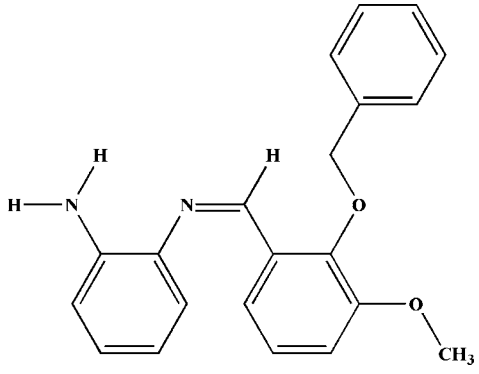
Received 31 May 2008; accepted 12 June 2008

Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.070; $wR$ factor = 0.192; data-to-parameter ratio = 16.6.

The title compound, $C_{21}H_{20}N_2O_2$, a Schiff base ligand, contains two independent molecules (*A* and *B*) in the asymmetric unit, with similar conformations. In molecule *A*, the central benzene ring forms dihedral angles of 30.79 (13) and 23.56 (13)°, respectively, with the amino and benzyl benzene rings, while in molecule *B* these angles are 32.30 (13) and 13.13 (12)°. The molecular structure is stabilized by intramolecular N—H···N and C—H···O hydrogen bonds. The crystal structure is stabilized by N—H···N hydrogen bonds and N—H···$\pi$ and C—H···$\pi$ interactions.

## Related literature

For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987). For related structures, see: Al-Douh *et al.* (2006*a*,*b*, 2007, 2008); Corden *et al.* (1996); Govindasamy *et al.* (1999); Pozharskii *et al.* (1966).




## Experimental

### Crystal data

$C_{21}H_{20}N_2O_2$
$M_r$ = 332.39
Monoclinic, $P2_1/c$
$a$ = 12.0932 (2) Å
$b$ = 13.7680 (3) Å
$c$ = 20.5249 (4) Å
$\beta$ = 99.149 (1)°
$V$ = 3373.90 (11) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 100.0 (1) K
0.36 × 0.18 × 0.07 mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker 2005)
$T_{min}$ = 0.970, $T_{max}$ = 0.994
37354 measured reflections
7737 independent reflections
4167 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.082

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.192
$S$ = 1.03
7737 reflections
465 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.87 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.38 e Å$^{-3}$

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

*Cg*1, *Cg*2, *Cg*3, *Cg*4, *Cg*5 and *Cg*6 are the centroids of the C1*A*–C6*A*, C8*A*–C13*A*, C15*A*–C20*A*, C1*B*–C6*B*, C8*B*–C13*B* and C15*B*–C20*B* rings, respectively.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2*A*—H2*AC*···N1*A* | 0.92 (3) | 2.31 (3) | 2.735 (4) | 108 (2) |
| N2*A*—H2*AC*···N2*B*$^{i}$ | 0.92 (3) | 2.49 (3) | 3.229 (4) | 138 (3) |
| N2*B*—H2*BC*···N1*B* | 0.90 (2) | 2.29 (3) | 2.726 (3) | 109 (2) |
| C7*A*—H7*A*···O1*A* | 0.95 | 2.43 | 2.765 (3) | 101 |
| C7*B*—H7*B*···O1*B* | 0.95 | 2.46 | 2.790 (3) | 100 |
| C14*A*—H14*A*···O2*A* | 0.99 | 2.43 | 2.895 (3) | 108 |
| C14*B*—H14*D*···O2*B* | 0.99 | 2.45 | 2.903 (3) | 107 |
| C21*A*—H21*C*···*Cg*1$^{ii}$ | 0.98 | 2.96 | 3.511 (3) | 117 |
| C21*B*—H21*F*···*Cg*2$^{iii}$ | 0.98 | 2.81 | 3.739 (3) | 159 |
| C10*A*—H10*A*···*Cg*3$^{ii}$ | 0.95 | 2.60 | 3.500 (3) | 159 |
| C21*B*—H21*E*···*Cg*4$^{iv}$ | 0.98 | 2.80 | 3.433 (3) | 123 |
| C21*A*—H21*B*···*Cg*5$^{v}$ | 0.98 | 2.96 | 3.844 (4) | 150 |
| C10*B*—H10*B*···*Cg*6$^{iv}$ | 0.95 | 2.66 | 3.587 (3) | 165 |
| N2*B*—H2*BC*···*Cg*6$^{vi}$ | 0.90 (2) | 2.83 (3) | 3.288 (3) | 113 (2) |

Symmetry codes: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x-1, y, z$; (iv) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (v) $x+1, y, z$; (vi) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

We thank the Malaysian Government and Universiti Sains Malaysia (USM) for an IRPA short-term grant (304/PKIMIA/638007) to conduct this work. MHA thanks the Yemen Government and Hadhramout University of Science and Technology (HUST) for financial scholarship support. HKF and RK thank the Malaysian Government and Universiti Sains Malaysia for Science Fund grant No. 305/PFIZIK/613312. RK thanks Universiti Sains Malaysia for a post-doctoral research fellowship.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2609).

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# supporting information

*Acta Cryst.* (2008). E**64**, o1290–o1291 [doi:10.1107/S1600536808017844]

## 2-Amino-*N*-(2-benzyloxy-3-methoxybenzylidene)aniline

**Mohammed H. Al-Douh, Shafida A. Hamid, Hasnah Osman, Reza Kia and Hoong-Kun Fun**

### S1. Comment

Mono-anil, is a Schiff base compound prepared from an equimolar amount of *o*-phenylenediamine and an aromatic or heterocyclic aldehyde as the first stage to produce 2-substituted benzimidazole derivatives following spontaneous oxidation by atmospheric oxygen (Pozharskii *et al.*, 1966). In our previous reports (Al-Douh *et al.*, 2007,2006a,b; Al-Douh *et al.*, 2008), we have reported crystal structures of 2-(2-benzyloxy -3-methoxyphenyl)-1-*H*-benzimidazole, benzyl *o*-vanillin and a derivative of the title compound, 2-amino-*N*-(2-hydroxy-3-methoxybenzylidene) benzeneamine. Continuing our investigation on the reaction mechanism of benzyl *o*-vanillin with *o*-phenylenediamine, we successfully synthesized the title compound, as a new amino benzeneamine derivative. We present here its crystal structure.

The bond lengths and angles in the title compound have normal values (Allen *et al.*, 1987) and are comparable with those a realated structure (Al-Douh *et al.*, 2008). The asymmetric unit contains two independent molecules [*A* and *B*] with almost similar conformations (Fig.1). In both A and B, the methoxy group is almost coplanar with the attached benzene ring [C21–O2–C12–C11 = -3.6 (4)° for A and -2.5 (4)° for B]. In molecule A, the C1-C6 and C15-C20 rings form dihedral angles of 30.79 (13)° and 23.56 (13)°, respectively, with the C8-C13 ring, while in B these angles are 32.30 (13)° and 13.13 (12)°. Intramolecular C—H···O and N—H···N hydrogen bonds involving O1, O2 and N1 atoms generate S(5) or S(6) ring motifs.

The crystal packing of the title compound is controlled by N—H···N hydrogen bonds, and N—H···$\pi$ and C—H···$\pi$ interactions (Table 1).

### S2. Experimental

The title compound was synthesized following procedures reported earlier (Al-Douh *et al.*, 2006a,b; Al-Douh *et al.*, 2007). Single crystals suitable for *X*-ray diffraction were obtained by slow evaporation of a hexane solution at room temperature.

### S3. Refinement

Amino H atoms were located in a difference map and their positional parameters were refined with N-H distances restrained to 0.90 (1)Å. C-bound H atoms were positioned geometrically and refined using a riding model with C-H = 0.95 Å for aromatic and methyine H, 0.99 Å for methylene H, and 0.98 Å for methyl H atoms. 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. The highest peak is located at 0.60 Å from H7A and the deepest hole is located at 0.71 Å from N2A.

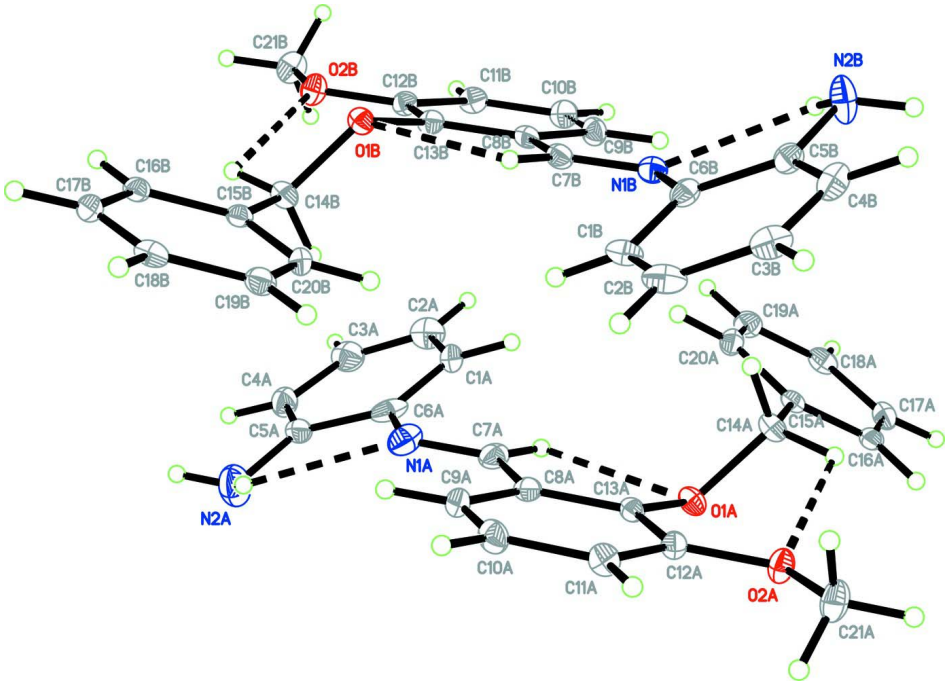


**Figure 1**

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. Intramolecular interactions are shown as dashed lines.

### 2-Amino-*N*-(2-benzyloxy-3-methoxybenzylidene)aniline

*Crystal data*

$C_{21}H_{20}N_2O_2$
$M_r = 332.39$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.0932\ (2)$ Å
$b = 13.7680\ (3)$ Å
$c = 20.5249\ (4)$ Å
$\beta = 99.149\ (1)°$
$V = 3373.90\ (11)$ Å$^3$
$Z = 8$
$F(000) = 1408$
$D_x = 1.309$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3259 reflections
$\theta = 2.4–22.7°$
$\mu = 0.09$ mm$^{-1}$
$T = 100$ K
Plate, yellow
0.36 × 0.18 × 0.07 mm

*Data collection*

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker 2005)
$T_{min} = 0.970$, $T_{max} = 0.994$
37354 measured reflections
7737 independent reflections
4167 reflections with $I > 2\sigma(I)$
$R_{int} = 0.082$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.7°$
$h = -15\rightarrow15$
$k = -17\rightarrow17$
$l = -26\rightarrow26$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.070$
$wR(F^2) = 0.192$
$S = 1.03$
7737 reflections
465 parameters
4 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0781P)^2 + 1.4666P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.87$ e Å$^{-3}$
$\Delta\rho_{min} = -0.38$ e Å$^{-3}$

*Special details*

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

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

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on $F^2$, conventional R-factors R are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2$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 | 0.99391 (15) | 0.97464 (12) | 0.31812 (8) | 0.0232 (4) |
| O2A | 1.17303 (15) | 0.85898 (13) | 0.35794 (9) | 0.0257 (5) |
| N1A | 0.7858 (2) | 0.94192 (17) | 0.14556 (13) | 0.0358 (6) |
| N2A | 0.7063 (3) | 0.9977 (2) | 0.01884 (15) | 0.0516 (8) |
| H2AB | 0.657 (2) | 1.000 (3) | −0.0199 (10) | 0.062* |
| H2AC | 0.748 (3) | 0.9432 (16) | 0.0317 (17) | 0.062* |
| C1A | 0.6378 (3) | 1.0482 (2) | 0.18465 (15) | 0.0353 (8) |
| H1A | 0.6636 | 1.0329 | 0.2296 | 0.042* |
| C2A | 0.5474 (3) | 1.1075 (2) | 0.16928 (18) | 0.0401 (8) |
| H2A | 0.5100 | 1.1320 | 0.2032 | 0.048* |
| C3A | 0.5108 (3) | 1.1317 (2) | 0.10576 (17) | 0.0395 (8) |
| H3A | 0.4500 | 1.1757 | 0.0954 | 0.047* |
| C4A | 0.5609 (3) | 1.0930 (2) | 0.05582 (15) | 0.0331 (7) |
| H4A | 0.5319 | 1.1097 | 0.0115 | 0.040* |
| C5A | 0.6517 (2) | 1.0309 (2) | 0.06765 (14) | 0.0283 (7) |
| C6A | 0.6950 (2) | 1.0082 (2) | 0.13495 (17) | 0.0344 (8) |
| C7A | 0.8502 (2) | 0.9488 (2) | 0.20040 (15) | 0.0311 (7) |
| H7A | 0.8354 | 0.9973 | 0.2308 | 0.037* |
| C8A | 0.9480 (2) | 0.88351 (19) | 0.21891 (13) | 0.0227 (6) |
| C9A | 0.9735 (2) | 0.8086 (2) | 0.17760 (13) | 0.0266 (7) |
| H9A | 0.9279 | 0.7987 | 0.1360 | 0.032* |
| C10A | 1.0642 (3) | 0.7494 (2) | 0.19684 (14) | 0.0283 (7) |
| H10A | 1.0797 | 0.6980 | 0.1688 | 0.034* |

| | | | | |
|---|---|---|---|---|
| C11A | 1.1335 (2) | 0.76356 (19) | 0.25672 (14) | 0.0258 (7) |
| H11A | 1.1967 | 0.7227 | 0.2691 | 0.031* |
| C12A | 1.1104 (2) | 0.83792 (19) | 0.29868 (13) | 0.0224 (6) |
| C13A | 1.0167 (2) | 0.89782 (18) | 0.27938 (13) | 0.0192 (6) |
| C14A | 0.9679 (2) | 0.94967 (19) | 0.38311 (13) | 0.0246 (6) |
| H14A | 1.0379 | 0.9411 | 0.4149 | 0.030* |
| H14B | 0.9249 | 0.8882 | 0.3808 | 0.030* |
| C15A | 0.9004 (2) | 1.03068 (18) | 0.40466 (12) | 0.0201 (6) |
| C16A | 0.9483 (2) | 1.09881 (19) | 0.45039 (13) | 0.0217 (6) |
| H16A | 1.0251 | 1.0934 | 0.4691 | 0.026* |
| C17A | 0.8843 (2) | 1.17526 (19) | 0.46915 (13) | 0.0253 (7) |
| H17A | 0.9171 | 1.2208 | 0.5013 | 0.030* |
| C18A | 0.7739 (2) | 1.1844 (2) | 0.44110 (14) | 0.0268 (7) |
| H18A | 0.7309 | 1.2373 | 0.4532 | 0.032* |
| C19A | 0.7249 (2) | 1.1172 (2) | 0.39544 (14) | 0.0302 (7) |
| H19A | 0.6486 | 1.1238 | 0.3760 | 0.036* |
| C20A | 0.7880 (2) | 1.0401 (2) | 0.37814 (13) | 0.0250 (6) |
| H20A | 0.7538 | 0.9929 | 0.3476 | 0.030* |
| C21A | 1.2661 (2) | 0.7965 (2) | 0.38025 (15) | 0.0322 (7) |
| H21A | 1.3063 | 0.8206 | 0.4224 | 0.048* |
| H21B | 1.3167 | 0.7956 | 0.3474 | 0.048* |
| H21C | 1.2388 | 0.7306 | 0.3862 | 0.048* |
| O1B | 0.50904 (15) | 0.75379 (12) | 0.18231 (9) | 0.0226 (4) |
| O2B | 0.33148 (15) | 0.87429 (13) | 0.14797 (9) | 0.0282 (5) |
| N1B | 0.71887 (19) | 0.77598 (16) | 0.35724 (11) | 0.0243 (5) |
| N2B | 0.7842 (2) | 0.7181 (2) | 0.48460 (13) | 0.0408 (7) |
| H2BB | 0.830 (2) | 0.720 (2) | 0.5241 (9) | 0.049* |
| H2BC | 0.738 (2) | 0.7680 (17) | 0.4697 (15) | 0.049* |
| C1B | 0.8724 (2) | 0.6776 (2) | 0.32288 (15) | 0.0288 (7) |
| H1B | 0.8507 | 0.6957 | 0.2780 | 0.035* |
| C2B | 0.9638 (3) | 0.6175 (2) | 0.34035 (16) | 0.0328 (7) |
| H2B | 1.0044 | 0.5943 | 0.3075 | 0.039* |
| C3B | 0.9958 (3) | 0.5914 (2) | 0.40519 (16) | 0.0324 (7) |
| H3B | 1.0582 | 0.5494 | 0.4169 | 0.039* |
| C4B | 0.9382 (2) | 0.6254 (2) | 0.45366 (16) | 0.0313 (7) |
| H4B | 0.9617 | 0.6071 | 0.4983 | 0.038* |
| C5B | 0.8457 (2) | 0.68672 (19) | 0.43727 (14) | 0.0257 (7) |
| C6B | 0.8112 (2) | 0.71220 (18) | 0.37070 (14) | 0.0249 (7) |
| C7B | 0.6539 (2) | 0.77124 (19) | 0.30195 (14) | 0.0234 (6) |
| H7B | 0.6680 | 0.7235 | 0.2709 | 0.028* |
| C8B | 0.5580 (2) | 0.83669 (19) | 0.28451 (13) | 0.0218 (6) |
| C9B | 0.5342 (2) | 0.9077 (2) | 0.32963 (14) | 0.0264 (7) |
| H9B | 0.5807 | 0.9139 | 0.3713 | 0.032* |
| C10B | 0.4435 (2) | 0.9681 (2) | 0.31328 (14) | 0.0289 (7) |
| H10B | 0.4284 | 1.0164 | 0.3437 | 0.035* |
| C11B | 0.3737 (2) | 0.95954 (19) | 0.25302 (14) | 0.0256 (6) |
| H11B | 0.3111 | 1.0016 | 0.2426 | 0.031* |
| C12B | 0.3950 (2) | 0.88960 (19) | 0.20775 (14) | 0.0227 (6) |

| | | | | |
|---|---|---|---|---|
| C13B | 0.4884 (2) | 0.82822 (18) | 0.22413 (13) | 0.0213 (6) |
| C14B | 0.5337 (2) | 0.78276 (19) | 0.11804 (13) | 0.0250 (7) |
| H14C | 0.5767 | 0.8443 | 0.1217 | 0.030* |
| H14D | 0.4634 | 0.7927 | 0.0868 | 0.030* |
| C15B | 0.6015 (2) | 0.70273 (18) | 0.09400 (13) | 0.0194 (6) |
| C16B | 0.5587 (2) | 0.64734 (18) | 0.03910 (13) | 0.0216 (6) |
| H16B | 0.4861 | 0.6607 | 0.0157 | 0.026* |
| C17B | 0.6221 (2) | 0.57224 (19) | 0.01840 (13) | 0.0242 (6) |
| H17B | 0.5935 | 0.5355 | −0.0197 | 0.029* |
| C18B | 0.7262 (2) | 0.55126 (19) | 0.05313 (14) | 0.0251 (6) |
| H18B | 0.7684 | 0.4989 | 0.0396 | 0.030* |
| C19B | 0.7695 (2) | 0.6061 (2) | 0.10765 (14) | 0.0254 (6) |
| H19B | 0.8417 | 0.5919 | 0.1315 | 0.030* |
| C20B | 0.7074 (2) | 0.68178 (19) | 0.12734 (13) | 0.0227 (6) |
| H20B | 0.7380 | 0.7200 | 0.1644 | 0.027* |
| C21B | 0.2325 (2) | 0.9329 (2) | 0.13189 (15) | 0.0323 (7) |
| H21D | 0.1931 | 0.9146 | 0.0881 | 0.048* |
| H21E | 0.2537 | 1.0015 | 0.1317 | 0.048* |
| H21F | 0.1833 | 0.9223 | 0.1648 | 0.048* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1A | 0.0304 (11) | 0.0202 (9) | 0.0203 (10) | 0.0033 (8) | 0.0083 (9) | 0.0007 (8) |
| O2A | 0.0230 (11) | 0.0288 (10) | 0.0235 (11) | 0.0054 (8) | −0.0019 (9) | −0.0040 (8) |
| N1A | 0.0313 (15) | 0.0302 (14) | 0.0435 (17) | −0.0047 (12) | −0.0018 (13) | 0.0055 (12) |
| N2A | 0.045 (2) | 0.071 (2) | 0.0371 (18) | 0.0098 (16) | 0.0005 (15) | −0.0018 (17) |
| C1A | 0.0352 (19) | 0.049 (2) | 0.0198 (16) | −0.0130 (16) | −0.0011 (14) | 0.0015 (14) |
| C2A | 0.041 (2) | 0.0316 (17) | 0.050 (2) | 0.0033 (15) | 0.0119 (17) | −0.0015 (16) |
| C3A | 0.044 (2) | 0.0312 (17) | 0.045 (2) | −0.0025 (15) | 0.0121 (17) | −0.0029 (16) |
| C4A | 0.0277 (18) | 0.0409 (18) | 0.0292 (17) | −0.0002 (14) | 0.0004 (14) | −0.0017 (14) |
| C5A | 0.0225 (16) | 0.0376 (17) | 0.0249 (16) | −0.0042 (13) | 0.0044 (13) | 0.0023 (13) |
| C6A | 0.0217 (17) | 0.0251 (15) | 0.055 (2) | −0.0074 (13) | 0.0005 (15) | 0.0126 (15) |
| C7A | 0.0273 (17) | 0.0327 (16) | 0.0312 (17) | −0.0103 (13) | −0.0021 (14) | 0.0136 (14) |
| C8A | 0.0199 (15) | 0.0256 (14) | 0.0234 (15) | −0.0034 (12) | 0.0056 (12) | 0.0027 (12) |
| C9A | 0.0276 (17) | 0.0319 (16) | 0.0197 (15) | −0.0084 (13) | 0.0018 (13) | −0.0022 (13) |
| C10A | 0.0361 (18) | 0.0251 (15) | 0.0253 (16) | −0.0009 (13) | 0.0093 (14) | −0.0064 (13) |
| C11A | 0.0270 (17) | 0.0244 (14) | 0.0267 (16) | 0.0039 (12) | 0.0061 (13) | 0.0001 (12) |
| C12A | 0.0235 (16) | 0.0238 (14) | 0.0197 (14) | −0.0034 (12) | 0.0029 (12) | −0.0002 (12) |
| C13A | 0.0216 (15) | 0.0181 (13) | 0.0188 (14) | −0.0012 (11) | 0.0058 (12) | 0.0011 (11) |
| C14A | 0.0303 (17) | 0.0243 (14) | 0.0202 (15) | 0.0018 (12) | 0.0069 (12) | 0.0025 (12) |
| C15A | 0.0224 (16) | 0.0228 (13) | 0.0168 (14) | 0.0004 (11) | 0.0080 (12) | 0.0044 (11) |
| C16A | 0.0199 (15) | 0.0252 (14) | 0.0204 (15) | −0.0014 (12) | 0.0041 (12) | 0.0064 (12) |
| C17A | 0.0361 (18) | 0.0204 (14) | 0.0198 (15) | −0.0012 (13) | 0.0057 (13) | −0.0003 (12) |
| C18A | 0.0299 (18) | 0.0248 (15) | 0.0284 (16) | 0.0083 (13) | 0.0127 (14) | 0.0050 (13) |
| C19A | 0.0198 (16) | 0.0418 (17) | 0.0297 (17) | 0.0042 (13) | 0.0061 (13) | 0.0057 (14) |
| C20A | 0.0218 (16) | 0.0308 (15) | 0.0224 (15) | −0.0021 (12) | 0.0031 (12) | −0.0040 (12) |
| C21A | 0.0276 (17) | 0.0351 (16) | 0.0301 (17) | 0.0101 (13) | −0.0070 (14) | −0.0010 (14) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O1B | 0.0265 (11) | 0.0201 (9) | 0.0221 (10) | 0.0013 (8) | 0.0070 (9) | −0.0013 (8) |
| O2B | 0.0255 (11) | 0.0281 (10) | 0.0292 (11) | 0.0050 (9) | −0.0010 (9) | −0.0041 (9) |
| N1B | 0.0229 (13) | 0.0244 (12) | 0.0266 (14) | −0.0005 (10) | 0.0068 (11) | 0.0008 (10) |
| N2B | 0.0474 (19) | 0.0516 (18) | 0.0213 (14) | 0.0191 (14) | −0.0011 (13) | −0.0062 (13) |
| C1B | 0.0287 (17) | 0.0257 (15) | 0.0348 (17) | −0.0035 (13) | 0.0136 (14) | 0.0047 (13) |
| C2B | 0.0287 (18) | 0.0246 (15) | 0.049 (2) | 0.0013 (13) | 0.0168 (15) | 0.0047 (14) |
| C3B | 0.0254 (17) | 0.0226 (15) | 0.049 (2) | 0.0021 (13) | 0.0063 (15) | 0.0020 (14) |
| C4B | 0.0290 (17) | 0.0251 (15) | 0.0366 (18) | 0.0001 (13) | −0.0045 (14) | −0.0028 (14) |
| C5B | 0.0254 (17) | 0.0235 (14) | 0.0278 (16) | −0.0014 (12) | 0.0030 (13) | −0.0046 (12) |
| C6B | 0.0242 (16) | 0.0185 (13) | 0.0309 (17) | −0.0037 (12) | 0.0013 (13) | −0.0016 (12) |
| C7B | 0.0272 (16) | 0.0232 (14) | 0.0216 (15) | −0.0023 (12) | 0.0093 (13) | −0.0011 (12) |
| C8B | 0.0211 (15) | 0.0233 (14) | 0.0230 (15) | −0.0019 (12) | 0.0092 (12) | 0.0012 (12) |
| C9B | 0.0280 (17) | 0.0293 (15) | 0.0223 (15) | 0.0006 (13) | 0.0055 (13) | −0.0036 (12) |
| C10B | 0.0327 (18) | 0.0238 (14) | 0.0321 (17) | −0.0001 (13) | 0.0114 (14) | −0.0079 (13) |
| C11B | 0.0226 (16) | 0.0236 (14) | 0.0320 (17) | 0.0036 (12) | 0.0088 (13) | −0.0031 (13) |
| C12B | 0.0221 (16) | 0.0216 (14) | 0.0249 (15) | −0.0008 (12) | 0.0056 (12) | −0.0011 (12) |
| C13B | 0.0232 (16) | 0.0164 (13) | 0.0256 (15) | −0.0015 (11) | 0.0076 (12) | −0.0026 (11) |
| C14B | 0.0290 (17) | 0.0240 (14) | 0.0232 (15) | 0.0012 (12) | 0.0074 (13) | 0.0015 (12) |
| C15B | 0.0194 (15) | 0.0197 (13) | 0.0196 (14) | −0.0018 (11) | 0.0050 (12) | 0.0032 (11) |
| C16B | 0.0195 (15) | 0.0255 (14) | 0.0198 (14) | −0.0025 (12) | 0.0033 (12) | 0.0052 (12) |
| C17B | 0.0292 (17) | 0.0229 (14) | 0.0216 (15) | −0.0069 (12) | 0.0071 (13) | −0.0035 (12) |
| C18B | 0.0268 (17) | 0.0223 (14) | 0.0289 (16) | 0.0013 (12) | 0.0131 (13) | 0.0039 (12) |
| C19B | 0.0211 (16) | 0.0320 (15) | 0.0239 (16) | −0.0003 (12) | 0.0060 (12) | 0.0049 (13) |
| C20B | 0.0240 (16) | 0.0271 (15) | 0.0173 (14) | −0.0034 (12) | 0.0042 (12) | −0.0024 (12) |
| C21B | 0.0266 (17) | 0.0299 (15) | 0.0381 (18) | 0.0077 (13) | −0.0018 (14) | 0.0012 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1A—C13A | 1.377 (3) | O1B—C13B | 1.385 (3) |
| O1A—C14A | 1.459 (3) | O1B—C14B | 1.454 (3) |
| O2A—C12A | 1.358 (3) | O2B—C12B | 1.357 (3) |
| O2A—C21A | 1.432 (3) | O2B—C21B | 1.437 (3) |
| N1A—C7A | 1.266 (4) | N1B—C7B | 1.275 (3) |
| N1A—C6A | 1.417 (4) | N1B—C6B | 1.413 (3) |
| N2A—C5A | 1.363 (4) | N2B—C5B | 1.383 (4) |
| N2A—H2AB | 0.917 (10) | N2B—H2BB | 0.905 (10) |
| N2A—H2AC | 0.921 (10) | N2B—H2BC | 0.905 (10) |
| C1A—C2A | 1.361 (4) | C1B—C2B | 1.381 (4) |
| C1A—C6A | 1.431 (4) | C1B—C6B | 1.403 (4) |
| C1A—H1A | 0.95 | C1B—H1B | 0.95 |
| C2A—C3A | 1.350 (4) | C2B—C3B | 1.374 (4) |
| C2A—H2A | 0.95 | C2B—H2B | 0.95 |
| C3A—C4A | 1.378 (4) | C3B—C4B | 1.384 (4) |
| C3A—H3A | 0.95 | C3B—H3B | 0.95 |
| C4A—C5A | 1.383 (4) | C4B—C5B | 1.399 (4) |
| C4A—H4A | 0.95 | C4B—H4B | 0.95 |
| C5A—C6A | 1.432 (4) | C5B—C6B | 1.408 (4) |
| C7A—C8A | 1.486 (4) | C7B—C8B | 1.467 (4) |

| | | | |
|---|---|---|---|
| C7A—H7A | 0.95 | C7B—H7B | 0.95 |
| C8A—C13A | 1.393 (4) | C8B—C13B | 1.388 (4) |
| C8A—C9A | 1.401 (4) | C8B—C9B | 1.408 (4) |
| C9A—C10A | 1.373 (4) | C9B—C10B | 1.374 (4) |
| C9A—H9A | 0.95 | C9B—H9B | 0.95 |
| C10A—C11A | 1.387 (4) | C10B—C11B | 1.387 (4) |
| C10A—H10A | 0.95 | C10B—H10B | 0.95 |
| C11A—C12A | 1.394 (4) | C11B—C12B | 1.391 (4) |
| C11A—H11A | 0.95 | C11B—H11B | 0.95 |
| C12A—C13A | 1.407 (4) | C12B—C13B | 1.407 (4) |
| C14A—C15A | 1.491 (4) | C14B—C15B | 1.503 (4) |
| C14A—H14A | 0.99 | C14B—H14C | 0.99 |
| C14A—H14B | 0.99 | C14B—H14D | 0.99 |
| C15A—C16A | 1.387 (4) | C15B—C20B | 1.383 (4) |
| C15A—C20A | 1.387 (4) | C15B—C16B | 1.391 (4) |
| C16A—C17A | 1.396 (4) | C16B—C17B | 1.393 (4) |
| C16A—H16A | 0.95 | C16B—H16B | 0.95 |
| C17A—C18A | 1.373 (4) | C17B—C18B | 1.374 (4) |
| C17A—H17A | 0.95 | C17B—H17B | 0.95 |
| C18A—C19A | 1.382 (4) | C18B—C19B | 1.383 (4) |
| C18A—H18A | 0.95 | C18B—H18B | 0.95 |
| C19A—C20A | 1.387 (4) | C19B—C20B | 1.381 (4) |
| C19A—H19A | 0.95 | C19B—H19B | 0.95 |
| C20A—H20A | 0.95 | C20B—H20B | 0.95 |
| C21A—H21A | 0.98 | C21B—H21D | 0.98 |
| C21A—H21B | 0.98 | C21B—H21E | 0.98 |
| C21A—H21C | 0.98 | C21B—H21F | 0.98 |

| | | | |
|---|---|---|---|
| C13A—O1A—C14A | 116.02 (19) | C13B—O1B—C14B | 116.28 (19) |
| C12A—O2A—C21A | 117.1 (2) | C12B—O2B—C21B | 116.9 (2) |
| C7A—N1A—C6A | 116.1 (3) | C7B—N1B—C6B | 119.9 (2) |
| C5A—N2A—H2AB | 107 (2) | C5B—N2B—H2BB | 109 (2) |
| C5A—N2A—H2AC | 112 (2) | C5B—N2B—H2BC | 112 (2) |
| H2AB—N2A—H2AC | 122 (3) | H2BB—N2B—H2BC | 122 (3) |
| C2A—C1A—C6A | 121.8 (3) | C2B—C1B—C6B | 120.7 (3) |
| C2A—C1A—H1A | 119.1 | C2B—C1B—H1B | 119.6 |
| C6A—C1A—H1A | 119.1 | C6B—C1B—H1B | 119.6 |
| C3A—C2A—C1A | 120.0 (3) | C3B—C2B—C1B | 120.0 (3) |
| C3A—C2A—H2A | 120.0 | C3B—C2B—H2B | 120.0 |
| C1A—C2A—H2A | 120.0 | C1B—C2B—H2B | 120.0 |
| C2A—C3A—C4A | 120.5 (3) | C2B—C3B—C4B | 120.7 (3) |
| C2A—C3A—H3A | 119.7 | C2B—C3B—H3B | 119.6 |
| C4A—C3A—H3A | 119.7 | C4B—C3B—H3B | 119.6 |
| C3A—C4A—C5A | 122.6 (3) | C3B—C4B—C5B | 120.4 (3) |
| C3A—C4A—H4A | 118.7 | C3B—C4B—H4B | 119.8 |
| C5A—C4A—H4A | 118.7 | C5B—C4B—H4B | 119.8 |
| N2A—C5A—C4A | 122.8 (3) | N2B—C5B—C4B | 121.2 (3) |
| N2A—C5A—C6A | 119.4 (3) | N2B—C5B—C6B | 119.6 (3) |

| | | | |
|---|---|---|---|
| C4A—C5A—C6A | 117.6 (3) | C4B—C5B—C6B | 119.1 (3) |
| N1A—C6A—C1A | 126.1 (3) | C1B—C6B—C5B | 119.1 (3) |
| N1A—C6A—C5A | 116.4 (3) | C1B—C6B—N1B | 124.2 (3) |
| C1A—C6A—C5A | 117.4 (3) | C5B—C6B—N1B | 116.6 (2) |
| N1A—C7A—C8A | 122.3 (3) | N1B—C7B—C8B | 122.5 (2) |
| N1A—C7A—H7A | 118.9 | N1B—C7B—H7B | 118.8 |
| C8A—C7A—H7A | 118.9 | C8B—C7B—H7B | 118.8 |
| C13A—C8A—C9A | 119.1 (3) | C13B—C8B—C9B | 119.1 (3) |
| C13A—C8A—C7A | 118.7 (2) | C13B—C8B—C7B | 120.7 (2) |
| C9A—C8A—C7A | 122.3 (3) | C9B—C8B—C7B | 120.2 (2) |
| C10A—C9A—C8A | 120.4 (3) | C10B—C9B—C8B | 119.9 (3) |
| C10A—C9A—H9A | 119.8 | C10B—C9B—H9B | 120.1 |
| C8A—C9A—H9A | 119.8 | C8B—C9B—H9B | 120.1 |
| C9A—C10A—C11A | 120.9 (3) | C9B—C10B—C11B | 121.0 (3) |
| C9A—C10A—H10A | 119.5 | C9B—C10B—H10B | 119.5 |
| C11A—C10A—H10A | 119.5 | C11B—C10B—H10B | 119.5 |
| C10A—C11A—C12A | 119.9 (3) | C10B—C11B—C12B | 120.2 (3) |
| C10A—C11A—H11A | 120.0 | C10B—C11B—H11B | 119.9 |
| C12A—C11A—H11A | 120.0 | C12B—C11B—H11B | 119.9 |
| O2A—C12A—C11A | 124.9 (2) | O2B—C12B—C11B | 125.0 (2) |
| O2A—C12A—C13A | 115.9 (2) | O2B—C12B—C13B | 116.1 (2) |
| C11A—C12A—C13A | 119.2 (2) | C11B—C12B—C13B | 118.9 (3) |
| O1A—C13A—C8A | 118.5 (2) | O1B—C13B—C8B | 118.1 (2) |
| O1A—C13A—C12A | 120.9 (2) | O1B—C13B—C12B | 120.9 (2) |
| C8A—C13A—C12A | 120.5 (2) | C8B—C13B—C12B | 120.8 (2) |
| O1A—C14A—C15A | 107.6 (2) | O1B—C14B—C15B | 107.4 (2) |
| O1A—C14A—H14A | 110.2 | O1B—C14B—H14C | 110.2 |
| C15A—C14A—H14A | 110.2 | C15B—C14B—H14C | 110.2 |
| O1A—C14A—H14B | 110.2 | O1B—C14B—H14D | 110.2 |
| C15A—C14A—H14B | 110.2 | C15B—C14B—H14D | 110.2 |
| H14A—C14A—H14B | 108.5 | H14C—C14B—H14D | 108.5 |
| C16A—C15A—C20A | 118.7 (3) | C20B—C15B—C16B | 118.9 (2) |
| C16A—C15A—C14A | 121.1 (2) | C20B—C15B—C14B | 120.1 (2) |
| C20A—C15A—C14A | 120.1 (2) | C16B—C15B—C14B | 121.0 (2) |
| C15A—C16A—C17A | 120.4 (3) | C15B—C16B—C17B | 120.1 (3) |
| C15A—C16A—H16A | 119.8 | C15B—C16B—H16B | 119.9 |
| C17A—C16A—H16A | 119.8 | C17B—C16B—H16B | 119.9 |
| C18A—C17A—C16A | 119.9 (3) | C18B—C17B—C16B | 120.1 (3) |
| C18A—C17A—H17A | 120.1 | C18B—C17B—H17B | 120.0 |
| C16A—C17A—H17A | 120.1 | C16B—C17B—H17B | 120.0 |
| C17A—C18A—C19A | 120.4 (3) | C17B—C18B—C19B | 120.2 (3) |
| C17A—C18A—H18A | 119.8 | C17B—C18B—H18B | 119.9 |
| C19A—C18A—H18A | 119.8 | C19B—C18B—H18B | 119.9 |
| C18A—C19A—C20A | 119.5 (3) | C20B—C19B—C18B | 119.7 (3) |
| C18A—C19A—H19A | 120.2 | C20B—C19B—H19B | 120.2 |
| C20A—C19A—H19A | 120.2 | C18B—C19B—H19B | 120.2 |
| C19A—C20A—C15A | 121.0 (3) | C19B—C20B—C15B | 121.1 (3) |
| C19A—C20A—H20A | 119.5 | C19B—C20B—H20B | 119.5 |

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|---|---|---|---|
| C15A—C20A—H20A | 119.5 | C15B—C20B—H20B | 119.5 |
| O2A—C21A—H21A | 109.5 | O2B—C21B—H21D | 109.5 |
| O2A—C21A—H21B | 109.5 | O2B—C21B—H21E | 109.5 |
| H21A—C21A—H21B | 109.5 | H21D—C21B—H21E | 109.5 |
| O2A—C21A—H21C | 109.5 | O2B—C21B—H21F | 109.5 |
| H21A—C21A—H21C | 109.5 | H21D—C21B—H21F | 109.5 |
| H21B—C21A—H21C | 109.5 | H21E—C21B—H21F | 109.5 |
| | | | |
| C6A—C1A—C2A—C3A | −1.4 (5) | C6B—C1B—C2B—C3B | −0.3 (4) |
| C1A—C2A—C3A—C4A | 3.1 (5) | C1B—C2B—C3B—C4B | −0.7 (4) |
| C2A—C3A—C4A—C5A | −1.9 (5) | C2B—C3B—C4B—C5B | 0.4 (4) |
| C3A—C4A—C5A—N2A | −175.4 (3) | C3B—C4B—C5B—N2B | 177.2 (3) |
| C3A—C4A—C5A—C6A | −1.0 (4) | C3B—C4B—C5B—C6B | 0.8 (4) |
| C7A—N1A—C6A—C1A | −30.8 (4) | C2B—C1B—C6B—C5B | 1.5 (4) |
| C7A—N1A—C6A—C5A | 154.2 (3) | C2B—C1B—C6B—N1B | 178.1 (3) |
| C2A—C1A—C6A—N1A | −176.5 (3) | N2B—C5B—C6B—C1B | −178.2 (3) |
| C2A—C1A—C6A—C5A | −1.6 (4) | C4B—C5B—C6B—C1B | −1.7 (4) |
| N2A—C5A—C6A—N1A | −7.4 (4) | N2B—C5B—C6B—N1B | 4.9 (4) |
| C4A—C5A—C6A—N1A | 178.1 (3) | C4B—C5B—C6B—N1B | −178.6 (2) |
| N2A—C5A—C6A—C1A | 177.2 (3) | C7B—N1B—C6B—C1B | 33.0 (4) |
| C4A—C5A—C6A—C1A | 2.7 (4) | C7B—N1B—C6B—C5B | −150.3 (3) |
| C6A—N1A—C7A—C8A | 179.2 (2) | C6B—N1B—C7B—C8B | −178.7 (2) |
| N1A—C7A—C8A—C13A | 178.0 (3) | N1B—C7B—C8B—C13B | −179.1 (3) |
| N1A—C7A—C8A—C9A | −1.7 (4) | N1B—C7B—C8B—C9B | −0.5 (4) |
| C13A—C8A—C9A—C10A | 0.8 (4) | C13B—C8B—C9B—C10B | −0.7 (4) |
| C7A—C8A—C9A—C10A | −179.4 (3) | C7B—C8B—C9B—C10B | −179.3 (3) |
| C8A—C9A—C10A—C11A | −1.3 (4) | C8B—C9B—C10B—C11B | 0.8 (4) |
| C9A—C10A—C11A—C12A | 1.0 (4) | C9B—C10B—C11B—C12B | −0.4 (4) |
| C21A—O2A—C12A—C11A | −3.6 (4) | C21B—O2B—C12B—C11B | −2.5 (4) |
| C21A—O2A—C12A—C13A | 177.3 (2) | C21B—O2B—C12B—C13B | 176.8 (2) |
| C10A—C11A—C12A—O2A | −179.3 (3) | C10B—C11B—C12B—O2B | 179.1 (3) |
| C10A—C11A—C12A—C13A | −0.1 (4) | C10B—C11B—C12B—C13B | −0.1 (4) |
| C14A—O1A—C13A—C8A | 119.4 (3) | C14B—O1B—C13B—C8B | −120.0 (3) |
| C14A—O1A—C13A—C12A | −63.8 (3) | C14B—O1B—C13B—C12B | 64.1 (3) |
| C9A—C8A—C13A—O1A | 176.9 (2) | C9B—C8B—C13B—O1B | −175.8 (2) |
| C7A—C8A—C13A—O1A | −2.9 (4) | C7B—C8B—C13B—O1B | 2.8 (4) |
| C9A—C8A—C13A—C12A | 0.0 (4) | C9B—C8B—C13B—C12B | 0.1 (4) |
| C7A—C8A—C13A—C12A | −179.7 (2) | C7B—C8B—C13B—C12B | 178.7 (2) |
| O2A—C12A—C13A—O1A | 2.1 (4) | O2B—C12B—C13B—O1B | −3.2 (4) |
| C11A—C12A—C13A—O1A | −177.1 (2) | C11B—C12B—C13B—O1B | 176.1 (2) |
| O2A—C12A—C13A—C8A | 178.8 (2) | O2B—C12B—C13B—C8B | −179.0 (2) |
| C11A—C12A—C13A—C8A | −0.4 (4) | C11B—C12B—C13B—C8B | 0.3 (4) |
| C13A—O1A—C14A—C15A | −156.0 (2) | C13B—O1B—C14B—C15B | 155.0 (2) |
| O1A—C14A—C15A—C16A | −102.4 (3) | O1B—C14B—C15B—C20B | −65.1 (3) |
| O1A—C14A—C15A—C20A | 76.5 (3) | O1B—C14B—C15B—C16B | 113.6 (3) |
| C20A—C15A—C16A—C17A | 0.0 (4) | C20B—C15B—C16B—C17B | −0.1 (4) |
| C14A—C15A—C16A—C17A | 178.8 (2) | C14B—C15B—C16B—C17B | −178.8 (2) |
| C15A—C16A—C17A—C18A | −1.5 (4) | C15B—C16B—C17B—C18B | 1.5 (4) |

| | | | |
|---|---|---|---|
| C16A—C17A—C18A—C19A | 1.4 (4) | C16B—C17B—C18B—C19B | −1.7 (4) |
| C17A—C18A—C19A—C20A | 0.1 (4) | C17B—C18B—C19B—C20B | 0.4 (4) |
| C18A—C19A—C20A—C15A | −1.7 (4) | C18B—C19B—C20B—C15B | 1.0 (4) |
| C16A—C15A—C20A—C19A | 1.6 (4) | C16B—C15B—C20B—C19B | −1.2 (4) |
| C14A—C15A—C20A—C19A | −177.3 (2) | C14B—C15B—C20B—C19B | 177.5 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2*A*—H2*AC*···N1*A* | 0.92 (3) | 2.31 (3) | 2.735 (4) | 108 (2) |
| N2*A*—H2*AC*···N2*B*$^{i}$ | 0.92 (3) | 2.49 (3) | 3.229 (4) | 138 (3) |
| N2*B*—H2*BC*···N1*B* | 0.90 (2) | 2.29 (3) | 2.726 (3) | 109 (2) |
| C7*A*—H7*A*···O1*A* | 0.95 | 2.43 | 2.765 (3) | 101 |
| C7*B*—H7*B*···O1*B* | 0.95 | 2.46 | 2.790 (3) | 100 |
| C14*A*—H14*A*···O2*A* | 0.99 | 2.43 | 2.895 (3) | 108 |
| C14*B*—H14*D*···O2*B* | 0.99 | 2.45 | 2.903 (3) | 107 |
| C21*A*—H21*C*···*Cg*1$^{ii}$ | 0.98 | 2.96 | 3.511 (3) | 117 |
| C21*B*—H21*F*···*Cg*2$^{iii}$ | 0.98 | 2.81 | 3.739 (3) | 159 |
| C10*A*—H10*A*···*Cg*3$^{ii}$ | 0.95 | 2.60 | 3.500 (3) | 159 |
| C21*B*—H21*E*···*Cg*4$^{iv}$ | 0.98 | 2.80 | 3.433 (3) | 123 |
| C21*A*—H21*B*···*Cg*5$^{v}$ | 0.98 | 2.96 | 3.844 (4) | 150 |
| C10*B*—H10*B*···*Cg*6$^{iv}$ | 0.95 | 2.66 | 3.587 (3) | 165 |
| N2*B*—H2*BC*···*Cg*6$^{vi}$ | 0.90 (2) | 2.83 (3) | 3.288 (3) | 113 (2) |

Symmetry codes: (i) *x*, −*y*+3/2, *z*−1/2; (ii) −*x*+2, *y*−1/2, −*z*+1/2; (iii) *x*−1, *y*, *z*; (iv) −*x*+1, *y*+1/2, −*z*+1/2; (v) *x*+1, *y*, *z*; (vi) *x*, −*y*+1/2, *z*−1/2.