# 6-(4-Bromophenyl)-2-ethoxy-4-(2,4,5-trimethoxyphenyl)nicotinonitrile[1]

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There are two molecules in the asymmetric unit of the title compound, $C_{23}H_{21}BrN_2O_4$, which differ in the conformation of their ethoxy residues, *i.e.* almost co-planar with the pyridine ring in one molecule [C—O—C—C = −174.0 (2)°] but almost perpendicular in the other [C—O—C—C = 92.8 (3)°]. The dihedral angles between the central pyridine ring and the 4-bromophenyl and 2,4,5-trimethoxyphenyl rings are 11.05 (12) and 63.78 (12)°, respectively, in one molecule; the corresponding angles in the other molecule are 30.38 (13) and 65.38 (13)°, respectively. In the crystal structure, pairs of molecules are arranged in a face-to-face sandwich structure which further stacks along the *b* axis. The crystal packing features C—H$\cdots\pi$ interactions and Br$\cdots$O [3.5417 (17) Å], Br$\cdots$C [3.748 (3) Å], C$\cdots$N [3.376 (4) Å] and C$\cdots$O [3.351 (3)–3.409 (3) Å] contacts. Finally, $\pi\cdots\pi$ interactions [centroid$\cdots$centroid distances = 3.6346 (19) and 3.6882 (19) Å] are observed.

## Related literature

For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the synthesis and applications of nicotinonitrile derivatives, see: Borgna *et al.* (1993); Goda *et al.* (2004). For related structures, see Chantrapromma *et al.* (2009, 2010). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).
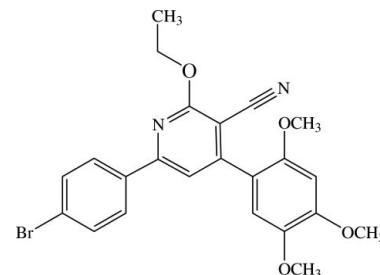


## Experimental

### Crystal data

| | |
|---|---|
| $C_{23}H_{21}BrN_2O_4$ | $\gamma$ = 99.586 (1)° |
| $M_r$ = 469.32 | $V$ = 2076.31 (9) Å$^3$ |
| Triclinic, $P\bar{1}$ | $Z$ = 4 |
| $a$ = 7.9631 (2) Å | Mo $K\alpha$ radiation |
| $b$ = 11.0499 (3) Å | $\mu$ = 2.01 mm$^{-1}$ |
| $c$ = 23.9690 (6) Å | $T$ = 100 K |
| $\alpha$ = 92.201 (1)° | 0.59 × 0.10 × 0.05 mm |
| $\beta$ = 91.968 (1)° | |

### Data collection

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 31800 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2005) | 9488 independent reflections |
| $T_{min}$ = 0.384, $T_{max}$ = 0.899 | 7074 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.043 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.036 | 549 parameters |
| $wR(F^2)$ = 0.098 | H-atom parameters constrained |
| $S$ = 1.07 | $\Delta\rho_{max}$ = 0.79 e Å$^{-3}$ |
| 9488 reflections | $\Delta\rho_{min}$ = −0.38 e Å$^{-3}$ |

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

$Cg1$ and $Cg2$ are the centroids of C7A–C11A/N1A and C12A–C17A rings, respectively.

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C22A—H22C$\cdots Cg2^i$ | 0.96 | 2.74 | 3.585 (3) | 147 |
| C22B—H22E$\cdots Cg1^{ii}$ | 0.96 | 2.68 | 3.511 (3) | 145 |

Symmetry codes: (i) $-x + 1, -y + 1, -z + 1$; (ii) $-x, -y + 1, -z + 1$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; 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, 2009).

# organic compounds

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# supporting information

## 6-(4-Bromophenyl)-2-ethoxy-4-(2,4,5-trimethoxyphenyl)nicotinonitrile

**Suchada Chantrapromma, Hoong-Kun Fun, Mahesh Padaki, Thitipone Suwunwong and Arun M. Isloor**

### S1. Comment

Substituted pyridine derivatives have been claimed to have several biological activities (Borgna *et al.*, 1993; Goda *et al.*, 2004). We have previously reported the syntheses and crystal structures of the nicotinonitrile derivatives (Chantrapromma *et al.*, 2009; 2010). In continuation of our research into the synthesis of antimicrobial agents, the title malononitrile derivative was synthesised and studied for its anti-bacterial activities. However, our results showed that the title compound does not possess anti-bacterial activities. Herein, we report the crystal structure of the title compound (I).

There are two crystallographic independent molecules *A* and *B* in the asymmetric unit of (I) (Fig. 1) with differences in conformation of the ethoxy group distinguishing them. In molecule *A* the ethoxy residue is almost co-planar with the pyridine ring [C11A–O1A–C18A–C19A = -174.0 (2) °] whereas it is almost perpendicular in molecule *B* [C11B–O1B–C18B–C19B = 92.8 (3) °]. The dihedral angles between the central pyridine ring and the 4-bromophenyl and 2,4,5-tri-methoxyphenyl rings are 11.05 (12) and 63.78 (12) ° respectively in molecule *A* whereas the corresponding pair of angles in molecule *B* are 30.38 (13) and 65.38 (13) °. All three methoxy groups are nearly co-planar with the attached benzene ring [torsion angles C20–O2–C13–C14 = -11.6 (4) °, C21–O3–C15–C16 = 180.0 (2) ° and C22–O4–C16–C17 = 8.1 (4) ° in molecule *A*; and the corresponding values are -5.5 (4), -175.5 (2) and -7.7 (4) ° in molecule *B*]. Weak intramolecular C1A—H1AA···N1A (in molecule *A*) and C18B–H18C—N1B (in molecule *B*) interactions generate S(5) ring motifs (Bernstein *et al.*, 1995). The bond distances are comparable with those in closely related structures (Chantrapromma *et al.*, 2009; 2010).

In the crystal structure (Fig. 2), the molecules are arranged into a face-to-face sandwich-like structure which further stack along the *b* axis. The crystal is consolidated by C—H···$\pi$ interactions (Table 1) and Br···O [3.5417 (17) Å], Br···C [3.748 (3) Å], C···N [3.376 (4) Å] and C···O [3.351 (3) - 3.409 (3) Å] contacts. Finally, $\pi$···$\pi$ interactions with the distances of Cg$_1$···Cg$_4$ = 3.6346 (15) Å (symmetry code: 1-x, 1-y, 1-z) and Cg$_2$···Cg$_3$ = 3.6882 (15) Å (symmetry code: -x, 1-y, 1-z) are observed; Cg$_1$, Cg$_2$, Cg$_3$ and Cg$_4$ are the centroids of C7A–C11A/N1A, C12A–C17A, C7B–C11B/N1B, and C12B–C17B rings, respectively.

### S2. Experimental

(*E*)-1-(4-Bromophenyl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one (0.57 g, 0.0015 mol) was added with continuous stirring to a freshly prepared sodium alkoxide solution (0.0014 mol of sodium in 100 ml of ethanol). Malononitrile (1.3 g, 0.02 mol) was then added with continuous stirring at room temperature until the precipitate separated out. The resulting solid was filtered (yield 68 %). Colorless needle-shaped single crystals of the title compound were obtained by recrystallization from ethanol by the slow evaporation of the solvent at room temperature after several days, Mp. 460-461 K.

## S3. Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with d(C—H) = 0.93 Å for aromatic-H, 0.97 for $CH_2$ and 0.96 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.
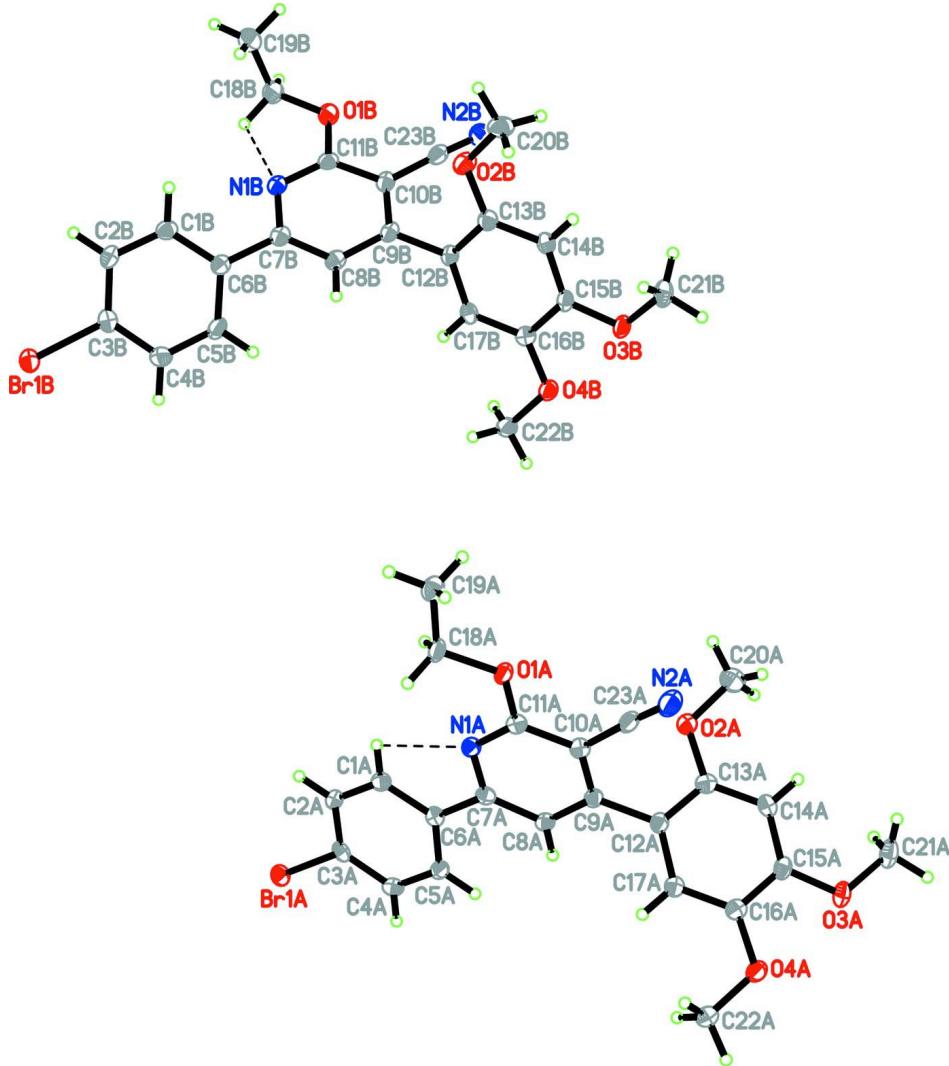
**Figure 1**

The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme. Intramolecular C—H⋯N interactions are shown as dashed lines.
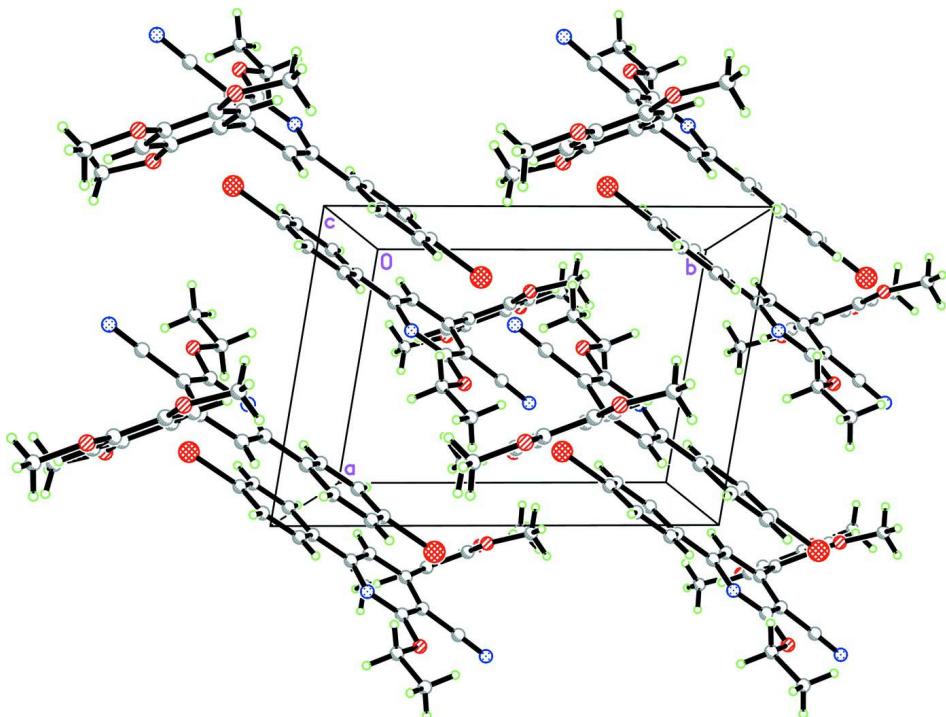
**Figure 2**
The crystal packing of the title compound viewed along the *c* axis.

### 6-(4-Bromophenyl)-2-ethoxy-4-(2,4,5-trimethoxyphenyl)nicotinonitrile

*Crystal data*

| | |
|---|---|
| $C_{23}H_{21}BrN_2O_4$ | $Z = 4$ |
| $M_r = 469.32$ | $F(000) = 960$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.501$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Melting point = 460–461 K |
| $a = 7.9631$ (2) Å | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $b = 11.0499$ (3) Å | Cell parameters from 9488 reflections |
| $c = 23.9690$ (6) Å | $\theta = 0.9$–27.5° |
| $\alpha = 92.201$ (1)° | $\mu = 2.01$ mm$^{-1}$ |
| $\beta = 91.968$ (1)° | $T = 100$ K |
| $\gamma = 99.586$ (1)° | Needle, colorless |
| $V = 2076.31$ (9) Å$^3$ | $0.59 \times 0.10 \times 0.05$ mm |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 31800 measured reflections |
| Radiation source: sealed tube | 9488 independent reflections |
| Graphite monochromator | 7074 reflections with $I > 2\sigma(I)$ |
| $\varphi$ and $\omega$ scans | $R_{int} = 0.043$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2005) | $\theta_{max} = 27.5°$, $\theta_{min} = 0.9°$ |
| $T_{min} = 0.384$, $T_{max} = 0.899$ | $h = -10{\rightarrow}10$ |
| | $k = -14{\rightarrow}14$ |
| | $l = -31{\rightarrow}31$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.036$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.098$ | |
| $S = 1.07$ | H-atom parameters constrained |
| 9488 reflections | $w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 0.7288P]$ |
| 549 parameters | where $P = (F_o^2 + 2F_c^2)/3$ |
| 0 restraints | $(\Delta/\sigma)_{max} = 0.001$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{max} = 0.79$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.38$ e Å$^{-3}$ |

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| Br1A | −0.17700 (4) | −0.35388 (2) | 0.439858 (11) | 0.02094 (8) |
| O1A | 0.5666 (2) | 0.35133 (16) | 0.42626 (7) | 0.0190 (4) |
| O2A | 0.2036 (3) | 0.48545 (17) | 0.28313 (7) | 0.0229 (4) |
| O3A | 0.2540 (3) | 0.46349 (17) | 0.08142 (7) | 0.0227 (4) |
| O4A | 0.3749 (3) | 0.26013 (17) | 0.08836 (7) | 0.0211 (4) |
| N1A | 0.3634 (3) | 0.18217 (19) | 0.40057 (8) | 0.0161 (5) |
| N2A | 0.6447 (4) | 0.5362 (2) | 0.30967 (10) | 0.0304 (6) |
| C1A | 0.1472 (3) | −0.0213 (2) | 0.43550 (10) | 0.0171 (6) |
| H1AA | 0.2118 | 0.0341 | 0.4613 | 0.021* |
| C2A | 0.0518 (4) | −0.1272 (2) | 0.45413 (11) | 0.0183 (6) |
| H2AA | 0.0519 | −0.1434 | 0.4919 | 0.022* |
| C3A | −0.0433 (3) | −0.2081 (2) | 0.41548 (11) | 0.0160 (5) |
| C4A | −0.0472 (3) | −0.1856 (2) | 0.35901 (11) | 0.0177 (6) |
| H4AA | −0.1134 | −0.2411 | 0.3337 | 0.021* |
| C5A | 0.0488 (4) | −0.0796 (2) | 0.34091 (10) | 0.0179 (6) |
| H5AA | 0.0470 | −0.0639 | 0.3031 | 0.022* |
| C6A | 0.1488 (3) | 0.0047 (2) | 0.37885 (10) | 0.0145 (5) |
| C7A | 0.2528 (3) | 0.1189 (2) | 0.36092 (10) | 0.0153 (5) |
| C8A | 0.2379 (3) | 0.1613 (2) | 0.30754 (10) | 0.0157 (5) |
| H8AA | 0.1637 | 0.1154 | 0.2809 | 0.019* |
| C9A | 0.3339 (4) | 0.2727 (2) | 0.29383 (10) | 0.0163 (5) |
| C10A | 0.4480 (3) | 0.3366 (2) | 0.33414 (10) | 0.0160 (5) |
| C11A | 0.4564 (3) | 0.2863 (2) | 0.38748 (10) | 0.0158 (5) |

| | | | |
|---|---|---|---|
| C12A | 0.3084 (3) | 0.3240 (2) | 0.23801 (10) | 0.0166 (6) |
| C13A | 0.2479 (3) | 0.4339 (2) | 0.23373 (11) | 0.0183 (6) |
| C14A | 0.2272 (3) | 0.4832 (2) | 0.18187 (11) | 0.0186 (6) |
| H14A | 0.1854 | 0.5566 | 0.1793 | 0.022* |
| C15A | 0.2695 (3) | 0.4223 (2) | 0.13403 (10) | 0.0180 (6) |
| C16A | 0.3318 (3) | 0.3113 (2) | 0.13770 (10) | 0.0180 (6) |
| C17A | 0.3479 (3) | 0.2623 (2) | 0.18950 (10) | 0.0166 (5) |
| H17A | 0.3856 | 0.1873 | 0.1920 | 0.020* |
| C18A | 0.5755 (4) | 0.2961 (2) | 0.48023 (10) | 0.0206 (6) |
| H18A | 0.6219 | 0.2205 | 0.4764 | 0.025* |
| H18B | 0.4625 | 0.2770 | 0.4949 | 0.025* |
| C19A | 0.6888 (4) | 0.3869 (3) | 0.51911 (11) | 0.0244 (6) |
| H19A | 0.6960 | 0.3531 | 0.5552 | 0.037* |
| H19B | 0.6423 | 0.4615 | 0.5224 | 0.037* |
| H19C | 0.8007 | 0.4042 | 0.5045 | 0.037* |
| C20A | 0.1635 (5) | 0.6051 (3) | 0.28312 (13) | 0.0425 (9) |
| H20A | 0.1407 | 0.6307 | 0.3204 | 0.064* |
| H20B | 0.0645 | 0.6053 | 0.2591 | 0.064* |
| H20C | 0.2579 | 0.6607 | 0.2698 | 0.064* |
| C21A | 0.1906 (4) | 0.5766 (3) | 0.07668 (12) | 0.0281 (7) |
| H21A | 0.1801 | 0.5945 | 0.0380 | 0.042* |
| H21B | 0.2683 | 0.6418 | 0.0960 | 0.042* |
| H21C | 0.0810 | 0.5695 | 0.0929 | 0.042* |
| C22A | 0.4189 (4) | 0.1406 (2) | 0.09113 (11) | 0.0243 (6) |
| H22A | 0.4428 | 0.1117 | 0.0544 | 0.036* |
| H22B | 0.3256 | 0.0854 | 0.1053 | 0.036* |
| H22C | 0.5179 | 0.1440 | 0.1155 | 0.036* |
| C23A | 0.5564 (4) | 0.4488 (3) | 0.32183 (10) | 0.0215 (6) |
| Br1B | 0.38606 (4) | 0.11796 (3) | 0.926074 (11) | 0.02560 (9) |
| O1B | 0.0191 (3) | 0.84937 (17) | 0.92736 (7) | 0.0231 (4) |
| O2B | 0.4260 (3) | 0.98663 (17) | 0.78188 (7) | 0.0240 (4) |
| O3B | 0.2913 (3) | 0.96201 (16) | 0.58180 (7) | 0.0210 (4) |
| O4B | 0.0815 (3) | 0.75855 (16) | 0.59168 (7) | 0.0209 (4) |
| N1B | 0.1491 (3) | 0.68209 (19) | 0.90306 (8) | 0.0164 (5) |
| N2B | −0.0051 (3) | 1.0323 (2) | 0.81419 (10) | 0.0279 (6) |
| C1B | 0.3117 (4) | 0.4800 (2) | 0.93221 (11) | 0.0199 (6) |
| H1BA | 0.3184 | 0.5436 | 0.9592 | 0.024* |
| C2B | 0.3487 (4) | 0.3679 (2) | 0.94771 (11) | 0.0202 (6) |
| H2BA | 0.3800 | 0.3556 | 0.9845 | 0.024* |
| C3B | 0.3378 (4) | 0.2743 (2) | 0.90675 (11) | 0.0199 (6) |
| C4B | 0.2924 (4) | 0.2911 (3) | 0.85171 (11) | 0.0230 (6) |
| H4BA | 0.2850 | 0.2270 | 0.8250 | 0.028* |
| C5B | 0.2584 (4) | 0.4043 (2) | 0.83709 (11) | 0.0226 (6) |
| H5BA | 0.2310 | 0.4170 | 0.8000 | 0.027* |
| C6B | 0.2645 (3) | 0.5004 (2) | 0.87740 (10) | 0.0173 (6) |
| C7B | 0.2157 (3) | 0.6191 (2) | 0.86213 (11) | 0.0178 (6) |
| C8B | 0.2394 (4) | 0.6627 (2) | 0.80881 (10) | 0.0187 (6) |
| H8BA | 0.2854 | 0.6167 | 0.7818 | 0.022* |

| | | | |
|---|---|---|---|
| C9B | 0.1946 (3) | 0.7745 (2) | 0.79583 (10) | 0.0165 (5) |
| C10B | 0.1183 (3) | 0.8366 (2) | 0.83705 (10) | 0.0179 (6) |
| C11B | 0.0976 (4) | 0.7856 (2) | 0.88999 (10) | 0.0179 (6) |
| C12B | 0.2257 (3) | 0.8253 (2) | 0.74001 (10) | 0.0164 (5) |
| C13B | 0.3413 (4) | 0.9333 (2) | 0.73404 (11) | 0.0185 (6) |
| C14B | 0.3669 (4) | 0.9808 (2) | 0.68134 (10) | 0.0178 (6) |
| H14B | 0.4443 | 1.0526 | 0.6774 | 0.021* |
| C15B | 0.2768 (4) | 0.9209 (2) | 0.63469 (10) | 0.0170 (6) |
| C16B | 0.1637 (3) | 0.8103 (2) | 0.64004 (10) | 0.0160 (5) |
| C17B | 0.1417 (3) | 0.7636 (2) | 0.69231 (10) | 0.0172 (6) |
| H17B | 0.0693 | 0.6893 | 0.6959 | 0.021* |
| C18B | −0.0121 (4) | 0.8016 (3) | 0.98201 (11) | 0.0262 (7) |
| H18C | −0.0237 | 0.7127 | 0.9796 | 0.031* |
| H18D | −0.1179 | 0.8227 | 0.9951 | 0.031* |
| C19B | 0.1320 (5) | 0.8537 (3) | 1.02274 (13) | 0.0367 (8) |
| H19D | 0.1053 | 0.8262 | 1.0594 | 0.055* |
| H19E | 0.1481 | 0.9418 | 1.0233 | 0.055* |
| H19F | 0.2346 | 0.8265 | 1.0115 | 0.055* |
| C20B | 0.5570 (4) | 1.0900 (3) | 0.77626 (12) | 0.0278 (7) |
| H20D | 0.6111 | 1.1153 | 0.8122 | 0.042* |
| H20E | 0.5081 | 1.1564 | 0.7614 | 0.042* |
| H20F | 0.6400 | 1.0679 | 0.7514 | 0.042* |
| C21B | 0.4143 (4) | 1.0690 (3) | 0.57435 (11) | 0.0233 (6) |
| H21D | 0.4166 | 1.0868 | 0.5355 | 0.035* |
| H21E | 0.5248 | 1.0550 | 0.5871 | 0.035* |
| H21F | 0.3845 | 1.1373 | 0.5955 | 0.035* |
| C22B | −0.0187 (4) | 0.6395 (2) | 0.59614 (11) | 0.0227 (6) |
| H22D | −0.0687 | 0.6101 | 0.5601 | 0.034* |
| H22E | −0.1074 | 0.6447 | 0.6218 | 0.034* |
| H22F | 0.0526 | 0.5839 | 0.6095 | 0.034* |
| C23B | 0.0514 (4) | 0.9469 (3) | 0.82524 (11) | 0.0212 (6) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1A | 0.02292 (16) | 0.01573 (13) | 0.02271 (14) | −0.00184 (12) | 0.00184 (12) | 0.00381 (10) |
| O1A | 0.0229 (11) | 0.0180 (9) | 0.0136 (8) | −0.0040 (8) | −0.0027 (8) | 0.0030 (7) |
| O2A | 0.0305 (12) | 0.0210 (10) | 0.0184 (9) | 0.0076 (9) | 0.0038 (9) | 0.0017 (8) |
| O3A | 0.0238 (11) | 0.0271 (10) | 0.0185 (9) | 0.0066 (9) | 0.0006 (8) | 0.0092 (8) |
| O4A | 0.0245 (11) | 0.0247 (10) | 0.0153 (9) | 0.0070 (9) | 0.0012 (8) | 0.0012 (7) |
| N1A | 0.0153 (12) | 0.0162 (11) | 0.0161 (10) | 0.0003 (10) | 0.0009 (9) | 0.0014 (8) |
| N2A | 0.0366 (16) | 0.0297 (14) | 0.0200 (12) | −0.0087 (13) | −0.0015 (12) | 0.0031 (10) |
| C1A | 0.0157 (14) | 0.0176 (13) | 0.0175 (12) | 0.0016 (11) | −0.0003 (11) | −0.0007 (10) |
| C2A | 0.0217 (15) | 0.0186 (13) | 0.0148 (12) | 0.0041 (12) | 0.0008 (11) | 0.0024 (10) |
| C3A | 0.0123 (13) | 0.0121 (12) | 0.0238 (13) | 0.0014 (11) | 0.0036 (11) | 0.0034 (10) |
| C4A | 0.0135 (14) | 0.0179 (13) | 0.0209 (13) | 0.0015 (11) | −0.0005 (11) | −0.0030 (10) |
| C5A | 0.0205 (15) | 0.0185 (13) | 0.0144 (12) | 0.0022 (12) | 0.0001 (11) | 0.0003 (10) |
| C6A | 0.0080 (13) | 0.0162 (12) | 0.0194 (12) | 0.0023 (11) | 0.0006 (11) | 0.0022 (10) |

| | | | | | |
|---|---|---|---|---|---|
| C7A | 0.0127 (13) | 0.0165 (12) | 0.0175 (12) | 0.0046 (11) | 0.0026 (11) | −0.0007 (10) |
| C8A | 0.0135 (14) | 0.0171 (12) | 0.0159 (12) | 0.0018 (11) | −0.0023 (11) | −0.0012 (10) |
| C9A | 0.0173 (14) | 0.0178 (13) | 0.0148 (12) | 0.0050 (11) | 0.0024 (11) | 0.0010 (10) |
| C10A | 0.0112 (13) | 0.0176 (13) | 0.0187 (12) | 0.0006 (11) | 0.0009 (11) | 0.0012 (10) |
| C11A | 0.0114 (13) | 0.0189 (13) | 0.0170 (12) | 0.0030 (11) | −0.0006 (11) | −0.0006 (10) |
| C12A | 0.0163 (14) | 0.0165 (12) | 0.0156 (12) | −0.0017 (11) | −0.0009 (11) | 0.0023 (10) |
| C13A | 0.0146 (14) | 0.0190 (13) | 0.0200 (13) | 0.0000 (12) | 0.0011 (11) | −0.0011 (10) |
| C14A | 0.0165 (14) | 0.0165 (13) | 0.0232 (13) | 0.0031 (12) | 0.0014 (12) | 0.0040 (10) |
| C15A | 0.0151 (14) | 0.0206 (13) | 0.0169 (12) | −0.0026 (12) | 0.0003 (11) | 0.0054 (10) |
| C16A | 0.0143 (14) | 0.0199 (13) | 0.0184 (13) | −0.0009 (12) | 0.0012 (11) | 0.0001 (10) |
| C17A | 0.0131 (14) | 0.0170 (12) | 0.0183 (12) | −0.0012 (11) | −0.0010 (11) | 0.0011 (10) |
| C18A | 0.0254 (16) | 0.0215 (13) | 0.0142 (12) | 0.0011 (13) | −0.0005 (12) | 0.0065 (10) |
| C19A | 0.0235 (16) | 0.0273 (15) | 0.0206 (14) | −0.0011 (13) | −0.0028 (12) | 0.0032 (11) |
| C20A | 0.071 (3) | 0.0301 (17) | 0.0321 (17) | 0.0255 (19) | 0.0053 (18) | 0.0008 (14) |
| C21A | 0.0297 (18) | 0.0338 (16) | 0.0237 (14) | 0.0107 (15) | 0.0022 (13) | 0.0138 (12) |
| C22A | 0.0315 (18) | 0.0239 (14) | 0.0173 (13) | 0.0054 (14) | −0.0009 (13) | −0.0013 (11) |
| C23A | 0.0262 (16) | 0.0238 (14) | 0.0126 (12) | −0.0010 (13) | −0.0007 (12) | 0.0013 (11) |
| Br1B | 0.03322 (19) | 0.02264 (15) | 0.02261 (14) | 0.00896 (13) | 0.00077 (13) | 0.00399 (11) |
| O1B | 0.0277 (12) | 0.0230 (10) | 0.0192 (9) | 0.0039 (9) | 0.0058 (9) | 0.0030 (8) |
| O2B | 0.0216 (11) | 0.0272 (10) | 0.0189 (9) | −0.0078 (9) | −0.0012 (8) | 0.0018 (8) |
| O3B | 0.0241 (11) | 0.0224 (10) | 0.0155 (9) | −0.0003 (9) | 0.0016 (8) | 0.0065 (7) |
| O4B | 0.0233 (11) | 0.0212 (9) | 0.0160 (9) | −0.0030 (9) | −0.0007 (8) | 0.0027 (7) |
| N1B | 0.0122 (11) | 0.0194 (11) | 0.0160 (10) | −0.0021 (10) | −0.0012 (9) | 0.0011 (9) |
| N2B | 0.0287 (15) | 0.0261 (13) | 0.0282 (13) | 0.0037 (12) | −0.0045 (11) | 0.0023 (10) |
| C1B | 0.0195 (15) | 0.0201 (13) | 0.0186 (13) | −0.0010 (12) | 0.0011 (12) | −0.0008 (10) |
| C2B | 0.0182 (15) | 0.0256 (14) | 0.0164 (12) | 0.0018 (12) | −0.0012 (12) | 0.0048 (11) |
| C3B | 0.0167 (15) | 0.0202 (13) | 0.0234 (14) | 0.0036 (12) | 0.0023 (12) | 0.0050 (11) |
| C4B | 0.0270 (17) | 0.0222 (14) | 0.0199 (13) | 0.0047 (13) | 0.0020 (12) | −0.0021 (11) |
| C5B | 0.0273 (16) | 0.0260 (14) | 0.0144 (12) | 0.0039 (13) | −0.0003 (12) | 0.0038 (11) |
| C6B | 0.0147 (14) | 0.0196 (13) | 0.0163 (12) | −0.0016 (11) | 0.0016 (11) | 0.0018 (10) |
| C7B | 0.0121 (14) | 0.0210 (13) | 0.0187 (13) | −0.0020 (11) | −0.0019 (11) | 0.0018 (10) |
| C8B | 0.0164 (14) | 0.0224 (14) | 0.0166 (12) | 0.0014 (12) | 0.0019 (11) | 0.0003 (10) |
| C9B | 0.0108 (13) | 0.0213 (13) | 0.0149 (12) | −0.0041 (11) | −0.0025 (10) | 0.0033 (10) |
| C10B | 0.0138 (14) | 0.0205 (13) | 0.0179 (12) | −0.0015 (12) | −0.0023 (11) | 0.0032 (10) |
| C11B | 0.0170 (14) | 0.0181 (13) | 0.0160 (12) | −0.0037 (12) | −0.0008 (11) | −0.0013 (10) |
| C12B | 0.0141 (14) | 0.0181 (13) | 0.0172 (12) | 0.0027 (11) | 0.0007 (11) | 0.0038 (10) |
| C13B | 0.0163 (14) | 0.0203 (13) | 0.0186 (13) | 0.0025 (12) | −0.0009 (11) | 0.0015 (10) |
| C14B | 0.0159 (14) | 0.0165 (13) | 0.0210 (13) | 0.0019 (11) | 0.0024 (11) | 0.0040 (10) |
| C15B | 0.0186 (15) | 0.0186 (13) | 0.0156 (12) | 0.0063 (12) | 0.0038 (11) | 0.0051 (10) |
| C16B | 0.0099 (13) | 0.0196 (13) | 0.0191 (13) | 0.0041 (11) | 0.0012 (11) | −0.0001 (10) |
| C17B | 0.0148 (14) | 0.0164 (12) | 0.0205 (13) | 0.0012 (11) | 0.0035 (11) | 0.0049 (10) |
| C18B | 0.0331 (18) | 0.0266 (15) | 0.0195 (13) | 0.0043 (14) | 0.0077 (13) | 0.0036 (11) |
| C19B | 0.049 (2) | 0.0237 (15) | 0.0343 (17) | −0.0022 (16) | −0.0071 (16) | 0.0035 (13) |
| C20B | 0.0288 (18) | 0.0264 (15) | 0.0237 (14) | −0.0074 (14) | 0.0019 (13) | −0.0040 (12) |
| C21B | 0.0173 (15) | 0.0282 (15) | 0.0238 (14) | −0.0005 (13) | 0.0019 (12) | 0.0110 (12) |
| C22B | 0.0263 (16) | 0.0195 (13) | 0.0205 (13) | −0.0015 (13) | 0.0006 (12) | 0.0001 (11) |
| C23B | 0.0206 (15) | 0.0254 (15) | 0.0153 (13) | −0.0024 (13) | −0.0013 (12) | 0.0012 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1A—C3A | 1.901 (2) | Br1B—C3B | 1.902 (3) |
| O1A—C11A | 1.354 (3) | O1B—C11B | 1.352 (3) |
| O1A—C18A | 1.456 (3) | O1B—C18B | 1.445 (3) |
| O2A—C13A | 1.377 (3) | O2B—C13B | 1.371 (3) |
| O2A—C20A | 1.411 (3) | O2B—C20B | 1.427 (3) |
| O3A—C15A | 1.366 (3) | O3B—C15B | 1.365 (3) |
| O3A—C21A | 1.431 (3) | O3B—C21B | 1.425 (3) |
| O4A—C16A | 1.370 (3) | O4B—C16B | 1.368 (3) |
| O4A—C22A | 1.426 (3) | O4B—C22B | 1.430 (3) |
| N1A—C11A | 1.316 (3) | N1B—C11B | 1.322 (3) |
| N1A—C7A | 1.362 (3) | N1B—C7B | 1.354 (3) |
| N2A—C23A | 1.150 (3) | N2B—C23B | 1.147 (4) |
| C1A—C2A | 1.384 (4) | C1B—C2B | 1.381 (4) |
| C1A—C6A | 1.398 (3) | C1B—C6B | 1.391 (3) |
| C1A—H1AA | 0.9300 | C1B—H1BA | 0.9300 |
| C2A—C3A | 1.376 (4) | C2B—C3B | 1.388 (4) |
| C2A—H2AA | 0.9300 | C2B—H2BA | 0.9300 |
| C3A—C4A | 1.386 (4) | C3B—C4B | 1.383 (4) |
| C4A—C5A | 1.381 (4) | C4B—C5B | 1.379 (4) |
| C4A—H4AA | 0.9300 | C4B—H4BA | 0.9300 |
| C5A—C6A | 1.402 (3) | C5B—C6B | 1.402 (4) |
| C5A—H5AA | 0.9300 | C5B—H5BA | 0.9300 |
| C6A—C7A | 1.477 (4) | C6B—C7B | 1.485 (4) |
| C7A—C8A | 1.387 (3) | C7B—C8B | 1.391 (3) |
| C8A—C9A | 1.393 (4) | C8B—C9B | 1.385 (4) |
| C8A—H8AA | 0.9300 | C8B—H8BA | 0.9300 |
| C9A—C10A | 1.390 (4) | C9B—C10B | 1.394 (4) |
| C9A—C12A | 1.494 (3) | C9B—C12B | 1.484 (3) |
| C10A—C11A | 1.417 (3) | C10B—C11B | 1.412 (3) |
| C10A—C23A | 1.435 (4) | C10B—C23B | 1.443 (4) |
| C12A—C13A | 1.384 (4) | C12B—C13B | 1.396 (4) |
| C12A—C17A | 1.398 (4) | C12B—C17B | 1.399 (4) |
| C13A—C14A | 1.392 (4) | C13B—C14B | 1.395 (3) |
| C14A—C15A | 1.387 (4) | C14B—C15B | 1.390 (4) |
| C14A—H14A | 0.9300 | C14B—H14B | 0.9300 |
| C15A—C16A | 1.402 (4) | C15B—C16B | 1.406 (4) |
| C16A—C17A | 1.384 (3) | C16B—C17B | 1.379 (3) |
| C17A—H17A | 0.9300 | C17B—H17B | 0.9300 |
| C18A—C19A | 1.503 (4) | C18B—C19B | 1.504 (4) |
| C18A—H18A | 0.9700 | C18B—H18C | 0.9700 |
| C18A—H18B | 0.9700 | C18B—H18D | 0.9700 |
| C19A—H19A | 0.9600 | C19B—H19D | 0.9600 |
| C19A—H19B | 0.9600 | C19B—H19E | 0.9600 |
| C19A—H19C | 0.9600 | C19B—H19F | 0.9600 |
| C20A—H20A | 0.9600 | C20B—H20D | 0.9600 |
| C20A—H20B | 0.9600 | C20B—H20E | 0.9600 |

| | | | |
|---|---|---|---|
| C20A—H20C | 0.9600 | C20B—H20F | 0.9600 |
| C21A—H21A | 0.9600 | C21B—H21D | 0.9600 |
| C21A—H21B | 0.9600 | C21B—H21E | 0.9600 |
| C21A—H21C | 0.9600 | C21B—H21F | 0.9600 |
| C22A—H22A | 0.9600 | C22B—H22D | 0.9600 |
| C22A—H22B | 0.9600 | C22B—H22E | 0.9600 |
| C22A—H22C | 0.9600 | C22B—H22F | 0.9600 |
| | | | |
| C11A—O1A—C18A | 115.60 (19) | C11B—O1B—C18B | 119.1 (2) |
| C13A—O2A—C20A | 118.5 (2) | C13B—O2B—C20B | 117.6 (2) |
| C15A—O3A—C21A | 116.7 (2) | C15B—O3B—C21B | 117.0 (2) |
| C16A—O4A—C22A | 115.9 (2) | C16B—O4B—C22B | 115.60 (19) |
| C11A—N1A—C7A | 118.5 (2) | C11B—N1B—C7B | 117.5 (2) |
| C2A—C1A—C6A | 121.6 (2) | C2B—C1B—C6B | 121.9 (2) |
| C2A—C1A—H1AA | 119.2 | C2B—C1B—H1BA | 119.1 |
| C6A—C1A—H1AA | 119.2 | C6B—C1B—H1BA | 119.1 |
| C3A—C2A—C1A | 118.5 (2) | C1B—C2B—C3B | 118.1 (2) |
| C3A—C2A—H2AA | 120.8 | C1B—C2B—H2BA | 121.0 |
| C1A—C2A—H2AA | 120.8 | C3B—C2B—H2BA | 121.0 |
| C2A—C3A—C4A | 121.9 (2) | C4B—C3B—C2B | 121.9 (2) |
| C2A—C3A—Br1A | 119.47 (19) | C4B—C3B—Br1B | 118.4 (2) |
| C4A—C3A—Br1A | 118.59 (19) | C2B—C3B—Br1B | 119.7 (2) |
| C5A—C4A—C3A | 119.0 (2) | C5B—C4B—C3B | 119.0 (2) |
| C5A—C4A—H4AA | 120.5 | C5B—C4B—H4BA | 120.5 |
| C3A—C4A—H4AA | 120.5 | C3B—C4B—H4BA | 120.5 |
| C4A—C5A—C6A | 120.9 (2) | C4B—C5B—C6B | 120.9 (2) |
| C4A—C5A—H5AA | 119.6 | C4B—C5B—H5BA | 119.6 |
| C6A—C5A—H5AA | 119.6 | C6B—C5B—H5BA | 119.6 |
| C1A—C6A—C5A | 118.1 (2) | C1B—C6B—C5B | 118.3 (2) |
| C1A—C6A—C7A | 119.7 (2) | C1B—C6B—C7B | 121.1 (2) |
| C5A—C6A—C7A | 122.3 (2) | C5B—C6B—C7B | 120.6 (2) |
| N1A—C7A—C8A | 121.5 (2) | N1B—C7B—C8B | 122.5 (2) |
| N1A—C7A—C6A | 115.7 (2) | N1B—C7B—C6B | 116.2 (2) |
| C8A—C7A—C6A | 122.7 (2) | C8B—C7B—C6B | 121.3 (2) |
| C7A—C8A—C9A | 120.1 (2) | C9B—C8B—C7B | 120.1 (2) |
| C7A—C8A—H8AA | 119.9 | C9B—C8B—H8BA | 119.9 |
| C9A—C8A—H8AA | 119.9 | C7B—C8B—H8BA | 119.9 |
| C10A—C9A—C8A | 118.3 (2) | C8B—C9B—C10B | 117.4 (2) |
| C10A—C9A—C12A | 121.2 (2) | C8B—C9B—C12B | 121.1 (2) |
| C8A—C9A—C12A | 120.5 (2) | C10B—C9B—C12B | 121.5 (2) |
| C9A—C10A—C11A | 118.0 (2) | C9B—C10B—C11B | 118.8 (2) |
| C9A—C10A—C23A | 121.0 (2) | C9B—C10B—C23B | 121.1 (2) |
| C11A—C10A—C23A | 121.0 (2) | C11B—C10B—C23B | 120.0 (2) |
| N1A—C11A—O1A | 119.7 (2) | N1B—C11B—O1B | 121.1 (2) |
| N1A—C11A—C10A | 123.5 (2) | N1B—C11B—C10B | 123.4 (2) |
| O1A—C11A—C10A | 116.8 (2) | O1B—C11B—C10B | 115.5 (2) |
| C13A—C12A—C17A | 119.3 (2) | C13B—C12B—C17B | 119.0 (2) |
| C13A—C12A—C9A | 120.6 (2) | C13B—C12B—C9B | 120.9 (2) |

| | | | |
|---|---|---|---|
| C17A—C12A—C9A | 120.1 (2) | C17B—C12B—C9B | 120.1 (2) |
| O2A—C13A—C12A | 115.6 (2) | O2B—C13B—C14B | 123.4 (2) |
| O2A—C13A—C14A | 123.6 (2) | O2B—C13B—C12B | 116.5 (2) |
| C12A—C13A—C14A | 120.7 (2) | C14B—C13B—C12B | 120.1 (2) |
| C15A—C14A—C13A | 119.6 (2) | C15B—C14B—C13B | 120.1 (2) |
| C15A—C14A—H14A | 120.2 | C15B—C14B—H14B | 120.0 |
| C13A—C14A—H14A | 120.2 | C13B—C14B—H14B | 120.0 |
| O3A—C15A—C14A | 123.9 (2) | O3B—C15B—C14B | 124.0 (2) |
| O3A—C15A—C16A | 115.8 (2) | O3B—C15B—C16B | 115.7 (2) |
| C14A—C15A—C16A | 120.4 (2) | C14B—C15B—C16B | 120.3 (2) |
| O4A—C16A—C17A | 124.8 (2) | O4B—C16B—C17B | 125.3 (2) |
| O4A—C16A—C15A | 116.0 (2) | O4B—C16B—C15B | 115.8 (2) |
| C17A—C16A—C15A | 119.2 (2) | C17B—C16B—C15B | 118.9 (2) |
| C16A—C17A—C12A | 120.8 (2) | C16B—C17B—C12B | 121.5 (2) |
| C16A—C17A—H17A | 119.6 | C16B—C17B—H17B | 119.2 |
| C12A—C17A—H17A | 119.6 | C12B—C17B—H17B | 119.2 |
| O1A—C18A—C19A | 107.7 (2) | O1B—C18B—C19B | 110.5 (2) |
| O1A—C18A—H18A | 110.2 | O1B—C18B—H18C | 109.6 |
| C19A—C18A—H18A | 110.2 | C19B—C18B—H18C | 109.6 |
| O1A—C18A—H18B | 110.2 | O1B—C18B—H18D | 109.6 |
| C19A—C18A—H18B | 110.2 | C19B—C18B—H18D | 109.6 |
| H18A—C18A—H18B | 108.5 | H18C—C18B—H18D | 108.1 |
| C18A—C19A—H19A | 109.5 | C18B—C19B—H19D | 109.5 |
| C18A—C19A—H19B | 109.5 | C18B—C19B—H19E | 109.5 |
| H19A—C19A—H19B | 109.5 | H19D—C19B—H19E | 109.5 |
| C18A—C19A—H19C | 109.5 | C18B—C19B—H19F | 109.5 |
| H19A—C19A—H19C | 109.5 | H19D—C19B—H19F | 109.5 |
| H19B—C19A—H19C | 109.5 | H19E—C19B—H19F | 109.5 |
| O2A—C20A—H20A | 109.5 | O2B—C20B—H20D | 109.5 |
| O2A—C20A—H20B | 109.5 | O2B—C20B—H20E | 109.5 |
| H20A—C20A—H20B | 109.5 | H20D—C20B—H20E | 109.5 |
| O2A—C20A—H20C | 109.5 | O2B—C20B—H20F | 109.5 |
| H20A—C20A—H20C | 109.5 | H20D—C20B—H20F | 109.5 |
| H20B—C20A—H20C | 109.5 | H20E—C20B—H20F | 109.5 |
| O3A—C21A—H21A | 109.5 | O3B—C21B—H21D | 109.5 |
| O3A—C21A—H21B | 109.5 | O3B—C21B—H21E | 109.5 |
| H21A—C21A—H21B | 109.5 | H21D—C21B—H21E | 109.5 |
| O3A—C21A—H21C | 109.5 | O3B—C21B—H21F | 109.5 |
| H21A—C21A—H21C | 109.5 | H21D—C21B—H21F | 109.5 |
| H21B—C21A—H21C | 109.5 | H21E—C21B—H21F | 109.5 |
| O4A—C22A—H22A | 109.5 | O4B—C22B—H22D | 109.5 |
| O4A—C22A—H22B | 109.5 | O4B—C22B—H22E | 109.5 |
| H22A—C22A—H22B | 109.5 | H22D—C22B—H22E | 109.5 |
| O4A—C22A—H22C | 109.5 | O4B—C22B—H22F | 109.5 |
| H22A—C22A—H22C | 109.5 | H22D—C22B—H22F | 109.5 |
| H22B—C22A—H22C | 109.5 | H22E—C22B—H22F | 109.5 |
| N2A—C23A—C10A | 176.9 (3) | N2B—C23B—C10B | 177.5 (3) |

| | | | |
|---|---|---|---|
| C6A—C1A—C2A—C3A | −0.1 (4) | C6B—C1B—C2B—C3B | 0.0 (4) |
| C1A—C2A—C3A—C4A | −0.7 (4) | C1B—C2B—C3B—C4B | 0.4 (4) |
| C1A—C2A—C3A—Br1A | −179.6 (2) | C1B—C2B—C3B—Br1B | −179.6 (2) |
| C2A—C3A—C4A—C5A | 0.7 (4) | C2B—C3B—C4B—C5B | 0.5 (5) |
| Br1A—C3A—C4A—C5A | 179.6 (2) | Br1B—C3B—C4B—C5B | −179.5 (2) |
| C3A—C4A—C5A—C6A | −0.1 (4) | C3B—C4B—C5B—C6B | −1.8 (5) |
| C2A—C1A—C6A—C5A | 0.7 (4) | C2B—C1B—C6B—C5B | −1.3 (4) |
| C2A—C1A—C6A—C7A | −180.0 (2) | C2B—C1B—C6B—C7B | 176.5 (3) |
| C4A—C5A—C6A—C1A | −0.6 (4) | C4B—C5B—C6B—C1B | 2.2 (4) |
| C4A—C5A—C6A—C7A | −180.0 (2) | C4B—C5B—C6B—C7B | −175.6 (3) |
| C11A—N1A—C7A—C8A | 0.6 (4) | C11B—N1B—C7B—C8B | 3.5 (4) |
| C11A—N1A—C7A—C6A | −178.3 (2) | C11B—N1B—C7B—C6B | −177.2 (2) |
| C1A—C6A—C7A—N1A | 10.6 (4) | C1B—C6B—C7B—N1B | −27.5 (4) |
| C5A—C6A—C7A—N1A | −170.1 (2) | C5B—C6B—C7B—N1B | 150.2 (3) |
| C1A—C6A—C7A—C8A | −168.3 (2) | C1B—C6B—C7B—C8B | 151.9 (3) |
| C5A—C6A—C7A—C8A | 11.0 (4) | C5B—C6B—C7B—C8B | −30.4 (4) |
| N1A—C7A—C8A—C9A | −1.8 (4) | N1B—C7B—C8B—C9B | 0.1 (4) |
| C6A—C7A—C8A—C9A | 177.1 (2) | C6B—C7B—C8B—C9B | −179.2 (2) |
| C7A—C8A—C9A—C10A | 2.4 (4) | C7B—C8B—C9B—C10B | −3.1 (4) |
| C7A—C8A—C9A—C12A | −175.0 (2) | C7B—C8B—C9B—C12B | 177.3 (2) |
| C8A—C9A—C10A—C11A | −1.8 (4) | C8B—C9B—C10B—C11B | 2.6 (4) |
| C12A—C9A—C10A—C11A | 175.5 (2) | C12B—C9B—C10B—C11B | −177.8 (2) |
| C8A—C9A—C10A—C23A | 177.0 (3) | C8B—C9B—C10B—C23B | −173.4 (3) |
| C12A—C9A—C10A—C23A | −5.7 (4) | C12B—C9B—C10B—C23B | 6.2 (4) |
| C7A—N1A—C11A—O1A | 179.6 (2) | C7B—N1B—C11B—O1B | 175.4 (2) |
| C7A—N1A—C11A—C10A | −0.1 (4) | C7B—N1B—C11B—C10B | −4.0 (4) |
| C18A—O1A—C11A—N1A | 1.7 (3) | C18B—O1B—C11B—N1B | −1.4 (4) |
| C18A—O1A—C11A—C10A | −178.6 (2) | C18B—O1B—C11B—C10B | 178.0 (2) |
| C9A—C10A—C11A—N1A | 0.7 (4) | C9B—C10B—C11B—N1B | 1.0 (4) |
| C23A—C10A—C11A—N1A | −178.1 (3) | C23B—C10B—C11B—N1B | 177.1 (2) |
| C9A—C10A—C11A—O1A | −179.0 (2) | C9B—C10B—C11B—O1B | −178.5 (2) |
| C23A—C10A—C11A—O1A | 2.2 (4) | C23B—C10B—C11B—O1B | −2.4 (4) |
| C10A—C9A—C12A—C13A | −61.4 (4) | C8B—C9B—C12B—C13B | −114.5 (3) |
| C8A—C9A—C12A—C13A | 115.8 (3) | C10B—C9B—C12B—C13B | 66.0 (4) |
| C10A—C9A—C12A—C17A | 117.6 (3) | C8B—C9B—C12B—C17B | 64.1 (4) |
| C8A—C9A—C12A—C17A | −65.2 (4) | C10B—C9B—C12B—C17B | −115.5 (3) |
| C20A—O2A—C13A—C12A | 171.4 (3) | C20B—O2B—C13B—C14B | −5.5 (4) |
| C20A—O2A—C13A—C14A | −11.6 (4) | C20B—O2B—C13B—C12B | 173.9 (2) |
| C17A—C12A—C13A—O2A | 176.7 (2) | C17B—C12B—C13B—O2B | −176.9 (2) |
| C9A—C12A—C13A—O2A | −4.2 (4) | C9B—C12B—C13B—O2B | 1.6 (4) |
| C17A—C12A—C13A—C14A | −0.3 (4) | C17B—C12B—C13B—C14B | 2.5 (4) |
| C9A—C12A—C13A—C14A | 178.7 (2) | C9B—C12B—C13B—C14B | −179.0 (3) |
| O2A—C13A—C14A—C15A | −177.5 (2) | O2B—C13B—C14B—C15B | 179.6 (2) |
| C12A—C13A—C14A—C15A | −0.7 (4) | C12B—C13B—C14B—C15B | 0.3 (4) |
| C21A—O3A—C15A—C14A | 0.2 (4) | C21B—O3B—C15B—C14B | 3.8 (4) |
| C21A—O3A—C15A—C16A | 180.0 (2) | C21B—O3B—C15B—C16B | −175.5 (2) |
| C13A—C14A—C15A—O3A | −179.9 (2) | C13B—C14B—C15B—O3B | 178.7 (2) |
| C13A—C14A—C15A—C16A | 0.3 (4) | C13B—C14B—C15B—C16B | −2.1 (4) |

| | | | | |
|---|---|---|---|---|
| C22A—O4A—C16A—C17A | 8.1 (4) | C22B—O4B—C16B—C17B | −7.7 (4) | |
| C22A—O4A—C16A—C15A | −172.8 (2) | C22B—O4B—C16B—C15B | 173.3 (2) | |
| O3A—C15A—C16A—O4A | 2.1 (4) | O3B—C15B—C16B—O4B | −0.6 (3) | |
| C14A—C15A—C16A—O4A | −178.0 (2) | C14B—C15B—C16B—O4B | −179.9 (2) | |
| O3A—C15A—C16A—C17A | −178.7 (2) | O3B—C15B—C16B—C17B | −179.6 (2) | |
| C14A—C15A—C16A—C17A | 1.1 (4) | C14B—C15B—C16B—C17B | 1.1 (4) | |
| O4A—C16A—C17A—C12A | 176.9 (2) | O4B—C16B—C17B—C12B | −177.2 (2) | |
| C15A—C16A—C17A—C12A | −2.1 (4) | C15B—C16B—C17B—C12B | 1.7 (4) | |
| C13A—C12A—C17A—C16A | 1.8 (4) | C13B—C12B—C17B—C16B | −3.5 (4) | |
| C9A—C12A—C17A—C16A | −177.3 (2) | C9B—C12B—C17B—C16B | 177.9 (2) | |
| C11A—O1A—C18A—C19A | −174.0 (2) | C11B—O1B—C18B—C19B | 92.8 (3) | |

*Hydrogen-bond geometry (Å, º)*

Cg1 and Cg2 are the centroids of C7A–C11A/N1A and C12A–C17A rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1*A*—H1*AA*···N1*A* | 0.93 | 2.43 | 2.770 (3) | 102 |
| C18*B*—H18*C*···N1*B* | 0.97 | 2.38 | 2.741 (4) | 101 |
| C22*A*—H22*C*···*Cg*2[i] | 0.96 | 2.74 | 3.585 (3) | 147 |
| C22*B*—H22*E*···*Cg*1[ii] | 0.96 | 2.68 | 3.511 (3) | 145 |

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*, −*y*+1, −*z*+1.