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# Ethyl 8-amino-7-(furan-2-yl)-5,6-dihydrothieno-[2,3-*b*]benzo[*h*]quinoline-9-carboxylate

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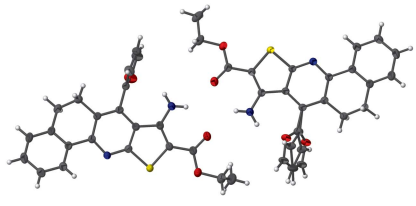
**CCDC reference**: 1519100

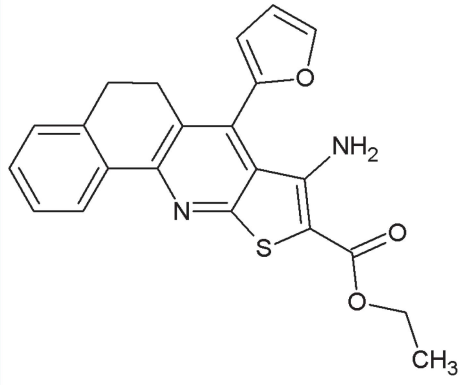
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{22}H_{18}N_2O_3S$, the two independent molecules in the asymmetric unit form a dimer *via* N—H···O hydrogen bonds. In the crystal, the molecular layers can be found in the (110) plane, connected by C—H···$\pi$ interactions. Atoms of the furan ring of one independent molecule are disordered over two sets of sites with an occupancy ratio 0.735 (3):0.265 (3).

**3D view**



**Chemical scheme**




## Structure description

The thiophene moiety is present in a large number of bioactive molecules having diverse biological activities such as anti-inflammatory (Murakami *et al.*, 1998), anticonvulsant (Kulandasamy *et al.*, 2009), antibacterial (Lu *et al.*, 2011) and antitumor (Kaushik *et al.*, 2012). The quinoline ring system is one of the most commonly encountered heterocycles in medicinal chemistry (Bouraiou *et al.*, 2007). Substituted quinolines possess diverse chemotherapeutic activities including antibacterial (Kidwai *et al.*, 2000), antifungal (Musiol *et al.*, 2006), antimalarial (Charris *et al.*, 2005; Cunico *et al.*, 2006) and antitumor (Chen *et al.*, 2006). As part of our studies in this area, we report herein the synthesis and crystal structure of the title compound.

In the asymmetric unit (Fig. 1), the two independent molecules *A* and *B* form a dimer *via* N—H···O hydrogen bonds (Table 1). In both molecules, the cyclohexene rings of the fused tetracyclic cores are puckered with $Q_T$ = 0.438 (2) Å, $\theta$ = 65.0 (2)°, $\varphi$ = 277.0 (3)° in *A* and $Q_T$ = 0.481 (2) Å, $\theta$ = 111.8 (2) °, $\varphi$ = 87.2 (2) ° in *B*. In both *A* and *B*, the molecular conformation is stabilized by an N—H···O hydrogen bonds.

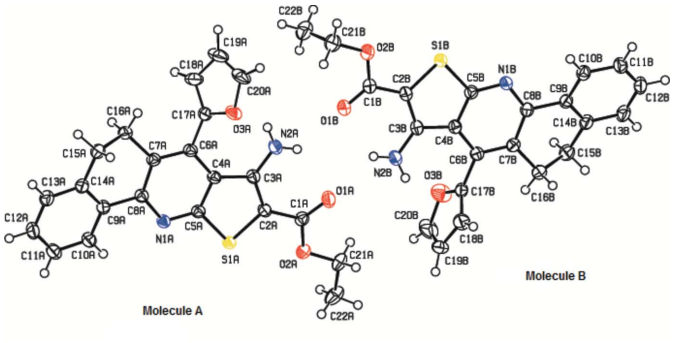



**Figure 1**
A view of molecules *A* and *B* in the asymmetric unit of the title compound, with displacement ellipsoids drawn at the 50% probability level. For clarity, only the major disorder component of the furan ring in molecule *A* is shown.

In the crystal, molecular layers can be found in the (110) plane which are connected by C—H···$\pi$ and C—H···N interactions (Fig. 2, Table 1). There is a $\pi$–$\pi$ interaction between the N1*A*/C4*A*–C8*A* and C9*A*–C14*A*($-x$, $-y+1$, $-z+2$) rings with a centroid–centroid distance of 3.7975 (10) Å.

## Synthesis and crystallization

To a mixture of 3-cyano-5,6-dihydro-4-(2-furyl)-benzo[*h*]qui-]quinoline-2(1*H*)-thione (10 mmol) and ethyl chloroacetate (10 mmol) in ethanol (20 ml) containing sodium ethoxide (20 mmol) was heated under reflux for one h and then allowed to cool. The solid that formed was collected and recrystallized from ethanol. Yield: 77%; m.p. 460–461 K. IR: 3490, 3360 ($NH_2$), 1665 (C═O) $cm^{-1.}$ $^1$H NMR ($CDCl_3$): 8.45 (*m*, 1H, CH–furyl); 6.60 (*m*, 2H, 2CH–furyl); 7.15–7.75 (*m*, 4H, ArH); 5.75 (*s*, 2H, $NH_2$); 4.02–4.45 (*q*, 2H, $OCH_2$); 2.85 (*t*, 4H, $CH_2$—$CH_2$); 1.30–1.45 (*t*, 3H, $CH_3$ of ester) p.p.m.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Atoms O3/C17–C20 atoms of the furan ring of molecule *A* are disordered over two sets of sites with an occupancy ratio 0.735 (3):0.265 (3).

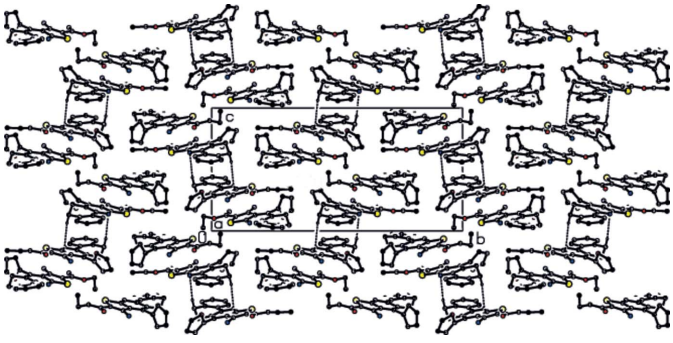



**Figure 2**
Packing of the title molecule, viewed down the *a* axis, with the hydrogen bonds shown by dotted lines. For clarity, the minor disorder component of the furan ring in molecule *A* is omitted.

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

*Cg*8, *Cg*9 and *Cg*11 are the centroids of the O3*B*/C17*B*–C20*B* furan, N1*B*/C4*B*–C8*B* pyridine and C9*B*–C14*B* benzene rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2*A*—H*N*2*A*···O1*A* | 0.83 (3) | 2.23 (3) | 2.839 (2) | 131 (2) |
| N2*A*—H*N*2*A*···O1*B* | 0.83 (3) | 2.33 (3) | 2.962 (2) | 134 (2) |
| N2*A*—H*N*2*B*···O3*A* | 0.86 (3) | 2.17 (3) | 2.869 (3) | 138 (2) |
| N2*B*—H*N*2*D*···O1*A* | 0.87 (3) | 2.33 (2) | 2.998 (2) | 134 (2) |
| N2*B*—H*N*2*D*···O1*B* | 0.87 (3) | 2.17 (2) | 2.802 (2) | 129 (2) |
| N2*B*—H*N*2*C*···*Cg*8 | 0.83 (3) | 2.55 (3) | 3.294 (2) | 150 (2) |
| C18*B*—H18*B*···*Cg*11$^{i}$ | 0.93 | 2.53 | 3.353 (2) | 148 |
| C21*A*—H21*A*···*Cg*9$^{i}$ | 0.97 | 2.96 | 3.718 (2) | 136 |
| C15*A*—H15*A*···N1*A*$^{ii}$ | 0.97 | 2.61 | 3.386 (2) | 137 |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{22}H_{18}N_2O_3S$ |
| $M_r$ | 390.44 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 173 |
| *a*, *b*, *c* (Å) | 11.5227 (1), 25.5293 (3), 12.4749 (1) |
| $\beta$ (°) | 90.038 (1) |
| *V* (Å$^3$) | 3669.70 (6) |
| *Z* | 8 |
| Radiation type | Cu $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 1.79 |
| Crystal size (mm) | 0.24 × 0.22 × 0.18 |
| | |
| Data collection | |
| Diffractometer | Rigaku Oxford Diffraction |
| Absorption correction | Multi-scan (*CrysAlis PRO*; Agilent, 2014) |
| $T_{min}$, $T_{max}$ | 0.850, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 26340, 7070, 6264 |
| $R_{int}$ | 0.041 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.615 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.042, 0.121, 1.02 |
| No. of reflections | 7070 |
| No. of parameters | 535 |
| No. of restraints | 6 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.51, −0.35 |

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

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# full crystallographic data

*IUCrData* (2016). **1**, x161884 [https://doi.org/10.1107/S2414314616018848]

## Ethyl 8-amino-7-(furan-2-yl)-5,6-dihydrothieno[2,3-*b*]benzo[*h*]quinoline-9-carboxylate

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*Crystal data*

$C_{22}H_{18}N_2O_3S$
$M_r$ = 390.44
Monoclinic, $P2_1/n$
$a$ = 11.5227 (1) Å
$b$ = 25.5293 (3) Å
$c$ = 12.4749 (1) Å
$\beta$ = 90.038 (1)°
$V$ = 3669.70 (6) Å$^3$
$Z$ = 8
$F(000)$ = 1632
$D_x$ = 1.413 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54184 Å
Cell parameters from 11878 reflections
$\theta$ = 4.0–71.5°
$\mu$ = 1.79 mm$^{-1}$
$T$ = 173 K
Prism, yellow
0.24 × 0.22 × 0.18 mm

*Data collection*

Rigaku Oxford Diffraction diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
$T_{min}$ = 0.850, $T_{max}$ = 1.000
26340 measured reflections
7070 independent reflections
6264 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041
$\theta_{max}$ = 71.6°, $\theta_{min}$ = 3.5°
$h$ = −14→14
$k$ = −31→31
$l$ = −15→9

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.121
$S$ = 1.02
7070 reflections
535 parameters
6 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0748P)^2 + 1.4658P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.51 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 e Å$^{-3}$

*Special details*

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

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| S1A | 0.22490 (3) | 0.33984 (2) | 0.86042 (3) | 0.02556 (12) | |
| O1A | 0.56095 (11) | 0.33865 (5) | 0.80644 (11) | 0.0341 (3) | |
| O2A | 0.42720 (11) | 0.27591 (5) | 0.83821 (10) | 0.0303 (3) | |
| N1A | 0.05971 (12) | 0.41276 (5) | 0.86245 (11) | 0.0241 (3) | |
| N2A | 0.46257 (14) | 0.43728 (7) | 0.75339 (14) | 0.0341 (3) | |
| HN2A | 0.522 (2) | 0.4191 (10) | 0.7475 (19) | 0.041* | |
| HN2B | 0.462 (2) | 0.4705 (10) | 0.7422 (19) | 0.041* | |
| C1A | 0.46067 (15) | 0.32571 (7) | 0.82123 (13) | 0.0257 (3) | |
| C2A | 0.36303 (14) | 0.36142 (6) | 0.82271 (13) | 0.0254 (3) | |
| C3A | 0.36690 (14) | 0.41373 (6) | 0.79308 (13) | 0.0245 (3) | |
| C4A | 0.25402 (14) | 0.43856 (6) | 0.80529 (13) | 0.0231 (3) | |
| C5A | 0.17046 (14) | 0.40254 (6) | 0.84125 (13) | 0.0232 (3) | |
| C6A | 0.21524 (14) | 0.49043 (6) | 0.78678 (13) | 0.0241 (3) | |
| C7A | 0.09879 (14) | 0.50196 (6) | 0.80572 (13) | 0.0241 (3) | |
| C8A | 0.02490 (14) | 0.46196 (6) | 0.84584 (12) | 0.0236 (3) | |
| C9A | −0.09666 (14) | 0.47437 (7) | 0.87498 (13) | 0.0249 (3) | |
| C10A | −0.17635 (15) | 0.43420 (7) | 0.89447 (14) | 0.0293 (4) | |
| H10A | −0.153863 | 0.399475 | 0.885679 | 0.035* | |
| C11A | −0.28851 (16) | 0.44565 (8) | 0.92675 (15) | 0.0338 (4) | |
| H11A | −0.341193 | 0.418752 | 0.939354 | 0.041* | |
| C12A | −0.32185 (16) | 0.49745 (8) | 0.94017 (15) | 0.0354 (4) | |
| H12A | −0.396979 | 0.505315 | 0.962087 | 0.042* | |
| C13A | −0.24327 (16) | 0.53752 (7) | 0.92095 (15) | 0.0324 (4) | |
| H13A | −0.266326 | 0.572119 | 0.930411 | 0.039* | |
| C14A | −0.13053 (15) | 0.52677 (7) | 0.88773 (13) | 0.0268 (3) | |
| C15A | −0.04349 (16) | 0.56975 (7) | 0.86893 (15) | 0.0303 (4) | |
| H15A | −0.003843 | 0.577505 | 0.935690 | 0.036* | |
| H15B | −0.083923 | 0.601183 | 0.846270 | 0.036* | |
| C16A | 0.04587 (15) | 0.55486 (6) | 0.78416 (14) | 0.0285 (3) | |
| H16A | 0.008902 | 0.554493 | 0.714280 | 0.034* | |
| H16B | 0.106769 | 0.581082 | 0.782748 | 0.034* | |
| C17A | 0.2979 (7) | 0.5314 (4) | 0.7524 (8) | 0.0262 (10) | 0.735 (3) |
| C18A | 0.2961 (3) | 0.56622 (11) | 0.6707 (2) | 0.0369 (6) | 0.735 (3) |
| H18A | 0.240017 | 0.569180 | 0.617413 | 0.044* | 0.735 (3) |
| C19A | 0.3992 (16) | 0.5979 (7) | 0.6830 (12) | 0.0446 (9) | 0.735 (3) |
| H19A | 0.422671 | 0.625051 | 0.638384 | 0.054* | 0.735 (3) |
| C20A | 0.4539 (2) | 0.58110 (10) | 0.7692 (3) | 0.0417 (6) | 0.735 (3) |
| H20A | 0.523515 | 0.594683 | 0.794691 | 0.050* | 0.735 (3) |
| O3A | 0.39379 (15) | 0.54085 (8) | 0.81596 (17) | 0.0337 (4) | 0.735 (3) |
| C17C | 0.282 (2) | 0.5346 (11) | 0.741 (2) | 0.0262 (10) | 0.265 (3) |
| C18C | 0.3788 (7) | 0.5585 (3) | 0.7729 (7) | 0.0369 (6) | 0.265 (3) |
| H18C | 0.422078 | 0.551525 | 0.834168 | 0.044* | 0.265 (3) |
| C19C | 0.402 (4) | 0.598 (2) | 0.692 (3) | 0.0446 (9) | 0.265 (3) |
| H19C | 0.462936 | 0.621598 | 0.691796 | 0.054* | 0.265 (3) |
| C20C | 0.3211 (7) | 0.5927 (3) | 0.6206 (7) | 0.0417 (6) | 0.265 (3) |

| | | | | | |
|---|---|---|---|---|---|
| H20C | 0.315117 | 0.614125 | 0.560551 | 0.050* | 0.265 (3) |
| O3C | 0.2450 (5) | 0.5525 (2) | 0.6428 (4) | 0.0337 (4) | 0.265 (3) |
| C21A | 0.51885 (17) | 0.23712 (7) | 0.83563 (16) | 0.0348 (4) | |
| H21A | 0.570214 | 0.241588 | 0.896586 | 0.042* | |
| H21B | 0.564068 | 0.240675 | 0.770478 | 0.042* | |
| C22A | 0.4620 (2) | 0.18439 (8) | 0.83956 (18) | 0.0457 (5) | |
| H22A | 0.417416 | 0.179079 | 0.775411 | 0.069* | |
| H22B | 0.411632 | 0.182600 | 0.900753 | 0.069* | |
| H22C | 0.520348 | 0.157701 | 0.845037 | 0.069* | |
| S1B | 1.02424 (3) | 0.42431 (2) | 0.56674 (3) | 0.02733 (12) | |
| O1B | 0.69672 (11) | 0.43020 (5) | 0.65658 (11) | 0.0366 (3) | |
| O2B | 0.82546 (11) | 0.49130 (5) | 0.60154 (12) | 0.0372 (3) | |
| O3B | 0.86546 (14) | 0.21442 (6) | 0.60904 (12) | 0.0471 (4) | |
| N1B | 1.18642 (12) | 0.34871 (5) | 0.56442 (11) | 0.0246 (3) | |
| N2B | 0.78963 (13) | 0.33034 (7) | 0.69322 (14) | 0.0326 (3) | |
| HN2C | 0.798 (2) | 0.3007 (10) | 0.7195 (19) | 0.039* | |
| HN2D | 0.730 (2) | 0.3500 (10) | 0.7069 (18) | 0.039* | |
| C1B | 0.79366 (15) | 0.44204 (7) | 0.62714 (14) | 0.0292 (4) | |
| C2B | 0.88844 (14) | 0.40521 (7) | 0.61652 (14) | 0.0267 (3) | |
| C3B | 0.88368 (14) | 0.35349 (7) | 0.64893 (13) | 0.0251 (3) | |
| C4B | 0.99295 (14) | 0.32699 (6) | 0.62983 (12) | 0.0238 (3) | |
| C5B | 1.07690 (14) | 0.36130 (6) | 0.58800 (13) | 0.0245 (3) | |
| C6B | 1.02569 (14) | 0.27431 (6) | 0.64358 (12) | 0.0236 (3) | |
| C7B | 1.13874 (14) | 0.25994 (6) | 0.61924 (13) | 0.0251 (3) | |
| C8B | 1.21695 (14) | 0.29883 (6) | 0.58245 (13) | 0.0243 (3) | |
| C9B | 1.33937 (14) | 0.28466 (7) | 0.56314 (13) | 0.0253 (3) | |
| C10B | 1.42585 (15) | 0.32303 (7) | 0.56302 (13) | 0.0276 (3) | |
| H10B | 1.406239 | 0.357947 | 0.574158 | 0.033* | |
| C11B | 1.54065 (15) | 0.30924 (8) | 0.54638 (14) | 0.0316 (4) | |
| H11B | 1.598095 | 0.334818 | 0.547796 | 0.038* | |
| C12B | 1.57021 (16) | 0.25741 (8) | 0.52763 (15) | 0.0361 (4) | |
| H12B | 1.647229 | 0.248335 | 0.515318 | 0.043* | |
| C13B | 1.48511 (17) | 0.21918 (8) | 0.52722 (15) | 0.0352 (4) | |
| H13B | 1.505379 | 0.184524 | 0.513931 | 0.042* | |
| C14B | 1.36936 (15) | 0.23194 (7) | 0.54647 (14) | 0.0290 (4) | |
| C15B | 1.27430 (17) | 0.19147 (7) | 0.54764 (16) | 0.0348 (4) | |
| H15C | 1.307342 | 0.157309 | 0.562736 | 0.042* | |
| H15D | 1.237743 | 0.189993 | 0.477643 | 0.042* | |
| C16B | 1.18314 (16) | 0.20466 (7) | 0.63247 (16) | 0.0331 (4) | |
| H16C | 1.118817 | 0.180319 | 0.626580 | 0.040* | |
| H16D | 1.216931 | 0.200740 | 0.703249 | 0.040* | |
| C17B | 0.94080 (14) | 0.23500 (6) | 0.68132 (14) | 0.0252 (3) | |
| C18B | 0.91781 (17) | 0.21757 (8) | 0.78011 (15) | 0.0365 (4) | |
| H18B | 0.956365 | 0.226416 | 0.843077 | 0.044* | |
| C19B | 0.82130 (19) | 0.18236 (9) | 0.7690 (2) | 0.0507 (6) | |
| H19B | 0.785630 | 0.163445 | 0.823494 | 0.061* | |
| C20B | 0.7931 (2) | 0.18204 (9) | 0.6666 (2) | 0.0536 (6) | |
| H20B | 0.732602 | 0.162626 | 0.637295 | 0.064* | |

| | | | | |
|---|---|---|---|---|
| C21B | 0.73855 (18) | 0.53200 (8) | 0.61779 (17) | 0.0404 (4) |
| H21C | 0.776869 | 0.565605 | 0.625701 | 0.048* |
| H21D | 0.696033 | 0.524921 | 0.683296 | 0.048* |
| C22B | 0.6554 (2) | 0.53445 (9) | 0.52547 (19) | 0.0481 (5) |
| H22D | 0.697369 | 0.541281 | 0.460532 | 0.072* |
| H22E | 0.600206 | 0.562013 | 0.537528 | 0.072* |
| H22F | 0.615224 | 0.501639 | 0.519249 | 0.072* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1A | 0.0241 (2) | 0.01813 (19) | 0.0345 (2) | −0.00011 (14) | 0.00498 (15) | 0.00198 (14) |
| O1A | 0.0239 (6) | 0.0310 (6) | 0.0474 (7) | 0.0021 (5) | 0.0016 (5) | −0.0010 (5) |
| O2A | 0.0304 (6) | 0.0227 (6) | 0.0377 (6) | 0.0045 (5) | 0.0024 (5) | 0.0018 (5) |
| N1A | 0.0226 (7) | 0.0211 (6) | 0.0286 (7) | −0.0009 (5) | 0.0026 (5) | −0.0010 (5) |
| N2A | 0.0227 (7) | 0.0253 (8) | 0.0543 (10) | 0.0005 (6) | 0.0072 (7) | 0.0045 (7) |
| C1A | 0.0276 (8) | 0.0244 (8) | 0.0252 (8) | 0.0026 (7) | 0.0009 (6) | −0.0006 (6) |
| C2A | 0.0224 (8) | 0.0232 (8) | 0.0305 (8) | −0.0006 (6) | 0.0032 (6) | −0.0006 (6) |
| C3A | 0.0230 (8) | 0.0226 (8) | 0.0280 (8) | −0.0010 (6) | 0.0013 (6) | −0.0024 (6) |
| C4A | 0.0235 (8) | 0.0213 (7) | 0.0247 (7) | −0.0018 (6) | 0.0028 (6) | −0.0012 (6) |
| C5A | 0.0249 (8) | 0.0192 (7) | 0.0255 (7) | −0.0010 (6) | 0.0014 (6) | −0.0010 (6) |
| C6A | 0.0255 (8) | 0.0204 (7) | 0.0263 (8) | −0.0012 (6) | 0.0031 (6) | −0.0004 (6) |
| C7A | 0.0258 (8) | 0.0212 (8) | 0.0254 (8) | 0.0002 (6) | 0.0018 (6) | 0.0004 (6) |
| C8A | 0.0235 (8) | 0.0225 (8) | 0.0247 (7) | −0.0009 (6) | 0.0008 (6) | −0.0012 (6) |
| C9A | 0.0229 (8) | 0.0260 (8) | 0.0258 (8) | 0.0006 (6) | −0.0002 (6) | 0.0001 (6) |
| C10A | 0.0258 (8) | 0.0291 (8) | 0.0329 (9) | −0.0020 (7) | 0.0016 (7) | −0.0011 (7) |
| C11A | 0.0254 (9) | 0.0390 (10) | 0.0370 (9) | −0.0054 (7) | 0.0027 (7) | 0.0014 (8) |
| C12A | 0.0227 (8) | 0.0456 (11) | 0.0377 (9) | 0.0060 (7) | 0.0044 (7) | 0.0028 (8) |
| C13A | 0.0299 (9) | 0.0330 (9) | 0.0344 (9) | 0.0074 (7) | 0.0033 (7) | 0.0020 (7) |
| C14A | 0.0255 (8) | 0.0281 (8) | 0.0270 (8) | 0.0034 (6) | 0.0005 (6) | 0.0018 (6) |
| C15A | 0.0302 (9) | 0.0211 (8) | 0.0396 (9) | 0.0048 (7) | 0.0055 (7) | 0.0014 (7) |
| C16A | 0.0279 (8) | 0.0229 (8) | 0.0346 (9) | 0.0018 (6) | 0.0054 (7) | 0.0051 (7) |
| C17A | 0.024 (3) | 0.0190 (14) | 0.036 (2) | 0.0028 (19) | 0.0079 (15) | 0.0007 (10) |
| C18A | 0.0445 (16) | 0.0279 (12) | 0.0384 (13) | −0.0023 (11) | 0.0120 (12) | 0.0092 (10) |
| C19A | 0.0494 (16) | 0.0260 (9) | 0.059 (3) | −0.0094 (10) | 0.0248 (18) | 0.0026 (18) |
| C20A | 0.0374 (13) | 0.0255 (12) | 0.0622 (17) | −0.0127 (10) | 0.0167 (12) | −0.0029 (11) |
| O3A | 0.0283 (8) | 0.0282 (9) | 0.0444 (10) | −0.0104 (7) | 0.0024 (7) | 0.0012 (8) |
| C17C | 0.024 (3) | 0.0190 (14) | 0.036 (2) | 0.0028 (19) | 0.0079 (15) | 0.0007 (10) |
| C18C | 0.0445 (16) | 0.0279 (12) | 0.0384 (13) | −0.0023 (11) | 0.0120 (12) | 0.0092 (10) |
| C19C | 0.0494 (16) | 0.0260 (9) | 0.059 (3) | −0.0094 (10) | 0.0248 (18) | 0.0026 (18) |
| C20C | 0.0374 (13) | 0.0255 (12) | 0.0622 (17) | −0.0127 (10) | 0.0167 (12) | −0.0029 (11) |
| O3C | 0.0283 (8) | 0.0282 (9) | 0.0444 (10) | −0.0104 (7) | 0.0024 (7) | 0.0012 (8) |
| C21A | 0.0384 (10) | 0.0273 (9) | 0.0386 (10) | 0.0110 (7) | −0.0054 (8) | −0.0009 (7) |
| C22A | 0.0592 (13) | 0.0262 (9) | 0.0518 (12) | 0.0084 (9) | −0.0151 (10) | 0.0008 (8) |
| S1B | 0.0224 (2) | 0.0226 (2) | 0.0370 (2) | 0.00243 (14) | 0.00525 (16) | 0.00390 (15) |
| O1B | 0.0248 (6) | 0.0362 (7) | 0.0488 (8) | 0.0053 (5) | 0.0069 (5) | 0.0077 (6) |
| O2B | 0.0293 (7) | 0.0292 (6) | 0.0531 (8) | 0.0070 (5) | 0.0080 (6) | 0.0060 (6) |
| O3B | 0.0457 (8) | 0.0517 (9) | 0.0440 (8) | −0.0184 (7) | −0.0076 (6) | −0.0019 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N1B | 0.0214 (7) | 0.0239 (7) | 0.0286 (7) | 0.0008 (5) | 0.0027 (5) | 0.0010 (5) |
| N2B | 0.0215 (7) | 0.0279 (8) | 0.0483 (9) | 0.0003 (6) | 0.0052 (6) | 0.0035 (7) |
| C1B | 0.0240 (8) | 0.0309 (9) | 0.0327 (9) | 0.0029 (7) | 0.0020 (7) | 0.0032 (7) |
| C2B | 0.0213 (8) | 0.0280 (8) | 0.0308 (8) | 0.0011 (6) | 0.0023 (6) | 0.0008 (6) |
| C3B | 0.0206 (8) | 0.0279 (8) | 0.0268 (8) | −0.0003 (6) | −0.0013 (6) | −0.0024 (6) |
| C4B | 0.0219 (8) | 0.0255 (8) | 0.0241 (7) | −0.0003 (6) | −0.0009 (6) | −0.0006 (6) |
| C5B | 0.0239 (8) | 0.0226 (8) | 0.0269 (8) | 0.0003 (6) | −0.0007 (6) | −0.0002 (6) |
| C6B | 0.0234 (8) | 0.0235 (8) | 0.0240 (7) | −0.0027 (6) | −0.0027 (6) | −0.0011 (6) |
| C7B | 0.0261 (8) | 0.0230 (8) | 0.0261 (8) | 0.0009 (6) | −0.0019 (6) | 0.0006 (6) |
| C8B | 0.0239 (8) | 0.0244 (8) | 0.0247 (7) | 0.0014 (6) | −0.0002 (6) | −0.0016 (6) |
| C9B | 0.0250 (8) | 0.0282 (8) | 0.0229 (7) | 0.0044 (6) | 0.0006 (6) | 0.0020 (6) |
| C10B | 0.0268 (8) | 0.0309 (8) | 0.0252 (8) | 0.0030 (7) | −0.0010 (6) | 0.0000 (6) |
| C11B | 0.0238 (8) | 0.0413 (10) | 0.0297 (8) | 0.0004 (7) | −0.0016 (6) | 0.0025 (7) |
| C12B | 0.0240 (8) | 0.0473 (11) | 0.0371 (9) | 0.0101 (8) | 0.0019 (7) | 0.0048 (8) |
| C13B | 0.0331 (10) | 0.0333 (9) | 0.0393 (10) | 0.0120 (7) | 0.0030 (7) | 0.0035 (8) |
| C14B | 0.0284 (9) | 0.0284 (8) | 0.0303 (8) | 0.0063 (7) | 0.0011 (7) | 0.0026 (7) |
| C15B | 0.0348 (9) | 0.0230 (8) | 0.0465 (10) | 0.0052 (7) | 0.0023 (8) | −0.0011 (7) |
| C16B | 0.0299 (9) | 0.0253 (9) | 0.0443 (10) | 0.0020 (7) | 0.0039 (7) | 0.0052 (7) |
| C17B | 0.0209 (7) | 0.0227 (8) | 0.0320 (8) | 0.0007 (6) | −0.0025 (6) | −0.0002 (6) |
| C18B | 0.0353 (10) | 0.0482 (11) | 0.0260 (8) | −0.0003 (8) | 0.0001 (7) | 0.0041 (8) |
| C19B | 0.0383 (11) | 0.0389 (11) | 0.0747 (16) | 0.0060 (9) | 0.0215 (11) | 0.0276 (11) |
| C20B | 0.0379 (11) | 0.0360 (11) | 0.0869 (18) | −0.0159 (9) | 0.0030 (11) | −0.0056 (11) |
| C21B | 0.0388 (10) | 0.0339 (10) | 0.0485 (11) | 0.0075 (8) | 0.0056 (9) | −0.0004 (8) |
| C22B | 0.0459 (12) | 0.0428 (12) | 0.0555 (13) | 0.0132 (9) | 0.0012 (10) | 0.0059 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1A—C5A | 1.7355 (16) | C21A—H21B | 0.9700 |
| S1A—C2A | 1.7489 (17) | C22A—H22A | 0.9600 |
| O1A—C1A | 1.216 (2) | C22A—H22B | 0.9600 |
| O2A—C1A | 1.345 (2) | C22A—H22C | 0.9600 |
| O2A—C21A | 1.448 (2) | S1B—C5B | 1.7395 (16) |
| N1A—C5A | 1.329 (2) | S1B—C2B | 1.7530 (17) |
| N1A—C8A | 1.335 (2) | O1B—C1B | 1.214 (2) |
| N2A—C3A | 1.350 (2) | O2B—C1B | 1.348 (2) |
| N2A—HN2A | 0.83 (3) | O2B—C21B | 1.457 (2) |
| N2A—HN2B | 0.86 (3) | O3B—C17B | 1.357 (2) |
| C1A—C2A | 1.448 (2) | O3B—C20B | 1.377 (3) |
| C2A—C3A | 1.386 (2) | N1B—C5B | 1.335 (2) |
| C3A—C4A | 1.455 (2) | N1B—C8B | 1.340 (2) |
| C4A—C5A | 1.405 (2) | N2B—C3B | 1.353 (2) |
| C4A—C6A | 1.416 (2) | N2B—HN2C | 0.83 (3) |
| C6A—C7A | 1.394 (2) | N2B—HN2D | 0.87 (3) |
| C6A—C17A | 1.479 (5) | C1B—C2B | 1.447 (2) |
| C6A—C17C | 1.480 (12) | C2B—C3B | 1.382 (2) |
| C7A—C8A | 1.421 (2) | C3B—C4B | 1.449 (2) |
| C7A—C16A | 1.506 (2) | C4B—C5B | 1.406 (2) |
| C8A—C9A | 1.482 (2) | C4B—C6B | 1.407 (2) |

| | | | |
|---|---|---|---|
| C9A—C10A | 1.398 (2) | C6B—C7B | 1.387 (2) |
| C9A—C14A | 1.403 (2) | C6B—C17B | 1.479 (2) |
| C10A—C11A | 1.385 (3) | C7B—C8B | 1.418 (2) |
| C10A—H10A | 0.9300 | C7B—C16B | 1.510 (2) |
| C11A—C12A | 1.387 (3) | C8B—C9B | 1.476 (2) |
| C11A—H11A | 0.9300 | C9B—C10B | 1.397 (2) |
| C12A—C13A | 1.387 (3) | C9B—C14B | 1.405 (2) |
| C12A—H12A | 0.9300 | C10B—C11B | 1.385 (2) |
| C13A—C14A | 1.391 (2) | C10B—H10B | 0.9300 |
| C13A—H13A | 0.9300 | C11B—C12B | 1.386 (3) |
| C14A—C15A | 1.505 (2) | C11B—H11B | 0.9300 |
| C15A—C16A | 1.525 (2) | C12B—C13B | 1.384 (3) |
| C15A—H15A | 0.9700 | C12B—H12B | 0.9300 |
| C15A—H15B | 0.9700 | C13B—C14B | 1.394 (3) |
| C16A—H16A | 0.9700 | C13B—H13B | 0.9300 |
| C16A—H16B | 0.9700 | C14B—C15B | 1.506 (3) |
| C17A—C18A | 1.352 (6) | C15B—C16B | 1.529 (3) |
| C17A—O3A | 1.381 (6) | C15B—H15C | 0.9700 |
| C18A—C19A | 1.445 (9) | C15B—H15D | 0.9700 |
| C18A—H18A | 0.9300 | C16B—H16C | 0.9700 |
| C19A—C20A | 1.317 (12) | C16B—H16D | 0.9700 |
| C19A—H19A | 0.9300 | C17B—C18B | 1.337 (3) |
| C20A—O3A | 1.370 (3) | C18B—C19B | 1.437 (3) |
| C20A—H20A | 0.9300 | C18B—H18B | 0.9300 |
| C17C—C18C | 1.335 (17) | C19B—C20B | 1.318 (4) |
| C17C—O3C | 1.37 (2) | C19B—H19B | 0.9300 |
| C18C—C19C | 1.442 (19) | C20B—H20B | 0.9300 |
| C18C—H18C | 0.9300 | C21B—C22B | 1.499 (3) |
| C19C—C20C | 1.30 (3) | C21B—H21C | 0.9700 |
| C19C—H19C | 0.9300 | C21B—H21D | 0.9700 |
| C20C—O3C | 1.379 (8) | C22B—H22D | 0.9600 |
| C20C—H20C | 0.9300 | C22B—H22E | 0.9600 |
| C21A—C22A | 1.498 (3) | C22B—H22F | 0.9600 |
| C21A—H21A | 0.9700 | | |

| | | | |
|---|---|---|---|
| C5A—S1A—C2A | 90.08 (8) | H21A—C21A—H21B | 108.5 |
| C1A—O2A—C21A | 115.70 (14) | C21A—C22A—H22A | 109.5 |
| C5A—N1A—C8A | 116.25 (14) | C21A—C22A—H22B | 109.5 |
| C3A—N2A—HN2A | 117.3 (17) | H22A—C22A—H22B | 109.5 |
| C3A—N2A—HN2B | 119.9 (16) | C21A—C22A—H22C | 109.5 |
| HN2A—N2A—HN2B | 122 (2) | H22A—C22A—H22C | 109.5 |
| O1A—C1A—O2A | 123.58 (15) | H22B—C22A—H22C | 109.5 |
| O1A—C1A—C2A | 124.71 (16) | C5B—S1B—C2B | 90.01 (8) |
| O2A—C1A—C2A | 111.72 (14) | C1B—O2B—C21B | 116.43 (15) |
| C3A—C2A—C1A | 125.29 (15) | C17B—O3B—C20B | 105.86 (17) |
| C3A—C2A—S1A | 113.86 (12) | C5B—N1B—C8B | 116.09 (14) |
| C1A—C2A—S1A | 120.82 (13) | C3B—N2B—HN2C | 118.1 (17) |
| N2A—C3A—C2A | 123.59 (16) | C3B—N2B—HN2D | 117.4 (16) |

| | | | |
|---|---|---|---|
| N2A—C3A—C4A | 125.07 (15) | HN2C—N2B—HN2D | 123 (2) |
| C2A—C3A—C4A | 111.28 (14) | O1B—C1B—O2B | 123.64 (16) |
| C5A—C4A—C6A | 116.60 (15) | O1B—C1B—C2B | 124.09 (17) |
| C5A—C4A—C3A | 111.16 (14) | O2B—C1B—C2B | 112.27 (14) |
| C6A—C4A—C3A | 132.24 (15) | C3B—C2B—C1B | 124.31 (15) |
| N1A—C5A—C4A | 126.37 (15) | C3B—C2B—S1B | 113.89 (12) |
| N1A—C5A—S1A | 120.04 (12) | C1B—C2B—S1B | 121.71 (13) |
| C4A—C5A—S1A | 113.57 (12) | N2B—C3B—C2B | 124.67 (16) |
| C7A—C6A—C4A | 118.25 (15) | N2B—C3B—C4B | 124.03 (16) |
| C7A—C6A—C17A | 121.3 (4) | C2B—C3B—C4B | 111.30 (14) |
| C4A—C6A—C17A | 120.4 (4) | C5B—C4B—C6B | 117.14 (15) |
| C7A—C6A—C17C | 113.9 (14) | C5B—C4B—C3B | 111.62 (14) |
| C4A—C6A—C17C | 127.7 (15) | C6B—C4B—C3B | 131.22 (15) |
| C6A—C7A—C8A | 119.02 (15) | N1B—C5B—C4B | 125.63 (15) |
| C6A—C7A—C16A | 123.28 (15) | N1B—C5B—S1B | 121.24 (12) |
| C8A—C7A—C16A | 117.69 (14) | C4B—C5B—S1B | 113.13 (12) |
| N1A—C8A—C7A | 123.43 (15) | C7B—C6B—C4B | 118.55 (15) |
| N1A—C8A—C9A | 116.55 (14) | C7B—C6B—C17B | 120.77 (15) |
| C7A—C8A—C9A | 119.99 (14) | C4B—C6B—C17B | 120.67 (15) |
| C10A—C9A—C14A | 119.81 (15) | C6B—C7B—C8B | 118.87 (15) |
| C10A—C9A—C8A | 120.47 (15) | C6B—C7B—C16B | 122.78 (15) |
| C14A—C9A—C8A | 119.66 (15) | C8B—C7B—C16B | 118.33 (15) |
| C11A—C10A—C9A | 120.58 (17) | N1B—C8B—C7B | 123.58 (15) |
| C11A—C10A—H10A | 119.7 | N1B—C8B—C9B | 117.15 (14) |
| C9A—C10A—H10A | 119.7 | C7B—C8B—C9B | 119.27 (15) |
| C10A—C11A—C12A | 119.66 (17) | C10B—C9B—C14B | 119.73 (16) |
| C10A—C11A—H11A | 120.2 | C10B—C9B—C8B | 120.65 (15) |
| C12A—C11A—H11A | 120.2 | C14B—C9B—C8B | 119.61 (15) |
| C13A—C12A—C11A | 120.09 (17) | C11B—C10B—C9B | 120.21 (17) |
| C13A—C12A—H12A | 120.0 | C11B—C10B—H10B | 119.9 |
| C11A—C12A—H12A | 120.0 | C9B—C10B—H10B | 119.9 |
| C12A—C13A—C14A | 121.05 (17) | C10B—C11B—C12B | 120.20 (17) |
| C12A—C13A—H13A | 119.5 | C10B—C11B—H11B | 119.9 |
| C14A—C13A—H13A | 119.5 | C12B—C11B—H11B | 119.9 |
| C13A—C14A—C9A | 118.81 (16) | C13B—C12B—C11B | 119.98 (17) |
| C13A—C14A—C15A | 121.67 (16) | C13B—C12B—H12B | 120.0 |
| C9A—C14A—C15A | 119.48 (15) | C11B—C12B—H12B | 120.0 |
| C14A—C15A—C16A | 112.13 (14) | C12B—C13B—C14B | 120.85 (17) |
| C14A—C15A—H15A | 109.2 | C12B—C13B—H13B | 119.6 |
| C16A—C15A—H15A | 109.2 | C14B—C13B—H13B | 119.6 |
| C14A—C15A—H15B | 109.2 | C13B—C14B—C9B | 119.00 (17) |
| C16A—C15A—H15B | 109.2 | C13B—C14B—C15B | 122.50 (16) |
| H15A—C15A—H15B | 107.9 | C9B—C14B—C15B | 118.48 (15) |
| C7A—C16A—C15A | 111.91 (14) | C14B—C15B—C16B | 110.83 (15) |
| C7A—C16A—H16A | 109.2 | C14B—C15B—H15C | 109.5 |
| C15A—C16A—H16A | 109.2 | C16B—C15B—H15C | 109.5 |
| C7A—C16A—H16B | 109.2 | C14B—C15B—H15D | 109.5 |
| C15A—C16A—H16B | 109.2 | C16B—C15B—H15D | 109.5 |

| | | | |
|---|---|---|---|
| H16A—C16A—H16B | 107.9 | H15C—C15B—H15D | 108.1 |
| C18A—C17A—O3A | 109.3 (3) | C7B—C16B—C15B | 111.29 (15) |
| C18A—C17A—C6A | 132.4 (5) | C7B—C16B—H16C | 109.4 |
| O3A—C17A—C6A | 118.1 (4) | C15B—C16B—H16C | 109.4 |
| C17A—C18A—C19A | 106.0 (5) | C7B—C16B—H16D | 109.4 |
| C17A—C18A—H18A | 127.0 | C15B—C16B—H16D | 109.4 |
| C19A—C18A—H18A | 127.0 | H16C—C16B—H16D | 108.0 |
| C20A—C19A—C18A | 107.3 (5) | C18B—C17B—O3B | 110.89 (16) |
| C20A—C19A—H19A | 126.3 | C18B—C17B—C6B | 130.61 (16) |
| C18A—C19A—H19A | 126.3 | O3B—C17B—C6B | 118.31 (15) |
| C19A—C20A—O3A | 110.5 (4) | C17B—C18B—C19B | 105.84 (18) |
| C19A—C20A—H20A | 124.8 | C17B—C18B—H18B | 127.1 |
| O3A—C20A—H20A | 124.8 | C19B—C18B—H18B | 127.1 |
| C20A—O3A—C17A | 106.9 (3) | C20B—C19B—C18B | 106.74 (18) |
| C18C—C17C—O3C | 111.9 (10) | C20B—C19B—H19B | 126.6 |
| C18C—C17C—C6A | 131.8 (15) | C18B—C19B—H19B | 126.6 |
| O3C—C17C—C6A | 116.1 (13) | C19B—C20B—O3B | 110.66 (19) |
| C17C—C18C—C19C | 105.3 (15) | C19B—C20B—H20B | 124.7 |
| C17C—C18C—H18C | 127.3 | O3B—C20B—H20B | 124.7 |
| C19C—C18C—H18C | 127.3 | O2B—C21B—C22B | 111.23 (17) |
| C20C—C19C—C18C | 106.2 (16) | O2B—C21B—H21C | 109.4 |
| C20C—C19C—H19C | 126.9 | C22B—C21B—H21C | 109.4 |
| C18C—C19C—H19C | 126.9 | O2B—C21B—H21D | 109.4 |
| C19C—C20C—O3C | 113.0 (11) | C22B—C21B—H21D | 109.4 |
| C19C—C20C—H20C | 123.5 | H21C—C21B—H21D | 108.0 |
| O3C—C20C—H20C | 123.5 | C21B—C22B—H22D | 109.5 |
| C17C—O3C—C20C | 103.3 (8) | C21B—C22B—H22E | 109.5 |
| O2A—C21A—C22A | 107.13 (16) | H22D—C22B—H22E | 109.5 |
| O2A—C21A—H21A | 110.3 | C21B—C22B—H22F | 109.5 |
| C22A—C21A—H21A | 110.3 | H22D—C22B—H22F | 109.5 |
| O2A—C21A—H21B | 110.3 | H22E—C22B—H22F | 109.5 |
| C22A—C21A—H21B | 110.3 | | |

| | | | |
|---|---|---|---|
| C21A—O2A—C1A—O1A | −1.3 (2) | C6A—C17C—C18C—C19C | 178 (5) |
| C21A—O2A—C1A—C2A | 178.60 (14) | C17C—C18C—C19C—C20C | −1 (6) |
| O1A—C1A—C2A—C3A | 9.5 (3) | C18C—C19C—C20C—O3C | −2 (6) |
| O2A—C1A—C2A—C3A | −170.43 (15) | C18C—C17C—O3C—C20C | −5 (3) |
| O1A—C1A—C2A—S1A | −172.33 (14) | C6A—C17C—O3C—C20C | 180 (2) |
| O2A—C1A—C2A—S1A | 7.7 (2) | C19C—C20C—O3C—C17C | 4 (4) |
| C5A—S1A—C2A—C3A | −2.08 (13) | C1A—O2A—C21A—C22A | −171.67 (15) |
| C5A—S1A—C2A—C1A | 179.55 (14) | C21B—O2B—C1B—O1B | 4.1 (3) |
| C1A—C2A—C3A—N2A | 3.6 (3) | C21B—O2B—C1B—C2B | −175.31 (16) |
| S1A—C2A—C3A—N2A | −174.69 (14) | O1B—C1B—C2B—C3B | −7.0 (3) |
| C1A—C2A—C3A—C4A | −179.28 (15) | O2B—C1B—C2B—C3B | 172.40 (16) |
| S1A—C2A—C3A—C4A | 2.43 (18) | O1B—C1B—C2B—S1B | 176.55 (15) |
| N2A—C3A—C4A—C5A | 175.54 (16) | O2B—C1B—C2B—S1B | −4.0 (2) |
| C2A—C3A—C4A—C5A | −1.5 (2) | C5B—S1B—C2B—C3B | 0.65 (14) |
| N2A—C3A—C4A—C6A | −3.6 (3) | C5B—S1B—C2B—C1B | 177.45 (15) |

| | | | |
|---|---|---|---|
| C2A—C3A—C4A—C6A | 179.29 (17) | C1B—C2B—C3B—N2B | 1.0 (3) |
| C8A—N1A—C5A—C4A | 1.3 (2) | S1B—C2B—C3B—N2B | 177.72 (14) |
| C8A—N1A—C5A—S1A | 179.82 (12) | C1B—C2B—C3B—C4B | −178.74 (16) |
| C6A—C4A—C5A—N1A | −2.1 (2) | S1B—C2B—C3B—C4B | −2.04 (18) |
| C3A—C4A—C5A—N1A | 178.59 (15) | N2B—C3B—C4B—C5B | −177.03 (16) |
| C6A—C4A—C5A—S1A | 179.31 (12) | C2B—C3B—C4B—C5B | 2.7 (2) |
| C3A—C4A—C5A—S1A | −0.02 (18) | N2B—C3B—C4B—C6B | 4.7 (3) |
| C2A—S1A—C5A—N1A | −177.56 (14) | C2B—C3B—C4B—C6B | −175.54 (16) |
| C2A—S1A—C5A—C4A | 1.15 (13) | C8B—N1B—C5B—C4B | 0.3 (2) |
| C5A—C4A—C6A—C7A | 0.3 (2) | C8B—N1B—C5B—S1B | −178.94 (12) |
| C3A—C4A—C6A—C7A | 179.43 (16) | C6B—C4B—C5B—N1B | −3.0 (2) |
| C5A—C4A—C6A—C17A | 177.9 (5) | C3B—C4B—C5B—N1B | 178.47 (15) |
| C3A—C4A—C6A—C17A | −2.9 (5) | C6B—C4B—C5B—S1B | 176.26 (11) |
| C5A—C4A—C6A—C17C | −174.5 (14) | C3B—C4B—C5B—S1B | −2.28 (18) |
| C3A—C4A—C6A—C17C | 4.6 (14) | C2B—S1B—C5B—N1B | −179.74 (14) |
| C4A—C6A—C7A—C8A | 2.0 (2) | C2B—S1B—C5B—C4B | 0.97 (13) |
| C17A—C6A—C7A—C8A | −175.6 (5) | C5B—C4B—C6B—C7B | 2.4 (2) |
| C17C—C6A—C7A—C8A | 177.5 (13) | C3B—C4B—C6B—C7B | −179.40 (16) |
| C4A—C6A—C7A—C16A | −177.02 (15) | C5B—C4B—C6B—C17B | −176.52 (14) |
| C17A—C6A—C7A—C16A | 5.4 (5) | C3B—C4B—C6B—C17B | 1.7 (3) |
| C17C—C6A—C7A—C16A | −1.5 (13) | C4B—C6B—C7B—C8B | 0.5 (2) |
| C5A—N1A—C8A—C7A | 1.3 (2) | C17B—C6B—C7B—C8B | 179.46 (14) |
| C5A—N1A—C8A—C9A | −176.71 (14) | C4B—C6B—C7B—C16B | 179.20 (15) |
| C6A—C7A—C8A—N1A | −2.9 (2) | C17B—C6B—C7B—C16B | −1.9 (2) |
| C16A—C7A—C8A—N1A | 176.12 (15) | C5B—N1B—C8B—C7B | 3.1 (2) |
| C6A—C7A—C8A—C9A | 174.99 (15) | C5B—N1B—C8B—C9B | −176.47 (14) |
| C16A—C7A—C8A—C9A | −5.9 (2) | C6B—C7B—C8B—N1B | −3.5 (2) |
| N1A—C8A—C9A—C10A | −14.4 (2) | C16B—C7B—C8B—N1B | 177.76 (15) |
| C7A—C8A—C9A—C10A | 167.52 (15) | C6B—C7B—C8B—C9B | 176.01 (14) |
| N1A—C8A—C9A—C14A | 162.75 (15) | C16B—C7B—C8B—C9B | −2.7 (2) |
| C7A—C8A—C9A—C14A | −15.3 (2) | N1B—C8B—C9B—C10B | 21.6 (2) |
| C14A—C9A—C10A—C11A | −0.3 (3) | C7B—C8B—C9B—C10B | −157.97 (15) |
| C8A—C9A—C10A—C11A | 176.87 (16) | N1B—C8B—C9B—C14B | −159.47 (15) |
| C9A—C10A—C11A—C12A | −0.2 (3) | C7B—C8B—C9B—C14B | 21.0 (2) |
| C10A—C11A—C12A—C13A | 0.2 (3) | C14B—C9B—C10B—C11B | 0.1 (2) |
| C11A—C12A—C13A—C14A | 0.2 (3) | C8B—C9B—C10B—C11B | 179.05 (15) |
| C12A—C13A—C14A—C9A | −0.7 (3) | C9B—C10B—C11B—C12B | 1.3 (3) |
| C12A—C13A—C14A—C15A | −178.61 (17) | C10B—C11B—C12B—C13B | −1.0 (3) |
| C10A—C9A—C14A—C13A | 0.7 (2) | C11B—C12B—C13B—C14B | −0.6 (3) |
| C8A—C9A—C14A—C13A | −176.44 (15) | C12B—C13B—C14B—C9B | 2.0 (3) |
| C10A—C9A—C14A—C15A | 178.67 (16) | C12B—C13B—C14B—C15B | −179.48 (18) |
| C8A—C9A—C14A—C15A | 1.5 (2) | C10B—C9B—C14B—C13B | −1.7 (2) |
| C13A—C14A—C15A—C16A | −150.95 (16) | C8B—C9B—C14B—C13B | 179.34 (15) |
| C9A—C14A—C15A—C16A | 31.2 (2) | C10B—C9B—C14B—C15B | 179.67 (15) |
| C6A—C7A—C16A—C15A | −142.57 (17) | C8B—C9B—C14B—C15B | 0.7 (2) |
| C8A—C7A—C16A—C15A | 38.4 (2) | C13B—C14B—C15B—C16B | 143.97 (17) |
| C14A—C15A—C16A—C7A | −50.0 (2) | C9B—C14B—C15B—C16B | −37.5 (2) |
| C7A—C6A—C17A—C18A | −53.5 (15) | C6B—C7B—C16B—C15B | 147.24 (16) |

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|---|---|---|---|
| C4A—C6A—C17A—C18A | 128.9 (11) | C8B—C7B—C16B—C15B | −34.1 (2) |
| C7A—C6A—C17A—O3A | 121.3 (7) | C14B—C15B—C16B—C7B | 52.9 (2) |
| C4A—C6A—C17A—O3A | −56.3 (12) | C20B—O3B—C17B—C18B | −0.7 (2) |
| O3A—C17A—C18A—C19A | 1.8 (15) | C20B—O3B—C17B—C6B | −176.30 (17) |
| C6A—C17A—C18A—C19A | 177.0 (16) | C7B—C6B—C17B—C18B | 87.1 (2) |
| C17A—C18A—C19A—C20A | −1 (2) | C4B—C6B—C17B—C18B | −94.0 (2) |
| C18A—C19A—C20A—O3A | −0.7 (19) | C7B—C6B—C17B—O3B | −98.35 (19) |
| C19A—C20A—O3A—C17A | 1.8 (14) | C4B—C6B—C17B—O3B | 80.6 (2) |
| C18A—C17A—O3A—C20A | −2.3 (10) | O3B—C17B—C18B—C19B | 1.1 (2) |
| C6A—C17A—O3A—C20A | −178.2 (7) | C6B—C17B—C18B—C19B | 175.93 (18) |
| C7A—C6A—C17C—C18C | 125 (4) | C17B—C18B—C19B—C20B | −1.0 (2) |
| C4A—C6A—C17C—C18C | −60 (5) | C18B—C19B—C20B—O3B | 0.6 (3) |
| C7A—C6A—C17C—O3C | −61 (3) | C17B—O3B—C20B—C19B | 0.1 (3) |
| C4A—C6A—C17C—O3C | 114 (2) | C1B—O2B—C21B—C22B | −82.2 (2) |
| O3C—C17C—C18C—C19C | 4 (4) | | |

*Hydrogen-bond geometry (Å, º)*

Cg8, Cg9 and Cg11 are the centroids of the O3*B*/C17*B*–C20*B* furan, N1*B*/C4*B*–C8*B* pyridine and C9*B*–C14*B* benzene rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2*A*—H*N*2*A*···O1*A* | 0.83 (3) | 2.23 (3) | 2.839 (2) | 131 (2) |
| N2*A*—H*N*2*A*···O1*B* | 0.83 (3) | 2.33 (3) | 2.962 (2) | 134 (2) |
| N2*A*—H*N*2*B*···O3*A* | 0.86 (3) | 2.17 (3) | 2.869 (3) | 138 (2) |
| N2*B*—H*N*2*D*···O1*A* | 0.87 (3) | 2.33 (2) | 2.998 (2) | 134 (2) |
| N2*B*—H*N*2*D*···O1*B* | 0.87 (3) | 2.17 (2) | 2.802 (2) | 129 (2) |
| N2*B*—H*N*2*C*···*Cg*8 | 0.83 (3) | 2.55 (3) | 3.294 (2) | 150 (2) |
| C18*B*—H18*B*···*Cg*11$^{i}$ | 0.93 | 2.53 | 3.353 (2) | 148 |
| C21*A*—H21*A*···*Cg*9$^{i}$ | 0.97 | 2.96 | 3.718 (2) | 136 |
| C15*A*—H15*A*···N1*A*$^{ii}$ | 0.97 | 2.61 | 3.386 (2) | 137 |

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