organic compounds

Acta Crystallographica Section E Structure Reports Online

ISSN 1600-5368

2-Bromo-5-*tert*-butyl-*N*-methyl-*N*-[2-(methylamino)phenyl]-3-(1-methyl-1*H*benzimidazol-2-yl)benzamide

Poonam Rajesh Prasad,^a Shikha Das,^a Harkesh B. Singh^a and Ray J. Butcher^{b*}

^aDepartment of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400 076, India, and ^bDepartment of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA Correspondence e-mail: rbutcher99@yahoo.com

Received 18 June 2014; accepted 19 June 2014

Key indicators: single-crystal X-ray study; T = 123 K; mean σ (C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.093; data-to-parameter ratio = 16.0.

In the title compound, $C_{27}H_{29}BrN_4O$, benzimidazole ring system and the amide moiety are planar [r.m.s. deviations = 0.016 (2) and 0.017 (1) Å, respectively]. The molecule adopts a conformation in which the amide linkage is almost perpendicular to the central ring [dihedral angle = 85.79 (8)°], while the benzimidazole ring system makes a dihedral angle of 70.26 (11)° with the central ring. In the crystal, the molecules form dimers through N-H···O hydrogen bonds and C-H···O interactions. These dimers are further linked into zigzag ribbons along [201] by weak C-H···Br interactions. As a result of the bulky nature of the molecule, as evidenced by the large dihedral angles between rings, there is little evidence for any π - π interactions.

Related literature

The metal binding properties of imidazole-containing pincer ligands can be modified by the type of donor atoms and the electron-withdrawing and electron-releasing character of their substituents, see: Selander & Szabó (2011). For the effect of *N*-substitution on the catalytic activity of phosphinoimidazolines in palladium-catalysed Heck reactions, see: Busacca *et al.* (2003). For the use of bromine-substituted benzimidazole in Heck reactions, see: Reddy & Krishna (2005). For standard bond lengths, see: Allen *et al.* (1987). For the preparation of the precursor, 2-bromo-5-(*tert*-butyl)isophthalic acid, see: Field *et al.* (2003).



Experimental

Crystal data $C_{27}H_{29}BrN_4O$ $M_r = 505.45$ Monoclinic, C2/c a = 34.4327 (13) Å b = 9.4152 (2) Å c = 17.1092 (7) Å $\beta = 118.312$ (5)°

Data collection

```
Agilent Xcalibur Ruby Gemini
diffractometer
Absorption correction: multi-scan
(CrysAlis PRO; Agilent, 2012)
T_{\rm min} = 0.788, T_{\rm max} = 1.000
```

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.034$ $wR(F^2) = 0.093$ S = 1.034929 reflections 308 parameters Cu $K\alpha$ radiation $\mu = 2.50 \text{ mm}^{-1}$ T = 123 K $0.38 \times 0.32 \times 0.23 \text{ mm}$

V = 4883.2 (3) Å³

Z = 8

CrossMark

9307 measured reflections 4929 independent reflections 4100 reflections with $I > 2\sigma(I)$ $R_{\rm int} = 0.028$

]	H atoms treated by a mixture of
	independent and constrained
	refinement
	$\Delta \rho_{\rm max} = 0.43 \ {\rm e} \ {\rm \AA}^{-3}$
	$\Delta \rho_{\rm min} = -0.35 \text{ e } \text{\AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$N3-H3B\cdotsO1^{i}$ $C4-H4A\cdotsBr^{ii}$ $C12-H12A\cdotsO1^{i}$	0.81 (3) 0.95 0.95	2.35 (3) 2.98 2.37	3.038 (3) 3.719 (3) 3.287 (3)	143 (3) 135 163
Summatry and as (i)	x + 1 $y = -1$	(33) $x + 3$ y	1 - 1 3	

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

RJB acknowledges the NSF MRI program (grant No. CHE-0619278) for funds to purchase an X-ray diffractometer.

Supporting information for this paper is available from the IUCr electronic archives (Reference: JJ2190).

References

- Agilent (2012). CrysalisAlis PRO and CrysAlis RED. Agilent Technologies, Yarnton, England.
- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). J. Chem. Soc. Perkin Trans. 2, pp. S1–19.
- Busacca, C. A., Grossbach, D., So, R. C., O'Brien, E. M. & Spinelli, E. M. (2003). Org. Lett. 5, 595–598.
- Field, J. E., Hill, T. J. & Venkataraman, D. J. (2003). J. Org. Chem. 68, 6071– 6078.
- Reddy, K. R. & Krishna, G. G. (2005). Tetrahedron Lett. 46, 661–663.
- Selander, N. J. & Szabó, K. (2011). Chem. Rev. 111, 2048-2076.
- Sheldrick, G. M. (2008). Acta Cryst. A64, 112–122.

supporting information

Acta Cryst. (2014). E70, o822-o823 [doi:10.1107/S1600536814014433]

2-Bromo-5-*tert*-butyl-*N*-methyl-*N*-[2-(methylamino)phenyl]-3-(1-methyl-1*H*-benzimidazol-2-yl)benzamide

Poonam Rajesh Prasad, Shikha Das, Harkesh B. Singh and Ray J. Butcher

1. Experimental

The methylation reaction of **2** (Fig. 1) was carried out by reacting **1** (0.5 g, 1.12 mmol) with an excess of methyl iodide (1.75 g, 10 eq), followed by the addition of KOH (0.125 g, 2.24 mmol) in dry acetone (20 mL) and some molecular sieves. The reaction mixture was refluxed for 2 h. Then, it was diluted with ethyl acetate and washed with water. The organic layer was dried over Na₂SO₄ and purified by column chromatography to afford **2** which was crystallized from a mixture of dichloromethane and ether. Anal. Calcd. for $C_{27}H_{29}BrON_4$: C, 64.16; H, 5.78; N, 11.08; found C, 64.30; H, 6.22; N, 9.17.

1.1. Refinement

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with a C—H distances of 0.95 and 0.98 Å $U_{iso}(H) = 1.2U_{eq}(C)$ and 0.96 Å for CH₃ [$U_{iso}(H) = 1.5U_{eq}(C)$]. The hydrogen atom attached to N3 was located in a difference Fourier and refined isotropically.

2. Comment

The presence of imidazole rings in any molecular framework provides excellent modification sites for the fine tuning of properties related to electronic and steric factors. It has been reported in the literature that the strong electronic effect can be modified by the type of donor atoms and the electron-withdrawing and electron-releasing character of their substituents (Selander, & Szabó, 2011). Recently the effect of *N*-substitution on the catalytic activities of phosphinoimidazolines in palladium catalyzed Heck reactions has been reported (Busacca *et al.*, 2003). Later, Reddy and co-workers (Reddy, & Krishna, 2005) have studied the use of bromine substituted benzimidazole in Heck reactions. Pincer ligands have immense scope in exploring different types of metal coordination chemistry and stabilizing unusual species. They provide the sites which can be easily fine tuned to synthesize a number of metal complexes/species, which can be stabilized by three coordinating/bonding units of the pincer ligands. There are no examples of selenium containing benzimidazoles known in the literature. Therefore, 2, 2'-(2-bromo-5-(*tert*-butyl)-1,3-diyl)bis(1H-benzimidazole) (1) and its derivatives, having two coordinating imidazole rings were designed to incorporate selenium at 2-position of the phenyl group. An attempted methylation of 1 led to cleavage of the one of the benzimidazole rings and resulted in the formation of unexpected compound **2** (Fig. 1). 2-Bromo-5-(*tert*-butyl)isophthalic acid, the precursor for synthesizing 1, was prepared according to literature procedure (Field, *et al.*, 2003). Compound 1 was synthesized by the reaction of 2-bromo-5-*tert*-butyl-isophthalic acid with 1,2-phenylenediamine in polyphosphoric acid at 240°C.

In view of the above, the structure of the title compound, $C_{27}H_{29}BrN_4O$, was determined (Fig. 2). The bond lengths and angles are all in the expected ranges (Allen *et al.*, 1987) for such compounds. All the aromatic groups and the amide moiety are planar (rms deviations of 0.006 (1), 0.008 (2), 0.016 (2), and 0.017 (1) for the central phenyl ring, the

substituent phenyl ring, the benzimidazole ring, and the amide moiety, respectively). The molecule adopts a conformation where the amide linkage is almost perpendicular to the central ring with a dihedral angle of $85.79 (8)^{\circ}$ between central ring (C9–C14) and amide moiety (C19/C20/C21/N4/O1) while the benzimidazole ring makes a dihedral angle of 70.26° with the central ring. The molecules form dimers through N3—H···O1 intermolecular hydrogen bonds (Fig. 3). These dimers are further linked into zig-zag ribbons in the [2 0 1] direction by weak C—H…Br interactions. Because of the bulky nature of the molecule, as evidenced by the large dihedral angles between rings, there is little evidence for any π - π interactions.



Figure 2

Figure 1

The molecular structure of $C_{27}H_{29}BrN_4O$, showing the atom numbering scheme and 30% probability displacement ellipsoids and the linking of the molecules into dimers by N-H-O hydrogen bonds (shown as dashed bonds).



Figure 3

The molecular packing for $C_{27}H_{29}BrN_4O$ viewed along the *b* axis showing linking of the hydrogen bonded dimers into zigzag chains in the [2 0 1] direction by C—H···Br interactions (N—H···O and C—H···Br interactions shown as dashed bonds).

2-Bromo-5-tert-butyl-N-methyl-N-[2-(methylamino)phenyl]-3-(1-methyl-1H-benzimidazol-2-yl)benzamide

Crystal data	
$C_{27}H_{29}BrN_{4}O$ $M_{r} = 505.45$ Monoclinic, C2/c Hall symbol: -C 2yc a = 34.4327 (13) Å b = 9.4152 (2) Å c = 17.1092 (7) Å $\beta = 118.312 (5)^{\circ}$ $V = 4883.2 (3) Å^{3}$ Z = 8	F(000) = 2096 $D_x = 1.375 \text{ Mg m}^{-3}$ Cu Ka radiation, $\lambda = 1.54184 \text{ Å}$ Cell parameters from 4036 reflections $\theta = 2.9-75.5^{\circ}$ $\mu = 2.50 \text{ mm}^{-1}$ T = 123 K Prism, colorless $0.38 \times 0.32 \times 0.23 \text{ mm}$
Data collection	
Agilent Xcalibur Ruby Gemini diffractometer Radiation source: Enhance (Cu) X-ray Source Graphite monochromator Detector resolution: 10.5081 pixels mm ⁻¹ ω scans	Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2012) $T_{min} = 0.788$, $T_{max} = 1.000$ 9307 measured reflections 4929 independent reflections 4100 reflections with $I > 2\sigma(I)$ $R_{int} = 0.028$

$\theta_{\rm max} = 75.6^\circ, \theta_{\rm min} = 2.9^\circ$	$k = -8 \rightarrow 11$
$h = -42 \rightarrow 42$	$l = -20 \rightarrow 21$
Refinement	
Refinement on F^2	Secondary atom site location: difference Fourier
Least-squares matrix: full	map
$R[F^2 > 2\sigma(F^2)] = 0.034$	Hydrogen site location: inferred from
$wR(F^2) = 0.093$	neighbouring sites
<i>S</i> = 1.03	H atoms treated by a mixture of independent
4929 reflections	and constrained refinement
308 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 0.4711P]$
0 restraints	where $P = (F_o^2 + 2F_c^2)/3$
Primary atom site location: structure-invariant	$(\Delta/\sigma)_{\rm max} = 0.004$
direct methods	$\Delta ho_{ m max} = 0.43 \ { m e} \ { m \AA}^{-3}$
	$\Delta \rho_{\rm min} = -0.35 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. ¹H NMR (400 MHz, CDCl₃): δ (ppm) 7.87-7.71 (1H, m), 7.46-7.31 (4H, m), 7.09-7.07 (1H, m), 6.54-6.48 (1H, m), 3.53 (2H, s), 3.45 (2H, s), 2.89 (2H, s), 1.38 (1H, s), 1.13 (6H, s). ¹³C NMR (CDCl₃): δ 29.4, 30.9, 31.1, 31.9, 31.2, 34.7, 35.1, 35.5, 53.9, 109.7, 109.9, 120.2, 122.1, 122.5, 122.7, 123.1, 123.3, 129.4, 129.7, 131.2, 133.0, 135.6, 142.8, 151.7, 152.6, 152.8.

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2 , conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ 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.

	x	у	Z	$U_{ m iso}$ */ $U_{ m eq}$
Br	0.630352 (8)	0.53882 (3)	0.543344 (15)	0.03435 (9)
01	0.52147 (5)	0.66100 (17)	0.36987 (11)	0.0338 (3)
N1	0.70366 (6)	0.3018 (2)	0.53797 (13)	0.0370 (4)
N2	0.65609 (7)	0.1320 (2)	0.53017 (14)	0.0380 (4)
N3	0.56938 (7)	0.7887 (2)	0.19074 (15)	0.0406 (5)
H3B	0.5490 (9)	0.765 (3)	0.1989 (18)	0.033 (7)*
N4	0.57538 (6)	0.78517 (19)	0.36118 (13)	0.0315 (4)
C1	0.72063 (8)	0.4328 (3)	0.52039 (19)	0.0447 (6)
H1A	0.6998	0.4684	0.4614	0.067*
H1B	0.7492	0.4142	0.5227	0.067*
H1C	0.7244	0.5039	0.5653	0.067*
C2	0.72791 (8)	0.2049 (3)	0.60366 (16)	0.0401 (5)
C3	0.77297 (9)	0.1991 (4)	0.66449 (19)	0.0541 (7)
H3A	0.7929	0.2717	0.6682	0.065*
C4	0.78664 (11)	0.0803 (4)	0.7190 (2)	0.0620 (9)
H4A	0.8171	0.0697	0.7600	0.074*
C5	0.75708 (12)	-0.0240 (4)	0.7155 (2)	0.0615 (8)
H5A	0.7679	-0.1020	0.7554	0.074*

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters $(Å^2)$

H6A 0.6929 -0.0892 0.6541 0.065^{++} C7 0.69805 (8) 0.1004 (3) 0.59819 (16) 0.0402 (5)C8 0.66112 (7) 0.2518 (2) 0.42009 (14) 0.0292 (4)C9 0.62557 (7) 0.3270 (2) 0.42009 (14) 0.0292 (4)C10 0.60873 (7) 0.2663 (2) 0.33589 (15) 0.0300 (4)H10A 0.6198 0.1769 0.3297 0.036^{++} C11 0.57614 (7) 0.3331 (2) 0.26044 (14) 0.0292 (4)C12 0.55997 (7) 0.4627 (2) 0.27251 (15) 0.0294 (4)H12A 0.5371 0.5266 (2) 0.35517 (14) 0.0264 (4)C13 0.57612 (6) 0.5266 (2) 0.16780 (16) 0.0358 (5)C16 0.59482 (11) 0.1859 (3) 0.15917 (19) 0.0543 (7)H16A 0.6042 0.1043 0.1996 0.081^{+} H16B 0.6200 0.2490 0.1744 0.081^{+} H16B 0.6200 0.2490 0.1744 0.081^{+} H17B 0.5328 0.0888 0.1979 0.104^{+} H17B 0.5328 0.0888 0.1979 0.104^{+} H17B 0.5326 0.3400 0.0387 0.054^{+} H18D 0.5306 0.3400 0.0387 0.054^{+} H18D 0.5362 0.3400 0.0387 0.054^{+} H17B 0.55254 (7) 0.6638 (2) 0.36324 (13) 0.0275 (4)C20 0.583836	H6A 0.6929 -0.0892 0.6541 0.0654° C7 $0.69805(8)$ $0.1004(3)$ $0.59819(16)$ $0.0402(5)$ C8 $0.66112(7)$ $0.2518(2)$ $0.4703(15)$ $0.0323(4)$ C9 $0.62557(7)$ $0.2270(2)$ $0.42009(14)$ $0.0292(4)$ C10 $0.60873(7)$ $0.2663(2)$ $0.33589(15)$ $0.0330(4)$ H10A 0.6198 0.1769 0.3297 0.036° C11 $0.57614(7)$ $0.3331(2)$ $0.26044(14)$ $0.0292(4)$ C12 $0.57612(7)$ $0.427(2)$ $0.27251(15)$ $0.0294(4)$ H12A 0.5371 $0.5266(2)$ $0.35517(14)$ $0.0226(4)$ C13 $0.57612(6)$ $0.5266(2)$ $0.35517(14)$ $0.0226(4)$ C14 $0.60895(7)$ $0.4577(2)$ $0.42851(14)$ $0.0276(4)$ C15 $0.55815(8)$ $0.2676(2)$ $0.16780(16)$ $0.0358(5)$ C16 $0.59482(11)$ $0.1859(3)$ 0.1996 0.081^{*} H168 0.6200 0.2490 0.1744 0.081^{*} H168 0.6200 0.2490 0.1744 0.081^{*} H177 $0.52108(12)$ $0.1646(4)$ $0.1534(2)$ $0.0693(11)$ H178 0.5328 0.0888 0.1979 0.104^{*} H178 0.5328 0.0888 0.1979 0.104^{*} H174 $0.5554(7)$ $0.6532(3)$ $0.3027(13)$ 0.054^{*} H175 $0.55254(7)$ 0.6532 $0.3331(2)$ $0.0936(5)$ C20 $0.55836(9)$ <	C6	0.71279 (11)	-0.0174 (3)	0.6561 (2)	0.0542 (7)
C7 $0.69805(8)$ $0.1004(3)$ $0.59819(16)$ $0.0402(5)$ C8 $0.66112(7)$ $0.2518(2)$ $0.49703(15)$ $0.0323(4)$ C9 $0.62557(7)$ $0.3270(2)$ $0.42009(14)$ $0.0292(4)$ C10 $0.60873(7)$ $0.2663(2)$ $0.33589(15)$ $0.0300(4)$ H10A 0.6198 0.1769 0.3297 0.036^* C11 $0.57614(7)$ $0.3331(2)$ $0.26044(14)$ $0.0292(4)$ C12 $0.5597(7)$ $0.4627(2)$ $0.7221(15)$ $0.0294(4)$ H12A 0.5371 0.5086 0.2224 0.035^* C13 $0.57612(6)$ $0.5266(2)$ $0.35517(14)$ $0.0264(4)$ C14 $0.60895(7)$ $0.4577(2)$ $0.4780(16)$ $0.0358(5)$ C15 $0.55815(8)$ $0.2676(2)$ $0.1578(16)$ $0.0358(5)$ C16 $0.59482(11)$ $0.1859(3)$ $0.15917(19)$ $0.0543(7)$ H16A 0.6042 0.1043 0.1996 0.081^* H16B 0.6200 0.2490 0.1744 0.081^* H17D $0.5218(12)$ $0.1646(4)$ $0.1534(2)$ $0.6693(11)$ H17A 0.4978 0.2157 0.1592 0.104^* H17B 0.5328 $0.3820(3)$ $0.090601(15)$ $0.0363(5)$ H18A 0.5131 0.4223 0.9925 0.054^* H18B $0.5366(9)$ $0.3216(2)$ $0.0426(6)$ C20 $0.55836(9)$ $0.9201(2)$ $0.35317(17)$ 0.054^* H18D 0.5622 0.9711 $0.33507(17)$	C70.69805 (8)0.1004 (3)0.59819 (16)0.0402 (5)C80.66112 (7)0.2518 (2)0.4703 (15)0.0323 (4)C90.62557 (7)0.3270 (2)0.42009 (14)0.0292 (4)C100.60873 (7)0.2663 (2)0.33589 (15)0.0300 (4)H10A0.61980.17690.32970.036*C110.57614 (7)0.3331 (2)0.26044 (14)0.0292 (4)L120.5597 (7)0.4627 (2)0.27251 (15)0.0294 (4)H12A0.53710.50860.22240.035*C130.57612 (6)0.5266 (2)0.35517 (14)0.0264 (4)C140.60895 (7)0.4577 (2)0.42851 (14)0.0276 (4)C150.55815 (8)0.2676 (2)0.16780 (16)0.0358 (5)C160.59482 (11)0.1859 (3)0.15917 (19)0.0543 (7)H16A0.60200.24900.17440.081*H16C0.58350.15240.09800.081*H16C0.58350.15240.09800.081*H17A0.49780.21570.15920.104*H17B0.53280.08880.10790.104*H17B0.53360.34000.03870.054*H18B0.53360.34000.03870.054*H18B0.53360.34000.03870.054*H18B0.53620.97110.39470.064*H20C0.58270.97510.41180.050*C210.65480.97130.319	H6A	0.6929	-0.0892	0.6541	0.065*
C8 0.66112 (7) 0.2518 (2) 0.49703 (15) 0.0323 (4)C9 0.62557 (7) 0.3270 (2) 0.42009 (14) 0.0292 (4)C10 0.60873 (7) 0.2663 (2) 0.33589 (15) 0.0300 (4)H10A 0.6198 0.1769 0.3297 0.036^* C11 0.57614 (7) 0.3331 (2) 0.26044 (14) 0.0292 (4)C12 0.55997 (7) 0.4627 (2) 0.27251 (15) 0.0294 (4)C13 0.57612 (6) 0.5266 (2) 0.35517 (14) 0.0294 (4)C14 0.60895 (7) 0.4577 (2) 0.42851 (14) 0.0276 (4)C15 0.55815 (8) 0.2676 (2) 0.16780 (16) 0.0358 (5)C16 0.59482 (11) 0.1889 (3) 0.15917 (19) 0.0543 (7)H16A 0.6042 0.1043 0.1996 $0.081*$ H16B 0.6200 0.2490 0.1744 $0.081*$ H17C 0.52188 0.2157 0.1592 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17B 0.5326 0.3420 (3) 0.09601 (15) 0.0363 (5)H18A 0.5131 0.4223 0.0925 $0.054*$ H18B 0.5362 0.9713 $0.104*$ $0.54*$ C18 0.5448 0.9743 0.3199 $0.064*$ H20A 0.5362 0.9713 0.35017 (17) 0.0326 (5)C22 0.4573 0.1108 <t< td=""><td>C8$0.66112$ (T)0.2518 (2)0.49703 (15)0.0323 (4)C9$0.62557$ (7)0.3270 (2)0.42009 (14)0.0292 (4)C10$0.60873$ (7)0.2663 (2)0.33589 (15)0.0300 (4)H10A$0.6198$$0.1769$$0.3297$$0.036^*$C11$0.57614$ (7)0.3331 (2)0.26044 (14)0.0292 (4)C12$0.55997$ (7)0.4627 (2)0.27251 (15)0.0294 (4)H12A$0.5371$$0.5086$$0.2224$$0.035^*$C13$0.57612$ (6)0.5266 (2)0.35517 (14)0.0264 (4)C14$0.60895$ (7)0.4577 (2)0.42851 (14)0.0276 (4)C15$0.55815$ (8)0.2676 (2)0.16780 (16)0.0584 (7)H16A$0.6042$$0.1043$$0.1996$$0.081^*$H16B$0.6200$$0.2490$$0.1744$$0.081^*$H17C$0.52108$ (12)0.1646 (4)0.1534 (2)0.0693 (11)H17A$0.4978$$0.2157$$0.1592$$0.104^*$H17C$0.5208$$0.1232$$0.0938$$0.104^*$H17C$0.5089$$0.1232$$0.0938$$0.104^*$H17A$0.4978$$0.2157$$0.1592$$0.054^*$H18A$0.5131$$0.4223$$0.0925$$0.054^*$H17B$0.5326$$0.3400$$0.0387$$0.054^*$H18C$0.5622$$0.4573$$0.1108$$0.0275$ (4)C19$0.55554$ (7)0.6638 (2)<td< td=""><td>C7</td><td>0.69805 (8)</td><td>0.1004 (3)</td><td>0.59819 (16)</td><td>0.0402 (5)</td></td<></td></t<>	C8 0.66112 (T) 0.2518 (2) 0.49703 (15) 0.0323 (4)C9 0.62557 (7) 0.3270 (2) 0.42009 (14) 0.0292 (4)C10 0.60873 (7) 0.2663 (2) 0.33589 (15) 0.0300 (4)H10A 0.6198 0.1769 0.3297 0.036^* C11 0.57614 (7) 0.3331 (2) 0.26044 (14) 0.0292 (4)C12 0.55997 (7) 0.4627 (2) 0.27251 (15) 0.0294 (4)H12A 0.5371 0.5086 0.2224 0.035^* C13 0.57612 (6) 0.5266 (2) 0.35517 (14) 0.0264 (4)C14 0.60895 (7) 0.4577 (2) 0.42851 (14) 0.0276 (4)C15 0.55815 (8) 0.2676 (2) 0.16780 (16) 0.0584 (7)H16A 0.6042 0.1043 0.1996 0.081^* H16B 0.6200 0.2490 0.1744 0.081^* H17C 0.52108 (12) 0.1646 (4) 0.1534 (2) 0.0693 (11)H17A 0.4978 0.2157 0.1592 0.104^* H17C 0.5208 0.1232 0.0938 0.104^* H17C 0.5089 0.1232 0.0938 0.104^* H17A 0.4978 0.2157 0.1592 0.054^* H18A 0.5131 0.4223 0.0925 0.054^* H17B 0.5326 0.3400 0.0387 0.054^* H18C 0.5622 0.4573 0.1108 0.0275 (4)C19 0.55554 (7) 0.6638 (2) <td< td=""><td>C7</td><td>0.69805 (8)</td><td>0.1004 (3)</td><td>0.59819 (16)</td><td>0.0402 (5)</td></td<>	C7	0.69805 (8)	0.1004 (3)	0.59819 (16)	0.0402 (5)
C9 0.62557 (7) 0.3270 (2) 0.42009 (14) 0.0292 (4)C10 0.60873 (7) 0.2663 (2) 0.33589 (15) 0.0300 (4)H10A 0.6198 0.1769 0.3297 0.036^* C11 0.57614 (7) 0.3331 (2) 0.26044 (14) 0.0292 (4)C12 0.55997 (7) 0.4627 (2) 0.27251 (15) 0.0294 (4)H12A 0.5371 0.5086 0.2224 0.035^* C13 0.57612 (6) 0.5266 (2) 0.35517 (14) 0.0264 (4)C14 0.60895 (7) 0.4577 (2) 0.42851 (14) 0.0276 (4)C15 0.55815 (8) 0.2676 (2) 0.16780 (16) 0.0388 (5)C16 0.59482 (11) 0.1899 (3) 0.15917 (19) 0.0543 (7)H16A 0.6042 0.1043 0.1996 0.081^* H16B 0.6200 0.2490 0.1744 0.081^* H16C 0.5335 0.1524 0.0980 0.081^* L17 0.52108 (12) 0.1646 (4) 0.1534 (2) 0.0693 (11)H17A 0.4978 0.2157 0.1592 0.104^* H17B 0.5328 0.3280 (3) 0.09601 (15) 0.0363 (5)L18A 0.5131 0.4223 0.0925 0.054^* H18D 0.5336 0.3400 0.3877 0.054^* H18C 0.5622 0.45733 0.1108 0.054^* L20 0.55554 (7) 0.6383 (2) 0.3612 (13) 0.0275 (4)L21 0.6458 <	C9 $0.62557(7)$ $0.3270(2)$ $0.42009(14)$ $0.0292(4)$ C10 $0.60873(7)$ $0.2663(2)$ $0.33589(15)$ $0.0300(4)$ H10A 0.6198 0.1769 0.3297 0.036^* C11 $0.57614(7)$ $0.3331(2)$ $0.26044(14)$ $0.0292(4)$ C12 $0.55997(7)$ $0.4627(2)$ $0.27251(15)$ $0.0294(4)$ H12A 0.3511 $0.5266(2)$ $0.35517(14)$ $0.0226(4)$ C13 $0.57612(6)$ $0.5266(2)$ $0.35517(14)$ $0.0226(4)$ C14 $0.60895(7)$ $0.4577(2)$ $0.42851(14)$ $0.0276(4)$ C15 $0.55815(8)$ $0.2676(2)$ $0.16780(16)$ $0.0358(5)$ C16 $0.59482(11)$ $0.1893(3)$ $0.15917(19)$ $0.0543(7)$ H16A 0.6042 0.1043 0.1996 $0.081*$ H16B 0.6200 0.2490 0.1744 $0.081*$ H16C 0.5835 0.1524 0.0980 $0.081*$ H17A 0.4978 0.2157 0.1592 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17B 0.5326 0.3400 0.0387 $0.054*$ H18B 0.5336 0.3400 0.0387 $0.054*$ H18B 0.5362 0.9011 0.3947 $0.064*$ L18A $0.5524(7)$ $0.6638(2)$ $0.35017(17)$ $0.0326(5)$ C20 $0.5584(7)$ 0.9711 $0.3217(4)$ $0.050*$ C21 0.6527 0.9711 $0.324(13)$ $0.0275(4)$ <td>C8</td> <td>0.66112 (7)</td> <td>0.2518 (2)</td> <td>0.49703 (15)</td> <td>0.0323 (4)</td>	C8	0.66112 (7)	0.2518 (2)	0.49703 (15)	0.0323 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C10 $0.60873 (7)$ $0.2663 (2)$ $0.33589 (15)$ $0.0300 (4)$ H10A 0.6198 0.1769 0.3297 $0.036*$ C11 $0.57614 (7)$ $0.3331 (2)$ $0.26044 (14)$ $0.0292 (4)$ C12 $0.5597 (7)$ $0.4627 (2)$ $0.27251 (15)$ $0.0294 (4)$ H12A 0.5371 0.5086 0.2224 $0.035*$ C13 $0.57612 (6)$ $0.5266 (2)$ $0.35517 (14)$ $0.0226 (4)$ C14 $0.60895 (7)$ $0.4577 (2)$ $0.42851 (14)$ $0.0276 (4)$ C15 $0.55815 (8)$ $0.2676 (2)$ $0.16780 (16)$ $0.0338 (5)$ C16 $0.59482 (11)$ $0.1859 (3)$ $0.15917 (19)$ $0.543 (7)$ H16A 0.6042 0.1043 0.1996 $0.081*$ H16C 0.5835 0.1524 0.0980 $0.081*$ C17 $0.52108 (12)$ $0.1646 (4)$ $0.1534 (2)$ $0.0693 (11)$ H17A 0.4978 0.2157 0.1592 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17B 0.5326 $0.3420 (3)$ $0.09601 (15)$ $0.0363 (5)$ H18A 0.5131 0.4223 0.0925 $0.054*$ H18B 0.5336 0.3400 0.0387 $0.054*$ H18B $0.5542 (7)$ $0.5913 (2)$ $0.35947 (2)$ $0.064*$ L20A 0.5622 0.4573 0.1108 $0.0275 (4)$ C20 $0.55836 (9)$ $0.9201 (2)$ $0.374 (2)$ $0.0664*$ H20A $0.5542 (7)$ $0.9751 ($	С9	0.62557 (7)	0.3270 (2)	0.42009 (14)	0.0292 (4)
H10A0.61980.17690.32970.036*C110.57614 (7)0.3331 (2)0.26044 (14)0.0292 (4)C120.55997 (7)0.4627 (2)0.27251 (15)0.0294 (4)H12A0.53710.50860.22240.035*C130.57612 (6)0.5266 (2)0.35517 (14)0.0264 (4)C140.60895 (7)0.4577 (2)0.42851 (14)0.0276 (4)C150.55815 (8)0.2676 (2)0.16780 (16)0.0358 (5)C160.59482 (11)0.1859 (3)0.15917 (19)0.0543 (7)H16A0.60420.10430.19960.081*H16B0.62000.24900.17440.081*H16C0.53350.15240.09800.081*C170.52108 (12)0.1646 (4)0.1534 (2)0.0693 (11)H17A0.49780.21570.15920.104*H17B0.53280.08880.19790.104*H17D0.50890.12320.09380.054*H18B0.53360.34000.03870.054*H18B0.53620.9201 (2)0.3754 (2)0.0426 (6)H20A0.53554 (7)0.6638 (2)0.36224 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.064*H20B0.54480.97430.31990.064*H20B0.5448 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8033 (3)0.42439 (18)0.0414 (5)H2A0.751 </td <td>H10A0.61980.17690.32970.036*C110.57614 (7)0.3331 (2)0.26044 (14)0.0292 (4)C120.55997 (7)0.4627 (2)0.27251 (15)0.0294 (4)H12A0.53710.50860.22240.035*C130.57612 (6)0.5266 (2)0.35517 (14)0.0264 (4)C140.60895 (7)0.4577 (2)0.42851 (14)0.0276 (4)C150.55815 (8)0.2676 (2)0.16780 (16)0.0358 (5)C160.59482 (11)0.1859 (3)0.15917 (19)0.0543 (7)H16A0.60420.10430.19960.081*H16B0.62000.24900.17440.081*H16C0.58350.15240.09800.081*C170.52108 (12)0.1646 (4)0.1534 (2)0.0693 (11)H17A0.49780.21570.15920.104*H17B0.53280.08880.19790.104*H17C0.50890.12320.09380.104*H17C0.50890.13220.03870.054*H18B0.53360.34000.03870.054*H18B0.53620.90110.3754 (2)0.0424 (6)H20A0.56220.45730.11080.054*C190.5554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.58270.97510.42120.064*C210.64480.97430.31990.064*C220.65527 (8)0.8083 (3)0.42439 (18)0.0</td> <td>C10</td> <td>0.60873 (7)</td> <td>0.2663 (2)</td> <td>0.33589 (15)</td> <td>0.0300 (4)</td>	H10A0.61980.17690.32970.036*C110.57614 (7)0.3331 (2)0.26044 (14)0.0292 (4)C120.55997 (7)0.4627 (2)0.27251 (15)0.0294 (4)H12A0.53710.50860.22240.035*C130.57612 (6)0.5266 (2)0.35517 (14)0.0264 (4)C140.60895 (7)0.4577 (2)0.42851 (14)0.0276 (4)C150.55815 (8)0.2676 (2)0.16780 (16)0.0358 (5)C160.59482 (11)0.1859 (3)0.15917 (19)0.0543 (7)H16A0.60420.10430.19960.081*H16B0.62000.24900.17440.081*H16C0.58350.15240.09800.081*C170.52108 (12)0.1646 (4)0.1534 (2)0.0693 (11)H17A0.49780.21570.15920.104*H17B0.53280.08880.19790.104*H17C0.50890.12320.09380.104*H17C0.50890.13220.03870.054*H18B0.53360.34000.03870.054*H18B0.53620.90110.3754 (2)0.0424 (6)H20A0.56220.45730.11080.054*C190.5554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.58270.97510.42120.064*C210.64480.97430.31990.064*C220.65527 (8)0.8083 (3)0.42439 (18)0.0	C10	0.60873 (7)	0.2663 (2)	0.33589 (15)	0.0300 (4)
C11 0.57614 (7) 0.3331 (2) 0.26044 (14) 0.0292 (4)C12 0.55997 (7) 0.4627 (2) 0.27251 (15) 0.0294 (4)H12A 0.5371 0.5086 0.2224 $0.035*$ C13 0.57612 (6) 0.5266 (2) 0.35517 (14) 0.0276 (4)C14 0.60895 (7) 0.4577 (2) 0.42851 (14) 0.0276 (4)C15 0.55815 (8) 0.2676 (2) 0.16780 (16) 0.0358 (5)C16 0.59482 (11) 0.1859 (3) 0.15917 (19) 0.0543 (7)H16A 0.6042 0.1043 0.1996 $0.081*$ H16B 0.6200 0.2490 0.1744 $0.081*$ H16C 0.5835 0.1524 0.0980 $0.081*$ H17A 0.4978 0.2157 0.1592 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17C 0.5089 0.1232 0.0938 $0.104*$ H17C 0.5089 0.1232 0.0925 $0.054*$ H18B 0.5336 0.3400 0.3877 $0.554*$ H18B 0.5362 0.9011 0.3947 $0.064*$ C19 0.5554 (7) 0.6638 (2) 0.36324 (13) 0.0275 (4)C20 0.55836 (9) 0.9201 (2) 0.3754 (2) $0.064*$ H20A 0.5362 0.9011 0.3947 $0.064*$ L214 0.6574 0.8092 0.4818 $0.050*$ C22 0.6527 (8) 0.8033 (3) 0.42439 (18) 0.0414 (5) </td <td>C11 0.57614 (7) 0.3331 (2) 0.26044 (14) 0.0292 (4) C12 0.55997 (7) 0.4627 (2) 0.27251 (15) 0.0294 (4) H12A 0.5371 0.5086 0.2224 0.035* C13 0.57612 (6) 0.5266 (2) 0.35517 (14) 0.0276 (4) C14 0.60895 (7) 0.4577 (2) 0.42851 (14) 0.0276 (4) C15 0.55815 (8) 0.2676 (2) 0.16780 (16) 0.0358 (5) C16 0.59482 (11) 0.1859 (3) 0.15917 (19) 0.0543 (7) H16A 0.6042 0.1043 0.1996 0.081* H16B 0.6200 0.2490 0.1744 0.081* H16C 0.5835 0.1524 0.0980 0.081* H17A 0.4978 0.2157 0.1592 0.104* H17A 0.5328 0.0888 0.1979 0.104* H17C 0.5089 0.1232 0.0925 0.054* H18D 0.5336 0.3400 0.0387 0.054*</td> <td>H10A</td> <td>0.6198</td> <td>0.1769</td> <td>0.3297</td> <td>0.036*</td>	C11 0.57614 (7) 0.3331 (2) 0.26044 (14) 0.0292 (4) C12 0.55997 (7) 0.4627 (2) 0.27251 (15) 0.0294 (4) H12A 0.5371 0.5086 0.2224 0.035* C13 0.57612 (6) 0.5266 (2) 0.35517 (14) 0.0276 (4) C14 0.60895 (7) 0.4577 (2) 0.42851 (14) 0.0276 (4) C15 0.55815 (8) 0.2676 (2) 0.16780 (16) 0.0358 (5) C16 0.59482 (11) 0.1859 (3) 0.15917 (19) 0.0543 (7) H16A 0.6042 0.1043 0.1996 0.081* H16B 0.6200 0.2490 0.1744 0.081* H16C 0.5835 0.1524 0.0980 0.081* H17A 0.4978 0.2157 0.1592 0.104* H17A 0.5328 0.0888 0.1979 0.104* H17C 0.5089 0.1232 0.0925 0.054* H18D 0.5336 0.3400 0.0387 0.054*	H10A	0.6198	0.1769	0.3297	0.036*
C12 0.55997 (7) 0.4627 (2) 0.27251 (15) 0.0294 (4)H12A 0.5371 0.5086 0.2224 $0.035*$ C13 0.57612 (6) 0.5266 (2) 0.35517 (14) 0.0276 (4)C14 0.60895 (7) 0.4577 (2) 0.42851 (14) 0.0276 (4)C15 0.55815 (8) 0.2676 (2) 0.16780 (16) 0.0338 (5)C16 0.59482 (11) 0.1859 (3) 0.15917 (19) 0.0543 (7)H16A 0.6042 0.1043 0.1996 $0.081*$ H16B 0.6200 0.2490 0.1744 $0.081*$ H17A 0.4978 0.2157 0.1592 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17B 0.5326 0.3820 (3) 0.90601 (15) 0.0363 (5)H18A 0.5131 0.4223 0.0925 $0.054*$ H18B 0.5366 0.3400 0.3877 $0.054*$ H18C 0.5554 (7) 0.6638 (2) 0.36324 (13) 0.0275 (4)C20 0.55836 (9) 0.9201 (2) 0.3754 (2) $0.064*$ H20A 0.5362 0.9711 0.3947 $0.064*$ H20A 0.5362 0.9711 0.3947 $0.064*$ H20A 0.5527 (8) 0.8033 (3) 0.42439 (18) 0.0414 (5)H22A 0.6574 0.9751 0.4212 $0.064*$ H22A 0.6574 0.8929 0.8333 0.3251 <td>C12$0.55997(7)$$0.4627(2)$$0.27251(15)$$0.0294(4)$H12A$0.5371$$0.5086$$0.2224$$0.035*$C13$0.57612(6)$$0.5266(2)$$0.35517(14)$$0.0276(4)$C14$0.60895(7)$$0.4577(2)$$0.42851(14)$$0.0276(4)$C15$0.55815(8)$$0.2676(2)$$0.16780(166)$$0.0388(5)$C16$0.59482(11)$$0.1859(3)$$0.15917(19)$$0.0543(7)$H16A$0.6042$$0.1043$$0.1996$$0.081*$H16B$0.6200$$0.2490$$0.1744$$0.081*$C17$0.52108(12)$$0.1646(4)$$0.1534(2)$$0.0693(11)$H17A$0.4978$$0.2157$$0.1592$$0.104*$H17B$0.5328$$0.0888$$0.1979$$0.104*$H17B$0.5328$$0.0888$$0.1979$$0.104*$H17C$0.5089$$0.1232$$0.0933$$0.104*$C18$0.54015(8)$$0.3820(3)$$0.9601(15)$$0.363(5)$H18A$0.5131$$0.4223$$0.0925$$0.054*$H18B$0.5362$$0.4573$$0.1108$$0.054*$C19$0.55554(7)$$0.6638(2)$$0.36324(13)$$0.0275(4)$C20$0.5836(9)$$0.9201(2)$$0.3754(2)$$0.064*$C21$0.64188(7)$$0.7711$$0.3326(5)$$0.2244(6)$H20B$0.5448$$0.9713$$0.3199$$0.064*$C21$0.65527(8)$$0.8083(3)$$0.42439(18)$$0.0511(7)$</td> <td>C11</td> <td>0.57614 (7)</td> <td>0.3331 (2)</td> <td>0.26044 (14)</td> <td>0.0292 (4)</td>	C12 $0.55997(7)$ $0.4627(2)$ $0.27251(15)$ $0.0294(4)$ H12A 0.5371 0.5086 0.2224 $0.035*$ C13 $0.57612(6)$ $0.5266(2)$ $0.35517(14)$ $0.0276(4)$ C14 $0.60895(7)$ $0.4577(2)$ $0.42851(14)$ $0.0276(4)$ C15 $0.55815(8)$ $0.2676(2)$ $0.16780(166)$ $0.0388(5)$ C16 $0.59482(11)$ $0.1859(3)$ $0.15917(19)$ $0.0543(7)$ H16A 0.6042 0.1043 0.1996 $0.081*$ H16B 0.6200 0.2490 0.1744 $0.081*$ C17 $0.52108(12)$ $0.1646(4)$ $0.1534(2)$ $0.0693(11)$ H17A 0.4978 0.2157 0.1592 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17C 0.5089 0.1232 0.0933 $0.104*$ C18 $0.54015(8)$ $0.3820(3)$ $0.9601(15)$ $0.363(5)$ H18A 0.5131 0.4223 0.0925 $0.054*$ H18B 0.5362 0.4573 0.1108 $0.054*$ C19 $0.55554(7)$ $0.6638(2)$ $0.36324(13)$ $0.0275(4)$ C20 $0.5836(9)$ $0.9201(2)$ $0.3754(2)$ $0.064*$ C21 $0.64188(7)$ 0.7711 $0.3326(5)$ $0.2244(6)$ H20B 0.5448 0.9713 0.3199 $0.064*$ C21 $0.65527(8)$ $0.8083(3)$ $0.42439(18)$ $0.0511(7)$	C11	0.57614 (7)	0.3331 (2)	0.26044 (14)	0.0292 (4)
H12A 0.5371 0.5086 0.2224 $0.035*$ C13 $0.57612 (6)$ $0.5266 (2)$ $0.35517 (14)$ $0.0264 (4)$ C14 $0.60895 (7)$ $0.4577 (2)$ $0.42851 (14)$ $0.0276 (4)$ C15 $0.55815 (8)$ $0.2676 (2)$ $0.16780 (16)$ $0.0358 (5)$ C16 $0.59482 (11)$ $0.1859 (3)$ $0.15917 (19)$ $0.0543 (7)$ H16A 0.6042 0.1043 0.1996 $0.081*$ H16B 0.6200 0.2490 0.1744 $0.081*$ C17 $0.52108 (12)$ $0.1646 (4)$ $0.1534 (2)$ $0.0693 (11)$ H17A 0.4978 0.2157 0.1592 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17C 0.5089 0.1232 0.0938 $0.104*$ H18D 0.5336 0.3400 0.0387 $0.054*$ H18B 0.5336 0.3400 0.0387 $0.054*$ H18B 0.5362 0.9011 0.3947 $0.064*$ L20A 0.5362 0.9713 0.3199 $0.064*$ H20A 0.5362 0.9713 0.3199 $0.064*$ H20B 0.5448 0.9743 0.3199 $0.064*$ H20A 0.65974 0.8033 0.3251 0.0507 C22 0.65577 0.8733 $0.315 (2)$ $0.0511 (7)$ H23A 0.7211 0.8336 0.4664 $0.061*$ C22 0.65974 $0.8098 (3)$ $0.2269 (2)$ $0.0445 (6)$ H24A 0.7151 <t< td=""><td>H12A$0.5371$$0.5086$$0.2224$$0.035*$C13$0.57612 (6)$$0.5266 (2)$$0.35517 (14)$$0.0264 (4)$C14$0.60895 (7)$$0.4577 (2)$$0.42851 (14)$$0.0276 (4)$C15$0.55815 (8)$$0.2676 (2)$$0.16780 (16)$$0.0358 (5)$C16$0.59482 (11)$$0.1859 (3)$$0.15917 (19)$$0.0543 (7)$H16A$0.6042$$0.1043$$0.1996$$0.081*$H16B$0.6200$$0.2490$$0.1744$$0.081*$C17$0.52108 (12)$$0.1646 (4)$$0.1534 (2)$$0.0693 (11)$H17A$0.4978$$0.2157$$0.1592$$0.104*$H17B$0.5328$$0.0888$$0.1979$$0.104*$H17C$0.5089$$0.1232$$0.0938$$0.104*$C18$0.54015 (8)$$0.3820 (3)$$0.09601 (15)$$0.0363 (5)$H18A$0.5131$$0.4223$$0.0925$$0.54*$H18B$0.5336$$0.3400$$0.3877$$0.054*$C19$0.55554 (7)$$0.6638 (2)$$0.3624 (13)$$0.0275 (4)$C20$0.5827 (0.9751)$$0.4212$$0.064*$L20A$0.5362$$0.9011$$0.3947$$0.064*$L20A$0.5327 (8)$$0.8033 (3)$$0.42439 (18)$$0.0414 (5)$H20B$0.5448 (7)$$0.7711$$0.326 (5)$$0.227 (2)$C22$0.65527 (8)$$0.8083 (3)$$0.42439 (18)$$0.061*$C24$0.68929 (8)$$0.8235 (3)$$0.3315 (2)$<td>C12</td><td>0.55997 (7)</td><td>0.4627 (2)</td><td>0.27251 (15)</td><td>0.0294 (4)</td></td></t<>	H12A 0.5371 0.5086 0.2224 $0.035*$ C13 $0.57612 (6)$ $0.5266 (2)$ $0.35517 (14)$ $0.0264 (4)$ C14 $0.60895 (7)$ $0.4577 (2)$ $0.42851 (14)$ $0.0276 (4)$ C15 $0.55815 (8)$ $0.2676 (2)$ $0.16780 (16)$ $0.0358 (5)$ C16 $0.59482 (11)$ $0.1859 (3)$ $0.15917 (19)$ $0.0543 (7)$ H16A 0.6042 0.1043 0.1996 $0.081*$ H16B 0.6200 0.2490 0.1744 $0.081*$ C17 $0.52108 (12)$ $0.1646 (4)$ $0.1534 (2)$ $0.0693 (11)$ H17A 0.4978 0.2157 0.1592 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17C 0.5089 0.1232 0.0938 $0.104*$ C18 $0.54015 (8)$ $0.3820 (3)$ $0.09601 (15)$ $0.0363 (5)$ H18A 0.5131 0.4223 0.0925 $0.54*$ H18B 0.5336 0.3400 0.3877 $0.054*$ C19 $0.55554 (7)$ $0.6638 (2)$ $0.3624 (13)$ $0.0275 (4)$ C20 $0.5827 (0.9751)$ 0.4212 $0.064*$ L20A 0.5362 0.9011 0.3947 $0.064*$ L20A $0.5327 (8)$ $0.8033 (3)$ $0.42439 (18)$ $0.0414 (5)$ H20B $0.5448 (7)$ 0.7711 $0.326 (5)$ $0.227 (2)$ C22 $0.65527 (8)$ $0.8083 (3)$ $0.42439 (18)$ $0.061*$ C24 $0.68929 (8)$ $0.8235 (3)$ $0.3315 (2)$ <td>C12</td> <td>0.55997 (7)</td> <td>0.4627 (2)</td> <td>0.27251 (15)</td> <td>0.0294 (4)</td>	C12	0.55997 (7)	0.4627 (2)	0.27251 (15)	0.0294 (4)
C13 $0.57612 (6)$ $0.5266 (2)$ $0.35517 (14)$ $0.0264 (4)$ C14 $0.60895 (7)$ $0.4577 (2)$ $0.42851 (14)$ $0.0276 (4)$ C15 $0.55815 (8)$ $0.2676 (2)$ $0.16780 (16)$ $0.0358 (5)$ C16 $0.59482 (11)$ $0.1859 (3)$ $0.15917 (19)$ $0.0543 (7)$ H16A 0.6042 0.1043 0.1996 0.081^* H16B 0.6200 0.2490 0.1744 0.081^* H16C 0.5835 0.1524 0.0980 0.081^* C17 $0.52108 (12)$ $0.1646 (4)$ $0.1534 (2)$ $0.693 (11)$ H17A 0.4978 0.2157 0.1592 0.104^* H17B 0.5328 0.0888 0.1979 0.104^* H17C 0.5089 0.1232 0.0938 0.104^* C18 $0.54015 (8)$ $0.3820 (3)$ $0.09601 (15)$ $0.0363 (5)$ H18A 0.5131 0.4223 0.0925 0.054^* C19 $0.55554 (7)$ $0.6638 (2)$ $0.36324 (13)$ $0.0275 (4)$ C20 $0.5826 (9)$ $0.9201 (2)$ $0.3754 (2)$ $0.0426 (6)$ H20A 0.5362 0.9011 0.3947 0.664^* C21 $0.61458 (7)$ $0.7918 (2)$ $0.35017 (17)$ $0.0326 (5)$ C23 $0.69305 (8)$ $0.8234 (3)$ $0.42439 (18)$ $0.0414 (5)$ H22A 0.6574 0.8092 0.4818 0.507^* C23 $0.69305 (8)$ $0.8235 (3)$ $0.3315 (2)$ $0.5011 (7)$ H3A 0.7211 <t< td=""><td>C13 0.57612 (6) 0.5266 (2) 0.35517 (14) 0.0264 (4) C14 0.60895 (7) 0.4577 (2) 0.42851 (14) 0.0276 (4) C15 0.55815 (8) 0.2676 (2) 0.16780 (16) 0.0338 (5) C16 0.59482 (11) 0.1859 (3) 0.15917 (19) 0.0543 (7) H16A 0.6042 0.1043 0.1996 0.081* H16B 0.6200 0.2490 0.1744 0.081* H16C 0.5835 0.1524 0.0980 0.081* C17 0.52108 (12) 0.1646 (4) 0.1534 (2) 0.0693 (11) H17A 0.4978 0.2157 0.1592 0.104* H17D 0.5328 0.0888 0.1979 0.104* H17C 0.5089 0.1232 0.0938 0.104* C18 0.54015 (8) 0.3820 (3) 0.0925 0.054* H18D 0.5336 0.3400 0.0337 0.054* C19 0.5554 (7) 0.6638 (2) 0.36324 (13) 0.0275 (4)</td><td>H12A</td><td>0.5371</td><td>0.5086</td><td>0.2224</td><td>0.035*</td></t<>	C13 0.57612 (6) 0.5266 (2) 0.35517 (14) 0.0264 (4) C14 0.60895 (7) 0.4577 (2) 0.42851 (14) 0.0276 (4) C15 0.55815 (8) 0.2676 (2) 0.16780 (16) 0.0338 (5) C16 0.59482 (11) 0.1859 (3) 0.15917 (19) 0.0543 (7) H16A 0.6042 0.1043 0.1996 0.081* H16B 0.6200 0.2490 0.1744 0.081* H16C 0.5835 0.1524 0.0980 0.081* C17 0.52108 (12) 0.1646 (4) 0.1534 (2) 0.0693 (11) H17A 0.4978 0.2157 0.1592 0.104* H17D 0.5328 0.0888 0.1979 0.104* H17C 0.5089 0.1232 0.0938 0.104* C18 0.54015 (8) 0.3820 (3) 0.0925 0.054* H18D 0.5336 0.3400 0.0337 0.054* C19 0.5554 (7) 0.6638 (2) 0.36324 (13) 0.0275 (4)	H12A	0.5371	0.5086	0.2224	0.035*
C14 0.60895 (7) 0.4577 (2) 0.42851 (14) 0.0276 (4)C15 0.55815 (8) 0.2676 (2) 0.16780 (16) 0.0358 (5)C16 0.59482 (11) 0.1859 (3) 0.15917 (19) 0.0543 (7)H16A 0.6042 0.1043 0.1996 $0.081*$ H16B 0.6200 0.2490 0.1744 $0.081*$ H16C 0.5835 0.1524 0.0980 $0.081*$ C17 0.52108 (12) 0.1646 (4) 0.1534 (2) 0.0693 (11)H17A 0.4978 0.2157 0.1592 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ C18 0.54015 (8) 0.3820 (3) 0.09601 (15) 0.0363 (5)H18A 0.5131 0.4223 0.0925 $0.054*$ C19 0.55554 (7) 0.6638 (2) 0.36324 (13) 0.0275 (4)C20 0.5836 (9) 0.9201 (2) 0.3754 (2) $0.044*$ H20B 0.5448 0.9743 0.3199 $0.064*$ H20C 0.5827 0.9711 0.3947 $0.064*$ C21 0.61458 (7) 0.7918 (2) 0.35017 (17) 0.0326 (5)C23 0.69305 (8) 0.8234 (3) 0.4155 (2) 0.0511 (7)H2AA 0.7111 0.8333 0.32511 $0.061*$ C24 0.68929 (8) 0.8235 (3) 0.3315 (2) 0.0507 (7)H2AA 0.7151 0.8998 (3) 0.2569 (2) 0.0435 (6)H2AA 0.721 0.66438 <td< td=""><td>C14$0.60895 (7)$$0.4577 (2)$$0.42851 (14)$$0.0276 (4)$C15$0.55815 (8)$$0.2676 (2)$$0.16780 (16)$$0.0358 (5)$C16$0.59482 (11)$$0.1859 (3)$$0.15917 (19)$$0.0543 (7)$H16A$0.6042$$0.1043$$0.1996$$0.081*$H16B$0.6200$$0.2490$$0.1744$$0.081*$C17$0.52108 (12)$$0.1646 (4)$$0.1534 (2)$$0.0693 (11)$H17A$0.4978$$0.2157$$0.1592$$0.104*$H17B$0.5328$$0.0888$$0.1979$$0.104*$H17C$0.5089$$0.1232$$0.0938$$0.104*$C18$0.54015 (8)$$0.3820 (3)$$0.09601 (15)$$0.0363 (5)$H18A$0.5131$$0.4223$$0.0925$$0.54*$H18B$0.5336$$0.3400$$0.3877$$0.054*$H18C$0.5622$$0.4573$$0.1108$$0.0275 (4)$C20$0.55836 (9)$$0.9201 (2)$$0.3754 (2)$$0.0426 (6)$H20A$0.5362$$0.9011$$0.3947$$0.064*$C21$0.61458 (7)$$0.7918 (2)$$0.35017 (17)$$0.0326 (5)$C22$0.65527 (8)$$0.8023 (3)$$0.4219 (18)$$0.0414 (5)$H22A$0.6574$$0.8092$$0.4818$$0.050*$C23$0.69305 (8)$$0.8234 (3)$$0.42439 (18)$$0.0414 (5)$H24A$0.7151$$0.8333$$0.3251 (0.061*$C24$0.68929 (8)$$0.8235 (3)$$0.315 (2)$</td><td>C13</td><td>0.57612 (6)</td><td>0.5266 (2)</td><td>0.35517 (14)</td><td>0.0264 (4)</td></td<>	C14 $0.60895 (7)$ $0.4577 (2)$ $0.42851 (14)$ $0.0276 (4)$ C15 $0.55815 (8)$ $0.2676 (2)$ $0.16780 (16)$ $0.0358 (5)$ C16 $0.59482 (11)$ $0.1859 (3)$ $0.15917 (19)$ $0.0543 (7)$ H16A 0.6042 0.1043 0.1996 $0.081*$ H16B 0.6200 0.2490 0.1744 $0.081*$ C17 $0.52108 (12)$ $0.1646 (4)$ $0.1534 (2)$ $0.0693 (11)$ H17A 0.4978 0.2157 0.1592 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17C 0.5089 0.1232 0.0938 $0.104*$ C18 $0.54015 (8)$ $0.3820 (3)$ $0.09601 (15)$ $0.0363 (5)$ H18A 0.5131 0.4223 0.0925 $0.54*$ H18B 0.5336 0.3400 0.3877 $0.054*$ H18C 0.5622 0.4573 0.1108 $0.0275 (4)$ C20 $0.55836 (9)$ $0.9201 (2)$ $0.3754 (2)$ $0.0426 (6)$ H20A 0.5362 0.9011 0.3947 $0.064*$ C21 $0.61458 (7)$ $0.7918 (2)$ $0.35017 (17)$ $0.0326 (5)$ C22 $0.65527 (8)$ $0.8023 (3)$ $0.4219 (18)$ $0.0414 (5)$ H22A 0.6574 0.8092 0.4818 $0.050*$ C23 $0.69305 (8)$ $0.8234 (3)$ $0.42439 (18)$ $0.0414 (5)$ H24A 0.7151 0.8333 $0.3251 (0.061*$ C24 $0.68929 (8)$ $0.8235 (3)$ $0.315 (2)$	C13	0.57612 (6)	0.5266 (2)	0.35517 (14)	0.0264 (4)
C15 0.55815 (8) 0.2676 (2) 0.16780 (16) 0.0358 (5)C16 0.59482 (11) 0.1859 (3) 0.15917 (19) 0.0543 (7)H16A 0.6042 0.1043 0.1996 $0.081*$ H16B 0.6200 0.2490 0.1744 $0.081*$ H16C 0.5835 0.1524 0.0980 $0.081*$ C17 0.52108 (12) 0.1646 (4) 0.1534 (2) 0.0693 (11)H17A 0.4978 0.2157 0.1592 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17C 0.5089 0.1232 0.0938 $0.104*$ C18 0.54015 (8) 0.3820 (3) 0.09601 (15) 0.0363 (5)H18A 0.5131 0.4223 0.0925 $0.054*$ H18B 0.5336 0.3400 0.0387 $0.054*$ H18E 0.5554 (7) 0.6638 (2) 0.36324 (13) 0.0275 (4)C20 0.55836 (9) 0.9201 (2) 0.3754 (2) $0.064*$ H20A 0.5622 0.9011 0.3947 $0.064*$ H20B 0.5448 0.9743 0.3199 $0.064*$ C21 0.61458 (7) 0.7918 (2) 0.35017 (17) 0.0326 (5)C22 0.65527 (8) 0.8083 (3) 0.42439 (18) 0.0414 (5)H22A 0.6574 0.8092 0.4818 $0.050*$ C23 0.69305 (8) 0.8234 (3) 0.4155 (2) 0.0511 (7)H23A 0.7211 0.8336 0.4664 $0.061*$ </td <td>C15$0.55815$ (8)0.2676 (2)0.16780 (16)0.0358 (5)C16$0.59482$ (11)0.1859 (3)0.15917 (19)0.0543 (7)H16A$0.6042$$0.1043$$0.1996$$0.081*$H16B$0.6200$$0.2490$$0.1744$$0.081*$H16C$0.5835$$0.1524$$0.0980$$0.081*$C17$0.52108$ (12)0.1646 (4)0.1534 (2)0.0693 (11)H17A$0.4978$$0.2157$$0.1592$$0.104*$H17B$0.5328$$0.0888$$0.1979$$0.104*$H17C$0.5089$$0.1232$$0.0938$$0.104*$C18$0.54015$ (8)0.3820 (3)0.09601 (15)0.0363 (5)H18A$0.5131$$0.4223$$0.0925$$0.054*$H18B$0.5336$$0.3400$$0.0387$$0.054*$C19$0.5554$ (7)0.6638 (2)0.36324 (13)0.0257 (4)C20$0.55836$ (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A$0.5362$$0.9011$$0.3947$$0.064*$H20B$0.5448$$0.9743$$0.3199$$0.644*$H20C$0.5827$$0.9751$$0.4212$$0.064*$C21$0.61458$ (7)0.7918 (2)0.35017 (17)0.0326 (5)C22$0.65574$$0.8092$$0.4818$$0.050*$C23$0.69305$ (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A$0.7111$$0.8333$$0.3251$$0.061*$<td< td=""><td>C14</td><td>0.60895 (7)</td><td>0.4577 (2)</td><td>0.42851 (14)</td><td>0.0276 (4)</td></td<></td>	C15 0.55815 (8) 0.2676 (2) 0.16780 (16) 0.0358 (5)C16 0.59482 (11) 0.1859 (3) 0.15917 (19) 0.0543 (7)H16A 0.6042 0.1043 0.1996 $0.081*$ H16B 0.6200 0.2490 0.1744 $0.081*$ H16C 0.5835 0.1524 0.0980 $0.081*$ C17 0.52108 (12) 0.1646 (4) 0.1534 (2) 0.0693 (11)H17A 0.4978 0.2157 0.1592 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17C 0.5089 0.1232 0.0938 $0.104*$ C18 0.54015 (8) 0.3820 (3) 0.09601 (15) 0.0363 (5)H18A 0.5131 0.4223 0.0925 $0.054*$ H18B 0.5336 0.3400 0.0387 $0.054*$ C19 0.5554 (7) 0.6638 (2) 0.36324 (13) 0.0257 (4)C20 0.55836 (9) 0.9201 (2) 0.3754 (2) 0.0426 (6)H20A 0.5362 0.9011 0.3947 $0.064*$ H20B 0.5448 0.9743 0.3199 $0.644*$ H20C 0.5827 0.9751 0.4212 $0.064*$ C21 0.61458 (7) 0.7918 (2) 0.35017 (17) 0.0326 (5)C22 0.65574 0.8092 0.4818 $0.050*$ C23 0.69305 (8) 0.8234 (3) 0.4155 (2) 0.0511 (7)H23A 0.7111 0.8333 0.3251 $0.061*$ <td< td=""><td>C14</td><td>0.60895 (7)</td><td>0.4577 (2)</td><td>0.42851 (14)</td><td>0.0276 (4)</td></td<>	C14	0.60895 (7)	0.4577 (2)	0.42851 (14)	0.0276 (4)
C16 0.59482 (1) 0.1859 (3) 0.15917 (19) 0.0543 (7)H16A 0.6042 0.1043 0.1996 $0.081*$ H16B 0.6200 0.2490 0.1744 $0.081*$ H16C 0.5835 0.1524 0.0980 $0.081*$ C17 0.52108 (12) 0.1646 (4) 0.1534 (2) 0.0693 (11)H17A 0.4978 0.2157 0.1592 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17C 0.5089 0.1232 0.0938 $0.104*$ C18 0.54015 (8) 0.3820 (3) 0.09601 (15) 0.0363 (5)H18A 0.5131 0.4223 0.0925 $0.054*$ H18B 0.5336 0.3400 0.0387 $0.054*$ H18C 0.5622 0.4573 0.1108 $0.054*$ C19 0.5554 (7) 0.6638 (2) 0.36324 (13) 0.0275 (4)C20 0.55836 (9) 0.9201 (2) 0.3754 (2) $0.064*$ H20B 0.5448 0.9743 0.3199 $0.064*$ L20C 0.5827 0.9751 0.4212 $0.664*$ C21 0.61458 (7) 0.7918 (2) 0.33517 (17) 0.0326 (5)C22 0.6574 0.8092 0.4818 $0.050*$ C23 0.69305 (8) 0.8234 (3) 0.4155 (2) 0.0511 (7)H23A 0.7211 0.8336 0.4664 $0.061*$ C24 0.68929 (8) 0.8235 (3) 0.3315 (2) 0.0507 (7)H23A <td>C16$0.59482(11)$$0.1859(3)$$0.15917(19)$$0.0543(7)$H16A$0.6042$$0.1043$$0.1996$$0.081*$H16B$0.6200$$0.2490$$0.1744$$0.081*$H16C$0.5835$$0.1524$$0.0980$$0.081*$C17$0.52108(12)$$0.1646(4)$$0.1534(2)$$0.0693(11)$H17A$0.4978$$0.2157$$0.1592$$0.104*$H17B$0.5328$$0.0888$$0.1979$$0.104*$H17C$0.5089$$0.1232$$0.0938$$0.104*$C18$0.54015(8)$$0.3820(3)$$0.99601(15)$$0.363(5)$H18A$0.5131$$0.4223$$0.0925$$0.054*$H18B$0.5336$$0.3400$$0.0387$$0.054*$H18C$0.5622$$0.4573$$0.1108$$0.054*$C19$0.5554(7)$$0.6638(2)$$0.36324(13)$$0.0275(4)$C20$0.55836(9)$$0.9201(2)$$0.3754(2)$$0.064*$H20B$0.5448$$0.9743$$0.3199$$0.064*$C21$0.61458(7)$$0.7918(2)$$0.35017(17)$$0.0326(5)$C22$0.65527(8)$$0.8083(3)$$0.42439(18)$$0.0414(5)$H22A$0.6574$$0.8092$$0.4818$$0.050*$C23$0.69305(8)$$0.8235(3)$$0.3315(2)$$0.0511(7)$H23A$0.7111$$0.8333$$0.3251$$0.061*$C24$0.68929(8)$$0.8235(3)$$0.3315(2)$$0.0507(7)$H23A$0.7211$<!--</td--><td>C15</td><td>0.55815 (8)</td><td>0.2676 (2)</td><td>0.16780 (16)</td><td>0.0358 (5)</td></td>	C16 $0.59482(11)$ $0.1859(3)$ $0.15917(19)$ $0.0543(7)$ H16A 0.6042 0.1043 0.1996 $0.081*$ H16B 0.6200 0.2490 0.1744 $0.081*$ H16C 0.5835 0.1524 0.0980 $0.081*$ C17 $0.52108(12)$ $0.1646(4)$ $0.1534(2)$ $0.0693(11)$ H17A 0.4978 0.2157 0.1592 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17C 0.5089 0.1232 0.0938 $0.104*$ C18 $0.54015(8)$ $0.3820(3)$ $0.99601(15)$ $0.363(5)$ H18A 0.5131 0.4223 0.0925 $0.054*$ H18B 0.5336 0.3400 0.0387 $0.054*$ H18C 0.5622 0.4573 0.1108 $0.054*$ C19 $0.5554(7)$ $0.6638(2)$ $0.36324(13)$ $0.0275(4)$ C20 $0.55836(9)$ $0.9201(2)$ $0.3754(2)$ $0.064*$ H20B 0.5448 0.9743 0.3199 $0.064*$ C21 $0.61458(7)$ $0.7918(2)$ $0.35017(17)$ $0.0326(5)$ C22 $0.65527(8)$ $0.8083(3)$ $0.42439(18)$ $0.0414(5)$ H22A 0.6574 0.8092 0.4818 $0.050*$ C23 $0.69305(8)$ $0.8235(3)$ $0.3315(2)$ $0.0511(7)$ H23A 0.7111 0.8333 0.3251 $0.061*$ C24 $0.68929(8)$ $0.8235(3)$ $0.3315(2)$ $0.0507(7)$ H23A 0.7211 </td <td>C15</td> <td>0.55815 (8)</td> <td>0.2676 (2)</td> <td>0.16780 (16)</td> <td>0.0358 (5)</td>	C15	0.55815 (8)	0.2676 (2)	0.16780 (16)	0.0358 (5)
H16A 0.6042 0.1043 0.1996 $0.081*$ H16B 0.6200 0.2490 0.1744 $0.081*$ H16C 0.5835 0.1524 0.0980 $0.081*$ C17 $0.52108 (12)$ $0.1646 (4)$ $0.1534 (2)$ $0.0693 (11)$ H17A 0.4978 0.2157 0.1592 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17C 0.5089 0.1232 0.0938 $0.104*$ C18 $0.54015 (8)$ $0.3820 (3)$ $0.09601 (15)$ $0.0363 (5)$ H18A 0.5131 0.4223 0.0925 $0.054*$ H18B 0.5336 0.3400 0.0387 $0.054*$ H18C 0.5622 0.4573 0.1108 $0.054*$ C19 $0.5554 (7)$ $0.6638 (2)$ $0.36324 (13)$ $0.0275 (4)$ C20 $0.55836 (9)$ $0.9201 (2)$ $0.3754 (2)$ $0.0426 (6)$ H20A 0.5362 0.9711 0.3947 $0.064*$ H20C 0.5827 0.9751 0.4212 $0.064*$ C21 $0.61458 (7)$ $0.7918 (2)$ $0.35017 (17)$ $0.0326 (5)$ C22 0.6574 0.8092 0.4818 $0.050*$ C23 $0.69305 (8)$ $0.8234 (3)$ $0.42439 (18)$ $0.0414 (5)$ H23A 0.7211 0.8333 0.3251 $0.061*$ C24 $0.68929 (8)$ $0.8235 (3)$ $0.3315 (2)$ $0.0507 (7)$ H24A 0.7151 0.8333 0.3251 $0.061*$ C25 0.6490	H16A 0.6042 0.1043 0.1996 $0.081*$ H16B 0.6200 0.2490 0.1744 $0.081*$ H16C 0.5835 0.1524 0.0980 $0.081*$ C17 0.52108 (12) 0.1646 (4) 0.1534 (2) 0.0693 (11)H17A 0.4978 0.2157 0.1592 $0.104*$ H17B 0.5328 0.0888 0.1979 $0.104*$ H17C 0.5089 0.1232 0.0938 $0.104*$ C18 0.54015 (8) 0.3820 (3) 0.09601 (15) 0.0363 (5)H18A 0.5131 0.4223 0.0925 $0.054*$ H18B 0.5336 0.3400 0.0387 $0.054*$ C19 0.55554 (7) 0.6638 (2) 0.3324 (13) 0.0275 (4)C20 0.55836 (9) 0.9201 (2) 0.3754 (2) $0.064*$ H20B 0.5448 0.9743 0.3199 $0.064*$ C21 0.61458 (7) 0.7918 (2) 0.35017 (17) 0.0326 (5)C22 0.6527 (8) 0.8083 (3) 0.42139 (18) 0.0414 (5)H22A 0.6574 0.8092 0.4818 $0.050*$ C23 0.69305 (8) 0.8234 (3) 0.4155 (2) 0.0511 (7)H23A 0.7211 0.8333 0.3251 $0.061*$ C24 0.68929 (8) 0.8235 (3) 0.3315 (2) 0.0517 (7)H24A 0.7151 0.8333 0.2259 (2) 0.0435 (6)H25A 0.6474 0.8101 0.2000 $0.52*$	C16	0.59482 (11)	0.1859 (3)	0.15917 (19)	0.0543 (7)
H16B 0.6200 0.2490 0.1744 0.081* H16C 0.5835 0.1524 0.0980 0.081* C17 0.52108 (12) 0.1646 (4) 0.1534 (2) 0.0693 (11) H17A 0.4978 0.2157 0.1592 0.104* H17B 0.5328 0.0888 0.1979 0.104* H17C 0.5089 0.1232 0.0938 0.104* C18 0.54015 (8) 0.3820 (3) 0.09601 (15) 0.0363 (5) H18B 0.5336 0.3400 0.0387 0.054* H18B 0.5336 0.3400 0.0387 0.054* H18C 0.5622 0.4573 0.1108 0.054* C19 0.55554 (7) 0.6638 (2) 0.36324 (13) 0.0275 (4) C20 0.55836 (9) 0.9201 (2) 0.3754 (2) 0.064* H20A 0.5362 0.9011 0.3947 0.064* C21 0.6557 (8) 0.8083 (3) 0.4212 0.064* C22 0.6557 (8)<	H16B0.62000.24900.17440.081*H16C0.58350.15240.09800.081*C170.52108 (12)0.1646 (4)0.1534 (2)0.0693 (11)H17A0.49780.21570.15920.104*H17B0.53280.08880.19790.104*H17C0.50890.12320.09380.104*C180.54015 (8)0.3820 (3)0.09601 (15)0.0363 (5)H18A0.51310.42230.09250.054*H18B0.53360.34000.03870.054*H18C0.56220.45730.11080.0275 (4)C200.5554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.064*H2080.54480.97430.31990.064*H2020.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8235 (3)0.3315 (2)0.0507 (7)H23A0.72110.83330.32510.061*C240.68929 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.3346 (5)C270.53230.77940.05880.070* <td>H16A</td> <td>0.6042</td> <td>0.1043</td> <td>0.1996</td> <td>0.081*</td>	H16A	0.6042	0.1043	0.1996	0.081*
H16C0.58350.15240.09800.081*C170.52108 (12)0.1646 (4)0.1534 (2)0.0693 (11)H17A0.49780.21570.15920.104*H17B0.53280.08880.19790.104*H17C0.50890.12320.09380.104*C180.54015 (8)0.3820 (3)0.09601 (15)0.363 (5)H18A0.51310.42230.09250.054*H18B0.53360.34000.03870.054*C190.55554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18) <t< td=""><td>H16C0.58350.15240.09800.081*C170.52108 (12)0.1646 (4)0.1534 (2)0.0693 (11)H17A0.49780.21570.15920.104*H17B0.53280.08880.19790.104*H17C0.50890.12320.09380.104*C180.54015 (8)0.3820 (3)0.09601 (15)0.0633 (5)H18A0.51310.42230.09250.054*H18B0.53360.34000.03870.054*C190.55554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65574 (8)0.80920.48180.050*C230.69305 (8)0.8234 (3)0.4125 (2)0.0511 (7)H23A0.72110.83360.3315 (2)0.0517 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.4336 (6)H25A0.64740.81010.20000.52*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.53230.79440.05880.070*H27B0.57950.70470.09450.070*<td>H16B</td><td>0.6200</td><td>0.2490</td><td>0.1744</td><td>0.081*</td></td></t<>	H16C0.58350.15240.09800.081*C170.52108 (12)0.1646 (4)0.1534 (2)0.0693 (11)H17A0.49780.21570.15920.104*H17B0.53280.08880.19790.104*H17C0.50890.12320.09380.104*C180.54015 (8)0.3820 (3)0.09601 (15)0.0633 (5)H18A0.51310.42230.09250.054*H18B0.53360.34000.03870.054*C190.55554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65574 (8)0.80920.48180.050*C230.69305 (8)0.8234 (3)0.4125 (2)0.0511 (7)H23A0.72110.83360.3315 (2)0.0517 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.4336 (6)H25A0.64740.81010.20000.52*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.53230.79440.05880.070*H27B0.57950.70470.09450.070* <td>H16B</td> <td>0.6200</td> <td>0.2490</td> <td>0.1744</td> <td>0.081*</td>	H16B	0.6200	0.2490	0.1744	0.081*
C17 0.52108 (12) 0.1646 (4) 0.1534 (2) 0.0693 (11) H17A 0.4978 0.2157 0.1592 0.104* H17B 0.5328 0.0888 0.1979 0.104* H17C 0.5089 0.1232 0.0938 0.104* C18 0.54015 (8) 0.3820 (3) 0.09601 (15) 0.0363 (5) H18A 0.5131 0.4223 0.0925 0.054* H18B 0.5336 0.3400 0.0387 0.054* H18B 0.55554 (7) 0.6638 (2) 0.36324 (13) 0.0275 (4) C20 0.55836 (9) 0.9201 (2) 0.3754 (2) 0.0426 (6) H20A 0.5362 0.9011 0.3947 0.064* H20B 0.5448 0.9743 0.3199 0.064* H20C 0.5827 0.9751 0.4212 0.064* C21 0.61458 (7) 0.7918 (2) 0.35017 (17) 0.0326 (5) C22 0.65527 (8) 0.8092 0.4818 0.050* C23	C170.52108 (12)0.1646 (4)0.1534 (2)0.0693 (11)H17A0.49780.21570.15920.104*H17B0.53280.08880.19790.104*H17C0.50890.12320.09380.104*C180.54015 (8)0.3820 (3)0.09601 (15)0.0363 (5)H18A0.51310.42230.09250.054*H18B0.53360.34000.03870.054*C190.5554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.315 (2)0.0511 (7)H23A0.72110.83360.32510.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2669 (2)0.4453 (6)H25A0.64740.81010.20000.52*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.7794	H16C	0.5835	0.1524	0.0980	0.081*
H17A0.49780.21570.15920.104*H17B0.53280.08880.19790.104*H17C0.50890.12320.09380.104*C180.54015 (8)0.3820 (3)0.09601 (15)0.0363 (5)H18A0.51310.42230.09250.054*H18B0.53360.34000.03870.054*C190.55554 (7)0.6638 (2)0.3624 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*H22A0.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.94550.070*	H17A0.49780.21570.15920.104*H17B0.53280.08880.19790.104*H17C0.50890.12320.09380.104*C180.54015 (8)0.3820 (3)0.09601 (15)0.0363 (5)H18A0.51310.42230.09250.054*H18B0.53360.34000.03870.054*H18C0.56220.45730.11080.0275 (4)C200.55554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.32510.061*C240.68929 (8)0.8235 (3)0.3256 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60901 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27B0.57580.70470.09450.070*H27C0.57580.70470.99550.70*	C17	0.52108 (12)	0.1646 (4)	0.1534 (2)	0.0693 (11)
H17B0.53280.08880.19790.104*H17C0.50890.12320.09380.104*C180.54015 (8)0.3820 (3)0.09601 (15)0.0363 (5)H18A0.51310.42230.09250.054*H18B0.53360.34000.03870.054*H18C0.56220.45730.11080.0275 (4)C200.5554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.044*H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8093 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8235 (3)0.3315 (2)0.0507 (7)H23A0.72110.83330.32510.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.3256 (17)0.0346 (5)C250.64900 (8)0.8098 (3)0.2569 (2)0.4355 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.7740.05	H17B0.53280.08880.19790.104*H17C0.50890.12320.09380.104*C180.54015 (8)0.3820 (3)0.09601 (15)0.0363 (5)H18A0.51310.42230.09250.054*H18B0.53360.34000.03870.054*C190.55554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.32510.061*C240.68929 (8)0.8235 (3)0.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.435 (6)H25A0.64740.81010.20000.052*C260.6091 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)C27 <t< td=""><td>H17A</td><td>0.4978</td><td>0.2157</td><td>0.1592</td><td>0.104*</td></t<>	H17A	0.4978	0.2157	0.1592	0.104*
H17C0.50890.12320.09380.104*C180.54015 (8)0.3820 (3)0.09601 (15)0.0363 (5)H18A0.51310.42230.09250.054*H18B0.53360.34000.03870.054*H18C0.56220.45730.11080.0275 (4)C200.5554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.50*C230.69305 (8)0.8235 (3)0.3315 (2)0.0511 (7)H23A0.72110.83330.32510.061*C240.68929 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.6091 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.94550.070*	H17C0.50890.12320.09380.104*C180.54015 (8)0.3820 (3)0.09601 (15)0.0363 (5)H18A0.51310.42230.09250.054*H18B0.53360.34000.03870.054*H18C0.56220.45730.11080.0275 (4)C200.5554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.50*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.4355 (6)L25A0.64740.81010.20000.52*C260.6091 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.70470.09450.070*H27B0.57580.70470.09450.070*	H17B	0.5328	0.0888	0.1979	0.104*
C180.54015 (8)0.3820 (3)0.09601 (15)0.0363 (5)H18A0.51310.42230.09250.054*H18B0.53360.34000.03870.054*H18C0.56220.45730.11080.0275 (4)C190.55554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.70470.09450.070*	C180.54015 (8)0.3820 (3)0.09601 (15)0.0363 (5)H18A0.51310.42230.09250.054*H18B0.53360.34000.03870.054*H18C0.56220.45730.11080.0275 (4)C190.55554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.50*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.435 (6)H25A0.64740.81010.20000.652*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.4644 (6)H27A0.53230.70470.09450.070*H27B0.57580.70470.99450.070*	H17C	0.5089	0.1232	0.0938	0.104*
H18A0.51310.42230.09250.054*H18B0.53360.34000.03870.054*H18C0.56220.45730.11080.0275 (4)C190.55554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.064*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.70470.09450.070*	H18A0.51310.42230.09250.054*H18B0.53360.34000.03870.054*H18C0.56220.45730.11080.0275 (4)C190.55554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.4335 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57580.70470.09450.070*	C18	0.54015 (8)	0.3820 (3)	0.09601 (15)	0.0363 (5)
H18B0.53360.34000.03870.054*H18C0.56220.45730.11080.054*C190.55554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	H18B0.53360.34000.03870.054*H18C0.56220.45730.11080.054*C190.55554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.50*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.70470.09450.070*H27B0.57580.87430.09050.070*	H18A	0.5131	0.4223	0.0925	0.054*
H18C0.56220.45730.11080.054*C190.55554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.70470.09450.070*	H18C0.56220.45730.11080.054*C190.55554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.6677 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	H18B	0.5336	0.3400	0.0387	0.054*
C190.55554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	C190.55554 (7)0.6638 (2)0.36324 (13)0.0275 (4)C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.70470.09450.070*H27B0.57580.87430.09050.070*	H18C	0.5622	0.4573	0.1108	0.054*
C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	C200.55836 (9)0.9201 (2)0.3754 (2)0.0426 (6)H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.70470.09450.070*H27B0.57580.87430.09050.070*	C19	0.55554 (7)	0.6638 (2)	0.36324 (13)	0.0275 (4)
H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	H20A0.53620.90110.39470.064*H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.70470.09450.070*H27B0.57580.87430.09050.070*	C20	0.55836 (9)	0.9201 (2)	0.3754 (2)	0.0426 (6)
H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	H20B0.54480.97430.31990.064*H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.70470.09450.070*H27B0.57580.87430.09050.070*	H20A	0.5362	0.9011	0.3947	0.064*
H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	H20C0.58270.97510.42120.064*C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57580.87430.09050.070*	H20B	0.5448	0.9743	0.3199	0.064*
C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	C210.61458 (7)0.7918 (2)0.35017 (17)0.0326 (5)C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57580.87430.09050.070*	H20C	0.5827	0.9751	0.4212	0.064*
C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	C220.65527 (8)0.8083 (3)0.42439 (18)0.0414 (5)H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*H27C0.57580.87430.09050.070*	C21	0.61458 (7)	0.7918 (2)	0.35017 (17)	0.0326 (5)
H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	H22A0.65740.80920.48180.050*C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*H27C0.57580.87430.09050.070*	C22	0.65527 (8)	0.8083 (3)	0.42439 (18)	0.0414 (5)
C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	C230.69305 (8)0.8234 (3)0.4155 (2)0.0511 (7)H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*H27C0.57580.87430.09050.070*	H22A	0.6574	0.8092	0.4818	0.050*
H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	H23A0.72110.83360.46640.061*C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*H27C0.57580.87430.09050.070*	C23	0.69305 (8)	0.8234 (3)	0.4155 (2)	0.0511 (7)
C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	C240.68929 (8)0.8235 (3)0.3315 (2)0.0507 (7)H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*H27C0.57580.87430.09050.070*	H23A	0.7211	0.8336	0.4664	0.061*
H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	H24A0.71510.83330.32510.061*C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*H27C0.57580.87430.09050.070*	C24	0.68929 (8)	0.8235 (3)	0.3315 (2)	0.0507 (7)
C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	C250.64900 (8)0.8098 (3)0.2569 (2)0.0435 (6)H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*H27C0.57580.87430.09050.070*	H24A	0.7151	0.8333	0.3251	0.061*
H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	H25A0.64740.81010.20000.052*C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*H27C0.57580.87430.09050.070*	C25	0.64900 (8)	0.8098 (3)	0.2569 (2)	0.0435 (6)
C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	C260.60991 (7)0.7951 (2)0.26395 (17)0.0346 (5)C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*H27C0.57580.87430.09050.070*	H25A	0.6474	0.8101	0.2000	0.052*
C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	C270.56379 (9)0.7866 (3)0.10141 (18)0.0464 (6)H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*H27C0.57580.87430.09050.070*	C26	0.60991 (7)	0.7951 (2)	0.26395 (17)	0.0346 (5)
H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*	H27A0.53230.77940.05880.070*H27B0.57950.70470.09450.070*H27C0.57580.87430.09050.070*	C27	0.56379 (9)	0.7866 (3)	0.10141 (18)	0.0464 (6)
H27B 0.5795 0.7047 0.0945 0.070*	H27B0.57950.70470.09450.070*H27C0.57580.87430.09050.070*	H27A	0.5323	0.7794	0.0588	0.070*
	H27C 0.5758 0.8743 0.0905 0.070*	H27B	0.5795	0.7047	0.0945	0.070*
H27C 0.5758 0.8743 0.0905 0.070*		H27C	0.5758	0.8743	0.0905	0.070*

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.03690 (13)	0.03680 (13)	0.02700 (13)	0.00268 (9)	0.01323 (10)	-0.00251 (9)
01	0.0297 (7)	0.0358 (8)	0.0387 (8)	-0.0016 (6)	0.0186 (7)	-0.0021 (7)
N1	0.0310 (9)	0.0397 (10)	0.0355 (10)	0.0022 (8)	0.0118 (8)	0.0008 (9)
N2	0.0409 (10)	0.0310 (9)	0.0377 (10)	0.0037 (8)	0.0151 (9)	0.0023 (8)
N3	0.0332 (10)	0.0481 (12)	0.0406 (11)	-0.0087 (9)	0.0175 (9)	-0.0048 (9)
N4	0.0269 (9)	0.0257 (8)	0.0416 (10)	0.0007 (7)	0.0159 (8)	-0.0004 (8)
C1	0.0359 (12)	0.0481 (14)	0.0495 (15)	-0.0062 (11)	0.0196 (12)	-0.0017 (12)
C2	0.0389 (12)	0.0445 (13)	0.0324 (12)	0.0115 (10)	0.0132 (10)	0.0003 (10)
C3	0.0398 (14)	0.072 (2)	0.0381 (14)	0.0112 (13)	0.0085 (12)	-0.0019 (14)
C4	0.0498 (16)	0.083 (2)	0.0357 (14)	0.0283 (16)	0.0059 (13)	0.0053 (15)
C5	0.071 (2)	0.0625 (19)	0.0414 (15)	0.0313 (17)	0.0189 (15)	0.0140 (14)
C6	0.0675 (19)	0.0453 (15)	0.0460 (15)	0.0195 (14)	0.0237 (15)	0.0108 (12)
C7	0.0439 (13)	0.0377 (12)	0.0349 (12)	0.0119 (10)	0.0153 (11)	0.0026 (10)
C8	0.0334 (11)	0.0304 (10)	0.0312 (11)	0.0043 (9)	0.0138 (9)	-0.0007 (9)
C9	0.0270 (10)	0.0282 (10)	0.0307 (11)	-0.0011 (8)	0.0124 (9)	0.0003 (8)
C10	0.0302 (10)	0.0243 (9)	0.0355 (11)	-0.0010 (8)	0.0155 (9)	-0.0012 (8)
C11	0.0321 (10)	0.0241 (9)	0.0313 (11)	-0.0072 (8)	0.0150 (9)	-0.0027 (8)
C12	0.0292 (10)	0.0267 (10)	0.0294 (10)	-0.0019 (8)	0.0115 (9)	0.0023 (8)
C13	0.0246 (9)	0.0239 (9)	0.0302 (10)	-0.0031 (8)	0.0125 (8)	-0.0007 (8)
C14	0.0279 (10)	0.0289 (10)	0.0249 (10)	-0.0031 (8)	0.0117 (8)	-0.0022 (8)
C15	0.0483 (13)	0.0268 (10)	0.0300 (11)	-0.0073 (10)	0.0167 (10)	-0.0028 (9)
C16	0.082 (2)	0.0392 (13)	0.0388 (14)	0.0177 (14)	0.0262 (15)	0.0001 (11)
C17	0.089 (2)	0.071 (2)	0.0360 (14)	-0.053 (2)	0.0204 (16)	-0.0103 (14)
C18	0.0436 (12)	0.0350 (11)	0.0307 (11)	0.0006 (10)	0.0179 (10)	-0.0003 (9)
C19	0.0249 (9)	0.0289 (10)	0.0242 (10)	0.0005 (8)	0.0080 (8)	-0.0015 (8)
C20	0.0406 (12)	0.0276 (11)	0.0617 (16)	0.0050 (10)	0.0261 (12)	0.0003 (11)
C21	0.0271 (10)	0.0223 (9)	0.0484 (13)	-0.0001 (8)	0.0179 (10)	0.0013 (9)
C22	0.0332 (12)	0.0383 (12)	0.0450 (14)	-0.0049 (10)	0.0123 (11)	0.0063 (11)
C23	0.0282 (12)	0.0508 (15)	0.0623 (18)	-0.0053 (11)	0.0116 (12)	0.0077 (13)
C24	0.0316 (12)	0.0470 (14)	0.077 (2)	-0.0034 (11)	0.0282 (13)	0.0031 (14)
C25	0.0407 (13)	0.0375 (12)	0.0617 (16)	-0.0055 (10)	0.0320 (13)	-0.0044 (12)
C26	0.0310 (11)	0.0244 (9)	0.0477 (13)	-0.0018 (8)	0.0182 (10)	-0.0021 (9)
C27	0.0515 (15)	0.0427 (13)	0.0443 (14)	-0.0125 (12)	0.0221 (12)	-0.0076 (11)

Geometric parameters (Å, °)

Br—C14	1.901 (2)	C12—C13	1.388 (3)	_
O1—C19	1.232 (3)	C12—H12A	0.9500	
N1—C8	1.373 (3)	C13—C14	1.389 (3)	
N1—C2	1.379 (3)	C13—C19	1.510 (3)	
N1-C1	1.456 (3)	C15—C18	1.526 (3)	
N2—C8	1.310 (3)	C15—C17	1.527 (3)	
N2—C7	1.391 (3)	C15—C16	1.545 (4)	
N3—C26	1.365 (3)	C16—H16A	0.9800	
N3—C27	1.447 (3)	C16—H16B	0.9800	

N3—H3B	0.81 (3)	C16—H16C	0.9800
N4—C19	1.340 (3)	С17—Н17А	0.9800
N4—C21	1.450 (3)	C17—H17B	0.9800
N4—C20	1.467 (3)	С17—Н17С	0.9800
C1—H1A	0.9800	C18—H18A	0.9800
C1—H1B	0.9800	C18—H18B	0.9800
C1—H1C	0.9800	C18—H18C	0.9800
C2—C7	1.394 (4)	C20—H20A	0.9800
C2—C3	1.401 (4)	C20—H20B	0.9800
C3—C4	1.388 (5)	C20—H20C	0.9800
C3—H3A	0.9500	$C_{21} - C_{22}$	1.383 (3)
C4—C5	1.395 (5)	$C_{21} - C_{26}$	1.406 (3)
C4—H4A	0.9500	C^{22} C^{23}	1.100(3) 1.387(3)
C5—C6	1 376 (5)	C22_H22A	0.9500
C5—H5A	0.9500	C^{23} C^{24}	1 379 (4)
C6-C7	1 412 (4)	C23—H23A	0.9500
C6—H6A	0.9500	C_{24} C_{25}	1.375(4)
	1 484 (3)	C24 C25	0.9500
C_{0} C_{14}	1 303 (3)	$C_{24} = 112471$	1.414(3)
C_{0} C_{10}	1.395 (3)	C25 H25A	0.9500
C_{10}	1.395 (3)	C27_H27A	0.9500
	0.9500	$C_{27} = H_{27}R$	0.9800
C_{11} C_{12}	1 306 (3)	C_{27} H27C	0.9800
$C_{11} = C_{12}$	1.530(3)	027-11270	0.9800
en—en	1.551 (5)		
C8—N1—C2	106.0 (2)	C18—C15—C11	111.07 (18)
C8—N1—C1	128.4 (2)	C17—C15—C11	108.6 (2)
C2—N1—C1	125.5 (2)	C18—C15—C16	108.3 (2)
C8—N2—C7	104.4 (2)	C17—C15—C16	109.0 (3)
C26—N3—C27	122.4 (2)	C11—C15—C16	110.6 (2)
C26—N3—H3B	117 (2)	C15—C16—H16A	109.5
C27—N3—H3B	119 (2)	C15—C16—H16B	109.5
C19—N4—C21	123.86 (18)	H16A—C16—H16B	109.5
C19—N4—C20	119.04 (18)	C15—C16—H16C	109.5
C21—N4—C20	117.02 (18)	H16A—C16—H16C	109.5
N1—C1—H1A	109.5	H16B—C16—H16C	109.5
N1—C1—H1B	109.5	С15—С17—Н17А	109.5
H1A—C1—H1B	109.5	С15—С17—Н17В	109.5
N1—C1—H1C	109.5	H17A—C17—H17B	109.5
H1A—C1—H1C	109.5	С15—С17—Н17С	109.5
H1B—C1—H1C	109.5	H17A—C17—H17C	109.5
N1-C2-C7	105.7(2)	H17B-C17-H17C	109.5
N1-C2-C3	131.4 (3)	C15—C18—H18A	109.5
C7—C2—C3	123.0 (3)	C15—C18—H18B	109.5
C4-C3-C2	115.7 (3)	H18A—C18—H18B	109.5
C4—C3—H3A	122.1	C15—C18—H18C	109.5
C2—C3—H3A	122.1	H18A - C18 - H18C	109.5
C_{3} C_{4} C_{5}	122.0(3)	H18B— $C18$ — $H18C$	109.5

C3—C4—H4A	119.0	O1C19N4	122.7 (2)
C5—C4—H4A	119.0	O1—C19—C13	119.92 (19)
C6—C5—C4	122.0 (3)	N4—C19—C13	117.37 (17)
С6—С5—Н5А	119.0	N4—C20—H20A	109.5
C4—C5—H5A	119.0	N4—C20—H20B	109.5
C5—C6—C7	117.2 (3)	H20A—C20—H20B	109.5
С5—С6—Н6А	121.4	N4—C20—H20C	109.5
С7—С6—Н6А	121.4	H20A—C20—H20C	109.5
N2—C7—C2	110.2 (2)	H20B—C20—H20C	109.5
N2—C7—C6	129.8 (3)	C22—C21—C26	121.5 (2)
C2—C7—C6	120.0 (3)	C22—C21—N4	119.1 (2)
N2—C8—N1	113.7 (2)	C26—C21—N4	119.1 (2)
N2—C8—C9	124.9 (2)	C21—C22—C23	120.3 (3)
N1—C8—C9	121.4 (2)	C21—C22—H22A	119.8
C14—C9—C10	118.6 (2)	C23—C22—H22A	119.8
C14—C9—C8	122.40 (19)	C24—C23—C22	119.0 (3)
C10—C9—C8	119.00 (19)	С24—С23—Н23А	120.5
C9—C10—C11	121.9 (2)	С22—С23—Н23А	120.5
C9—C10—H10A	119.0	C25—C24—C23	121.4 (2)
C11—C10—H10A	119.0	C25—C24—H24A	119.3
C10—C11—C12	117.3 (2)	C23—C24—H24A	119.3
C10—C11—C15	121.96 (19)	C24—C25—C26	120.8 (3)
C12—C11—C15	120.7 (2)	С24—С25—Н25А	119.6
C13—C12—C11	122.3 (2)	С26—С25—Н25А	119.6
C13—C12—H12A	118.8	N3—C26—C21	121.4 (2)
C11—C12—H12A	118.8	N3—C26—C25	121.8 (2)
C12—C13—C14	118.62 (19)	C21—C26—C25	116.8 (2)
C12—C13—C19	119.05 (19)	N3—C27—H27A	109.5
C14—C13—C19	122.21 (19)	N3—C27—H27B	109.5
C13—C14—C9	121.17 (19)	H27A—C27—H27B	109.5
C13—C14—Br	119.78 (16)	N3—C27—H27C	109.5
C9—C14—Br	119.01 (16)	H27A—C27—H27C	109.5
C18—C15—C17	109.2 (2)	H27B—C27—H27C	109.5
C8—N1—C2—C7	0.1 (2)	C12—C13—C14—Br	-177.74 (14)
C1—N1—C2—C7	177.6 (2)	C19—C13—C14—Br	-1.6 (3)
C8—N1—C2—C3	178.1 (3)	C10-C9-C14-C13	0.4 (3)
C1—N1—C2—C3	-4.3 (4)	C8—C9—C14—C13	179.08 (19)
N1-C2-C3-C4	-176.7 (3)	C10-C9-C14-Br	178.12 (15)
C7—C2—C3—C4	1.0 (4)	C8—C9—C14—Br	-3.2 (3)
C2—C3—C4—C5	-2.2 (4)	C10-C11-C15-C18	-154.3 (2)
C3—C4—C5—C6	1.9 (5)	C12—C11—C15—C18	26.3 (3)
C4—C5—C6—C7	-0.2 (5)	C10-C11-C15-C17	85.6 (3)
C8—N2—C7—C2	-0.3 (3)	C12—C11—C15—C17	-93.8 (3)
C8—N2—C7—C6	-178.8 (3)	C10-C11-C15-C16	-34.1 (3)
N1-C2-C7-N2	0.1 (3)	C12-C11-C15-C16	146.5 (2)
C3—C2—C7—N2	-178.1 (2)	C21—N4—C19—O1	-177.7 (2)
N1—C2—C7—C6	178.7 (2)	C20—N4—C19—O1	5.7 (3)

C3—C2—C7—C6	0.5 (4)	C21—N4—C19—C13	1.1 (3)
C5—C6—C7—N2	177.4 (3)	C20-N4-C19-C13	-175.5 (2)
C5—C6—C7—C2	-0.9 (4)	C12-C13-C19-O1	82.7 (3)
C7—N2—C8—N1	0.4 (3)	C14—C13—C19—O1	-93.4 (2)
C7—N2—C8—C9	177.9 (2)	C12-C13-C19-N4	-96.1 (2)
C2—N1—C8—N2	-0.3 (3)	C14—C13—C19—N4	87.7 (2)
C1—N1—C8—N2	-177.8 (2)	C19—N4—C21—C22	-98.6 (3)
C2—N1—C8—C9	-177.9 (2)	C20—N4—C21—C22	78.2 (3)
C1—N1—C8—C9	4.6 (4)	C19—N4—C21—C26	87.6 (3)
N2-C8-C9-C14	112.4 (3)	C20—N4—C21—C26	-95.7 (3)
N1-C8-C9-C14	-70.3 (3)	C26—C21—C22—C23	-2.4 (4)
N2-C8-C9-C10	-68.9 (3)	N4—C21—C22—C23	-176.1 (2)
N1-C8-C9-C10	108.4 (2)	C21—C22—C23—C24	0.8 (4)
C14—C9—C10—C11	0.4 (3)	C22—C23—C24—C25	0.4 (4)
C8—C9—C10—C11	-178.28 (19)	C23—C24—C25—C26	0.1 (4)
C9—C10—C11—C12	-1.6 (3)	C27—N3—C26—C21	-177.6 (2)
C9—C10—C11—C15	179.03 (19)	C27—N3—C26—C25	4.3 (4)
C10-C11-C12-C13	2.0 (3)	C22-C21-C26-N3	-175.4 (2)
C15—C11—C12—C13	-178.63 (19)	N4-C21-C26-N3	-1.7 (3)
C11—C12—C13—C14	-1.2 (3)	C22—C21—C26—C25	2.8 (3)
C11—C12—C13—C19	-177.46 (18)	N4-C21-C26-C25	176.5 (2)
C12—C13—C14—C9	0.0 (3)	C24—C25—C26—N3	176.5 (2)
C19—C13—C14—C9	176.10 (18)	C24—C25—C26—C21	-1.6 (4)

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H··· A	
N3—H3 <i>B</i> …O1 ⁱ	0.81 (3)	2.35 (3)	3.038 (3)	143 (3)	
C4—H4A···Br ⁱⁱ	0.95	2.98	3.719 (3)	135	
C12—H12A…O1 ⁱ	0.95	2.37	3.287 (3)	163	

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