organic compounds

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Bis[3-methyl-5-(pyridin-2-yl)-1*H*-pyrazol-4-yl] selenide methanol hemisolvate

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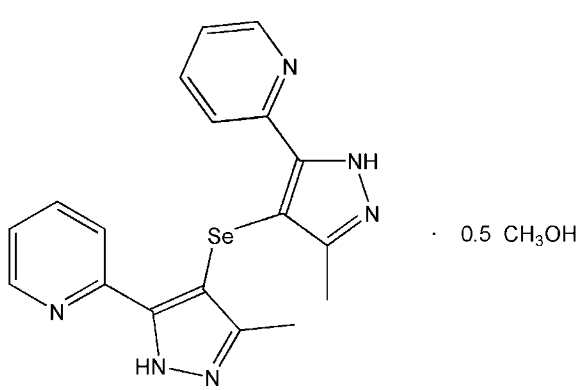
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.006 Å; R factor = 0.032; wR factor = 0.078; data-to-parameter ratio = 15.4.

The asymmetric unit of the title compound, $C_{18}H_{16}N_6Se\cdot 0.5CH_3OH$, contains two independent molecules of bis[3-methyl-5-(pyridin-2-yl)-1*H*-pyrazol-4-yl] selenide with similar C—Se—C bond angles [99.30 (14) and 98.26 (13)°], and a methanol molecule of solvation. In one molecule, the dihedral angles between pyrazole and neighbouring pyridine rings are 18.3 (2) and 15.8 (2)°, and the corresponding angles in the other molecule are 13.5 (2) and 8.3 (2)°. In the crystal, the selenide and solvent molecules are linked by classical O—H⋯N and N—H⋯N hydrogen bonds, as well as by weak C—H⋯O and C—H⋯π interactions, forming a three-dimensional supramolecular architecture.

Related literature

For structural studies of related pyrazol-4-ylselenides, see: Seredyuk *et al.* (2010) and for structural studies of *d*-metal complexes of pyrazol-4-ylselenide, see: Seredyuk *et al.* (2007, 2009, 2013). For related structures, see: Krämer *et al.* (2002); Penkova *et al.* (2008, 2009, 2010).



Experimental

Crystal data

$2C_{18}H_{16}N_6Se\cdot CH_4O$
M_r = 822.70
Monoclinic, Cc
a = 24.386 (5) Å
b = 10.784 (2) Å
c = 15.139 (3) Å
β = 118.59 (3)°
V = 3495.8 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.17 mm^{-1}
T = 120 K
0.36 × 0.24 × 0.13 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.545, T_{max} = 0.767
11797 measured reflections
7632 independent reflections
6581 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.078
S = 0.97
7632 reflections
494 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}
Absolute structure: Flack (1983), 3629 Friedel pairs
Absolute structure parameter: −0.018 (6)

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

*Cg*7 is the centroid of the N21*A*-containing pyridine ring.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O1—H1*O*1⋯N4*A*	0.91 (5)	2.03 (5)	2.839 (5)	148 (5)
N1*A*—H1*A*⋯N21*A*^{i}	0.78 (4)	2.33 (4)	3.040 (4)	151 (4)
N1*B*—H1*B*⋯N21*B*^{ii}	0.73 (4)	2.32 (4)	2.988 (5)	153 (4)
N3*A*—H3*A*⋯N2*A*^{iii}	0.83 (4)	2.06 (4)	2.863 (4)	165 (4)
N3*B*—H3*B*⋯N2*B*^{iv}	0.77 (3)	2.01 (4)	2.770 (4)	170 (3)
C27*B*—H27*F*⋯O1^{v}	0.96	2.32	3.273 (5)	171
C14*B*—H14*B*⋯*Cg*7^{v}	0.93	2.61	3.315 (4)	133

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5749).

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supplementary materials

Acta Cryst. (2014). E**70**, o127–o128 [doi:10.1107/S1600536813034624]

Bis[3-methyl-5-(pyridin-2-yl)-1*H*-pyrazol-4-yl] selenide methanol hemisolvate

Maksym Seredyuk, Natalia O. Sharkina, Elzbieta Gumienna-Kontecka and Anatoly A. Kapshuk

1. Comment

Pyrazole–derived ligands are widely used in molecular magnetism, bioinspired catalysis and supramolecular chemistry due to their bridging nature and possibility for facile functionalization with various chelating groups (Krämer *et al.*, 2002; Penkova *et al.*, 2009). As a part of our synthetic and structural study of bis(1*H*–pyrazol–4–yl)selenides (Seredyuk *et al.*, 2010) and their complexes with *d*–metals (Seredyuk *et al.*, 2007, 2009, 2013), we report here the molecular and crystal structures of the title compound (Fig. 1).

The molecule of the title compound is a symmetric organic selenide. The asymmetric unit of the title compound contains two independent molecules with the angles of C—Se—C fragments equal to 99.30 (14) and 98.26 (13)°. Additionally there is one molecule of methanol forming hydrogen bond with one of the selenide molecules [*d*(O1···N4A) = 2.839 (5) Å]. In one molecule, the dihedral angles between pyrazole and neighboring pyridine rings are 18.3 (2) and 15.8 (2)°, and the corresponding angles in another molecule are 13.5 (2) and 8.3 (2)°. The C—C, C—N, N—N bond lengths in the pyrazole ring exhibit normal values (Penkova *et al.*, 2008, 2010). The selenide molecules are united through hydrogen bonds between pyrazoles [*d*(N1A···N21A) = 2.863 (4) Å; *d*(N1B···N21B) = 2.988 (5) Å] and pyrazole and pyridine moieties [*d*(N3A···N2A) = 2.863 (4) Å; *d*(N3B···N2B) = 2.770 (4) Å] with neighboring molecules forming two different zigzag chains running along [001] (Fig. 2). Also, there are weak C—H···O and C—H···π interactions, forming the three dimensional supramolecular architecture. No π-π stacking interactions are observed between the neighboring molecules, however, there are two intermolecular contacts between pyrazole and pyridine moieties of neighbouring chains [*d*(C14B···N1A) = 3.197 (6) and *d*(C14B···C1A) = 3.393 (5) Å].

2. Experimental

A concentrated hot solution of bis(5-methyl-3-(pyridin-2-yl)-1*H*-pyrazol-4-yl)selenide (Seredyuk *et al.*, 2010) in methanol was cooled on air and kept overnight at ambient temperature in a sealed vial. Obtained well formed colourless crystals were filtered off and air dried. $C_{18.5}H_{18}N_6O_{0.5}Se$ requires: C, 54.02; H, 4.41; N, 20.43. Found: C, 54.05; H, 4.37; N, 20.93.

3. Refinement

The H atoms from NH and OH were located from the difference Fourier map but were constrained to ride on their parent atom, with U_{iso} = 1.2U_{eq}(parent atom) for the N—H atoms and U_{is} = 1.5U_{eq}(parent atom) for the O—H atoms. The methyl and aromatic H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.96 Å and U_{iso} = 1.5U_{eq}(C) for the methyl H atoms and C—H = 0.93 Å and U_{iso} = 1.2U_{eq}(C) for the aromatic H atoms.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97*

(Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

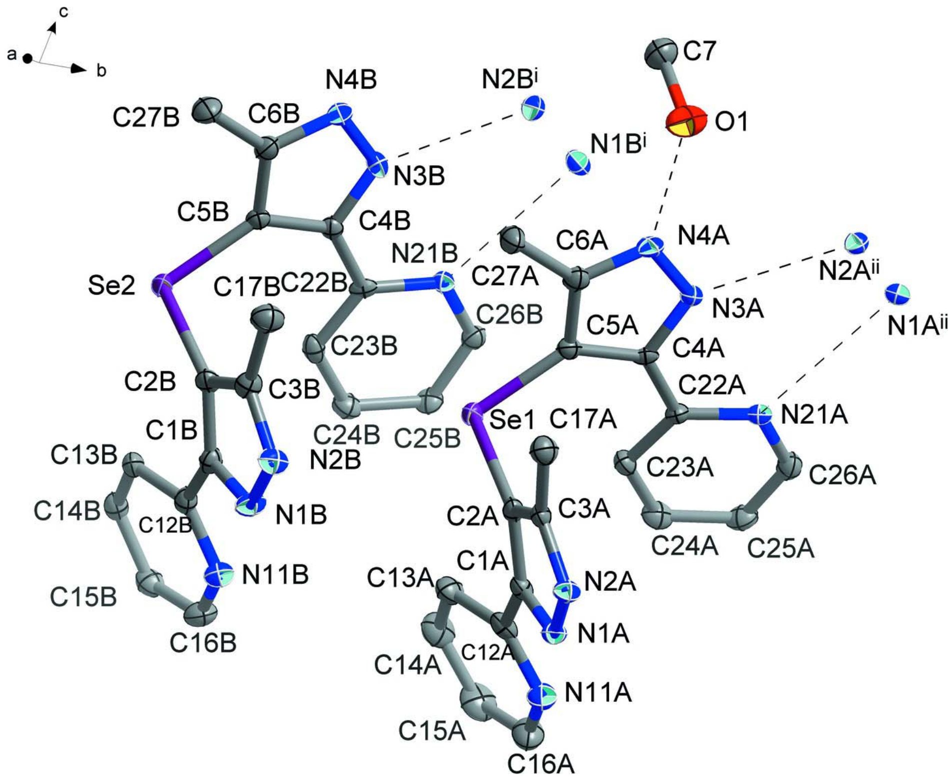

Figure 1

The crystal structure of the title compound showing the labeling scheme and 50% probability displacement ellipsoids. Hydrogen bonds are indicated by dashed lines. H atoms are omitted for clarity [symmetry code: (i) *x*, 1 - *y*, 0.5 + *z*; (ii) *x*, 2 - *y*, 0.5 + *z*].

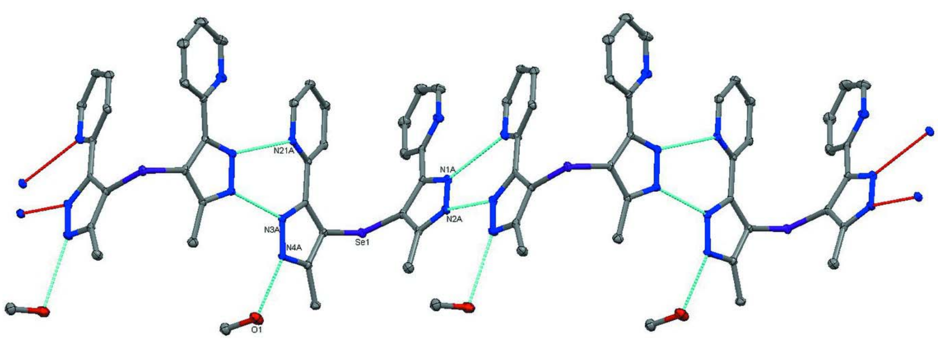

Figure 2

A fragment of the crystal packing showing a zigzag chain along [001] formed due to hydrogen bonding NH···N (dashed lines). Only one of the two selenide molecules is shown.

Bis[3-methyl-5-(pyridin-2-yl)-1*H*-pyrazol-4-yl] selenide methanol hemisolvate

Crystal data

$2C_{18}H_{16}N_6Se \cdot CH_4O$
$M_r = 822.70$
Monoclinic, *Cc*
Hall symbol: C -2yc
$a = 24.386$ (5) Å
$b = 10.784$ (2) Å
$c = 15.139$ (3) Å
$\beta = 118.59$ (3)°
$V = 3495.8$ (16) Å^3
$Z = 4$
$F(000) = 1672$
$D_x = 1.563$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3138 reflections
$\theta = 3.6–27.6°$
$\mu = 2.17$ mm^{-1}
$T = 120$ K
Block, colorless
0.36 × 0.24 × 0.13 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Horizontally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm^{-1}
φ scans and ω scans with κ offset
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.545$, $T_{max} = 0.767$
11797 measured reflections
7632 independent reflections
6581 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 28.5°$, $\theta_{min} = 3.6°$
$h = -32 \rightarrow 32$
$k = -8 \rightarrow 14$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.078$
$S = 0.97$
7632 reflections
494 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -0.81$ e Å^{-3}
Absolute structure: Flack (1983), 3629 Friedel pairs
Absolute structure parameter: −0.018 (6)

Special details

Experimental. The H atoms from NH and OH were located from the difference Fourier map but were constrained to ride on their parent atom, with $U_{iso} = 1.2U_{eq}$(parent atom) for the N—H atoms and $U_{is} = 1.5U_{eq}$(parent atom) for the O—H atoms. The methyl and aromatic H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.96 Å and $U_{iso} = 1.5U_{eq}$(C) for the methyl H atoms and C—H = 0.93 Å and $U_{iso} = 1.2U_{eq}$(C) for the aromatic H atoms.

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.

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

	x	y	z	U_{iso}*/U_{eq}
Se1	0.355504 (12)	0.63083 (3)	0.018781 (17)	0.01693 (11)
Se2	0.429962 (12)	0.13792 (3)	0.106831 (16)	0.01682 (11)
O1	0.54984 (14)	0.9478 (3)	0.4101 (2)	0.0366 (7)
N1A	0.29572 (16)	0.8389 (3)	−0.2336 (3)	0.0171 (7)
N1B	0.36479 (18)	0.3522 (3)	−0.1434 (3)	0.0219 (9)
N2A	0.35458 (15)	0.8832 (3)	−0.1848 (3)	0.0175 (7)
N2B	0.42002 (16)	0.4077 (3)	−0.0902 (3)	0.0208 (7)
N3A	0.37107 (15)	0.9089 (3)	0.2126 (2)	0.0168 (7)
N3B	0.43950 (16)	0.4036 (3)	0.3037 (3)	0.0185 (7)
N4A	0.43116 (16)	0.8668 (3)	0.2581 (3)	0.0199 (8)
N4B	0.50018 (16)	0.3670 (3)	0.3518 (3)	0.0200 (8)
N11A	0.17652 (13)	0.7566 (3)	−0.3020 (2)	0.0240 (6)
N11B	0.25090 (12)	0.2489 (3)	−0.2249 (2)	0.0216 (6)
N21A	0.24727 (12)	0.9800 (2)	0.09135 (19)	0.0177 (5)
N21B	0.31604 (12)	0.4718 (2)	0.18315 (19)	0.0158 (5)
C1A	0.28369 (17)	0.7508 (3)	−0.1820 (3)	0.0154 (7)
C1B	0.35530 (18)	0.2556 (3)	−0.0949 (3)	0.0168 (7)
C2A	0.33882 (17)	0.7373 (3)	−0.0920 (3)	0.0166 (8)
C2B	0.40936 (18)	0.2493 (3)	−0.0023 (3)	0.0169 (8)
C3A	0.38170 (18)	0.8204 (3)	−0.0981 (3)	0.0155 (7)
C3B	0.4480 (2)	0.3469 (4)	−0.0026 (3)	0.0193 (9)
C4A	0.33359 (19)	0.8424 (4)	0.1301 (3)	0.0136 (7)
C4B	0.40427 (18)	0.3416 (3)	0.2179 (3)	0.0146 (7)
C5A	0.37217 (17)	0.7535 (3)	0.1200 (3)	0.0162 (7)
C5B	0.44480 (17)	0.2577 (3)	0.2088 (3)	0.0154 (7)
C6A	0.43134 (18)	0.7730 (3)	0.2017 (3)	0.0189 (8)
C6B	0.50331 (17)	0.2784 (3)	0.2931 (3)	0.0200 (8)
C7	0.55599 (18)	0.8730 (3)	0.4891 (3)	0.0303 (8)
H7A	0.5975	0.8808	0.5444	0.045*
H7B	0.5484	0.7882	0.4673	0.045*
H7C	0.5263	0.8983	0.5102	0.045*
C12A	0.22154 (16)	0.6938 (3)	−0.2267 (3)	0.0184 (7)
C12B	0.29543 (16)	0.1904 (3)	−0.1438 (3)	0.0181 (7)
C13A	0.21192 (17)	0.5802 (3)	−0.1921 (3)	0.0245 (7)
H13A	0.2448	0.5369	−0.1411	0.029*
C13B	0.28421 (15)	0.0781 (3)	−0.1087 (2)	0.0174 (6)
H13B	0.3159	0.0389	−0.0529	0.021*
C14A	0.15067 (17)	0.5340 (3)	−0.2372 (3)	0.0303 (8)
H14A	0.1420	0.4595	−0.2154	0.036*
C14B	0.22572 (15)	0.0272 (3)	−0.1579 (2)	0.0195 (7)
H14B	0.2173	−0.0468	−0.1353	0.023*
C15A	0.10368 (18)	0.5995 (4)	−0.3138 (3)	0.0344 (9)
H15A	0.0626	0.5715	−0.3438	0.041*
C15B	0.17929 (16)	0.0859 (3)	−0.2412 (3)	0.0232 (7)
H15B	0.1392	0.0530	−0.2754	0.028*
C16A	0.11907 (17)	0.7087 (3)	−0.3452 (3)	0.0326 (9)
H16A	0.0876	0.7508	−0.3993	0.039*

C16B	0.19462 (16)	0.1959 (3)	−0.2721 (3)	0.0256 (7)
H16B	0.1638	0.2349	−0.3290	0.031*
C17A	0.4486 (2)	0.8426 (4)	−0.0230 (4)	0.0239 (9)
H17A	0.4662	0.9025	−0.0492	0.036*
H17B	0.4714	0.7662	−0.0099	0.036*
H17C	0.4512	0.8733	0.0384	0.036*
C17B	0.51041 (19)	0.3890 (4)	0.0777 (3)	0.0267 (9)
H17D	0.5278	0.4470	0.0498	0.040*
H17E	0.5377	0.3188	0.1042	0.040*
H17F	0.5058	0.4283	0.1307	0.040*
C22A	0.26647 (16)	0.8694 (3)	0.0726 (3)	0.0146 (7)
C22B	0.33795 (19)	0.3707 (3)	0.1561 (3)	0.0137 (8)
C23A	0.22481 (15)	0.7835 (3)	0.0046 (2)	0.0182 (6)
H23A	0.2393	0.7077	−0.0054	0.022*
C23B	0.29889 (14)	0.2977 (3)	0.0742 (2)	0.0179 (6)
H23B	0.3145	0.2273	0.0585	0.021*
C24A	0.16218 (15)	0.8117 (3)	−0.0476 (3)	0.0226 (7)
H24A	0.1340	0.7558	−0.0937	0.027*
C24B	0.23644 (16)	0.3303 (3)	0.0160 (3)	0.0215 (7)
H24B	0.2102	0.2832	−0.0399	0.026*
C25A	0.14153 (15)	0.9257 (3)	−0.0306 (2)	0.0231 (7)
H25A	0.0996	0.9476	−0.0650	0.028*
C25B	0.21373 (14)	0.4343 (3)	0.0424 (2)	0.0188 (7)
H25B	0.1723	0.4589	0.0049	0.023*
C26A	0.18575 (15)	1.0048 (3)	0.0394 (2)	0.0208 (7)
H26A	0.1720	1.0802	0.0513	0.025*
C26B	0.25535 (14)	0.4998 (3)	0.1269 (2)	0.0188 (6)
H26B	0.2401	0.5680	0.1459	0.023*
C27A	0.49055 (17)	0.7012 (3)	0.2310 (3)	0.0237 (8)
H27A	0.5259	0.7535	0.2697	0.036*
H27B	0.4916	0.6740	0.1714	0.036*
H27C	0.4919	0.6305	0.2704	0.036*
C27B	0.56453 (17)	0.2152 (4)	0.3213 (3)	0.0256 (9)
H27D	0.5982	0.2650	0.3696	0.038*
H27E	0.5693	0.2049	0.2624	0.038*
H27F	0.5652	0.1354	0.3500	0.038*
H1A	0.2724 (18)	0.868 (3)	−0.285 (3)	0.018 (10)*
H1B	0.3444 (19)	0.377 (3)	−0.193 (3)	0.021 (11)*
H3A	0.3594 (18)	0.969 (4)	0.234 (3)	0.032 (11)*
H3B	0.4296 (14)	0.455 (3)	0.329 (2)	0.007 (8)*
H1O1	0.508 (2)	0.943 (5)	0.375 (4)	0.068 (17)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Se1	0.0222 (2)	0.01311 (19)	0.0151 (2)	0.00129 (14)	0.0086 (2)	0.00062 (14)
Se2	0.0222 (2)	0.01314 (19)	0.0158 (2)	0.00342 (15)	0.0097 (2)	0.00146 (15)
O1	0.0315 (15)	0.0364 (15)	0.0316 (14)	−0.0089 (12)	0.0068 (13)	0.0070 (12)
N1A	0.0182 (15)	0.0185 (15)	0.0125 (14)	0.0000 (12)	0.0058 (13)	0.0008 (12)
N1B	0.0228 (19)	0.0223 (17)	0.0177 (18)	−0.0013 (13)	0.0073 (16)	0.0057 (13)

N2A	0.0160 (15)	0.0192 (15)	0.0149 (15)	−0.0034 (11)	0.0056 (13)	−0.0006 (12)
N2B	0.0212 (17)	0.0208 (17)	0.0187 (17)	−0.0070 (14)	0.0082 (15)	−0.0001 (14)
N3A	0.0173 (16)	0.0173 (15)	0.0128 (15)	0.0033 (13)	0.0047 (14)	−0.0010 (13)
N3B	0.0222 (16)	0.0171 (15)	0.0179 (15)	0.0008 (13)	0.0110 (14)	−0.0043 (13)
N4A	0.0130 (15)	0.0256 (17)	0.0146 (15)	0.0047 (12)	0.0013 (13)	0.0010 (12)
N4B	0.0138 (15)	0.0221 (16)	0.0169 (16)	0.0048 (12)	0.0015 (13)	−0.0003 (12)
N11A	0.0199 (14)	0.0250 (15)	0.0224 (15)	0.0004 (11)	0.0065 (13)	−0.0011 (12)
N11B	0.0213 (15)	0.0240 (15)	0.0188 (14)	0.0006 (11)	0.0089 (13)	0.0029 (12)
N21A	0.0185 (13)	0.0191 (13)	0.0119 (12)	0.0011 (10)	0.0045 (11)	0.0007 (10)
N21B	0.0214 (13)	0.0143 (12)	0.0138 (12)	0.0010 (10)	0.0100 (12)	0.0005 (10)
C1A	0.0183 (16)	0.0146 (15)	0.0143 (15)	−0.0028 (12)	0.0087 (14)	−0.0039 (13)
C1B	0.0195 (17)	0.0137 (15)	0.0191 (17)	0.0009 (12)	0.0107 (15)	0.0020 (13)
C2A	0.024 (2)	0.0120 (15)	0.0171 (17)	0.0008 (13)	0.0131 (17)	−0.0005 (13)
C2B	0.023 (2)	0.0155 (17)	0.0156 (18)	−0.0009 (14)	0.0122 (17)	0.0007 (14)
C3A	0.0185 (19)	0.0126 (16)	0.0148 (17)	−0.0009 (14)	0.0075 (16)	−0.0025 (14)
C3B	0.020 (2)	0.0191 (19)	0.021 (2)	0.0001 (16)	0.0119 (19)	0.0018 (16)
C4A	0.0144 (18)	0.0171 (16)	0.0092 (17)	0.0000 (14)	0.0055 (16)	0.0039 (14)
C4B	0.0177 (18)	0.0142 (16)	0.0145 (17)	0.0002 (13)	0.0098 (16)	0.0008 (13)
C5A	0.0171 (18)	0.0160 (16)	0.0135 (16)	−0.0015 (14)	0.0056 (16)	0.0009 (14)
C5B	0.0181 (17)	0.0148 (16)	0.0132 (15)	0.0013 (13)	0.0074 (15)	0.0018 (13)
C6A	0.0216 (18)	0.0191 (17)	0.0176 (17)	0.0011 (13)	0.0106 (15)	0.0025 (13)
C6B	0.0217 (18)	0.0202 (17)	0.0188 (17)	0.0050 (14)	0.0102 (16)	0.0036 (14)
C7	0.033 (2)	0.029 (2)	0.0290 (18)	0.0012 (16)	0.0145 (18)	0.0032 (16)
C12A	0.0210 (17)	0.0202 (17)	0.0173 (17)	−0.0065 (13)	0.0118 (15)	−0.0065 (14)
C12B	0.0211 (17)	0.0151 (15)	0.0205 (17)	0.0021 (13)	0.0120 (15)	−0.0001 (14)
C13A	0.0258 (17)	0.0222 (18)	0.0203 (16)	−0.0049 (15)	0.0068 (15)	−0.0041 (15)
C13B	0.0220 (16)	0.0131 (15)	0.0162 (15)	0.0008 (13)	0.0085 (14)	−0.0014 (12)
C14A	0.0307 (19)	0.0266 (19)	0.033 (2)	−0.0112 (15)	0.0143 (18)	−0.0045 (16)
C14B	0.0250 (17)	0.0160 (15)	0.0219 (16)	−0.0015 (13)	0.0147 (15)	−0.0020 (13)
C15A	0.0237 (19)	0.035 (2)	0.040 (2)	−0.0127 (16)	0.0119 (18)	−0.0100 (18)
C15B	0.0199 (17)	0.0254 (17)	0.0223 (17)	−0.0027 (14)	0.0084 (15)	−0.0047 (14)
C16A	0.0221 (18)	0.030 (2)	0.033 (2)	0.0001 (15)	0.0029 (17)	−0.0064 (17)
C16B	0.0227 (17)	0.0296 (19)	0.0188 (16)	0.0022 (15)	0.0053 (15)	0.0038 (15)
C17A	0.025 (2)	0.0212 (19)	0.023 (2)	−0.0025 (16)	0.010 (2)	−0.0007 (16)
C17B	0.027 (2)	0.0283 (19)	0.0236 (19)	−0.0030 (16)	0.0115 (17)	0.0012 (16)
C22A	0.0142 (15)	0.0148 (16)	0.0120 (16)	0.0015 (12)	0.0042 (14)	0.0012 (12)
C22B	0.0130 (18)	0.0184 (18)	0.0117 (17)	−0.0012 (13)	0.0075 (16)	0.0041 (13)
C23A	0.0212 (16)	0.0156 (15)	0.0162 (14)	−0.0019 (12)	0.0076 (14)	−0.0031 (12)
C23B	0.0230 (16)	0.0156 (15)	0.0208 (16)	−0.0011 (12)	0.0152 (15)	−0.0022 (13)
C24A	0.0212 (17)	0.0233 (17)	0.0212 (17)	−0.0073 (14)	0.0085 (15)	−0.0009 (14)
C24B	0.0214 (17)	0.0221 (17)	0.0192 (16)	−0.0039 (13)	0.0082 (15)	−0.0027 (14)
C25A	0.0164 (16)	0.0296 (18)	0.0206 (16)	0.0041 (14)	0.0066 (14)	0.0037 (14)
C25B	0.0127 (15)	0.0224 (16)	0.0200 (16)	0.0006 (12)	0.0068 (14)	0.0004 (13)
C26A	0.0224 (17)	0.0191 (16)	0.0227 (17)	0.0038 (13)	0.0122 (15)	0.0013 (13)
C26B	0.0210 (16)	0.0177 (15)	0.0178 (15)	0.0033 (12)	0.0095 (14)	0.0036 (13)
C27A	0.0207 (18)	0.0246 (18)	0.0220 (19)	0.0055 (14)	0.0072 (16)	−0.0035 (15)
C27B	0.0188 (18)	0.029 (2)	0.023 (2)	0.0044 (15)	0.0054 (16)	0.0000 (16)

Geometric parameters (Å, º)

Se1—C2A	1.908 (4)	C7—H7B	0.9600
Se1—C5A	1.915 (4)	C7—H7C	0.9600
Se2—C2B	1.905 (4)	C12A—C13A	1.396 (5)
Se2—C5B	1.910 (4)	C12B—C13B	1.401 (5)
O1—C7	1.390 (4)	C13A—C14A	1.404 (5)
O1—H1O1	0.91 (5)	C13A—H13A	0.9300
N1A—C1A	1.347 (5)	C13B—C14B	1.369 (4)
N1A—N2A	1.349 (5)	C13B—H13B	0.9300
N1A—H1A	0.78 (4)	C14A—C15A	1.373 (6)
N1B—N2B	1.335 (5)	C14A—H14A	0.9300
N1B—C1B	1.356 (5)	C14B—C15B	1.380 (5)
N1B—H1B	0.73 (4)	C14B—H14B	0.9300
N2A—C3A	1.337 (5)	C15A—C16A	1.387 (5)
N2B—C3B	1.337 (5)	C15A—H15A	0.9300
N3A—C4A	1.348 (5)	C15B—C16B	1.390 (5)
N3A—N4A	1.365 (5)	C15B—H15B	0.9300
N3A—H3A	0.83 (4)	C16A—H16A	0.9300
N3B—C4B	1.343 (5)	C16B—H16B	0.9300
N3B—N4B	1.358 (5)	C17A—H17A	0.9600
N3B—H3B	0.77 (3)	C17A—H17B	0.9600
N4A—C6A	1.325 (5)	C17A—H17C	0.9600
N4B—C6B	1.332 (5)	C17B—H17D	0.9600
N11A—C12A	1.328 (4)	C17B—H17E	0.9600
N11A—C16A	1.334 (4)	C17B—H17F	0.9600
N11B—C16B	1.335 (4)	C22A—C23A	1.397 (4)
N11B—C12B	1.345 (4)	C22B—C23B	1.390 (5)
N21A—C26A	1.346 (4)	C23A—C24A	1.377 (5)
N21A—C22A	1.359 (4)	C23A—H23A	0.9300
N21B—C26B	1.342 (4)	C23B—C24B	1.391 (5)
N21B—C22B	1.361 (4)	C23B—H23B	0.9300
C1A—C2A	1.391 (5)	C24A—C25A	1.398 (5)
C1A—C12A	1.467 (5)	C24A—H24A	0.9300
C1B—C2B	1.393 (5)	C24B—C25B	1.392 (4)
C1B—C12B	1.462 (5)	C24B—H24B	0.9300
C2A—C3A	1.413 (5)	C25A—C26A	1.386 (5)
C2B—C3B	1.414 (5)	C25A—H25A	0.9300
C3A—C17A	1.496 (6)	C25B—C26B	1.387 (4)
C3B—C17B	1.494 (6)	C25B—H25B	0.9300
C4A—C5A	1.402 (5)	C26A—H26A	0.9300
C4A—C22A	1.469 (5)	C26B—H26B	0.9300
C4B—C5B	1.395 (5)	C27A—H27A	0.9600
C4B—C22B	1.464 (6)	C27A—H27B	0.9600
C5A—C6A	1.396 (5)	C27A—H27C	0.9600
C5B—C6B	1.404 (5)	C27B—H27D	0.9600
C6A—C27A	1.506 (5)	C27B—H27E	0.9600
C6B—C27B	1.505 (5)	C27B—H27F	0.9600
C7—H7A	0.9600		

C2A—Se1—C5A	99.30 (14)	C14B—C13B—H13B	120.6
C2B—Se2—C5B	98.26 (13)	C12B—C13B—H13B	120.6
C7—O1—H1O1	96 (3)	C15A—C14A—C13A	119.5 (3)
C1A—N1A—N2A	113.7 (3)	C15A—C14A—H14A	120.3
C1A—N1A—H1A	128 (3)	C13A—C14A—H14A	120.3
N2A—N1A—H1A	119 (3)	C13B—C14B—C15B	119.9 (3)
N2B—N1B—C1B	113.7 (4)	C13B—C14B—H14B	120.0
N2B—N1B—H1B	117 (3)	C15B—C14B—H14B	120.0
C1B—N1B—H1B	130 (3)	C14A—C15A—C16A	118.2 (3)
C3A—N2A—N1A	104.8 (3)	C14A—C15A—H15A	120.9
N1B—N2B—C3B	105.5 (3)	C16A—C15A—H15A	120.9
C4A—N3A—N4A	112.2 (3)	C14B—C15B—C16B	117.6 (3)
C4A—N3A—H3A	124 (3)	C14B—C15B—H15B	121.2
N4A—N3A—H3A	123 (3)	C16B—C15B—H15B	121.2
C4B—N3B—N4B	113.7 (3)	N11A—C16A—C15A	123.6 (3)
C4B—N3B—H3B	129 (2)	N11A—C16A—H16A	118.2
N4B—N3B—H3B	117 (2)	C15A—C16A—H16A	118.2
C6A—N4A—N3A	105.2 (3)	N11B—C16B—C15B	124.0 (3)
C6B—N4B—N3B	104.3 (3)	N11B—C16B—H16B	118.0
C12A—N11A—C16A	117.8 (3)	C15B—C16B—H16B	118.0
C16B—N11B—C12B	117.5 (3)	C3A—C17A—H17A	109.5
C26A—N21A—C22A	116.8 (3)	C3A—C17A—H17B	109.5
C26B—N21B—C22B	117.5 (3)	H17A—C17A—H17B	109.5
N1A—C1A—C2A	105.4 (3)	C3A—C17A—H17C	109.5
N1A—C1A—C12A	119.5 (3)	H17A—C17A—H17C	109.5
C2A—C1A—C12A	135.2 (3)	H17B—C17A—H17C	109.5
N1B—C1B—C2B	104.9 (3)	C3B—C17B—H17D	109.5
N1B—C1B—C12B	118.9 (3)	C3B—C17B—H17E	109.5
C2B—C1B—C12B	136.1 (3)	H17D—C17B—H17E	109.5
C1A—C2A—C3A	105.5 (3)	C3B—C17B—H17F	109.5
C1A—C2A—Se1	128.6 (3)	H17D—C17B—H17F	109.5
C3A—C2A—Se1	125.8 (3)	H17E—C17B—H17F	109.5
C1B—C2B—C3B	105.8 (3)	N21A—C22A—C23A	122.3 (3)
C1B—C2B—Se2	129.3 (3)	N21A—C22A—C4A	116.6 (3)
C3B—C2B—Se2	124.9 (3)	C23A—C22A—C4A	121.1 (3)
N2A—C3A—C2A	110.6 (3)	N21B—C22B—C23B	121.5 (3)
N2A—C3A—C17A	120.8 (4)	N21B—C22B—C4B	116.8 (3)
C2A—C3A—C17A	128.6 (4)	C23B—C22B—C4B	121.7 (3)
N2B—C3B—C2B	110.1 (4)	C24A—C23A—C22A	119.5 (3)
N2B—C3B—C17B	119.7 (4)	C24A—C23A—H23A	120.3
C2B—C3B—C17B	130.1 (4)	C22A—C23A—H23A	120.3
N3A—C4A—C5A	105.8 (3)	C22B—C23B—C24B	119.8 (3)
N3A—C4A—C22A	120.8 (4)	C22B—C23B—H23B	120.1
C5A—C4A—C22A	133.3 (4)	C24B—C23B—H23B	120.1
N3B—C4B—C5B	105.3 (3)	C23A—C24A—C25A	119.2 (3)
N3B—C4B—C22B	120.8 (3)	C23A—C24A—H24A	120.4
C5B—C4B—C22B	133.9 (4)	C25A—C24A—H24A	120.4
C6A—C5A—C4A	105.3 (3)	C23B—C24B—C25B	119.1 (3)
C6A—C5A—Se1	123.1 (3)	C23B—C24B—H24B	120.4

C4A—C5A—Se1	131.5 (3)
C4B—C5B—C6B	105.5 (3)
C4B—C5B—Se2	130.5 (3)
C6B—C5B—Se2	124.0 (3)
N4A—C6A—C5A	111.4 (3)
N4A—C6A—C27A	120.1 (3)
C5A—C6A—C27A	128.5 (3)
N4B—C6B—C5B	111.3 (3)
N4B—C6B—C27B	120.1 (3)
C5B—C6B—C27B	128.6 (3)
O1—C7—H7A	109.5
O1—C7—H7B	109.5
H7A—C7—H7B	109.5
O1—C7—H7C	109.5
H7A—C7—H7C	109.5
H7B—C7—H7C	109.5
N11A—C12A—C13A	123.4 (3)
N11A—C12A—C1A	115.4 (3)
C13A—C12A—C1A	121.1 (3)
N11B—C12B—C13B	122.2 (3)
N11B—C12B—C1B	114.2 (3)
C13B—C12B—C1B	123.5 (3)
C12A—C13A—C14A	117.4 (3)
C12A—C13A—H13A	121.3
C14A—C13A—H13A	121.3
C14B—C13B—C12B	118.8 (3)
C25B—C24B—H24B	120.4
C26A—C25A—C24A	117.7 (3)
C26A—C25A—H25A	121.1
C24A—C25A—H25A	121.1
C26B—C25B—C24B	117.4 (3)
C26B—C25B—H25B	121.3
C24B—C25B—H25B	121.3
N21A—C26A—C25A	124.5 (3)
N21A—C26A—H26A	117.8
C25A—C26A—H26A	117.8
N21B—C26B—C25B	124.7 (3)
N21B—C26B—H26B	117.7
C25B—C26B—H26B	117.7
C6A—C27A—H27A	109.5
C6A—C27A—H27B	109.5
H27A—C27A—H27B	109.5
C6A—C27A—H27C	109.5
H27A—C27A—H27C	109.5
H27B—C27A—H27C	109.5
C6B—C27B—H27D	109.5
C6B—C27B—H27E	109.5
H27D—C27B—H27E	109.5
C6B—C27B—H27F	109.5
H27D—C27B—H27F	109.5
H27E—C27B—H27F	109.5

C1A—N1A—N2A—C3A	0.3 (4)
C1B—N1B—N2B—C3B	−0.9 (5)
C4A—N3A—N4A—C6A	0.9 (4)
C4B—N3B—N4B—C6B	0.5 (4)
N2A—N1A—C1A—C2A	0.6 (4)
N2A—N1A—C1A—C12A	−179.6 (3)
N2B—N1B—C1B—C2B	0.3 (5)
N2B—N1B—C1B—C12B	177.5 (3)
N1A—C1A—C2A—C3A	−1.2 (4)
C12A—C1A—C2A—C3A	179.0 (4)
N1A—C1A—C2A—Se1	178.8 (3)
C12A—C1A—C2A—Se1	−1.0 (6)
C5A—Se1—C2A—C1A	−116.8 (3)
C5A—Se1—C2A—C3A	63.2 (3)
N1B—C1B—C2B—C3B	0.4 (4)
C12B—C1B—C2B—C3B	−176.1 (4)
N1B—C1B—C2B—Se2	179.3 (3)
C12B—C1B—C2B—Se2	2.8 (7)
C5B—Se2—C2B—C1B	−122.5 (4)
C5B—Se2—C2B—C3B	56.2 (4)
N1A—N2A—C3A—C2A	−1.1 (4)
N1A—N2A—C3A—C17A	179.1 (3)
N3B—N4B—C6B—C5B	−0.7 (4)
N3B—N4B—C6B—C27B	179.1 (3)
C4B—C5B—C6B—N4B	0.8 (4)
Se2—C5B—C6B—N4B	−179.9 (3)
C4B—C5B—C6B—C27B	−179.1 (4)
Se2—C5B—C6B—C27B	0.2 (5)
C16A—N11A—C12A—C13A	1.1 (5)
C16A—N11A—C12A—C1A	−180.0 (3)
N1A—C1A—C12A—N11A	−18.1 (5)
C2A—C1A—C12A—N11A	161.6 (4)
N1A—C1A—C12A—C13A	160.8 (3)
C2A—C1A—C12A—C13A	−19.4 (6)
C16B—N11B—C12B—C13B	−0.1 (5)
C16B—N11B—C12B—C1B	−178.7 (3)
N1B—C1B—C12B—N11B	−12.2 (5)
C2B—C1B—C12B—N11B	164.0 (4)
N1B—C1B—C12B—C13B	169.3 (3)
C2B—C1B—C12B—C13B	−14.5 (7)
N11A—C12A—C13A—C14A	−2.8 (5)
C1A—C12A—C13A—C14A	178.3 (3)
N11B—C12B—C13B—C14B	−0.9 (5)
C1B—C12B—C13B—C14B	177.6 (3)

C1A—C2A—C3A—N2A	1.5 (4)	C12A—C13A—C14A—C15A	1.4 (5)
Se1—C2A—C3A—N2A	−178.5 (3)	C12B—C13B—C14B—C15B	0.7 (5)
C1A—C2A—C3A—C17A	−178.7 (4)	C13A—C14A—C15A—C16A	1.4 (6)
Se1—C2A—C3A—C17A	1.3 (6)	C13B—C14B—C15B—C16B	0.4 (5)
N1B—N2B—C3B—C2B	1.1 (5)	C12A—N11A—C16A—C15A	2.0 (5)
N1B—N2B—C3B—C17B	−177.3 (4)	C14A—C15A—C16A—N11A	−3.3 (6)
C1B—C2B—C3B—N2B	−1.0 (5)	C12B—N11B—C16B—C15B	1.3 (5)
Se2—C2B—C3B—N2B	−180.0 (3)	C14B—C15B—C16B—N11B	−1.4 (5)
C1B—C2B—C3B—C17B	177.2 (4)	C26A—N21A—C22A—C23A	−1.4 (5)
Se2—C2B—C3B—C17B	−1.8 (6)	C26A—N21A—C22A—C4A	−179.5 (3)
N4A—N3A—C4A—C5A	−1.5 (4)	N3A—C4A—C22A—N21A	15.2 (5)
N4A—N3A—C4A—C22A	177.4 (3)	C5A—C4A—C22A—N21A	−166.2 (4)
N4B—N3B—C4B—C5B	0.0 (4)	N3A—C4A—C22A—C23A	−162.9 (3)
N4B—N3B—C4B—C22B	−179.2 (3)	C5A—C4A—C22A—C23A	15.6 (6)
N3A—C4A—C5A—C6A	1.4 (4)	C26B—N21B—C22B—C23B	−1.0 (5)
C22A—C4A—C5A—C6A	−177.3 (4)	C26B—N21B—C22B—C4B	179.8 (3)
N3A—C4A—C5A—Se1	−176.2 (3)	N3B—C4B—C22B—N21B	7.5 (5)
C22A—C4A—C5A—Se1	5.1 (7)	C5B—C4B—C22B—N21B	−171.4 (4)
C2A—Se1—C5A—C6A	−110.9 (3)	N3B—C4B—C22B—C23B	−171.6 (4)
C2A—Se1—C5A—C4A	66.4 (4)	C5B—C4B—C22B—C23B	9.5 (7)
N3B—C4B—C5B—C6B	−0.4 (4)	N21A—C22A—C23A—C24A	1.6 (5)
C22B—C4B—C5B—C6B	178.6 (4)	C4A—C22A—C23A—C24A	179.7 (3)
N3B—C4B—C5B—Se2	−179.7 (3)	N21B—C22B—C23B—C24B	2.4 (5)
C22B—C4B—C5B—Se2	−0.7 (7)	C4B—C22B—C23B—C24B	−178.5 (3)
C2B—Se2—C5B—C4B	64.7 (4)	C22A—C23A—C24A—C25A	−0.7 (5)
C2B—Se2—C5B—C6B	−114.4 (3)	C22B—C23B—C24B—C25B	−1.6 (5)
N3A—N4A—C6A—C5A	0.0 (4)	C23A—C24A—C25A—C26A	−0.4 (5)
N3A—N4A—C6A—C27A	−178.6 (3)	C23B—C24B—C25B—C26B	−0.3 (5)
C4A—C5A—C6A—N4A	−0.9 (4)	C22A—N21A—C26A—C25A	0.2 (5)
Se1—C5A—C6A—N4A	177.0 (3)	C24A—C25A—C26A—N21A	0.7 (5)
C4A—C5A—C6A—C27A	177.6 (4)	C22B—N21B—C26B—C25B	−1.1 (5)
Se1—C5A—C6A—C27A	−4.5 (5)	C24B—C25B—C26B—N21B	1.8 (5)

Hydrogen-bond geometry (Å, º)

Cg7 is the centroid of the N21A-containing pyridine ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*1···N4*A*	0.91 (5)	2.03 (5)	2.839 (5)	148 (5)
N1*A*—H1*A*···N21*A*^{i}	0.78 (4)	2.33 (4)	3.040 (4)	151 (4)
N1*B*—H1*B*···N21*B*^{ii}	0.73 (4)	2.32 (4)	2.988 (5)	153 (4)
N3*A*—H3*A*···N2*A*^{iii}	0.83 (4)	2.06 (4)	2.863 (4)	165 (4)
N3*B*—H3*B*···N2*B*^{iv}	0.77 (3)	2.01 (4)	2.770 (4)	170 (3)
C27*B*—H27*F*···O1^{v}	0.96	2.32	3.273 (5)	171
C14*B*—H14*B*···*Cg*7^{v}	0.93	2.61	3.315 (4)	133

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