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3,3′-[(2-Bromo-1,3-phenylene)bis(methylene)]-bis(1-butyl-2,3-dihydro-1*H*-imidazole-2-selone)

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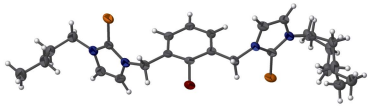
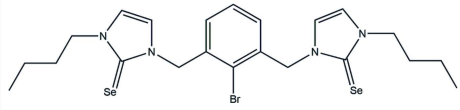
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{22}H_{29}BrN_4Se_2$, the two Se atoms are directed in opposite directions with respect to the central benzene ring. The C=Se bond lengths at 1.848 (5) and 1.851 (5) Å are on the long side for a double bond but shorter than expected for a C—Se single bond. In the crystal, Br···Br intermolecular interactions [3.4685 (12) Å] link the molecules into a zigzag chain propagating along the *b*-axis direction. In addition, there are C—H···Se intermolecular interactions present, linking the chains to form slabs parallel to the *ab* plane. One of the two butyl side chains is disordered over two conformations with occupancies of 0.777 (9) and 0.223 (9).

3D view



Chemical scheme



Structure description

Selones, the Se-analogues of ketones, have generated considerable interest due to their promising utility in many domains, including homogeneous catalysis (see for example: Prabhu *et al.*, 2014; Babu *et al.*, 2016; Sharma *et al.*, 2017), photocatalysis (Jin *et al.*, 2013), and biological fields (see for example: Roy *et al.*, 2013; Palmer & Parkin, 2015; Banerjee *et al.*, 2015).

Recently, our group has reported the syntheses and crystal structures of [2 + 2] binuclear palladium(II) and platinum(II) self-assembled 24-membered metallomacrocycles resulting from the reaction $Pd(COD)Cl_2$ and $Pt(COD)Cl_2$ with 3,3′-[(2-bromo-1,3-phenylene)bis(methylene)]bis(1-mesityl-1,3-dihydro-2*H*-imidazole-2-selone), and of a mononuclear gold(III) complex formed with $AuCl(SMe_2)$ (Rani *et al.*, 2017). Herein, we report on the synthesis and crystal structure of the related title compound, 3,3′-[(2-bromo-1,3-phenylene)bis(methylene)]bis(1-butyl-2,3-dihydro-1*H*-imidazole-2-selone).

In the title compound, Fig. 1, one of the two butyl side chains (atoms C11–C14) is disordered over two conformations with occupancies of 0.777 (9)/0.223 (9). The molecule

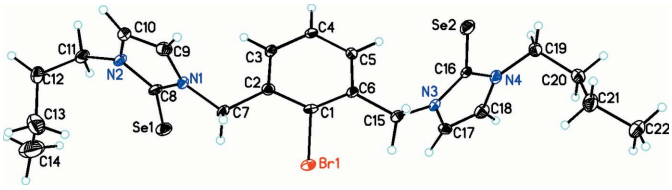


Figure 1
The molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. For the disordered *n*-butyl substituent (atoms C11–C14) only the major component is shown.

adopts a conformation in which the two Se atoms are directed in opposite directions with respect to the central benzene ring. Atom Br1 deviates from the plane of the benzene ring by 0.044 (6) Å, and the Se atoms deviate from the plane of the imidazole ring to which they are attached by 0.041 (7) Å for atom Se1 and 0.044 (7) Å for atom Se2. Each imidazole ring is almost perpendicular to the central benzene ring with dihedral angles of 87.9 (1) and 81.2 (1)° for rings N1/N2/C8–C10 and N3/N4/C16–C18, respectively, and they are inclined to one another by 57.0 (3)°. The C═Se bond lengths, Se1—C8 = 1.848 (5) and Se2—C16 =1.851 (5) Å, are on the long side for a double bond but shorter than expected for a C—Se single bond (Murai *et al.*, 1995). The butyl side chains do not have extended conformations as indicated by their internal N—C—C—C and C—C—C—CH_3 torsion angles, which are N2—C11*A*—C12*A*—C13*A* = 71.2 (14) ° and C11*A*—C12*A*—C13*A*—C14*A* = 66.6 (12) ° (major component), and N4—C19—C20—C21 = 58.1 (7) ° and C19—C20—C21—C22 = 178.1 (5) °.

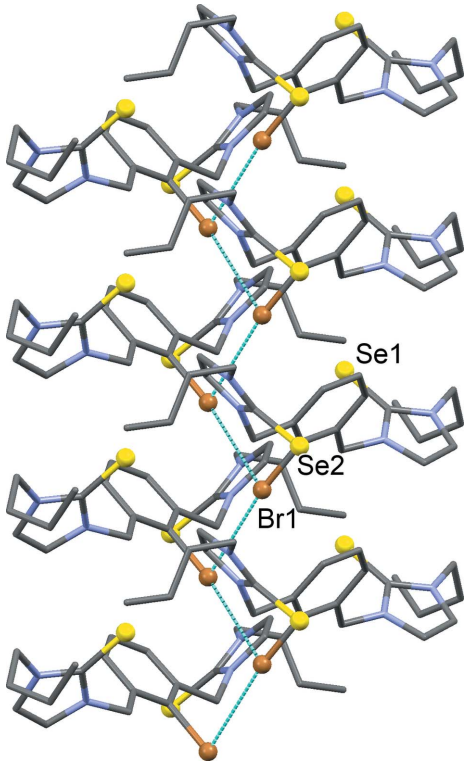


Figure 2
Diagram showing the Br···Br intermolecular interactions (as dashed lines), linking the molecules into zigzag chains propagating along the *b* axis direction. For the disordered *n*-butyl substituent only the major component is shown, and H atoms have been omitted for clarity.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10*A*···Se2^{i}	0.95	2.97	3.823 (5)	150
C12*A*—H12*B*···Se2^{i}	0.99	2.79	3.590 (7)	139
C19—H19*A*···Se2^{ii}	0.99	2.94	3.708 (5)	136

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

In the crystal, molecules are linked by Br···Br^{i,ii} [= 3.4685 (12) Å], intermolecular interactions forming zigzag chains propagating along the *b*-axis direction (Fig. 2; symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$). In addition, there are C—H···Se2 intermolecular interactions present (Table 1). The latter link the chains to form slabs parallel to the *ab* plane (Fig. 3).

A search of the Cambridge Structural Database for analogous structures gave only one hit (QUNCOT: Ghavale *et al.*, 2015) where, instead of an imidazole-type moiety, benzimidazole moieties are present.

Synthesis and crystallization

To a solution of 1,1′-[(2-bromo-1,3-phenylene)bis(methylene)]bis(3-mesityl-1*H*-imidazol-3-ium) dibromide (1.5 g, 2.53 mmol) in dry methanol (50 ml) was added Se powder (0.46 g, 5.82 mmol) followed by K_2CO_3 (0.874 g, 6.33 mmol). The reaction mixture was refluxed for 48 h. A white coloured precipitate deposited near the walls. The reaction mixture was filtered through a Whatman filter paper to remove unconsumed selenium powder. The solvent was evaporated and the residue was redissolved in $CHCl_3$ to remove the leftover salt, which is insoluble in $CHCl_3$. The solvent was evaporated and

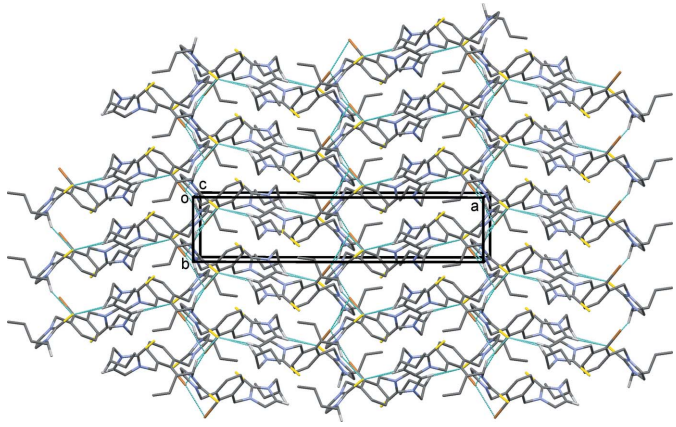


Figure 3
A view along the *c* axis of the crystal packing of the title compound. The Br···Br and C—H···Se interactions are shown as dashed lines (see Table 1). For the disordered *n*-butyl substituent only the major component is shown, and, for clarity, only the H atoms involved in the C—H···Se interactions have been included.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{29}BrN_4Se_2$
M_r	587.32
Crystal system, space group	Monoclinic, *I*2/*a*
Temperature (K)	100
a, *b*, *c* (Å)	23.767 (3), 5.1425 (3), 39.806 (10)
β (°)	102.61 (2)
V (Å^3)	4747.8 (14)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	4.81
Crystal size (mm)	0.23 × 0.17 × 0.09
Data collection	
Diffractometer	Rigaku CCD
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.581, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34850, 7195, 4099
R_{int}	0.113
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.726
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.062, 0.146, 1.02
No. of reflections	7195
No. of parameters	302
No. of restraints	311
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.65, −1.00

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2017* (Sheldrick, 2015*b*), *SHELXTL* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008) and *PLATON* (Spek, 2009).

the sample was dried under *vacuo* (yield 1.20 g, 81%; m.p. 436 K). Colourless prismatic crystals were obtained by slow evaporation of a chloroform solution of the compound at room temperature.

^{1}H NMR (500 MHz, $CDCl_3$, 298 K): δ 7.24 (*t*, *J* = 7.5 Hz, 1H), 7.09–7.07 (*d*, *J* = 7.5 Hz, 2H,), 6.88 (*d*, *J* = 2.0 Hz, 2H), 6.81 (*d*, *J* = 2.0 Hz, 2H), 5.51 (*s*, 4H), 4.18 (*t*, *J* = 7.5 Hz, 4H), 1.82–1.79 (*m*, 4H), 1.42–1.37 (*m*, 4H), 0.98 (*t*, *J* = 7.0 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$, 298 K): 156.8, 136.2, 129.8, 128.3, 124.3, 119.3, 118.8, 53.4, 49.9, 31.3, 19.9, 13.8. ^{77}Se NMR (95.4 MHz, $CDCl_3$, 298 K): δ 0.5 p.p.m. Analysis calculated for $C_{22}H_{31}N_4BrSe_2$ (587.3260): C 44.84, H 5.13, N, 9.51. found C 45.03, H 5.01, N 8.31. ESI–MS: *m*/*z* calculated 626.9542; found 626.9500 $[M + K]^+$. FT–IR (KBr, cm^{-1}): 3158(*w*), 3077(*m*), 2957(*s*), 2931(*s*), 2871(*m*), 1677(*w*), 1566(*m*), 1458(*s*), 1407(*s*), 1357(*w*), 1284(*w*), 1236(*s*), 1218(*s*), 1181(*m*), 1132(*m*), 1055(*m*), 1025(*m*, C═Se), 761(*m*), 714(*m*), 668(*w*).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. One of the two butyl side chains is disordered over two conformations (C11*A*–C14*A*/C11*B*–C14*B*) with a refined occupancy ratio of 0.777 (9): 0.223 (9) and both were constrained to have similar metrical parameters.

Funding information

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full crystallographic data

IUCrData (2017). **2**, x171746 [https://doi.org/10.1107/S2414314617017461]

3,3′-[(2-Bromo-1,3-phenylene)bis(methylene)]bis(1-butyl-2,3-dihydro-1*H*-imidazole-2-selone)

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3,3′-[(2-Bromo-1,3-phenylene)bis(methylene)]bis(1-butyl-2,3-dihydro-1*H*-imidazole-2-selone)

Crystal data

$C_{22}H_{29}BrN_4Se_2$
M_r = 587.32
Monoclinic, *I*2/*a*
a = 23.767 (3) Å
b = 5.1425 (3) Å
c = 39.806 (10) Å
β = 102.61 (2)°
V = 4747.8 (14) Å^3
Z = 8
F(000) = 2336
D_x = 1.643 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 7207 reflections
θ = 2.2–28.9°
μ = 4.81 mm^{-1}
T = 100 K
Prism, colorless
0.23 × 0.17 × 0.09 mm

Data collection

Rigaku CCD diffractometer
Radiation source: fine-focus sealed X-ray tube
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.581, T_{max} = 1.000
34850 measured reflections
7195 independent reflections
4099 reflections with $I > 2\sigma(I)$
R_{int} = 0.113
θ_{max} = 31.1°, θ_{min} = 2.2°
h = −34→32
k = −7→7
l = −54→57

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.146
S = 1.02
7195 reflections
302 parameters
311 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.058P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −1.00 e Å^{-3}

Special details

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

Refinement. The H atoms were positioned geometrically and allowed to ride on their parent atoms: C—H = 0.95–0.99 Å with U_{iso}(H) = 1.5U_{eq}(*C*-methyl) and 1.2U_{eq}(C) for other C-bound H atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1	0.03432 (2)	0.42252 (9)	0.23314 (2)	0.03175 (14)	
Se1	0.13904 (2)	−0.26010 (11)	0.34617 (2)	0.04244 (16)	
Se2	0.08179 (2)	0.17304 (11)	0.09546 (2)	0.04280 (17)	
N1	0.18882 (16)	0.1338 (8)	0.31010 (10)	0.0316 (9)	
N2	0.25023 (16)	−0.0141 (8)	0.35460 (10)	0.0333 (9)	
N3	0.00557 (16)	−0.0457 (8)	0.13496 (10)	0.0317 (9)	
N4	−0.00708 (16)	−0.2196 (8)	0.08424 (10)	0.0331 (9)	
C1	0.08406 (18)	0.1496 (9)	0.22385 (12)	0.0278 (10)	
C2	0.12891 (19)	0.0756 (9)	0.25105 (12)	0.0283 (10)	
C3	0.16548 (19)	−0.1204 (9)	0.24409 (12)	0.0312 (10)	
H3A	0.196352	−0.178879	0.261858	0.037*	
C4	0.15725 (19)	−0.2312 (9)	0.21144 (12)	0.0314 (10)	
H4A	0.182993	−0.361719	0.207026	0.038*	
C5	0.11175 (19)	−0.1523 (9)	0.18535 (13)	0.0318 (10)	
H5A	0.106484	−0.229836	0.163219	0.038*	
C6	0.07374 (18)	0.0393 (9)	0.19125 (12)	0.0288 (10)	
C7	0.13510 (19)	0.1943 (10)	0.28618 (12)	0.0353 (11)	
H7A	0.131785	0.385518	0.283642	0.042*	
H7B	0.102736	0.133754	0.296168	0.042*	
C8	0.19483 (19)	−0.0397 (10)	0.33649 (13)	0.0327 (11)	
C9	0.2400 (2)	0.2678 (10)	0.31233 (14)	0.0378 (12)	
H9A	0.246848	0.401618	0.297264	0.045*	
C10	0.2781 (2)	0.1749 (10)	0.33961 (13)	0.0362 (11)	
H10A	0.317070	0.228839	0.347217	0.043*	
C11A	0.2772 (6)	−0.150 (4)	0.3877 (2)	0.0415 (18)	0.777 (9)
H11A	0.314525	−0.227601	0.385894	0.050*	0.777 (9)
H11B	0.251583	−0.292610	0.392113	0.050*	0.777 (9)
C12A	0.2866 (3)	0.0431 (17)	0.41745 (18)	0.0459 (18)	0.777 (9)
H12A	0.312305	−0.038945	0.437571	0.055*	0.777 (9)
H12B	0.307207	0.195545	0.410878	0.055*	0.777 (9)
C13A	0.2347 (4)	0.138 (2)	0.4285 (2)	0.058 (2)	0.777 (9)
H13A	0.207640	0.212700	0.408279	0.070*	0.777 (9)
H13B	0.246190	0.279971	0.445444	0.070*	0.777 (9)
C14A	0.2031 (3)	−0.0743 (18)	0.4447 (2)	0.068 (3)	0.777 (9)
H14A	0.169133	0.001099	0.451154	0.102*	0.777 (9)
H14B	0.229140	−0.144843	0.465166	0.102*	0.777 (9)
H14C	0.190994	−0.214146	0.427911	0.102*	0.777 (9)
C15	0.0234 (2)	0.1316 (10)	0.16346 (13)	0.0360 (11)	
H15A	−0.009932	0.163767	0.174104	0.043*	
H15B	0.033920	0.299565	0.154351	0.043*	
C16	0.02429 (19)	−0.0392 (9)	0.10495 (12)	0.0313 (10)	
C17	−0.0368 (2)	−0.2339 (10)	0.13295 (14)	0.0360 (11)	

H17A	−0.056450	−0.279112	0.150487	0.043*	
C18	−0.0446 (2)	−0.3398 (10)	0.10158 (14)	0.0368 (11)	
H18A	−0.071160	−0.473955	0.092722	0.044*	
C19	−0.0022 (2)	−0.2783 (11)	0.04901 (13)	0.0414 (12)	
H19A	0.009974	−0.461625	0.047847	0.050*	
H19B	0.028133	−0.166725	0.043003	0.050*	
C20	−0.0580 (2)	−0.2359 (11)	0.02291 (14)	0.0469 (14)	
H20A	−0.051574	−0.278474	−0.000216	0.056*	
H20B	−0.087093	−0.359333	0.027889	0.056*	
C21	−0.0822 (2)	0.0339 (12)	0.02194 (14)	0.0503 (14)	
H21A	−0.053011	0.159054	0.017564	0.060*	
H21B	−0.090319	0.075274	0.044720	0.060*	
C22	−0.1373 (3)	0.0678 (15)	−0.00551 (16)	0.070 (2)	
H22A	−0.152009	0.244755	−0.004373	0.105*	
H22B	−0.166194	−0.057673	−0.001584	0.105*	
H22C	−0.129043	0.038010	−0.028284	0.105*	
C11B	0.274 (2)	−0.165 (14)	0.3813 (8)	0.048 (4)	0.223 (9)
H11C	0.315587	−0.187117	0.380908	0.057*	0.223 (9)
H11D	0.256154	−0.339009	0.377563	0.057*	0.223 (9)
C12B	0.2706 (12)	−0.073 (6)	0.4171 (6)	0.056 (4)	0.223 (9)
H12C	0.270102	−0.228140	0.431643	0.067*	0.223 (9)
H12D	0.306396	0.024516	0.426880	0.067*	0.223 (9)
C13B	0.2211 (12)	0.093 (8)	0.4200 (5)	0.059 (4)	0.223 (9)
H13C	0.185392	−0.011671	0.414007	0.070*	0.223 (9)
H13D	0.217749	0.236373	0.403042	0.070*	0.223 (9)
C14B	0.2259 (11)	0.211 (6)	0.4562 (6)	0.059 (6)	0.223 (9)
H14D	0.187460	0.220141	0.461396	0.089*	0.223 (9)
H14E	0.242222	0.386475	0.456853	0.089*	0.223 (9)
H14F	0.250942	0.101579	0.473348	0.089*	0.223 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0238 (2)	0.0309 (3)	0.0410 (3)	0.00448 (19)	0.00805 (19)	0.0010 (2)
Se1	0.0290 (3)	0.0445 (3)	0.0546 (4)	−0.0049 (2)	0.0109 (2)	−0.0029 (3)
Se2	0.0278 (3)	0.0556 (4)	0.0433 (3)	−0.0039 (2)	0.0039 (2)	0.0106 (3)
N1	0.0225 (18)	0.040 (2)	0.031 (2)	0.0018 (16)	0.0020 (15)	−0.0011 (18)
N2	0.0243 (18)	0.038 (2)	0.035 (2)	0.0038 (17)	0.0025 (16)	−0.0007 (18)
N3	0.0247 (19)	0.036 (2)	0.033 (2)	0.0032 (16)	0.0024 (16)	−0.0002 (17)
N4	0.028 (2)	0.037 (2)	0.033 (2)	0.0007 (17)	0.0033 (17)	0.0045 (18)
C1	0.021 (2)	0.027 (2)	0.036 (2)	0.0039 (18)	0.0098 (18)	0.000 (2)
C2	0.025 (2)	0.029 (2)	0.032 (2)	0.0003 (18)	0.0079 (18)	0.002 (2)
C3	0.024 (2)	0.038 (3)	0.031 (2)	0.0067 (19)	0.0040 (19)	0.006 (2)
C4	0.025 (2)	0.038 (3)	0.034 (3)	0.004 (2)	0.0113 (19)	0.002 (2)
C5	0.029 (2)	0.036 (3)	0.032 (3)	0.002 (2)	0.0094 (19)	0.001 (2)
C6	0.021 (2)	0.036 (3)	0.030 (2)	0.0012 (18)	0.0075 (17)	0.003 (2)
C7	0.026 (2)	0.041 (3)	0.035 (3)	0.012 (2)	−0.001 (2)	−0.001 (2)
C8	0.022 (2)	0.038 (3)	0.038 (3)	0.0029 (19)	0.0050 (19)	0.001 (2)

C9	0.030 (2)	0.039 (3)	0.045 (3)	−0.001 (2)	0.010 (2)	0.004 (2)
C10	0.025 (2)	0.049 (3)	0.035 (3)	−0.002 (2)	0.0066 (19)	−0.005 (2)
C11A	0.027 (3)	0.065 (4)	0.031 (4)	0.007 (3)	0.003 (3)	0.012 (4)
C12A	0.032 (3)	0.071 (5)	0.031 (3)	−0.010 (3)	0.000 (3)	0.007 (3)
C13A	0.054 (4)	0.082 (5)	0.033 (4)	0.004 (4)	−0.002 (3)	−0.008 (4)
C14A	0.040 (4)	0.111 (7)	0.053 (5)	0.000 (4)	0.011 (4)	0.007 (5)
C15	0.030 (2)	0.042 (3)	0.034 (3)	0.011 (2)	0.004 (2)	−0.001 (2)
C16	0.022 (2)	0.040 (3)	0.031 (2)	0.0041 (19)	0.0039 (18)	0.008 (2)
C17	0.031 (2)	0.041 (3)	0.039 (3)	0.001 (2)	0.013 (2)	0.008 (2)
C18	0.033 (2)	0.035 (3)	0.041 (3)	−0.006 (2)	0.006 (2)	0.003 (2)
C19	0.039 (3)	0.048 (3)	0.036 (3)	0.008 (2)	0.008 (2)	−0.002 (2)
C20	0.048 (3)	0.059 (3)	0.034 (3)	0.007 (3)	0.009 (2)	−0.003 (3)
C21	0.048 (3)	0.062 (4)	0.036 (3)	0.008 (3)	−0.001 (2)	−0.004 (3)
C22	0.050 (4)	0.105 (6)	0.049 (4)	0.026 (4)	−0.001 (3)	0.002 (4)
C11B	0.035 (7)	0.069 (7)	0.033 (6)	0.008 (6)	−0.005 (6)	0.007 (6)
C12B	0.047 (7)	0.079 (7)	0.037 (5)	0.005 (6)	−0.002 (6)	0.005 (6)
C13B	0.049 (7)	0.085 (8)	0.037 (7)	0.004 (7)	0.000 (6)	−0.006 (7)
C14B	0.045 (10)	0.093 (12)	0.040 (9)	−0.018 (10)	0.008 (9)	−0.009 (9)

Geometric parameters (Å, º)

Br1—C1	1.922 (4)	C12A—H12A	0.9900
Br1—Br1^{i}	3.4688 (7)	C12A—H12B	0.9900
Br1—Br1^{ii}	3.4688 (7)	C13A—C14A	1.545 (12)
Se1—C8	1.848 (5)	C13A—H13A	0.9900
Se2—C16	1.851 (5)	C13A—H13B	0.9900
N1—C8	1.362 (6)	C14A—H14A	0.9800
N1—C9	1.383 (6)	C14A—H14B	0.9800
N1—C7	1.450 (5)	C14A—H14C	0.9800
N2—C11B	1.34 (5)	C15—H15A	0.9900
N2—C8	1.363 (6)	C15—H15B	0.9900
N2—C10	1.383 (6)	C17—C18	1.338 (7)
N2—C11A	1.508 (12)	C17—H17A	0.9500
N3—C16	1.363 (6)	C18—H18A	0.9500
N3—C17	1.386 (6)	C19—C20	1.512 (7)
N3—C15	1.445 (6)	C19—H19A	0.9900
N4—C16	1.352 (6)	C19—H19B	0.9900
N4—C18	1.386 (6)	C20—C21	1.500 (8)
N4—C19	1.464 (6)	C20—H20A	0.9900
C1—C6	1.388 (6)	C20—H20B	0.9900
C1—C2	1.396 (6)	C21—C22	1.520 (7)
C2—C3	1.397 (6)	C21—H21A	0.9900
C2—C7	1.503 (6)	C21—H21B	0.9900
C3—C4	1.393 (6)	C22—H22A	0.9800
C3—H3A	0.9500	C22—H22B	0.9800
C4—C5	1.387 (6)	C22—H22C	0.9800
C4—H4A	0.9500	C11B—C12B	1.523 (12)
C5—C6	1.391 (6)	C11B—H11C	0.9900

C5—H5A	0.9500	C11B—H11D	0.9900
C6—C15	1.518 (6)	C12B—C13B	1.478 (10)
C7—H7A	0.9900	C12B—H12C	0.9900
C7—H7B	0.9900	C12B—H12D	0.9900
C9—C10	1.342 (7)	C13B—C14B	1.545 (13)
C9—H9A	0.9500	C13B—H13C	0.9900
C10—H10A	0.9500	C13B—H13D	0.9900
C11A—C12A	1.524 (11)	C14B—H14D	0.9800
C11A—H11A	0.9900	C14B—H14E	0.9800
C11A—H11B	0.9900	C14B—H14F	0.9800
C12A—C13A	1.479 (9)		

C1—Br1—Br1^{i}	83.93 (13)	C13A—C14A—H14B	109.5
C1—Br1—Br1^{ii}	167.60 (15)	H14A—C14A—H14B	109.5
Br1^{i}—Br1—Br1^{ii}	95.68 (3)	C13A—C14A—H14C	109.5
C8—N1—C9	109.5 (4)	H14A—C14A—H14C	109.5
C8—N1—C7	125.2 (4)	H14B—C14A—H14C	109.5
C9—N1—C7	124.8 (4)	N3—C15—C6	115.1 (4)
C11B—N2—C8	124 (3)	N3—C15—H15A	108.5
C11B—N2—C10	126 (3)	C6—C15—H15A	108.5
C8—N2—C10	109.8 (4)	N3—C15—H15B	108.5
C8—N2—C11A	126.5 (8)	C6—C15—H15B	108.5
C10—N2—C11A	123.5 (8)	H15A—C15—H15B	107.5
C16—N3—C17	109.8 (4)	N4—C16—N3	106.0 (4)
C16—N3—C15	125.2 (4)	N4—C16—Se2	127.8 (4)
C17—N3—C15	124.8 (4)	N3—C16—Se2	126.2 (4)
C16—N4—C18	109.3 (4)	C18—C17—N3	106.8 (4)
C16—N4—C19	125.2 (4)	C18—C17—H17A	126.6
C18—N4—C19	125.4 (4)	N3—C17—H17A	126.6
C6—C1—C2	124.2 (4)	C17—C18—N4	108.1 (4)
C6—C1—Br1	119.2 (3)	C17—C18—H18A	126.0
C2—C1—Br1	116.6 (3)	N4—C18—H18A	126.0
C3—C2—C1	116.5 (4)	N4—C19—C20	112.8 (4)
C3—C2—C7	122.6 (4)	N4—C19—H19A	109.0
C1—C2—C7	120.9 (4)	C20—C19—H19A	109.0
C4—C3—C2	120.9 (4)	N4—C19—H19B	109.0
C4—C3—H3A	119.6	C20—C19—H19B	109.0
C2—C3—H3A	119.6	H19A—C19—H19B	107.8
C5—C4—C3	120.4 (4)	C21—C20—C19	115.2 (5)
C5—C4—H4A	119.8	C21—C20—H20A	108.5
C3—C4—H4A	119.8	C19—C20—H20A	108.5
C4—C5—C6	120.7 (5)	C21—C20—H20B	108.5
C4—C5—H5A	119.7	C19—C20—H20B	108.5
C6—C5—H5A	119.7	H20A—C20—H20B	107.5
C1—C6—C5	117.3 (4)	C20—C21—C22	112.9 (5)
C1—C6—C15	120.2 (4)	C20—C21—H21A	109.0
C5—C6—C15	122.4 (4)	C22—C21—H21A	109.0
N1—C7—C2	114.6 (4)	C20—C21—H21B	109.0

N1—C7—H7A	108.6	C22—C21—H21B	109.0
C2—C7—H7A	108.6	H21A—C21—H21B	107.8
N1—C7—H7B	108.6	C21—C22—H22A	109.5
C2—C7—H7B	108.6	C21—C22—H22B	109.5
H7A—C7—H7B	107.6	H22A—C22—H22B	109.5
N2—C8—N1	105.7 (4)	C21—C22—H22C	109.5
N2—C8—Se1	127.1 (4)	H22A—C22—H22C	109.5
N1—C8—Se1	127.1 (3)	H22B—C22—H22C	109.5
C10—C9—N1	107.7 (4)	N2—C11B—C12B	117 (3)
C10—C9—H9A	126.2	N2—C11B—H11C	108.0
N1—C9—H9A	126.2	C12B—C11B—H11C	108.0
C9—C10—N2	107.2 (4)	N2—C11B—H11D	108.0
C9—C10—H10A	126.4	C12B—C11B—H11D	108.0
N2—C10—H10A	126.4	H11C—C11B—H11D	107.2
N2—C11A—C12A	109.7 (11)	C13B—C12B—C11B	117.6 (10)
N2—C11A—H11A	109.7	C13B—C12B—H12C	107.9
C12A—C11A—H11A	109.7	C11B—C12B—H12C	107.9
N2—C11A—H11B	109.7	C13B—C12B—H12D	107.9
C12A—C11A—H11B	109.7	C11B—C12B—H12D	107.9
H11A—C11A—H11B	108.2	H12C—C12B—H12D	107.2
C13A—C12A—C11A	117.1 (6)	C12B—C13B—C14B	113.8 (10)
C13A—C12A—H12A	108.0	C12B—C13B—H13C	108.8
C11A—C12A—H12A	108.0	C14B—C13B—H13C	108.8
C13A—C12A—H12B	108.0	C12B—C13B—H13D	108.8
C11A—C12A—H12B	108.0	C14B—C13B—H13D	108.8
H12A—C12A—H12B	107.3	H13C—C13B—H13D	107.7
C12A—C13A—C14A	113.7 (7)	C13B—C14B—H14D	109.5
C12A—C13A—H13A	108.8	C13B—C14B—H14E	109.5
C14A—C13A—H13A	108.8	H14D—C14B—H14E	109.5
C12A—C13A—H13B	108.8	C13B—C14B—H14F	109.5
C14A—C13A—H13B	108.8	H14D—C14B—H14F	109.5
H13A—C13A—H13B	107.7	H14E—C14B—H14F	109.5
C13A—C14A—H14A	109.5		

C6—C1—C2—C3	0.8 (7)	C8—N2—C10—C9	0.4 (6)
Br1—C1—C2—C3	−179.1 (3)	C11A—N2—C10—C9	−174.9 (6)
C6—C1—C2—C7	−176.5 (4)	C8—N2—C11A—C12A	−108.0 (11)
Br1—C1—C2—C7	3.5 (6)	C10—N2—C11A—C12A	66.5 (10)
C1—C2—C3—C4	0.7 (7)	N2—C11A—C12A—C13A	71.2 (14)
C7—C2—C3—C4	178.0 (4)	C11A—C12A—C13A—C14A	66.6 (12)
C2—C3—C4—C5	−1.3 (7)	C16—N3—C15—C6	−93.5 (5)
C3—C4—C5—C6	0.3 (7)	C17—N3—C15—C6	92.2 (5)
C2—C1—C6—C5	−1.8 (7)	C1—C6—C15—N3	−161.1 (4)
Br1—C1—C6—C5	178.2 (3)	C5—C6—C15—N3	20.2 (6)
C2—C1—C6—C15	179.4 (4)	C18—N4—C16—N3	−0.8 (5)
Br1—C1—C6—C15	−0.6 (6)	C19—N4—C16—N3	179.2 (4)
C4—C5—C6—C1	1.2 (7)	C18—N4—C16—Se2	178.5 (3)
C4—C5—C6—C15	180.0 (4)	C19—N4—C16—Se2	−1.6 (7)

C8—N1—C7—C2	−104.3 (5)	C17—N3—C16—N4	1.1 (5)
C9—N1—C7—C2	84.6 (6)	C15—N3—C16—N4	−174.0 (4)
C3—C2—C7—N1	13.2 (7)	C17—N3—C16—Se2	−178.2 (3)
C1—C2—C7—N1	−169.6 (4)	C15—N3—C16—Se2	6.8 (6)
C11B—N2—C8—N1	−175.0 (13)	C16—N3—C17—C18	−0.9 (5)
C10—N2—C8—N1	0.3 (5)	C15—N3—C17—C18	174.1 (4)
C11A—N2—C8—N1	175.4 (6)	N3—C17—C18—N4	0.4 (5)
C11B—N2—C8—Se1	5.9 (15)	C16—N4—C18—C17	0.2 (5)
C10—N2—C8—Se1	−178.7 (4)	C19—N4—C18—C17	−179.7 (4)
C11A—N2—C8—Se1	−3.6 (9)	C16—N4—C19—C20	−120.4 (5)
C9—N1—C8—N2	−0.9 (5)	C18—N4—C19—C20	59.5 (6)
C7—N1—C8—N2	−173.1 (4)	N4—C19—C20—C21	58.1 (7)
C9—N1—C8—Se1	178.1 (4)	C19—C20—C21—C22	178.1 (5)
C7—N1—C8—Se1	5.9 (7)	C8—N2—C11B—C12B	−92 (6)
C8—N1—C9—C10	1.2 (6)	C10—N2—C11B—C12B	94 (5)
C7—N1—C9—C10	173.4 (4)	N2—C11B—C12B—C13B	28 (8)
N1—C9—C10—N2	−0.9 (6)	C11B—C12B—C13B—C14B	−171 (5)
C11B—N2—C10—C9	175.7 (16)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10*A*···Se2^{iii}	0.95	2.97	3.823 (5)	150
C12*A*—H12*B*···Se2^{iii}	0.99	2.79	3.590 (7)	139
C19—H19*A*···Se2^{iv}	0.99	2.94	3.708 (5)	136

Symmetry codes: (iii) −*x*+1/2, −*y*+1/2, −*z*+1/2; (iv) *x*, *y*−1, *z*.