Crystal structure, Hirshfeld surface analysis and DFT study of 2,2''-[[((1E,1'E)-(diselanediyi)bis(2,1-phenylene))bis(methaneylelylidene)]bis(azaneyleyldene))bis[3',6'-bis(diethylamino)-4a',9a'-dihydrospiro[isoindoline-1,9'-xanthen]-3-one]

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The title compound, C70H70N8O4Se2, is a spiro bicyclic diselenide, made up of two [SeC6H4CH=N—N(CO)C6H4(C)C6H3NEt2(O)C6H3NEt2] units related by a twofold crystallographic symmetry element bisecting the diselenide bond. The compound crystallizes in a non-centrosymmetric polar space group (tetragonal, P4b2) and the structure was refined as an inversion twin. The two diethyl amine groups and their attached phenyl groups of the xanthene ring are disordered over two orientations, with occupancies of 0.664 (19)/0.336 (19) and 0.665 (11)/0.335 (11), respectively. The dihedral angles between the mean planes of the central isoindoline and the phenyl rings are 26.8 (2) and 2.5 (4)°, respectively. The mean plane of the central xanthene ring forms dihedral angles of 2.0 (5), 8.8 (5), 1.7 (5) and 7.9 (6)° with the peripheral phenyl rings. The isoindoline and xanthene rings subtend a dihedral angle of 89.8 (2)°. The molecular conformation is stabilized by an intramolecular C—H⋯O hydrogen bond generating an S(6) ring motif. In the crystal, molecules are linked by C—H⋯O hydrogen bonds together with C—H⋯C (ring) interactions, forming a three-dimensional network. A Hirshfeld surface analysis of the crystal structure indicates that the most important contributions to the crystal packing are from H⋯H (68.1%), C⋯H/H⋯C (21.2%) and O⋯H/H⋯O (8.7%) contacts. The optimized structure calculated using density functional theory (DFT) at the B3LYP/6-31G(d) level is compared with the experimentally determined molecular structure in the solid state. The HOMO–LUMO behaviour was used to determine the energy gap and the molecular electrostatic potential (MEP) of the compound was investigated.

1. Chemical context

Diaryl diselenides and aryl selenolates have been previously used as ligand precursors for the synthesis of transition-metal complexes (Khandelwal & Gupta, 1989; Gupta & Parihar, 1995, 1998; Gupta et al., 1998). Selenospirocyclic compounds are a class of heterocyclic compounds with a wide variety of uses in organic synthesis (Aho et al., 2005; Kotha et al., 2009; James et al., 1991), biological activities (Mugesh et al., 2001; Nogueira et al., 2004; Press et al., 2008; Alberto et al., 2009) and photoluminescence properties (Singh et al., 2011; Shi et al., 2010). However, the formation of spirobicyclic diselenides is rare and to the best of our knowledge, not reported in the literature. There are very few reports of the formation of selenospiroyclic derivatives which have been structurally characterized (Singh et al., 2011; Shi et al., 2010). Very recently, organoselenium compounds containing both N and Se have
been reported with interesting intra- and intermolecular interactions (Saravanan et al., 2021). Although the synthetic and structural studies of various diselenides (see section 4, Database survey) are known in the literature, to the best of our knowledge, a synthesis and structural data have not yet been published for the title compound. Herein we report the crystal structure, DFT and Hirshfeld surface analysis of 2,2\textsuperscript{00}-(\{(1E,1\textsuperscript{0}E)-(diselanediyl)bis(2,1-phenylene)\}bis(methaneylylidene))bis[3,6\textsuperscript{0}bis(diethylamino)-4a',9a'-dihydrospirorbis(1,9\textsuperscript{0}0-xanthen)-3-one], isolated from the condensation of rhodamine B hydrazide with bis(o-formylphenyl)diselenide.

2. Structural commentary

The title compound (Fig. 1), a rare example of spiro bicyclic diselenide, crystallizes in the non-centrosymmetric polar tetragonal space group, \(P\bar{4}b2\), as a racemic mixture. There is a half-molecule in the asymmetric unit (\(Z = 4\)), and the structure was refined as an inversion twin [Flack parameter 0.05 (2); Parsons et al., 2013]. The Se–Se unit is coplanar with both phenyl rings but the Se–aryl planes are essentially perpendicular to each other [C–Se–Se–C torsion angle of \(-88.9 (3)^\circ\)]. The diethyl amine groups and their attached phenyl groups (C16–C21, N3/C18–C20/C22–C25 and C26–C31, N4/C32–C35) of the xanthene rings are disordered over two conformations with occupancies of 0.664 (19)/0.336 (19) and 0.665 (11)/0.335 (11), respectively. In both major and minor components, the diethyl amine nitrogens are planar with the sum of the bond angles at N3/N3\textsuperscript{A} being 358.5 and 359.5\(^\circ\) and at N4/N4\textsuperscript{A} being 357.5 and 357.4\(^\circ\), respectively. In order to investigate the pyramidal nature of the amine N atoms, the dihedral angles between the respective N–C\textsubscript{2} groups and the attached phenyl rings were calculated and found to be 14.3 (7) and 14.8 (5) for N3 and N4, respectively. The Se–Se bond length of 2.3517 (17) \(\AA\) and Se–C bond length of 1.939 (7) \(\AA\) fall within the literature ranges of 2.287 to 3.051 \(\AA\) and 1.91–1.97 \(\AA\), respectively (see CSD survey). The C–Se–Se–C torsion angle typically falls in the range of ca 73–128\(^\circ\) (Dickson et al., 1999). The observed C–Se–Se–C torsion angle, \(-88.9 (3)^\circ\), results from the \(\text{syn}\) conformation around the Se–Se bridge. This conformation can be rationalized in terms of repulsion of the 4p lone pairs at the Se centres. The dihedral angles between the mean planes of the central isoindoline (N2/C8/C9/C14/C15) and the phenyl rings (C1–C6 and C9–C14), are 26.8 (2) and 2.5 (4)\(^\circ\), respectively. The mean plane of the central xanthene ring (O2/C21/C16/C15/C31/C26) forms dihedral angles of 2.0 (5), 8.8 (9) and 1.7 (5), 7.9 (6)\(^\circ\) with the peripheral phenyl rings (C16–C21, C16A–C21A and C26–C31, C26A–C31A, respectively). The isoindoline (N2/C8/C9/C14/C15) and xanthene (O2/C21/C16/C15/C31/C26) rings are essentially perpendicular to each other [dihedral angle of 89.8 (6)\(^\circ\)].

3. Supramolecular features

The crystal packing of the title compound viewed along the \(c\) axis is presented in Fig. 2. The title compound packs in a way that allows close contacts between the oxygen atoms and hydrogen atoms of adjacent molecules, leading to a network of C–H···O interactions involving donor atoms C7 (azomethine carbon) and C12 (aromatic carbon) with carbonyl oxygen O1 as acceptor with D···A distances of 3.391 (10) and 3.447 (10) \(\AA\), respectively (symmetry codes: \(y + \frac{1}{2}, x - \frac{1}{2}, -z + 2; 1 + y, 1 - x, 2 - z\)) between neighbouring molecules (Table 1). An intramolecular C–H···O hydrogen bond involving carbonyl oxygen, O1 and methine hydrogen, H7 with D···A

Figure 1
Diagram showing: (a) a half molecule showing the disorder, (b) the major component of the title compound [symmetry operation: \(\frac{1}{2} + y, -\frac{1}{2} + x, 1 - z\)]. Displacement ellipsoids are shown at the 30\% probability level.
distance of 2.940 (9) Å leading to an S(6) ring motif (Bernstein et al., 1995) is also present. Furthermore, there exists a C—H/C1/C1/C1/C25 interaction between the H25 C atom of the methyl carbon C25 and the centroid of the C16–C21 phenyl ring; symmetry code 1/C0 y, C0 1+x, C0 z. These interactions play a vital role in stabilizing the crystal packing within the crystal structure.

4. Hirshfeld surface analysis

Hirshfeld surface (HS) calculations (Spackman & Jayatilaka, 2009) were performed on the title compound to further investigate the intermolecular interactions. The Hirshfeld surface plotted over $d_{norm}$ in the range $[1.0432$ to $+2.0960$ a.u. generated using CrystalExplorer 21.5 (Spackman et al., 2021) is shown in Fig. 3. The red spots that appear around O1 are caused by the intermolecular C7—H7/C1/C1/C1/C1 O1 and C12—H12/C1/C1/C1/C1 O1 interactions, which are important in the packing of the title molecule. An intramolecular C—H/C1/C1/C1 O hydrogen bond is also indicated by the red spots near the hydrogen and oxygen atoms (Fig. 3b). Bright-red spots on top and bottom of the HS near N3 indicate an intermolecular C—H/C1/C1/C1/C25 (ring) interaction involving H25B of the C25 methyl group and a benzene ring (Fig. 3c).

The two-dimensional fingerprint plots (McKinnon et al., 2007) were generated using CrystalExplorer 21.5 encompassing all intermolecular contacts, as well as the delineated specific contacts (Fig. 4). More significant contacts and their percentage contributions to the Hirshfeld surface are given in Table 2. The most important interaction is H···H, contributing 68.1% to the overall crystal packing. The presence of C—H···π interactions is indicated by pairs of characteristic wings in the fingerprint plot representing C···H/H/C1/C1/C1 contacts.

Table 1

| Hydrogen-bond geometry (Å, °) | $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|-------------------------------|-------------|-------|--------|---------|-------------|
| C2—H2A···Se1i                 | 0.95        | 2.82  | 3.436  (8) | 124     |
| C7—H7A···O1                  | 0.95        | 2.43  | 2.940  (9) | 114     |
| C7—H7A···O1ii                | 0.95        | 2.63  | 3.391  (10) | 137     |
| C12—H12A···O1iii             | 0.95        | 2.56  | 3.447  (10) | 156     |
| C33A—H33E···Se1i             | 0.98        | 3.04  | 4.00   (3) | 168     |

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

Table 2

| Contact | Percentage contribution |
|---------|-------------------------|
| H···H   | 68.1                    |
| C···H/C1/C1/C1/C1 ···O   | 21.2                    |
| O···H/C1/C1/C1/C1 ···O   | 8.7                     |
| N···H/C1/C1/C1/C1 ···N   | 1.6                     |
| Se···H/C1/C1/C1/C1 ···Se | 0.4                     |

Figure 2

Packing diagram of (a) the title compound viewed along c axis and (b) partial packing showing the formation of C—H···π interactions (symmetry code: 1−y, −1+x, 1−z).

Figure 3

(a) A view of the three-dimensional Hirshfeld surface mapped over $d_{norm}$ in the range $−1.0432$ to $+2.0960$ a.u. and views showing (b) C—H···O and (c) C—H···π interactions.
with a 21.2% contribution to the HS. Pairs of scattered points of spikes are seen in the fingerprint plot delineated into O/C1/C1/H/C1/C1/O contacts (8.7% contribution to the HS). The lowest contributions are from N/C1/C1/H/C1/C1/N (1.6%) and Se/C1/C1/H/C1/C1/Se (0.4%) contacts. These interactions play a crucial role in the overall stabilization of the crystal packing.

5. DFT Calculations

A density functional theory (DFT) geometry-optimized molecular orbital calculation (WebMOPro; Polik & Schmidt, 2021) with the GAUSSIAN 16 programme package (Frisch et al., 2019) employing the B3LYP functional and 6-31G(d) basis set (Becke, 1993) was performed on the title compound. Starting geometries were taken from the X-ray refinement data. Theoretical and experimental results related to bond lengths and angles are in good agreement (Table 3).

Calculated molecular orbital energies (eV) for the surfaces of the frontier molecular orbitals of the title compound are shown in Fig. 5. The HOMO (highest occupied molecular orbital) acts as an electron donor and the LUMO (lowest

![Figure 4](https://example.com/figure4.png)

**Figure 4** A view of the two-dimensional fingerprint plots for the title compound, showing (a) all interactions, and those delineated into (b) H···H (c) C···H/H···C (d) O···H/H···O (e) N···H/H···N and (f) Se···H/H···Se interactions. The $d_i$ and $d_e$ values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

![Table 3](https://example.com/table3.png)

**Table 3** Comparison of selected (X-ray and DFT) bond lengths and angles (Å, °).

| Bonds/Angles               | X-ray   | B3LYP/6-31G(d) |
|----------------------------|---------|----------------|
| Se1—C1                    | 1.939 (7) | 1.941 |
| Se1—Se1'                  | 2.3517 (17) | 2.356 |
| O1—C8                     | 1.222 (9) | 1.224 |
| O2—C21                    | 1.315 (12) | 1.374 |
| O2—C26                    | 1.349 (13) | 1.368 |
| N1—C7                     | 1.280 (9) | 1.291 |
| N1—N2                     | 1.380 (8) | 1.353 |
| N2—C8                     | 1.378 (10) | 1.392 |
| N2—C15                    | 1.507 (9) | 1.513 |
| C1—C6                     | 1.415 (11) | 1.42 |
| C19—N3                    | 1.426 (7) | 1.383 |
| C22—N3                    | 1.446 (13) | 1.464 |
| C24—N3                    | 1.466 (12) | 1.461 |
| N4—C28                    | 1.423 (10) | 1.39 |
| N4—C32                    | 1.543 (14) | 1.461 |
| N4—C34                    | 1.481 (13) | 1.462 |
| C1—Se1—Se1'               | 103.5 (2) | 102.711 |
| C26—O2—C21                | 119.4 (9) | 119.241 |
| C7—N1—N2                  | 121.3 (6) | 122.983 |
| N1—N2—C15                 | 115.5 (5) | 116.391 |
| C2—C1—Se1                 | 122.5 (6) | 121.361 |
| C6—C1—Se1                 | 119.2 (5) | 119.262 |
| O1—C8—N2                  | 125.8 (6) | 126.543 |
| C8—N2—C15                 | 115.3 (5) | 114.337 |
| O1—C8—C9                  | 129.0 (7) | 128.268 |
| N2—C8—C9                  | 105.2 (6) | 105.19 |
| C19—N3—C22                | 120.9 (7) | 120.635 |
| C19—N3—C24                | 119.4 (7) | 120.99 |
| C22—N3—C24                | 118.2 (7) | 118.187 |
| C28—N4—C32                | 120.2 (7) | 120.875 |
| C28—N4—C34                | 120.1 (8) | 120.772 |
| C32—N4—C34                | 117.2 (9) | 117.917 |
| C1—Se1—Se1—C1'            | −88.9 (6) | −73.195 |

![Figure 5](https://example.com/figure5.png)

**Figure 5** Calculated frontier molecular orbitals of the title compound.
The molecular electrostatic potential (MEP) map (Fig. 6) was calculated at the B3LYP/6–31G(d) level of theory. In the MEP diagram, the molecular electrostatic potential is in the range −0.0833 to 0.0321 a.u. and the different electrostatic potentials at the surface of the molecule are represented by different colours. Electrostatic potentials increase in the order red < yellow < green < blue, and red indicates the electron rich region and blue indicates the electron-deficient region. As shown in Fig. 6, the carbonyl groups are surrounded by negative charges, indicating some possible nucleophilic sites, whereas the positive charge regions are located on the H atoms indicating possible electrophilic sites.

6. Database survey
A search of the Cambridge Structural Database (CSD, Version 5.42, update May 2021; Groom et al., 2016) for the basic skeleton of this compound gave no hits. However, a CSD search on phenyl–Se–Se–phenyl compounds gave 152 hits and 199 observations with the Se–Se distance ranging from 2.287 to 3.051 Å (with a mean value of 2.393 Å and a standard deviation 0.162). In the structures of CATWEB01, REDGAK, REDGEO and REDGUE (Panda et al., 2012), the torsional angles of the selenium-attached phenyl ring (C–Se–Se–C) are ca 81° and those of CIDXET and CIDXUJ (Kulcsar et al., 2007) are 80.9 and 114.0°, respectively.

7. Synthesis and crystallization
The title compound was obtained by the condensation of rhodamine B hydrazide (Leite et al., 2013) and bis(o-formyl-phenyl)diselenide (Panda et al., 2005) (see Fig. 7). In a typical experiment, a solution of rhodamine B hydrazide (0.228 g, 0.5 mmol) in ethanol (30 mL) was added dropwise to a solution of bis(o-formylphenyl)diselenide (0.184 g, 0.5 mmol) in ethanol (30 mL) over approximately 45 minutes in a dropping funnel. The solution mixture was stirred further for 4 h at room temperature. After cooling, the solid was filtered and washed three times with cold ethanol. Pale-yellow crystals of the title compound suitable for single-crystal X-ray diffraction study were obtained from chloroform/pentane (1:1 mixture), yield 0.461 g, 81%, m.p. 519 K (Fig. 7). FT–IR (ATR): (ν, cm⁻¹) = 3387, 2967, 1613, 1514, 1218, 1117, 753. 1H NMR [300 MHz, CDCl3, δ (ppm)]: 1.15 (24H, t, J = 7.2 Hz, NCH2CH3), 3.33 (16H, q, J = 7.2 Hz, NCH2CH3), 6.29 (4H, s, H-Ar), 6.43 (4H, d, J = 2.7 Hz, H-Ar), 6.46 (4H, d, J = 2.7 Hz, H-Ar), 7.09 (2H, m, H-Ar), 7.19 (4H, m, H-Ar), 7.43 (4H, m, H-Ar), 7.92 (4H, m, H-Ar), 8.60 (2H, s, N––C––H). 13C NMR [75 MHz, CDCl3, δ (ppm)]: 12.7 (NCH2CH3), 44.5 (NCH2CH3), 66.1 (spiro carbon), 98.2, 104.7, 108.2, 123.1, 123.9, 130.9, 132.6, 149.1, 151.7, 154.0, 166.3 (C––O).

8. Refinement
Crystal data, data collection and structure refinement details are summarized in Table 5. All H atoms were positioned geometrically with C–H bond distances of 0.95 Å (aromatic...
H), 0.99 Å (methylene H), 0.98 Å (methyl H) and were refined as riding with isotropic displacement parameters 1.2 and 1.5 times that of the adjacent carbon atoms. The title compound crystallized with disorder in the two diethyl amine groups attached to the xanthene ring. The disorder model included the phenyl rings to which these amine groups were attached. For these groups, the occupancy factors are 0.664 (19)/0.336 (19) and 0.665 (11)/0.335 (11). All atoms in the diethyl amine groups (N3/C18/C19/C20/C22/C23/C24/C25 and N4/C32/C33/C34/C35) were subject to displacement and positional restraints using SIMU and SAME instructions. For the SIMU command the esd’s used were 0.005 while for the SAME command the esd’s used were 0.003.

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Figure 7
Scheme showing the reaction sequence for the synthesis of the title compound.

Table 5
Experimental details.

| Crystal data | Chemical formula | C70H70N8O4Se2 |
|--------------|------------------|----------------|
| Crystal system, space group | Tetragonal, P4321 |
| Temperature (K) | 100 |
| a, c (Å) | 21.507 (4), 13.434 (4) |
| V (Å³) | 6214 (3) |
| Z | 4 |
| Radiation type | Mo Kα |
| μ (mm⁻¹) | 1.25 |
| Crystal size (mm) | 0.27 × 0.23 × 0.08 |
| Data collection | Bruker APEXII CCD |
| Absorption correction | Multi-scan (SADABS; Krause et al., 2015) |
| T_max, T_min | 0.566, 0.746 |
| No. of measured, independent and observed [I > 2σ(I)] reflections | 7696, 7696, 6090 |
| R(int) | 0.119 |
| (sin θ/λ)max (Å⁻¹) | 0.666 |
| Reﬁnement | R[F2 > 2σ(F2)], wR(F2), S |
| No. of reﬂections | 7696 |
| No. of parameters | 540 |
| No. of restraints | 696 |
| H-atom treatment | H-atom parameters constrained |
| Δρ_max, Δρ_min (e Å⁻³) | 0.52, -0.97 |
| Absolute structure | Refined as an inversion twin |
| Absolute structure parameter | 0.05 (2) |

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Crystal structure, Hirshfeld surface analysis and DFT study of

2,2′′-(((([(1E,1′E)-(diselanediyl)bis(2,1-phenylene)]bis(methaneylylidene))bis(aza-
neylylidene))bis[3′,6′-bis(diethylamino)-4a′,9a′-dihydrospiro[isoindoline-1,9′-
xanthen]-3-one]

Manzoor Ahmad Malla, Ravi Bansal, Ray J. Butcher and Sushil K. Gupta

Computing details

Data collection: APEX2 (Bruker 2005); cell refinement: SAINT (Bruker 2005); data reduction: SAINT (Bruker 2005); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: SHELXL2018/3 (Sheldrick, 2015b); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL (Sheldrick, 2008), publCIF (Westrip (2010).

2,2′′-(((1E,1′E)-(Diselanediyl)bis(2,1-phenylene)]bis(methaneylylidene))bis(aza-
neylylidene))bis[3′,6′-bis(diethylamino)-4a′,9a′-dihydrospiro[isoindoline-1,9′-
xanthen]-3-one]

Crystal data

C_{70}H_{70}N_{8}O_{4}Se_{2}

Mr = 1245.26

Tetragonal, P4b2

a = 21.507 (4) Å

c = 13.434 (4) Å

V = 6214 (3) Å^3

Z = 4

F(000) = 2584

Data collection

Bruker APEXII CCD
diffractometer

φ and ω scans

Absorption correction: multi-scan

(SADABS; Krause et al., 2015)

T_{min} = 0.566, T_{max} = 0.746

7696 measured reflections

Refinement

Refinement on F^2

Least-squares matrix: full

R[F^2 > 2σ(F^2)] = 0.070

wR(F^2) = 0.142

S = 1.08

7696 reflections

540 parameters

696 restraints

Primary atom site location: dual

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
w = \frac{1}{\sigma^2(F_o^2) + (0.040P)^2 + 13.6633P} \\
\quad \text{where } P = (F_o^2 + 2F_c^2)/3 \\
\Delta \rho_{\text{max}} = 0.96 \text{ e Å}^{-3} \\
\Delta \rho_{\text{min}} = -0.96 \text{ e Å}^{-3} \\
\left(\Delta / \sigma^2\right)_{\text{max}} = 0.001 \\
\text{Absolute structure: Refined as an inversion twin} \\
\text{Absolute structure parameter: 0.05 (2)}

**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.** Refined as a 2-component inversion twin.

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

|         | x            | y            | z            | U_iso*/U_eq | Occ. (<1) |
|---------|--------------|--------------|--------------|------------|-----------|
| Se1     | 0.70568 (3)  | 0.18183 (3)  | 0.58326 (6)  | 0.01973 (16) |           |
| O1      | 0.7532 (2)   | 0.1249 (2)   | 0.9772 (4)   | 0.0257 (12) |           |
| O2      | 0.8536 (3)   | 0.2775 (2)   | 0.6006 (4)   | 0.0307 (13) |           |
| N1      | 0.7287 (3)   | 0.1778 (3)   | 0.7778 (5)   | 0.0218 (13) |           |
| N2      | 0.7820 (3)   | 0.1786 (3)   | 0.8351 (5)   | 0.0215 (13) |           |
| C1      | 0.6247 (3)   | 0.1743 (3)   | 0.6457 (6)   | 0.0209 (15) |           |
| C2      | 0.5709 (3)   | 0.1704 (3)   | 0.5920 (7)   | 0.0269 (17) |           |
| H2A     | 0.573364     | 0.172617     | 0.521440     | 0.032*      |           |
| C3      | 0.5136 (4)   | 0.1636 (4)   | 0.6348 (6)   | 0.0305 (19) |           |
| H3A     | 0.477457     | 0.160360     | 0.594590     | 0.037*      |           |
| C4      | 0.5089 (3)   | 0.1615 (4)   | 0.7383 (7)   | 0.0303 (19) |           |
| H4A     | 0.469386     | 0.156737     | 0.768954     | 0.036*      |           |
| C5      | 0.5619 (3)   | 0.1662 (4)   | 0.7962 (6)   | 0.0253 (17) |           |
| H5A     | 0.558725     | 0.165049     | 0.866677     | 0.030*      |           |
| C6      | 0.6207 (3)   | 0.1729 (3)   | 0.7508 (6)   | 0.0215 (16) |           |
| C7      | 0.6747 (3)   | 0.1760 (3)   | 0.8178 (6)   | 0.0222 (16) |           |
| H7A     | 0.669701     | 0.176542     | 0.888011     | 0.027*      |           |
| C8      | 0.7925 (3)   | 0.1505 (3)   | 0.9257 (6)   | 0.0232 (15) |           |
| C9      | 0.8604 (3)   | 0.1565 (3)   | 0.9431 (5)   | 0.0228 (17) |           |
| C10     | 0.8957 (4)   | 0.1375 (4)   | 1.0242 (6)   | 0.0306 (19) |           |
| H10A    | 0.877362     | 0.115811     | 1.078296     | 0.037*      |           |
| C11     | 0.9584 (4)   | 0.1513 (4)   | 1.0233 (7)   | 0.037 (2)   |           |
| H11A    | 0.983691     | 0.137835     | 1.077174     | 0.044*      |           |
| C12     | 0.9853 (4)   | 0.1842 (4)   | 0.9463 (6)   | 0.037 (2)   |           |
| H12A    | 1.028150     | 0.194827     | 0.949810     | 0.045*      |           |
| C13     | 0.9506 (4)   | 0.2021 (4)   | 0.8633 (7)   | 0.0317 (19) |           |
| H13A    | 0.969281     | 0.223137     | 0.808773     | 0.038*      |           |
| C14     | 0.8875 (3)   | 0.1879 (3)   | 0.8636 (6)   | 0.0251 (17) |           |
| C15     | 0.8387 (3)   | 0.2057 (3)   | 0.7855 (6)   | 0.0221 (16) |           |
| C16     | 0.8320 (7)   | 0.2769 (4)   | 0.7760 (12)  | 0.0246 (13) | 0.664 (19) |
| C17     | 0.8171 (5)   | 0.3120 (4)   | 0.8595 (9)   | 0.0261 (14) | 0.664 (19) |
| H17A    | 0.810023     | 0.292093     | 0.921568     | 0.031*      | 0.664 (19) |
| C18     | 0.8125 (5)   | 0.3763 (4)   | 0.8522 (7)   | 0.0276 (14) | 0.664 (19) |
| H18A    | 0.802296     | 0.400347     | 0.909233     | 0.033*      | 0.664 (19) |
| Atom | x    | y    | z    | U11  | U22  | U33  | U12  | U13  | U23  |
|------|------|------|------|------|------|------|------|------|------|
| C19  | 0.8228 (6) | 0.4055 (4) | 0.7613 (7) | 0.0267 (12) | 0.664 (19) |
| C20  | 0.8377 (8) | 0.3704 (5) | 0.6778 (8) | 0.0253 (12) | 0.664 (19) |
| H20A | 0.844811 | 0.390334 | 0.615758 | 0.030* | 0.664 (19) |
| C21  | 0.8423 (9) | 0.3061 (5) | 0.6852 (10) | 0.0245 (12) | 0.664 (19) |
| N3   | 0.8171 (5) | 0.4714 (4) | 0.7552 (8) | 0.0295 (13) | 0.664 (19) |
| C22  | 0.8049 (7) | 0.5092 (5) | 0.8399 (10) | 0.0306 (16) | 0.664 (19) |
| H22A | 0.772449 | 0.488677 | 0.880586 | 0.037* | 0.664 (19) |
| H22B | 0.788165 | 0.549841 | 0.817849 | 0.037* | 0.664 (19) |
| C23  | 0.8617 (8) | 0.5205 (6) | 0.9047 (11) | 0.037 (3) | 0.664 (19) |
| H23A | 0.852407 | 0.553040 | 0.953573 | 0.056* | 0.664 (19) |
| H23B | 0.896586 | 0.533822 | 0.862790 | 0.056* | 0.664 (19) |
| H23C | 0.872832 | 0.482036 | 0.939413 | 0.056* | 0.664 (19) |
| C24  | 0.8381 (7) | 0.5024 (6) | 0.6620 (9) | 0.0298 (15) | 0.664 (19) |
| H24A | 0.822744 | 0.545818 | 0.662541 | 0.036* | 0.664 (19) |
| H24B | 0.819286 | 0.481215 | 0.604023 | 0.036* | 0.664 (19) |
| C25  | 0.9087 (8) | 0.5033 (12) | 0.6489 (16) | 0.031 (3) | 0.664 (19) |
| H25A | 0.919134 | 0.524192 | 0.586220 | 0.047* | 0.664 (19) |
| H25B | 0.924392 | 0.460560 | 0.647392 | 0.047* | 0.664 (19) |
| H25C | 0.927740 | 0.525770 | 0.704517 | 0.047* | 0.664 (19) |
| C16A | 0.8351 (14) | 0.2773 (7) | 0.780 (2) | 0.0248 (14) | 0.336 (19) |
| C17A | 0.8317 (11) | 0.3109 (8) | 0.8683 (19) | 0.0261 (15) | 0.336 (19) |
| H17B | 0.830645 | 0.289786 | 0.930371 | 0.031* | 0.336 (19) |
| C18A | 0.8300 (11) | 0.3755 (8) | 0.8657 (14) | 0.0266 (15) | 0.336 (19) |
| H18B | 0.827661 | 0.398511 | 0.925919 | 0.032* | 0.336 (19) |
| C19A | 0.8316 (11) | 0.4064 (7) | 0.7749 (13) | 0.0270 (12) | 0.336 (19) |
| C20A | 0.8350 (16) | 0.3728 (9) | 0.6867 (14) | 0.0254 (13) | 0.336 (19) |
| H20B | 0.836078 | 0.393930 | 0.624620 | 0.030* | 0.336 (19) |
| C21A | 0.8367 (18) | 0.3082 (9) | 0.689 (2) | 0.0246 (13) | 0.336 (19) |
| N3A  | 0.8297 (10) | 0.4726 (8) | 0.7720 (13) | 0.0291 (13) | 0.336 (19) |
| C22A | 0.8308 (12) | 0.5089 (9) | 0.8626 (17) | 0.0309 (17) | 0.336 (19) |
| H22C | 0.800367 | 0.491063 | 0.910067 | 0.037* | 0.336 (19) |
| H22D | 0.817367 | 0.551850 | 0.847216 | 0.037* | 0.336 (19) |
| C23A | 0.8943 (14) | 0.5112 (12) | 0.9123 (19) | 0.038 (3) | 0.336 (19) |
| H23D | 0.889360 | 0.523101 | 0.982309 | 0.057* | 0.336 (19) |
| H23E | 0.920456 | 0.541792 | 0.878306 | 0.057* | 0.336 (19) |
| H23F | 0.913845 | 0.470107 | 0.908442 | 0.057* | 0.336 (19) |
| C24A | 0.8356 (12) | 0.5051 (11) | 0.6767 (15) | 0.0298 (16) | 0.336 (19) |
| H24C | 0.819079 | 0.547850 | 0.684418 | 0.036* | 0.336 (19) |
| H24D | 0.809503 | 0.483585 | 0.626721 | 0.036* | 0.336 (19) |
| C25A | 0.9021 (15) | 0.509 (3) | 0.637 (3) | 0.031 (3) | 0.336 (19) |
| H25D | 0.901289 | 0.520804 | 0.566831 | 0.047* | 0.336 (19) |
| H25E | 0.922335 | 0.468488 | 0.644552 | 0.047* | 0.336 (19) |
| H25F | 0.925212 | 0.540334 | 0.675210 | 0.047* | 0.336 (19) |
| C26 | 0.8598 (9) | 0.2150 (6) | 0.5998 (10) | 0.0279 (16) | 0.665 (11) |
| C27 | 0.8741 (5) | 0.1898 (4) | 0.5073 (8) | 0.0299 (16) | 0.665 (11) |
| H27A | 0.880123 | 0.216328 | 0.451607 | 0.036* | 0.665 (11) |
| C28 | 0.8797 (5) | 0.1258 (4) | 0.4964 (6) | 0.0323 (14) | 0.665 (11) |
| C29 | 0.8709 (5) | 0.0870 (5) | 0.5780 (7) | 0.0310 (16) | 0.665 (11) |
| Atomic displacement parameters (Å²) |
|-------------------------------------|
|                                      |
| Se1                                 |
|                                      |
| U¹¹ 0.0141 (3) 0.00190 (3) 0.0260 (3) | 0.0019 (3) 0.0068 (3) 0.0070 (3) |

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| Atom | u1   | u2   | u3   | u4   | u5   | u6   |
|------|------|------|------|------|------|------|
| O1   | 0.023 (3) | 0.022 (3) | 0.031 (3) | -0.001 (2) | -0.005 (2) | 0.010 (2) |
| O2   | 0.046 (3) | 0.019 (3) | 0.027 (3) | -0.009 (2) | -0.002 (3) | 0.006 (2) |
| N1   | 0.017 (3) | 0.022 (3) | 0.027 (3) | 0.000 (2) | -0.008 (2) | 0.007 (3) |
| N2   | 0.018 (3) | 0.020 (3) | 0.027 (3) | -0.003 (2) | -0.007 (2) | 0.012 (3) |
| C1   | 0.017 (3) | 0.013 (3) | 0.033 (4) | 0.003 (3) | -0.006 (3) | 0.002 (3) |
| C2   | 0.017 (3) | 0.037 (4) | 0.027 (4) | 0.004 (3) | -0.003 (3) | -0.003 (4) |
| C3   | 0.019 (4) | 0.037 (5) | 0.036 (6) | 0.005 (3) | -0.008 (3) | -0.006 (4) |
| C4   | 0.012 (3) | 0.036 (5) | 0.043 (5) | 0.000 (3) | 0.001 (4) | -0.004 (4) |
| C5   | 0.016 (4) | 0.029 (4) | 0.031 (4) | 0.005 (3) | -0.002 (3) | -0.002 (3) |
| C6   | 0.019 (3) | 0.013 (3) | 0.032 (4) | 0.000 (3) | -0.002 (3) | 0.002 (3) |
| C7   | 0.022 (4) | 0.018 (3) | 0.026 (4) | 0.000 (3) | -0.003 (3) | 0.004 (3) |
| C8   | 0.026 (3) | 0.012 (3) | 0.032 (4) | -0.002 (2) | -0.009 (4) | 0.005 (3) |
| C9   | 0.027 (4) | 0.019 (3) | 0.022 (4) | -0.001 (3) | -0.011 (3) | 0.003 (3) |
| C10  | 0.037 (5) | 0.028 (4) | 0.027 (4) | -0.003 (3) | -0.016 (4) | 0.006 (4) |
| C11  | 0.033 (5) | 0.041 (5) | 0.036 (5) | 0.007 (4) | -0.018 (4) | 0.005 (4) |
| C12  | 0.028 (4) | 0.046 (5) | 0.038 (5) | -0.004 (4) | -0.014 (4) | 0.003 (4) |
| C13  | 0.025 (4) | 0.024 (4) | 0.046 (5) | -0.003 (3) | -0.012 (4) | 0.001 (4) |
| C14  | 0.021 (4) | 0.018 (4) | 0.036 (5) | -0.003 (3) | -0.009 (3) | 0.003 (3) |
| C15  | 0.015 (3) | 0.014 (3) | 0.037 (4) | -0.002 (3) | -0.010 (3) | 0.011 (3) |
| C16  | 0.022 (3) | 0.020 (2) | 0.032 (3) | -0.002 (2) | -0.004 (2) | 0.008 (2) |
| C17  | 0.025 (3) | 0.022 (2) | 0.032 (3) | -0.001 (2) | -0.003 (3) | 0.008 (2) |
| C18  | 0.028 (3) | 0.023 (2) | 0.033 (3) | 0.000 (2) | -0.002 (3) | 0.006 (2) |
| C19  | 0.027 (2) | 0.021 (2) | 0.032 (3) | 0.000 (2) | -0.001 (2) | 0.007 (2) |
| C20  | 0.025 (3) | 0.020 (2) | 0.031 (3) | -0.002 (2) | -0.003 (2) | 0.009 (2) |
| C21  | 0.022 (3) | 0.020 (2) | 0.031 (3) | -0.002 (2) | -0.004 (2) | 0.008 (2) |
| C22  | 0.033 (3) | 0.021 (2) | 0.034 (3) | 0.000 (2) | -0.001 (2) | 0.005 (2) |
| C23  | 0.034 (3) | 0.023 (3) | 0.035 (3) | 0.000 (3) | 0.000 (3) | 0.005 (3) |
| C24  | 0.043 (5) | 0.033 (4) | 0.036 (5) | 0.004 (4) | -0.006 (5) | 0.005 (4) |
| C25  | 0.035 (3) | 0.020 (3) | 0.035 (3) | 0.000 (2) | -0.001 (3) | 0.007 (3) |
| C26  | 0.027 (4) | 0.024 (2) | 0.039 (3) | -0.002 (3) | -0.007 (3) | 0.002 (2) |
| C27  | 0.028 (4) | 0.025 (2) | 0.040 (3) | -0.001 (3) | -0.008 (3) | 0.004 (2) |
| C28  | 0.026 (3) | 0.024 (2) | 0.039 (3) | -0.001 (3) | -0.008 (3) | 0.005 (2) |
| C29  | 0.024 (3) | 0.021 (2) | 0.037 (3) | -0.002 (2) | -0.009 (2) | 0.005 (2) |
| N3A  | 0.033 (3) | 0.033 (3) | 0.035 (3) | 0.000 (2) | -0.001 (3) | 0.005 (3) |
| C30  | 0.027 (3) | 0.023 (3) | 0.034 (3) | 0.000 (3) | -0.001 (3) | 0.005 (3) |
| Atom  | U(1)  | U(2)  | U(3)  | U(4)  | U(5)  | U(6)  |
|-------|-------|-------|-------|-------|-------|-------|
| C32   | 0.036 | 0.038 | 0.050 | 0.001 | −0.008| −0.007|
| C33   | 0.041 | 0.051 | 0.056 | −0.004| −0.005| −0.015|
| C34   | 0.038 | 0.036 | 0.050 | −0.001| −0.008| −0.002|
| C35   | 0.050 | 0.050 | 0.063 | 0.003 | −0.009| −0.003|
| C26A  | 0.026 | 0.022 | 0.038 | −0.002| −0.009| 0.004 |
| C27A  | 0.028 | 0.024 | 0.039 | −0.002| −0.009| 0.003 |
| C28A  | 0.030 | 0.027 | 0.042 | −0.001| −0.009| 0.002 |
| C29A  | 0.028 | 0.025 | 0.040 | −0.001| −0.008| 0.004 |
| C30A  | 0.026 | 0.024 | 0.039 | −0.001| −0.008| 0.005 |
| C31A  | 0.025 | 0.022 | 0.037 | −0.002| −0.009| 0.005 |
| N4A   | 0.035 | 0.034 | 0.047 | −0.001| −0.008| −0.003|
| C32A  | 0.036 | 0.037 | 0.049 | −0.001| −0.008| −0.006|
| C33A  | 0.038 | 0.045 | 0.051 | 0.000 | −0.007| −0.010|
| C34A  | 0.037 | 0.035 | 0.050 | −0.001| −0.008| −0.003|
| C35A  | 0.049 | 0.040 | 0.063 | −0.002| −0.006| −0.002|

**Geometric parameters (Å, °)**

| Bond                   | Distance | Angle   |
|------------------------|----------|---------|
| Se1—C1                 | 1.939 (7) | C18A—H18B 0.9500 |
| Se1—Se1i               | 2.3517 (17) | C19A—C20A 1.3900 |
| O1—C8                  | 1.222 (9)  | C19A—N3A 1.425 (8) |
| O2—C21                 | 1.315 (12) | C20A—C21A 1.3900 |
| O2—C26A                | 1.35 (3)   | C20A—H20B 0.9500 |
| O2—C26                 | 1.349 (13) | N3A—C22A 1.446 (13) |
| O2—C21A                | 1.41 (2)   | N3A—C24A 1.465 (12) |
| N1—C7                  | 1.280 (9)  | C22A—C23A 1.521 (17) |
| N1—N2                  | 1.380 (8)  | C22A—H22C 0.9900 |
| N2—C8                  | 1.378 (10) | C22A—H22D 0.9900 |
| N2—C15                 | 1.507 (9)  | C23A—H23D 0.9800 |
| C1—C2                  | 1.367 (10) | C23A—H23E 0.9800 |
| C1—C6                  | 1.415 (11) | C23A—H23F 0.9800 |
| C2—C3                  | 1.368 (11) | C24A—C25A 1.527 (12) |
| C2—H2A                 | 0.9500     | C24A—H24C 0.9900 |
| C3—C4                  | 1.394 (12) | C24A—H24D 0.9900 |
| C3—H3A                 | 0.9500     | C25A—H25D 0.9800 |
| C4—C5                  | 1.384 (11) | C25A—H25E 0.9800 |
| C4—H4A                 | 0.9500     | C25A—H25F 0.9800 |
| C5—C6                  | 1.411 (10) | C26—C27 1.3900 |
| C5—H5A                 | 0.9500     | C26—C31 1.3900 |
| C6—C7                  | 1.471 (10) | C27—C28 1.3900 |
| C7—H7A                 | 0.9500     | C27—H27A 0.9500 |
| C8—C9                  | 1.484 (10) | C28—C29 1.3900 |
| C9—C10                 | 1.389 (10) | C28—N4 1.423 (10) |
| C9—C14                 | 1.392 (11) | C29—C30 1.3900 |
| C10—C11                | 1.381 (12) | C29—H29A 0.9500 |
| C10—H10A               | 0.9500     | C30—C31 1.3900 |
| C11—C12                | 1.381 (12) | C30—H30A 0.9500 |
| C11—H11A               | 0.9500     | N4—C34 1.481 (13) |
| Bond                  | Length (Å) | Bond                  | Length (Å) |
|-----------------------|------------|-----------------------|------------|
| C12—C13               | 1.397 (11) | N4—C32                | 1.543 (14) |
| C12—H12A              | 0.9500     | C32—C33               | 1.448 (16) |
| C13—C14               | 1.391 (11) | C32—H32A              | 0.9900     |
| C13—H13A              | 0.9500     | C32—H32B              | 0.9900     |
| C14—C15               | 1.534 (10) | C33—H33A              | 0.9800     |
| C15—C31A              | 1.537 (18) | C33—H33B              | 0.9800     |
| C15—C16A              | 1.542 (17) | C33—H33C              | 0.9800     |
| C15—C31               | 1.543 (10) | C34—C35               | 1.616 (19) |
| C16—C17               | 1.3900     | C34—H34A              | 0.9900     |
| C16—C21               | 1.3900     | C34—H34B              | 0.9900     |
| C17—C18               | 1.3900     | C35—H35A              | 0.9800     |
| C17—H17A              | 0.9500     | C35—H35B              | 0.9800     |
| C18—C19               | 1.3900     | C35—H35C              | 0.9800     |
| C18—H18A              | 0.9500     | C26A—C27A             | 1.3900     |
| C19—C20               | 1.3900     | C26A—C31A             | 1.3900     |
| C19—N3                | 1.426 (7)  | C27A—C28A             | 1.3900     |
| C20—C21               | 1.3900     | C27A—H27B             | 0.9500     |
| C20—H20A              | 0.9500     | C28A—C29A             | 1.3900     |
| N3—C22                | 1.446 (13) | C28A—N4A              | 1.424 (11) |
| N3—C24                | 1.466 (12) | C29A—C30A             | 1.3900     |
| C22—C23               | 1.520 (17) | C30A—C31A             | 1.3900     |
| C22—H22A              | 0.9900     | C30A—H30B             | 0.9500     |
| C22—H22B              | 0.9900     | N4A—C34A              | 1.481 (13) |
| C23—H23A              | 0.9800     | N4A—C32A              | 1.543 (15) |
| C23—H23B              | 0.9800     | C32A—C33A             | 1.448 (17) |
| C23—H23C              | 0.9800     | C32A—H32C             | 0.9900     |
| C24—C25               | 1.528 (12) | C32A—H32D             | 0.9900     |
| C24—H24A              | 0.9900     | C33A—H33D             | 0.9800     |
| C24—H24B              | 0.9900     | C33A—H33E             | 0.9800     |
| C25—H25A              | 0.9800     | C33A—H33F             | 0.9800     |
| C25—H25B              | 0.9800     | C34A—C35A             | 1.615 (19) |
| C25—H25C              | 0.9800     | C34A—H34C             | 0.9900     |
| C16A—C17A             | 1.3900     | C34A—H34D             | 0.9900     |
| C16A—C21A             | 1.3900     | C35A—H35D             | 0.9800     |
| C17A—C18A             | 1.3900     | C35A—H35E             | 0.9800     |
| C17A—H17B             | 0.9500     | C35A—H35F             | 0.9800     |
| C18A—C19A             | 1.3900     |                       |            |
|                       |            |                       |            |
| C1—Se1—Se1i           | 103.5 (2)  | C20A—C21A—C16A        | 120.0      |
| C21—O2—C26            | 119.4 (9)  | C20A—C21A—O2          | 117.0 (15) |
| C26A—O2—C21A          | 118.8 (16) | C16A—C21A—O2          | 121.6 (15) |
| C7—N1—N2              | 121.3 (6)  | C19A—N3A—C22A         | 121.1 (8)  |
| C8—N2—N1              | 128.5 (6)  | C19A—N3A—C24A         | 119.9 (8)  |
| C8—N2—C15             | 115.3 (5)  | C22A—N3A—C24A         | 118.5 (8)  |
| N1—N2—C15             | 115.5 (5)  | N3A—C22A—C23A         | 113.7 (11) |
| C2—C1—C6              | 118.3 (7)  | N3A—C22A—H22C         | 108.8      |
| C2—C1—Se1             | 122.5 (6)  | C23A—C22A—H22C        | 108.8      |
C6—C1—Se1 119.2 (5) N3A—C22A—H22D 108.8
C1—C2—C3 123.2 (8) C23A—C22A—H22D 108.8
C1—C2—H2A 118.4 H22C—C22A—H22D 107.7
C3—C2—H2A 118.4 C22A—C23A—H23D 109.5
C2—C3—C4 119.3 (7) C22A—C23A—H23E 109.5
C2—C3—H3A 120.4 H23D—C23A—H23E 109.5
C4—C3—H3A 120.4 C22A—C23A—H23F 109.5
C5—C4—C3 119.8 (7) H23D—C23A—H23F 109.5
C5—C4—H4A 120.1 H23E—C23A—H23F 109.5
C3—C4—H4A 120.1 N3A—C24A—C25A 114.2 (9)
C3—C4—H4A 120.1 N3A—C24A—C25B 114.2 (9)
C4—C5—C6 117.5 (7) N3A—C24A—C25C 114.2 (9)
C4—C5—H5A 121.3 N3A—C24A—C25D 114.2 (9)
C5—C6—C1 121.3 C25A—C24A—C25D 109.5
C5—C6—C7 116.6 (7) C25A—C24A—C25E 109.5
C1—C6—C7 124.1 (7) C25A—C24A—C25F 109.5
N1—C7—C6 117.5 (7) C25A—C24A—C25G 109.5
N1—C7—H7A 121.3 C25A—C24A—C25H 109.5
C6—C7—H7A 121.3 C25A—C24A—C25I 109.5
O1—C8—N2 125.8 (6) C24A—C25A—C25B 109.5
O1—C8—C9 129.0 (7) C24A—C25A—C25C 109.5
N2—C8—C9 105.2 (6) C24A—C25A—C25D 109.5
C10—C9—C14 121.0 (7) C24A—C25A—C25E 109.5
C10—C9—C8 129.5 (7) C24A—C25A—C25F 109.5
C14—C9—C14 109.5 (6) C24A—C25A—C25G 109.5
C10—C11—H11A 119.2 C24A—C25A—C25H 109.5
C11—C10—C9 117.7 (8) C24A—C25A—C25I 109.5
C11—C10—H10A 121.1 C24A—C25A—C25J 109.5
C9—C10—H10A 121.1 C24A—C25A—C25K 109.5
C12—C11—C10 121.7 (8) C24A—C25A—C25L 109.5
C12—C11—C11A 119.2 C24A—C25A—C25M 109.5
C10—C11—C11A 119.2 C24A—C25A—C25N 109.5
C11—C12—C13 121.0 (8) C24A—C25A—C25O 109.5
C11—C12—H12A 119.5 C24A—C25A—C25P 109.5
C13—C12—H12A 119.5 C24A—C25A—C25Q 109.5
C14—C13—C12 117.3 (8) C24A—C25A—C25R 109.5
C14—C13—H13A 121.3 C24A—C25A—C25S 109.5
C12—C13—H13A 121.3 C24A—C25A—C25T 109.5
C13—C14—C9 121.2 (7) C24A—C25A—C25U 109.5
C13—C14—C15 127.6 (7) C24A—C25A—C25V 109.5
C9—C14—C15 111.1 (6) C24A—C25A—C25W 109.5
N2—C15—C14 98.9 (6) C24A—C25A—C25X 109.5
N2—C15—C31A 111.4 (18) C24A—C25A—C25Y 109.5
C14—C15—C31A 114.5 (18) C24A—C25A—C25Z 109.5
N2—C15—C16A 111.5 (12) C24A—C25A—C25A 109.5
C14—C15—C16A 108.3 (13) C24A—C25A—C25B 109.5
C31A—C15—C16A 111.6 (18) C24A—C25A—C25C 109.5
N2—C15—C16 110.2 (7) C24A—C25A—C25D 109.5
C14—C15—C16 111.6 (8) C24A—C25A—C25E 109.5
C13—C14—C9 121.2 (7) C24A—C25A—C25F 109.5
C13—C14—C15 127.6 (7) C24A—C25A—C25G 109.5
C9—C14—C15 111.1 (6) C24A—C25A—C25H 109.5
N2—C15—C14 98.9 (6) C24A—C25A—C25I 109.5
N2—C15—C31A 111.4 (18) C24A—C25A—C25J 109.5
C14—C15—C31A 114.5 (18) C24A—C25A—C25K 109.5
N2—C15—C16A 111.5 (12) C24A—C25A—C25L 109.5
C14—C15—C16A 108.3 (13) C24A—C25A—C25M 109.5
C31A—C15—C16A 111.6 (18) C24A—C25A—C25N 109.5
N2—C15—C16 110.2 (7) C24A—C25A—C25O 109.5
C14—C15—C16 111.6 (8) C24A—C25A—C25P 109.5

Acta Cryst. (2022). E78, 1-7
N2—C15—C31 112.2 (10) C32—C33—H33A 109.5
C14—C15—C31 113.3 (10) C32—C33—H33B 109.5
C16—C15—C31 110.2 (10) H33A—C33—H33B 109.5
C17—C16—C21 120.0 C32—C33—H33C 109.5
C17—C16—C15 119.6 (9) H33A—C33—H33C 109.5
C21—C16—C15 120.4 (9) H33B—C33—H33C 109.5
C16—C17—C18 120.0 N4—C34—C35 107.2 (9)
C16—C17—H17A 120.0 N4—C34—H34A 110.3
C18—C17—H17A 120.0 C35—C34—H34A 110.3
C19—C18—C17 120.0 C35—C34—H34B 110.3
C19—C18—H18A 120.0 H34A—C34—H34B 108.5
C17—C18—H18A 120.0 C34—C35—H35A 109.5
C18—C19—C20 120.0 C34—C35—H35B 109.5
C18—C19—N3 120.2 (5) C34—C35—H35C 109.5
C20—C19—N3 119.8 (5) O2—C21—O2—C26A—C27A 115.1 (16)
C21—C20—C19 120.0 C26A—C27A—C28A 120.0
C21—C20—H20A 120.0 C26A—C27A—N4A 121.3 (6)
C19—C20—H20A 120.0 C28A—C29A—N4A 121.3 (6)
O2—C21—C20 114.7 (8) C29A—C28A—C27A 120.0
O2—C21—C16 125.2 (8) C29A—C28A—N4A 121.3 (6)
C20—C21—C16 120.0 C30A—C31A—C26A 120.0
C19—N3—C22 120.9 (7) C30A—C31A—C15 119.8 (19)
C19—N3—C24 119.4 (7) C31A—C30A—C26A 120.0
C22—N3—C24 118.2 (7) C31A—C30A—C15 119.8 (19)
N3—C22—C23 113.9 (10) C33A—C32A—C34A 119.9 (9)
N3—C22—H22A 108.8 C33A—C32A—H32C 110.9
C23—C22—H22A 108.8 C33A—C32A—H32D 110.9
N3—C22—H22B 108.8 C33A—C32A—H32E 109.5
C23—C22—H22B 108.8 C33A—C32A—H32F 109.5
H22A—C22—H22B 107.7 C33A—C32A—H32G 109.5
C22—C23—H23A 109.5 C33A—C32A—H32H 109.5
C22—C23—H23B 109.5 C33A—C32A—H32I 109.5
H23A—C23—H23B 109.5 C33A—C32A—H32J 109.5
C22—C23—H23C 109.5 C33A—C32A—H32K 109.5
H23A—C23—H23C 109.5 C33A—C32A—H32L 109.5
C22—C23—C24—C25 114.1 (8) C33A—C32A—H32M 109.5
N3—C24—C25 108.7 C33A—C32A—H32N 109.5
C25—C24—C25—H24A 108.7 C33A—C32A—H32O 109.5
N3—C24—C25—H24B 108.7 C33A—C32A—H32P 109.5
C25—C24—C25—H24B 108.7 C33A—C32A—H32Q 109.5
H24A—C24—C25—H25A 107.6 C33A—C32A—H32R 109.5
C24—C25—H25A 109.5 C33A—C32A—H32S 109.5
C24—C25—H25B 109.5 C33A—C32A—H32T 109.5
H25A—C25—H25B 109.5 C33A—C32A—H32U 109.5
C24—C25—H25C 109.5 C33A—C32A—H32V 109.5
H25A—C25—H25C 109.5 C33A—C32A—H32W 109.5
H25B—C25—H25C 109.5 C33A—C32A—H32X 109.5

Acta Cryst. (2022). E78, 1-7
| Bond/Angle/Distance | Value |
|---------------------|-------|
| C17A—C16A—C21A     | 120.0 |
| C17A—C16A—C15      | 118.9 (16) |
| C21A—C16A—C15      | 121.1 (16) |
| C16A—C17A—C18A     | 120.0 |
| C16A—C17A—H17B     | 120.0 |
| C18A—C17A—H17B     | 120.0 |
| C19A—C18A—C17A     | 120.0 |
| C19A—C18A—H18B     | 120.0 |
| C17A—C18A—H18B     | 120.0 |
| C18A—C19A—C20A     | 120.0 |
| C18A—C19A—N3A      | 120.1 (6) |
| C20A—C19A—N3A      | 119.9 (6) |
| C21A—C20A—C19A     | 120.0 |
| C21A—C20A—H20B     | 120.0 |
| C19A—C20A—H20B     | 120.0 |
| C7—N1—N2—C8        | 33.2 (11) |
| C7—N1—N2—C15       | −156.7 (7) |
| C6—C1—C2—C3        | −1.9 (11) |
| Se1—C1—C2—C3       | 178.4 (6) |
| C1—C2—C3—C4        | 1.2 (12) |
| C2—C3—C4—C5        | 0.0 (12) |
| C3—C4—C5—C6        | −0.4 (12) |
| C4—C5—C6—C7        | −0.3 (11) |
| C4—C5—C6—C7        | −178.4 (7) |
| C2—C1—C6—C5        | 1.4 (10) |
| Se1—C1—C6—C5       | −178.8 (5) |
| C2—C1—C6—C7        | 179.4 (6) |
| Se1—C1—C6—C7       | −0.9 (9) |
| N2—N1—C7—C6        | −177.8 (6) |
| C5—C6—C7—N1        | 175.5 (7) |
| C1—C6—C7—N1        | −2.5 (10) |
| N1—N2—C8—O1        | −8.7 (12) |
| C15—N2—C8—O1       | −178.8 (7) |
| N1—N2—C8—C9        | 169.5 (7) |
| C15—N2—C8—C9       | −0.6 (8) |
| O1—C8—C9—C10       | −3.6 (14) |
| N2—C8—C9—C10       | 178.3 (8) |
| O1—C8—C9—C14       | 178.3 (8) |
| N2—C8—C9—C14       | 0.3 (8) |
| C14—C9—C10—C11     | 0.5 (12) |
| C8—C9—C10—C11      | −177.3 (8) |
| C9—C10—C11—C12     | 1.6 (13) |
| C10—C11—C12—C13    | −3.4 (15) |
| C11—C12—C13—C14    | 2.8 (13) |
| C12—C13—C14—C9     | −0.7 (12) |
| C12—C13—C14—C15    | 175.9 (8) |
| C10—C9—C14—C13     | −1.0 (12) |
| Bond                  | Angle (deg) |
|----------------------|-------------|
| C8—C9—C14—C13       | 177.2 (7)   |
| C10—C9—C14—C15      | -178.1 (7)  |
| C8—C9—C14—C15       | 0.1 (9)     |
| C8—N2—C15—C14       | 0.7 (8)     |
| N1—N2—C15—C14       | -170.8 (6)  |
| C8—N2—C15—C31A      | 121.4 (18)  |
| N1—N2—C15—C31A      | -50.0 (18)  |
| C8—N2—C15—C16A      | -113.1 (14) |
| N1—N2—C15—C16A      | 75.4 (14)   |
| C8—N2—C15—C16       | -163.6 (9)  |
| N1—N2—C15—C16       | 72.2 (9)    |
| C8—N2—C15—C31       | 120.4 (10)  |
| N1—N2—C15—C31       | -51.0 (11)  |
| C13—C14—C15—N2      | -177.3 (8)  |
| C9—C14—C15—N2       | -0.5 (8)    |
| C13—C14—C15—C31A    | 64 (2)      |
| C9—C14—C15—C31A     | -118.9 (18) |
| C13—C14—C15—C16A    | -61.1 (15)  |
| C13—C14—C15—C16     | 115.8 (13)  |
| C13—C14—C15—C16     | -61.4 (12)  |
| C9—C14—C15—C16      | 115.5 (9)   |
| C13—C14—C15—C31     | 63.7 (13)   |
| C9—C14—C15—C31      | -119.4 (11) |
| N2—C15—C16—C17      | 51.8 (11)   |
| C14—C15—C16—C17     | -57.0 (11)  |
| C31—C15—C16—C21     | 128.6 (12)  |
| N2—C15—C16—C21      | -129.8 (7)  |
| C14—C15—C16—C21     | 121.4 (8)   |
| C31—C15—C16—C21     | -5.4 (13)   |
| C21—C16—C17—C18     | 0.0         |
| C15—C16—C17—C18     | 178.4 (11)  |
| C16—C17—C18—C19     | 0.0         |
| C17—C18—C19—C20     | 0.0         |
| C17—C18—C19—N3      | 178.9 (10)  |
| C18—C19—C20—C21     | 0.0         |
| N3—C19—C20—C21      | -178.9 (10) |
| C26—O2—C21—C20      | 179.1 (11)  |
| C26—O2—C21—C16      | -4.4 (18)   |
| C19—C20—C21—O2      | 168.6 (15)  |
| C19—C20—C21—O2      | 0.0         |
| C17—C16—C21—O2      | -176.4 (16) |
| C15—C16—C21—O2      | 5.2 (13)    |
| C17—C16—C21—C20     | 0.0         |
| C15—C16—C21—C20     | -178.4 (11) |
| C18—C19—N3—C22      | 4.3 (15)    |
| C20—C19—N3—C22      | -176.7 (9)  |
| C18—C19—N3—C24      | 169.8 (9)   |
| C20—C19—N3—C24      | -11.2 (13)  |

| Bond                  | Angle (deg) |
|----------------------|-------------|
| C26—C27—C28—N4      | -175.1 (11) |
| C27—C28—C29—C30     | 0.0         |
| N4—C28—C30—C31      | 175.0 (11)  |
| C28—C29—C30—C31     | 0.0         |
| O2—C26—C31—C30      | 177.7 (14)  |
| C27—C26—C31—C30     | 0.0         |
| O2—C26—C31—C15      | -5.7 (10)   |
| C27—C26—C31—C15     | 176.6 (17)  |
| N2—C15—C31—C30      | -54.6 (13)  |
| C14—C15—C31—C30     | 56.3 (13)   |
| C16—C15—C31—C30     | -177.8 (9)  |
| N2—C15—C31—C26      | 128.8 (8)   |
| C14—C15—C31—C26     | -120.3 (9)  |
| C16—C15—C31—C26     | 5.6 (15)    |
| C29—C28—N4—C34      | 17.8 (13)   |
| C27—C28—N4—C34      | -167.2 (9)  |
| C29—C28—N4—C32      | 179.1 (9)   |
| C27—C28—N4—C32      | -5.9 (12)   |
| C28—N4—C32—C33      | -73.2 (14)  |
| C31—C15—C16—C20     | 51.8 (11)   |
| C32—N4—C32—C33      | 88.6 (12)   |
| C31—C15—C16—C20     | 63.9 (14)   |
| C32—N4—C32—C33      | -98.0 (12)  |
| C31—C15—C16—C20     | 0.0         |
| C21A—O2—C26A—C27A   | 167 (2)     |
| C21A—O2—C26A—C31A   | -15 (3)     |
| C31A—C26A—C27A—C28A | 178 (3)     |
| C31A—C26A—C27A—C28A | 0.0         |
| C26A—C27A—C28A—C29A | 0.0         |
| C26A—C27A—C28A—N4A  | -176 (2)    |
| C27A—C28A—C29A—C30A | 0.0         |
| C26A—C27A—C28A—C29A | 0.0         |
| N4A—C28A—C29A—C30A  | 176 (2)     |
| C28A—C29A—C30A—C31A | 0.0         |
| C28A—C29A—C30A—C31A | 0.0         |
| C29A—C30A—C31A—C32A | 176 (2)     |
| C29A—C30A—C31A—C32A | 0.0         |
Symmetry code: (i) \(y+1/2, x-1/2, -z+1\).

Hydrogen-bond geometry (Å, °)

| D—H···A     | D—H | H···A | D···A  | D—H···A |
|-------------|-----|-------|--------|---------|
| C2—H2A···Se1\(^{i}\) | 0.95 | 2.82  | 3.436 (8) | 124     |
| C7—H7A···O1   | 0.95 | 2.43  | 2.940 (9) | 114     |
| C7—H7A···O1\(^{ii}\) | 0.95 | 2.63  | 3.391 (10)| 137     |
| C12—H12A···O1\(^{iii}\) | 0.95 | 2.56  | 3.447 (10)| 156     |
| C33A—H33E···Se1\(^{i}\) | 0.98 | 3.04  | 4.00 (3)  | 168     |

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

Percentage contributions of interatomic contacts to the Hirshfeld surface for the title compound

| Contact | Percentage contribution |
|---------|-------------------------|
| H···H   | 68.1                    |
| C···H/H···C | 21.2                |
| O···H/H···O | 8.7                   |
| N···H/H···N | 1.6                   |
| Se···H/H···Se | 0.4               |

Comparison of selected (X-ray and DFT) bond lengths and angles (Å, °)

|                  | X-ray     | B3LYP/6-31G(d) |
|------------------|-----------|----------------|
| Se1—C1           | 1.939 (7) | 1.941          |
| Se1—Se1’         | 2.3517 (17)| 2.356         |
| O1—C8            | 1.222 (9) | 1.224          |
| O2—C21           | 1.315 (12) | 1.374        |
| O2—C26           | 1.349 (13) | 1.368        |
| N1—C7            | 1.280 (9) | 1.291          |
| N1—N2            | 1.380 (8) | 1.353          |
| N2—C8            | 1.378 (10) | 1.392        |
| N2—C15           | 1.507 (9) | 1.513          |
| C1—C6            | 1.415 (11) | 1.42       |
| C19—N3           | 1.426 (7) | 1.383          |
| C22—N3           | 1.446 (13) | 1.464        |
| C24—N3           | 1.466 (12) | 1.461        |
| N4—C28           | 1.423 (10) | 1.39       |
| N4—C32           | 1.543 (14) | 1.461        |
| N4—C34           | 1.481 (13) | 1.462        |
| C1—Se1—Se1’      | 103.5 (2) | 102.711       |
| C26—O2—C21       | 119.4 (9) | 119.241       |
| Bond                  | Bond Angle (°) | Bond Angle (°) |
|-----------------------|----------------|----------------|
| C7—N1—N2              | 121.3 (6)      | 122.983        |
| N1—N2—C15             | 115.5 (5)      | 116.391        |
| C2—C1—Se1             | 122.5 (6)      | 121.361        |
| C6—C1—Se1             | 119.2 (5)      | 119.262        |
| O1—C8—N2              | 125.8 (6)      | 126.543        |
| C8—N2—C15             | 115.3 (5)      | 114.337        |
| O1—C8—C9              | 129.0 (7)      | 128.268        |
| N2—C8—C9              | 105.2 (6)      | 105.19         |
| C19—N3—C22            | 120.9 (7)      | 120.635        |
| C19—N3—C24            | 119.4 (7)      | 120.99         |
| C22—N3—C24            | 118.2 (7)      | 118.187        |
| C28—N4—C32            | 120.2 (7)      | 120.875        |
| C28—N4—C34            | 120.1 (8)      | 120.772        |
| C32—N4—C34            | 117.2 (9)      | 117.917        |
| C1—Se1—Se1’—C1’      | -88.9 (6)      | -73.195        |

Symmetry code: (i) 1/2 + y, x - 1/2, 1 - z.