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# 1-(2-Naphthyl)-3-phenyl-3-(4,5,6,7-tetrahydro-1,2,3-benzoselenadiazol-4-yl)-propan-1-one

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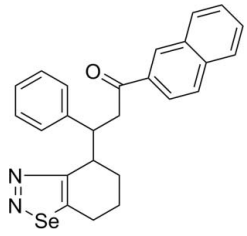
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.038; $wR$ factor = 0.096; data-to-parameter ratio = 13.7.

In the title compound, $C_{25}H_{22}N_2OSe$, the fused six-membered cyclohexene ring of the 4,5,6,7-tetrahydro-1,2,3-benzoselenadiazole group adopts a near half-chair conformation and the five-membered 1,2,3-selenadiazole ring is essentially planar (r.m.s. deviation = 0.004 Å). There are weak intermolecular C—H···O and C—H···$\pi$ interactions in the crystal structure. Intermolecular $\pi$–$\pi$ stacking is also observed between the naphthyl units, with a centroid–centroid distance of 3.529 (15) Å.

## Related literature

For the biological importance of 1,2,3-selenadiazole derivatives, see: Kuroda *et al.* (2001); El-Bahaie *et al.* (1990); El-Kashef *et al.* (1986); Plano *et al.* (2010). For ring puckering analysis, see: Cremer & Pople (1975). For synthetic procedures, see: Al Arab (1989); Li *et al.* (2003); Qian *et al.* (2008); Xu *et al.* (2009).




## Experimental

### Crystal data

$C_{25}H_{22}N_2OSe$
$M_r$ = 445.41
Triclinic, $P\overline{1}$
$a$ = 8.0600 (4) Å
$b$ = 10.1215 (5) Å
$c$ = 13.0827 (6) Å
$\alpha$ = 81.479 (4)°
$\beta$ = 76.478 (4)°
$\gamma$ = 82.087 (4)°
$V$ = 1020.33 (9) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.86 mm$^{-1}$
$T$ = 293 K
0.4 × 0.3 × 0.2 mm

### Data collection

Oxford Diffraction Xcalibur E diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
$T_{min}$ = 0.658, $T_{max}$ = 1.000
6762 measured reflections
3594 independent reflections
2770 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.096
$S$ = 1.01
3594 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.41 e Å$^{-3}$

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

*Cg* is the centroid of the C16–C21 ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C20—H20···O1$^{i}$ | 0.93 | 2.56 | 3.381 (3) | 147 |
| C22—H22···O1$^{i}$ | 0.93 | 2.58 | 3.392 (4) | 146 |
| C4—H4$A$···$Cg^{ii}$ | 0.97 | 2.63 | 3.584 (3) | 167 |

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2375).

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# supporting information

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# 1-(2-Naphthyl)-3-phenyl-3-(4,5,6,7-tetrahydro-1,2,3-benzoselenadiazol-4-yl)propan-1-one

**J. Muthukumaran, M. Nachiappan, S. Chitra, P. Manisankar, Suman Bhattacharya, S. Muthusubramanian, R. Krishna and J. Jeyakanthan**

## S1. Comment

Selenium containing heterocyclic compounds are of interest due to their biological applications. They posses various beneficial activities such as anti-fungal (Kuroda *et al.*, 2001), anti-bacterial (El-Kashef *et al.*, 1986), anti-microbial (El-Bahaie *et al.*, 1990), and anti-cancer (Plano *et al.*, 2010). Considering the importances of 1,2,3-selenadiazole derivatives, we report the structure of the title compound (Fig. 1). The five-membered 1,2,3-selenadiazole moiety (C1/N1/N2/Se1/C2) of the title compound adopts a planar conformation (r.m.s. deviation = 0.004 Å). Cremer & Pople puckering analysis (Cremer & Pople, 1975) cannot be performed to this moiety, for its weighted average absolute torsion angle is 0.62°, which is less than 5.0°. However, the fused six-membered ring (C1/C2/C3/C4/C5/C6) of 4,5,6,7-tetrahydrobenzo[*d*][1,2,3]selenadiazole group adopts a near to half-chair conformation with puckering parameters of Q = 0.489 (3) Å, $\theta$ = 48.9 (4)° and Φ = 218.1 (5)°. The stabilization of crystal packing is mainly governed by intermolecular hydrogen bonding interactions such as C20–H20···O1 (*x* - 1, *y*, *z*) and C22—H22···O1 (Fig. 2). The C—H···$\pi$ interaction (Fig. 3) is observed between C4—H4A···*Cg* (–x,1 - *y*,1 - *z*) *[Cg* is the centroid of C16—C21 ring, C···*Cg* distance: 3.584 (3) Å, H···*Cg* 2.63 Å, H-Perp: 2.61 Å], which also contribute to the crystal packing. The crystal packing also exhibits intermolecular $\pi$–$\pi$ stacking interaction between naphthyl units with a centroid-centroid distance of 3.529 (15) Å.

## S2. Experimental

Diastereomerically pure racemic cyclic 1,5-diketones,(*2S*,1'R**)-2-[3-(2-naphthyl)-3-oxo-1-phenylpropyl]cyclohexan-1-one, were obtained via a simple Michael addition of cyclohexanone with substituted chalcones by a known method (Al Arab, 1989; Li *et al.*, 2003; Xu *et al.*, 2009; Qian *et al.*, 2008). A mixture of (*2S*,1'R**)- 2-[3-(2-naphthyl)-3-oxo-1-phenylpropyl]-1-cyclohexanone (1 mmol, 0.36 g) and semicarbazide hydrochloride (1 mmol, 0.11 g) in ethanol (10 ml) was refluxed for 3 h. After completion of the reaction as monitored by TLC, the mixture was poured into ice-cold water (50 ml) and the resulting mono-semicarbazone solid was filtered off. The mono-semicarbazone (1 mmol, 0.41 g) and $SeO_2$ (2 mmol, 0.44 g) in THF(10 ml) was refluxed on a water bath for 30 minutes and on completion of the reaction the mixture was filtered to remove selenium powder. The filtrate was concentrated under vacuum, and the residue was subjected to column chromatography using petroleum ether/ethyl acetate mixture (95:5; *v*/*v*) as eluent to afford the racemic mixture of the pure product (Yield: 70%, m.p.: 404-405 K). Dissolving the pure compound in 3:1 mixture of dichloromethane/ethyl acetate and on keeping for slow evaporation of the solvents provides crystals for X-ray analysis.

## S3. Refinement

The hydrogen atoms were placed in calculated positions (C–H = 0.93–0.98 Å) and included in the refinement in riding-model approximation with $U_{iso}$(H) = 1.2$U_{eq}$(C).

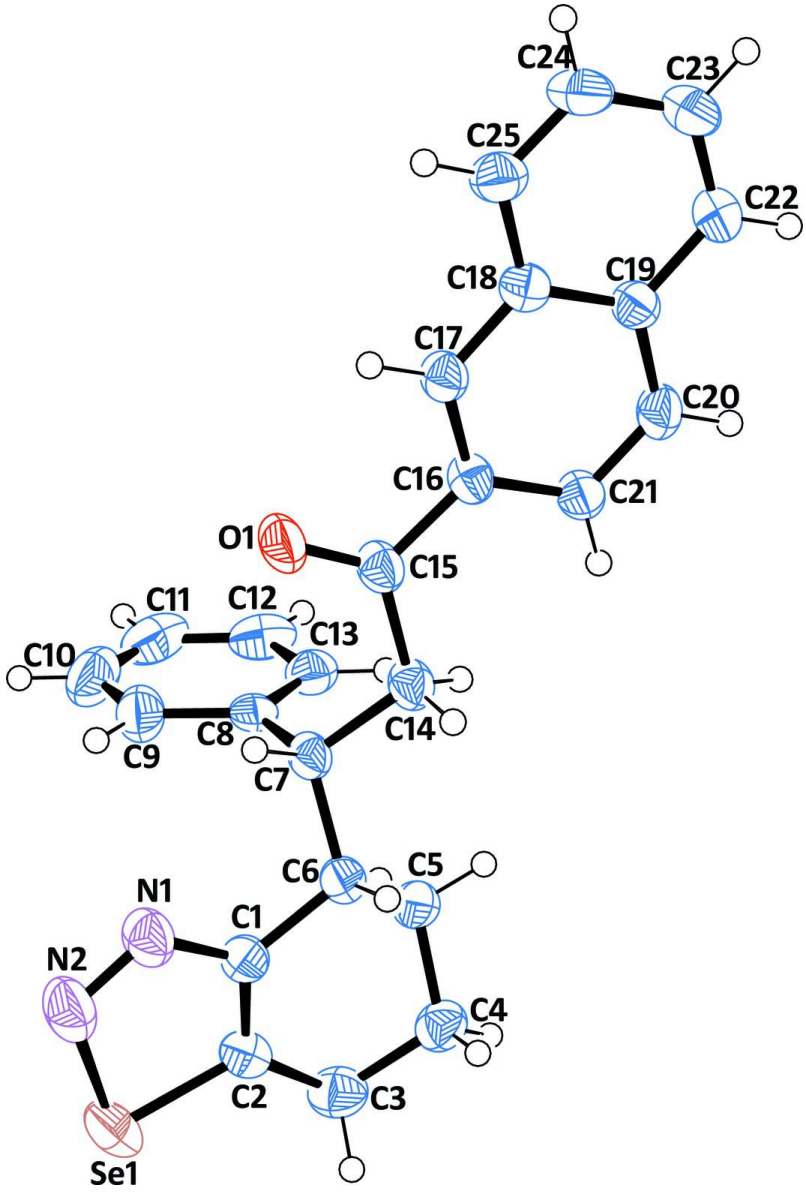


**Figure 1**

Molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level.

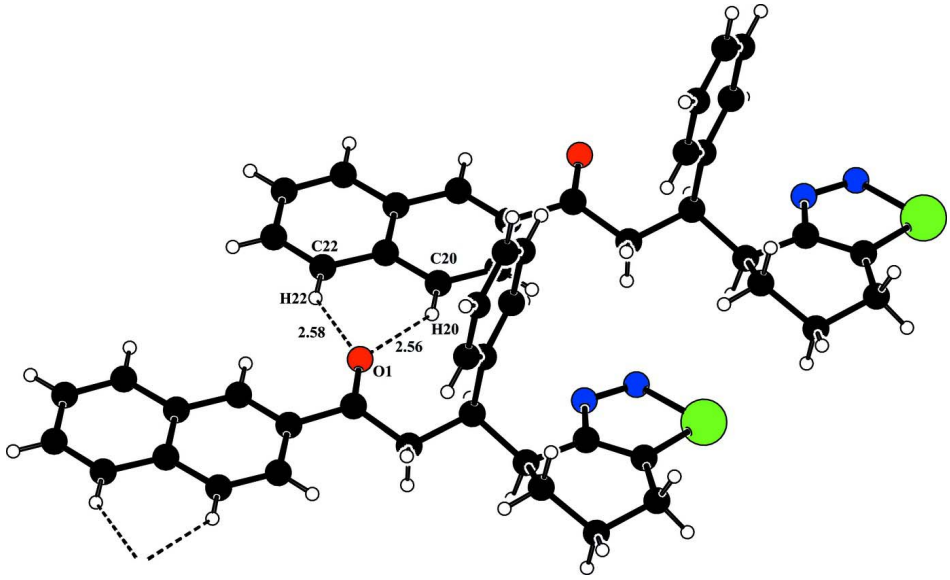


**Figure 2**

A weak intermolecular C—H···O interaction in title compound.

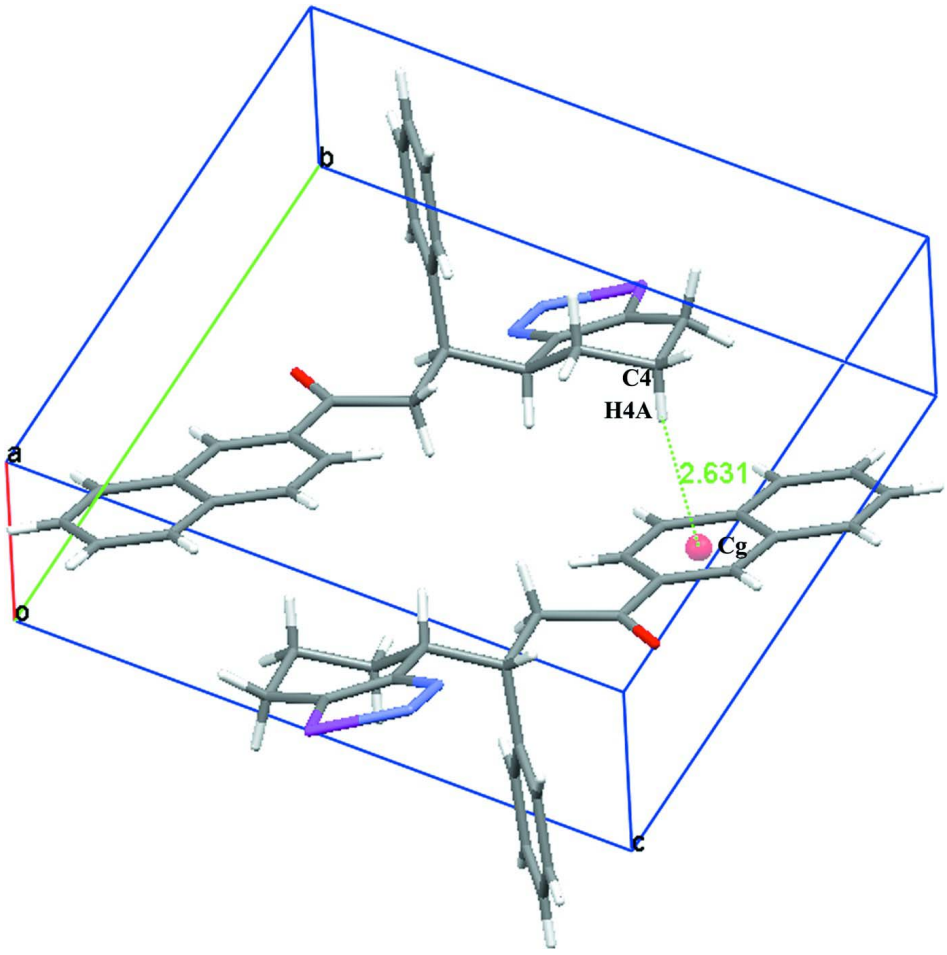


**Figure 3**

A weak intermolecular C—H···$\pi$ interaction in title compound. *Cg* is the centroid of C16—C21 ring.

**1-(2-Naphthyl)-3-phenyl-3-(4,5,6,7-tetrahydro-1,2,3-benzoselenadiazol- 4-yl)propan-1-one**

*Crystal data*

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Hall symbol: -P 1
$a = 8.0600$ (4) Å
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$\alpha = 81.479$ (4)°
$\beta = 76.478$ (4)°
$\gamma = 82.087$ (4)°
$V = 1020.33$ (9) Å$^3$
$Z = 2$
$F(000) = 456$
$D_x = 1.450$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3065 reflections
$\theta = 2.6$–29.3°
$\mu = 1.86$ mm$^{-1}$
$T = 293$ K
Block, blue
0.4 × 0.3 × 0.2 mm

*Data collection*

Oxford Diffraction Xcalibur E diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 15.9821 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)

$T_{min}$ = 0.658, $T_{max}$ = 1.000
6762 measured reflections
3594 independent reflections
2770 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025

$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.6°
$h$ = −9→9
$k$ = −12→12
$l$ = −12→15

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.096
$S$ = 1.01
3594 reflections
262 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.050P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.41 e Å$^{-3}$

*Special details*

**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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Se1 | 0.62678 (4) | 0.82915 (3) | 0.61536 (3) | 0.06072 (16) |
| O1 | 0.3614 (3) | 0.5213 (2) | 0.20388 (17) | 0.0633 (6) |
| N1 | 0.5844 (3) | 0.6746 (2) | 0.48187 (19) | 0.0476 (6) |
| N2 | 0.7071 (3) | 0.7047 (3) | 0.5160 (2) | 0.0587 (7) |
| C1 | 0.4227 (3) | 0.7366 (2) | 0.5202 (2) | 0.0344 (6) |
| C2 | 0.4117 (4) | 0.8232 (3) | 0.5918 (2) | 0.0395 (7) |
| C3 | 0.2505 (4) | 0.8991 (3) | 0.6443 (2) | 0.0485 (7) |
| H3A | 0.2499 | 0.9934 | 0.6163 | 0.058* |
| H3B | 0.2451 | 0.8916 | 0.7197 | 0.058* |
| C4 | 0.0939 (4) | 0.8443 (3) | 0.62557 (19) | 0.0422 (7) |
| H4A | 0.0714 | 0.7629 | 0.6736 | 0.051* |
| H4B | −0.0057 | 0.9098 | 0.6406 | 0.051* |
| C5 | 0.1215 (3) | 0.8137 (3) | 0.5122 (2) | 0.0398 (6) |
| H5A | 0.1464 | 0.8947 | 0.4642 | 0.048* |
| H5B | 0.0169 | 0.7858 | 0.5016 | 0.048* |
| C6 | 0.2686 (3) | 0.7034 (3) | 0.48589 (19) | 0.0339 (6) |
| H6 | 0.2328 | 0.6210 | 0.5303 | 0.041* |
| C7 | 0.3076 (3) | 0.6729 (2) | 0.36983 (19) | 0.0331 (6) |
| H7 | 0.4113 | 0.6089 | 0.3604 | 0.040* |
| C8 | 0.3471 (3) | 0.7946 (3) | 0.28883 (18) | 0.0334 (6) |

| | | | | |
|---|---|---|---|---|
| C9 | 0.5157 (4) | 0.8233 (3) | 0.2486 (2) | 0.0480 (7) |
| H9 | 0.6049 | 0.7671 | 0.2711 | 0.058* |
| C10 | 0.5519 (5) | 0.9349 (3) | 0.1752 (2) | 0.0606 (9) |
| H10 | 0.6651 | 0.9530 | 0.1493 | 0.073* |
| C11 | 0.4227 (5) | 1.0187 (3) | 0.1405 (2) | 0.0601 (9) |
| H11 | 0.4479 | 1.0933 | 0.0912 | 0.072* |
| C12 | 0.2555 (5) | 0.9919 (3) | 0.1790 (2) | 0.0533 (8) |
| H12 | 0.1669 | 1.0484 | 0.1560 | 0.064* |
| C13 | 0.2194 (4) | 0.8812 (3) | 0.2518 (2) | 0.0415 (7) |
| H13 | 0.1057 | 0.8639 | 0.2770 | 0.050* |
| C14 | 0.1634 (3) | 0.6015 (3) | 0.3511 (2) | 0.0376 (6) |
| H14A | 0.1320 | 0.5334 | 0.4105 | 0.045* |
| H14B | 0.0635 | 0.6662 | 0.3483 | 0.045* |
| C15 | 0.2124 (4) | 0.5363 (3) | 0.2507 (2) | 0.0375 (6) |
| C16 | 0.0773 (3) | 0.4844 (2) | 0.2104 (2) | 0.0334 (6) |
| C17 | 0.1294 (3) | 0.4041 (2) | 0.13129 (19) | 0.0358 (6) |
| H17 | 0.2463 | 0.3836 | 0.1048 | 0.043* |
| C18 | 0.0114 (3) | 0.3514 (2) | 0.08876 (19) | 0.0340 (6) |
| C19 | −0.1658 (3) | 0.3833 (3) | 0.12857 (19) | 0.0352 (6) |
| C20 | −0.2175 (3) | 0.4677 (3) | 0.2103 (2) | 0.0410 (7) |
| H20 | −0.3339 | 0.4906 | 0.2366 | 0.049* |
| C21 | −0.1000 (3) | 0.5157 (3) | 0.2508 (2) | 0.0367 (6) |
| H21 | −0.1367 | 0.5694 | 0.3055 | 0.044* |
| C22 | −0.2856 (4) | 0.3321 (3) | 0.0848 (2) | 0.0485 (8) |
| H22 | −0.4026 | 0.3538 | 0.1098 | 0.058* |
| C23 | −0.2302 (4) | 0.2516 (3) | 0.0068 (2) | 0.0550 (9) |
| H23 | −0.3095 | 0.2182 | −0.0214 | 0.066* |
| C24 | −0.0545 (4) | 0.2186 (3) | −0.0316 (2) | 0.0532 (8) |
| H24 | −0.0184 | 0.1623 | −0.0845 | 0.064* |
| C25 | 0.0639 (4) | 0.2670 (3) | 0.0068 (2) | 0.0441 (7) |
| H25 | 0.1802 | 0.2450 | −0.0205 | 0.053* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Se1 | 0.0506 (2) | 0.0778 (3) | 0.0659 (2) | −0.01457 (18) | −0.02624 (18) | −0.01871 (18) |
| O1 | 0.0281 (12) | 0.0930 (17) | 0.0786 (15) | −0.0050 (11) | −0.0061 (11) | −0.0520 (13) |
| N1 | 0.0352 (14) | 0.0520 (15) | 0.0575 (15) | 0.0042 (12) | −0.0141 (12) | −0.0141 (12) |
| N2 | 0.0365 (15) | 0.0715 (18) | 0.0714 (18) | 0.0003 (13) | −0.0198 (14) | −0.0115 (14) |
| C1 | 0.0340 (16) | 0.0341 (14) | 0.0349 (14) | −0.0014 (12) | −0.0092 (12) | −0.0025 (12) |
| C2 | 0.0424 (17) | 0.0410 (15) | 0.0380 (15) | −0.0054 (13) | −0.0138 (13) | −0.0049 (12) |
| C3 | 0.056 (2) | 0.0458 (17) | 0.0457 (17) | −0.0006 (15) | −0.0107 (15) | −0.0160 (14) |
| C4 | 0.0400 (17) | 0.0445 (16) | 0.0394 (16) | 0.0021 (14) | −0.0051 (14) | −0.0081 (13) |
| C5 | 0.0312 (15) | 0.0499 (16) | 0.0382 (15) | 0.0044 (13) | −0.0075 (13) | −0.0130 (13) |
| C6 | 0.0320 (15) | 0.0353 (14) | 0.0352 (14) | −0.0048 (12) | −0.0076 (12) | −0.0053 (11) |
| C7 | 0.0261 (14) | 0.0340 (14) | 0.0404 (15) | 0.0014 (11) | −0.0080 (12) | −0.0119 (12) |
| C8 | 0.0378 (16) | 0.0356 (14) | 0.0307 (13) | −0.0041 (12) | −0.0073 (12) | −0.0163 (11) |
| C9 | 0.0389 (17) | 0.0519 (18) | 0.0536 (18) | −0.0098 (14) | −0.0043 (15) | −0.0126 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10 | 0.061 (2) | 0.065 (2) | 0.0523 (19) | −0.028 (2) | 0.0107 (18) | −0.0137 (17) |
| C11 | 0.088 (3) | 0.051 (2) | 0.0368 (17) | −0.017 (2) | 0.0017 (19) | −0.0073 (15) |
| C12 | 0.078 (2) | 0.0471 (18) | 0.0356 (16) | −0.0009 (17) | −0.0170 (17) | −0.0052 (14) |
| C13 | 0.0439 (17) | 0.0452 (16) | 0.0364 (15) | −0.0020 (14) | −0.0086 (13) | −0.0110 (13) |
| C14 | 0.0313 (15) | 0.0372 (15) | 0.0463 (16) | −0.0039 (12) | −0.0066 (13) | −0.0138 (12) |
| C15 | 0.0301 (16) | 0.0372 (15) | 0.0474 (16) | −0.0004 (12) | −0.0108 (14) | −0.0114 (12) |
| C16 | 0.0299 (15) | 0.0296 (13) | 0.0413 (15) | −0.0013 (11) | −0.0090 (12) | −0.0064 (12) |
| C17 | 0.0289 (14) | 0.0379 (15) | 0.0413 (15) | 0.0016 (12) | −0.0093 (12) | −0.0089 (12) |
| C18 | 0.0374 (16) | 0.0317 (14) | 0.0331 (14) | −0.0025 (12) | −0.0103 (12) | −0.0010 (11) |
| C19 | 0.0359 (16) | 0.0373 (14) | 0.0337 (14) | −0.0076 (12) | −0.0097 (12) | −0.0018 (12) |
| C20 | 0.0276 (15) | 0.0471 (16) | 0.0471 (16) | −0.0019 (13) | −0.0038 (13) | −0.0106 (13) |
| C21 | 0.0330 (15) | 0.0361 (14) | 0.0428 (15) | −0.0019 (12) | −0.0068 (13) | −0.0141 (12) |
| C22 | 0.0384 (17) | 0.066 (2) | 0.0453 (17) | −0.0154 (15) | −0.0092 (14) | −0.0096 (15) |
| C23 | 0.057 (2) | 0.071 (2) | 0.0461 (17) | −0.0244 (18) | −0.0162 (16) | −0.0134 (16) |
| C24 | 0.065 (2) | 0.061 (2) | 0.0414 (16) | −0.0106 (17) | −0.0159 (16) | −0.0187 (15) |
| C25 | 0.0448 (18) | 0.0493 (17) | 0.0398 (16) | −0.0006 (14) | −0.0099 (14) | −0.0135 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Se1—C2 | 1.840 (3) | C20—C21 | 1.362 (3) |
| Se1—N2 | 1.888 (3) | C20—C19 | 1.417 (4) |
| O1—C15 | 1.214 (3) | C20—H20 | 0.9300 |
| C1—C2 | 1.355 (4) | C5—H5A | 0.9700 |
| C1—N1 | 1.381 (3) | C5—H5B | 0.9700 |
| C1—C6 | 1.509 (3) | C13—C12 | 1.375 (4) |
| N1—N2 | 1.264 (3) | C13—H13 | 0.9300 |
| C14—C15 | 1.503 (3) | C21—H21 | 0.9300 |
| C14—C7 | 1.533 (3) | C18—C25 | 1.421 (4) |
| C14—H14A | 0.9700 | C18—C19 | 1.411 (4) |
| C14—H14B | 0.9700 | C25—C24 | 1.353 (4) |
| C15—C16 | 1.499 (3) | C25—H25 | 0.9300 |
| C17—C16 | 1.365 (3) | C9—C10 | 1.385 (4) |
| C17—C18 | 1.404 (3) | C9—H9 | 0.9300 |
| C17—H17 | 0.9300 | C19—C22 | 1.419 (3) |
| C7—C8 | 1.518 (3) | C22—C23 | 1.356 (4) |
| C7—C6 | 1.546 (3) | C22—H22 | 0.9300 |
| C7—H7 | 0.9800 | C10—C11 | 1.369 (5) |
| C6—C5 | 1.526 (4) | C10—H10 | 0.9300 |
| C6—H6 | 0.9800 | C12—C11 | 1.373 (5) |
| C8—C13 | 1.386 (4) | C12—H12 | 0.9300 |
| C8—C9 | 1.392 (4) | C3—H3A | 0.9700 |
| C16—C21 | 1.412 (4) | C3—H3B | 0.9700 |
| C2—C3 | 1.488 (4) | C23—C24 | 1.398 (5) |
| C4—C5 | 1.520 (3) | C23—H23 | 0.9300 |
| C4—C3 | 1.529 (3) | C24—H24 | 0.9300 |
| C4—H4A | 0.9700 | C11—H11 | 0.9300 |
| C4—H4B | 0.9700 | | |

| | | | |
|---|---|---|---|
| C2—Se1—N2 | 86.70 (11) | C4—C5—C6 | 112.0 (2) |
| C2—C1—N1 | 116.2 (2) | C4—C5—H5A | 109.2 |
| C2—C1—C6 | 123.1 (2) | C6—C5—H5A | 109.2 |
| N1—C1—C6 | 120.6 (2) | C4—C5—H5B | 109.2 |
| N2—N1—C1 | 117.3 (2) | C6—C5—H5B | 109.2 |
| C15—C14—C7 | 113.2 (2) | H5A—C5—H5B | 107.9 |
| C15—C14—H14A | 108.9 | C12—C13—C8 | 122.1 (3) |
| C7—C14—H14A | 108.9 | C12—C13—H13 | 119.0 |
| C15—C14—H14B | 108.9 | C8—C13—H13 | 119.0 |
| C7—C14—H14B | 108.9 | C20—C21—C16 | 120.3 (2) |
| H14A—C14—H14B | 107.8 | C20—C21—H21 | 119.8 |
| O1—C15—C16 | 119.7 (2) | C16—C21—H21 | 119.8 |
| O1—C15—C14 | 120.5 (2) | C17—C18—C25 | 122.4 (2) |
| C16—C15—C14 | 119.8 (2) | C17—C18—C19 | 119.0 (2) |
| C16—C17—C18 | 121.8 (2) | C25—C18—C19 | 118.6 (2) |
| C16—C17—H17 | 119.1 | C24—C25—C18 | 120.3 (3) |
| C18—C17—H17 | 119.1 | C24—C25—H25 | 119.9 |
| C8—C7—C14 | 112.5 (2) | C18—C25—H25 | 119.9 |
| C8—C7—C6 | 113.86 (19) | C10—C9—C8 | 120.6 (3) |
| C14—C7—C6 | 110.17 (19) | C10—C9—H9 | 119.7 |
| C8—C7—H7 | 106.6 | C8—C9—H9 | 119.7 |
| C14—C7—H7 | 106.6 | C22—C19—C20 | 122.3 (3) |
| C6—C7—H7 | 106.6 | C22—C19—C18 | 119.3 (2) |
| N1—N2—Se1 | 110.7 (2) | C20—C19—C18 | 118.4 (2) |
| C1—C6—C5 | 108.8 (2) | C23—C22—C19 | 120.3 (3) |
| C1—C6—C7 | 113.7 (2) | C23—C22—H22 | 119.9 |
| C5—C6—C7 | 114.0 (2) | C19—C22—H22 | 119.9 |
| C1—C6—H6 | 106.6 | C11—C10—C9 | 120.7 (3) |
| C5—C6—H6 | 106.6 | C11—C10—H10 | 119.6 |
| C7—C6—H6 | 106.6 | C9—C10—H10 | 119.7 |
| C13—C8—C9 | 117.2 (3) | C11—C12—C13 | 119.8 (3) |
| C13—C8—C7 | 122.2 (2) | C11—C12—H12 | 120.1 |
| C9—C8—C7 | 120.6 (3) | C13—C12—H12 | 120.1 |
| C17—C16—C21 | 119.2 (2) | C2—C3—C4 | 110.6 (2) |
| C17—C16—C15 | 118.1 (2) | C2—C3—H3A | 109.5 |
| C21—C16—C15 | 122.7 (2) | C4—C3—H3A | 109.5 |
| C1—C2—C3 | 125.2 (2) | C2—C3—H3B | 109.5 |
| C1—C2—Se1 | 109.2 (2) | C4—C3—H3B | 109.5 |
| C3—C2—Se1 | 125.65 (19) | H3A—C3—H3B | 108.1 |
| C5—C4—C3 | 111.4 (2) | C22—C23—C24 | 120.4 (3) |
| C5—C4—H4A | 109.3 | C22—C23—H23 | 119.8 |
| C3—C4—H4A | 109.3 | C24—C23—H23 | 119.8 |
| C5—C4—H4B | 109.3 | C25—C24—C23 | 121.2 (3) |
| C3—C4—H4B | 109.3 | C25—C24—H24 | 119.4 |
| H4A—C4—H4B | 108.0 | C23—C24—H24 | 119.4 |
| C21—C20—C19 | 121.2 (3) | C10—C11—C12 | 119.6 (3) |
| C21—C20—H20 | 119.4 | C10—C11—H11 | 120.2 |
| C19—C20—H20 | 119.4 | C12—C11—H11 | 120.2 |

| | | | |
|---|---|---|---|
| C2—C1—N1—N2 | −0.6 (4) | C3—C4—C5—C6 | 63.3 (3) |
| C6—C1—N1—N2 | −178.3 (2) | C1—C6—C5—C4 | −49.3 (3) |
| C7—C14—C15—O1 | 13.6 (4) | C7—C6—C5—C4 | −177.3 (2) |
| C7—C14—C15—C16 | −168.8 (2) | C9—C8—C13—C12 | −0.5 (4) |
| C15—C14—C7—C8 | 67.1 (3) | C7—C8—C13—C12 | 179.5 (2) |
| C15—C14—C7—C6 | −164.7 (2) | C19—C20—C21—C16 | 1.3 (4) |
| C1—N1—N2—Se1 | 0.9 (3) | C17—C16—C21—C20 | −0.9 (4) |
| C2—Se1—N2—N1 | −0.8 (2) | C15—C16—C21—C20 | 179.0 (2) |
| C2—C1—C6—C5 | 19.6 (3) | C16—C17—C18—C25 | −179.6 (2) |
| N1—C1—C6—C5 | −162.9 (2) | C16—C17—C18—C19 | 0.4 (4) |
| C2—C1—C6—C7 | 147.8 (2) | C17—C18—C25—C24 | 179.9 (3) |
| N1—C1—C6—C7 | −34.7 (3) | C19—C18—C25—C24 | −0.1 (4) |
| C8—C7—C6—C1 | −69.0 (3) | C13—C8—C9—C10 | 0.5 (4) |
| C14—C7—C6—C1 | 163.5 (2) | C7—C8—C9—C10 | −179.5 (2) |
| C8—C7—C6—C5 | 56.5 (3) | C21—C20—C19—C22 | −179.9 (2) |
| C14—C7—C6—C5 | −71.0 (3) | C21—C20—C19—C18 | −0.9 (4) |
| C14—C7—C8—C13 | 39.2 (3) | C17—C18—C19—C22 | 179.1 (2) |
| C6—C7—C8—C13 | −87.1 (3) | C25—C18—C19—C22 | −0.9 (4) |
| C14—C7—C8—C9 | −140.8 (2) | C17—C18—C19—C20 | 0.0 (3) |
| C6—C7—C8—C9 | 92.9 (3) | C25—C18—C19—C20 | −179.9 (2) |
| C18—C17—C16—C21 | 0.0 (4) | C20—C19—C22—C23 | −179.9 (3) |
| C18—C17—C16—C15 | −179.9 (2) | C18—C19—C22—C23 | 1.0 (4) |
| O1—C15—C16—C17 | 9.8 (4) | C8—C9—C10—C11 | −0.3 (4) |
| C14—C15—C16—C17 | −167.9 (2) | C8—C13—C12—C11 | 0.3 (4) |
| O1—C15—C16—C21 | −170.1 (3) | C1—C2—C3—C4 | 12.4 (4) |
| C14—C15—C16—C21 | 12.3 (4) | Se1—C2—C3—C4 | −166.41 (18) |
| N1—C1—C2—C3 | −179.1 (2) | C5—C4—C3—C2 | −41.7 (3) |
| C6—C1—C2—C3 | −1.5 (4) | C19—C22—C23—C24 | −0.2 (4) |
| N1—C1—C2—Se1 | −0.1 (3) | C18—C25—C24—C23 | 1.0 (4) |
| C6—C1—C2—Se1 | 177.50 (18) | C22—C23—C24—C25 | −0.8 (5) |
| N2—Se1—C2—C1 | 0.47 (19) | C9—C10—C11—C12 | 0.1 (5) |
| N2—Se1—C2—C3 | 179.4 (2) | C13—C12—C11—C10 | −0.1 (4) |

*Hydrogen-bond geometry (Å, º)*

Cg is the centroid of the C16–C21 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C20—H20···O1$^{i}$ | 0.93 | 2.56 | 3.381 (3) | 147 |
| C22—H22···O1$^{i}$ | 0.93 | 2.58 | 3.392 (4) | 146 |
| C4—H4*A*···*Cg*$^{ii}$ | 0.97 | 2.63 | 3.584 (3) | 167 |

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