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Ethyl 2-phenyl-3-(4-phenyl-1,2,3-selenadiazol-5-yl)-3-*p*-tolylpropanoate

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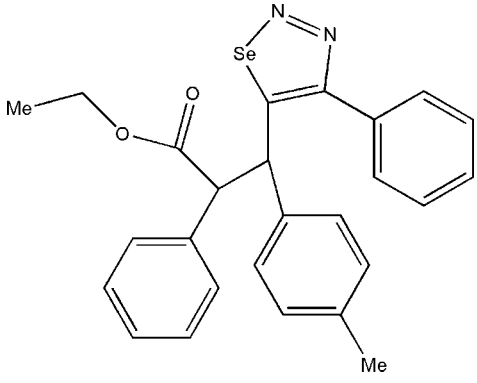
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.042; wR factor = 0.114; data-to-parameter ratio = 20.4.

In the title compound, $C_{26}H_{24}N_2O_2Se$, the selenadiazole ring is essentially planar [maximum deviation = 0.004 (3) Å]. The dihedral angle between the selenadiazole ring and the attached benzene ring is 50.17 (1)°. The crystal packing is stabilized by intermolecular C—H···N interactions.

Related literature

For general background to selenadiazol derivatives, see: El-Bahaie *et al.* (1990); El-Kashef *et al.* (1986); Khanna (2005); Kuroda *et al.* (2001); Padmavathi *et al.* (2002); Plano *et al.* (2010); Stadtman (1991).



Experimental

Crystal data

$C_{26}H_{24}N_2O_2Se$ M_r = 475.43
Monoclinic, $P2_1/c$
a = 12.148 (5) Å
b = 12.333 (5) Å
c = 16.522 (5) Å
β = 108.768 (5)°
V = 2343.7 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.63 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX CCD detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.715, T_{max} = 0.784
21985 measured reflections
5739 independent reflections
3536 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.114
S = 1.02
5739 reflections
282 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C20—H20···N1^{i}	0.93	2.61	3.522 (4)	165

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5750).

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supporting information

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Ethyl 2-phenyl-3-(4-phenyl-1,2,3-selenadiazol-5-yl)-3-*p*-tolylpropanoate

S. Sankari, P. Sugumar, T. Manisankar, S. Muthusubramanian and M. N. Ponnuswamy

S1. Comment

Selenadiazoles, having one selenium and two nitrogen atoms in a five membered ring, are the important class of organoselenium compounds utilized in the synthesis of semiconductor nanoparticles (Khanna, 2005). 1,2,3-Selenadiazoles are of interest owing to their chemical properties and biological applications such as anti-fungal (Kuroda *et al.*, 2001), anti-bacterial (El-Kashef *et al.*, 1986), anti-microbial (El-Bahaie *et al.*,1990), anti-cancer (Plano *et al.*, 2010) and insecticidal (Padmavathi *et al.*, 2002) properties.

Glutathione peroxidases(GPx) are the antioxidant selenoenzymes protecting various organisms from oxidative stress by catalyzing the reduction of hydroperoxides at the expense of glutathione(GSH) (Stadtman, 1991). In view of the above important properties of selenium containing compounds, an attempt is made to determine the crystal structure of the title compound.

The *ORTEP* plot of the molecule is shown in Fig.1. The selenadiazol ring is planar and oriented at an angle of 50.17 (1)° with the attached phenyl ring. The planar phenyl rings are twisted away across the propanyl bond at an angle of 73.7 (1)°. The propanoate group assumes partially an extended conformation which can seen from the torsion angle value of [C9—C16—C23—O2] 138.0 (2)°. The molecular packing is controlled by C—H···N intermolecular interactions in addition to van der Waals forces.

S2. Experimental

A mixture of ethyl-5-oxo-2,5-diphenyl-3-*p*-tolylpentanoate (1 mmol), semicarbazide hydrochloride(2 mmol) and anhydrous sodium acetate (3 mmol) in ethanol (10 ml) was refluxed for 4 hrs. After completion of the reaction as monitored by TLC, the mixture was poured into ice cold water and the resulting semicarbazone was filtered off. Then, a mixture of semicarbazone (1 mmol) and SeO_2 (2 mmol) in tetrahydrofuran (10 ml) were refluxed on a water bath for 1hr. The selenium deposited on cooling was removed by filtration, and the filtrate was poured into crushed ice, extracted with dichloromethane, and purified by column chromatography using silica gel (60–120 mesh) with 97:3 petroleum ether: ethyl acetate as eluent to give ethyl-2-phenyl-3-(4-phenyl-1,2, 3-selenadiazol-5-yl)-3-*p*-tolylpropanoate.

S3. Refinement

H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and allowed to ride on their parent atoms,with U_{iso}(H) = 1.5U_{eq}(C) for methyl H 1.2U_{eq}(C) for other H atoms.

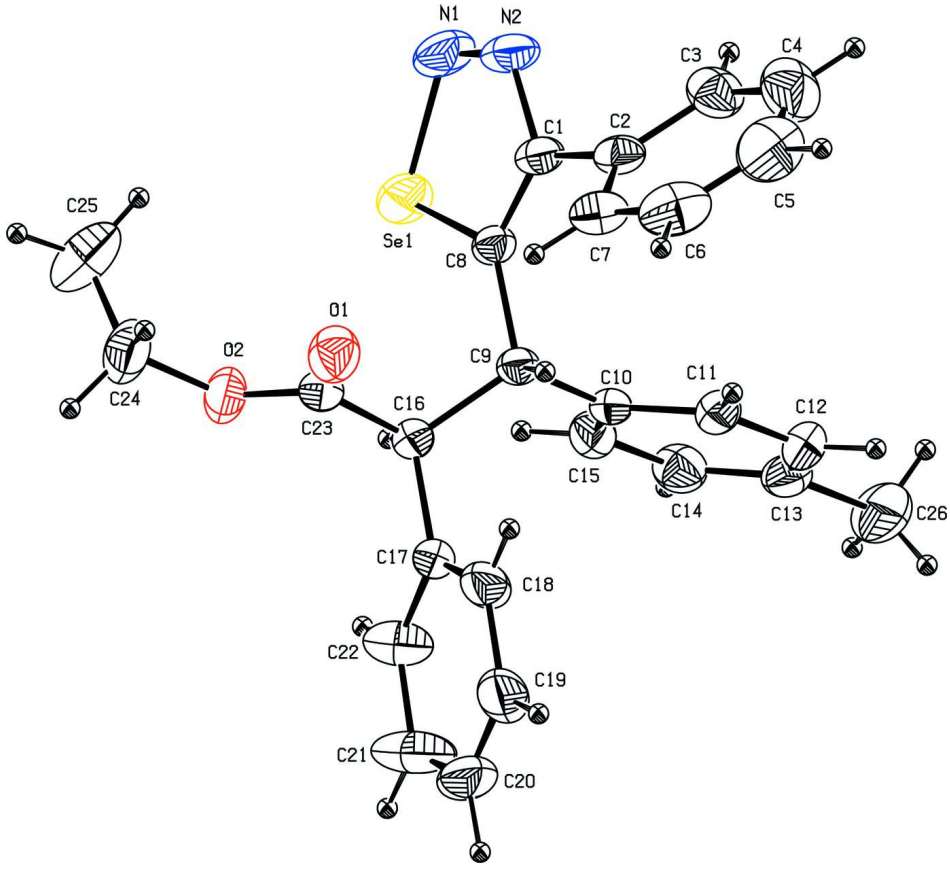

Figure 1

The molecular structure of the title compound, showing the atomic numbering and displacement ellipsoids drawn at the 30% probability level.

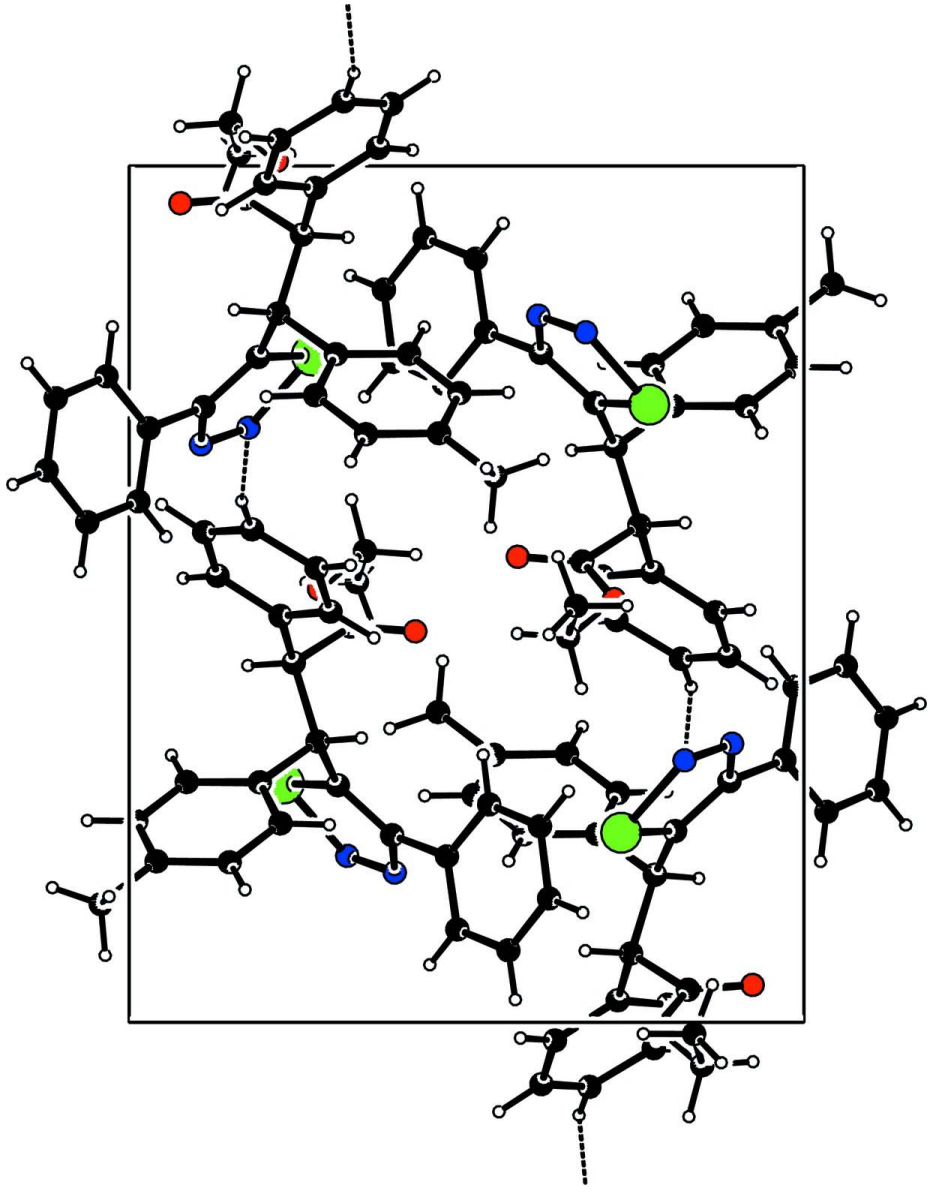

Figure 2

The packing of the molecules viewed down the b-axis.

Ethyl 2-phenyl-3-(4-phenyl-1,2,3-selenadiazol-5-yl)-3-*p*-tolylpropanoate

Crystal data

$C_{26}H_{24}N_2O_2Se$
$M_r = 475.43$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.148\ (5)$ Å
$b = 12.333\ (5)$ Å
$c = 16.522\ (5)$ Å
$\beta = 108.768\ (5)°$
$V = 2343.7\ (15)$ Å^3
$Z = 4$
$F(000) = 976$
$D_x = 1.347$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3536 reflections
$\theta = 1.8–28.3°$
$\mu = 1.63$ mm^{-1}
$T = 293$ K
Block, white crystalline
0.20 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX CCD detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.715, T_{max} = 0.784
21985 measured reflections
5739 independent reflections
3536 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 28.3°, θ_{min} = 1.8°
h = −16→16
k = −16→15
l = −22→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.114
S = 1.02
5739 reflections
282 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
$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 0.8234P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 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}
C1	0.6317 (3)	0.4864 (2)	0.10829 (19)	0.0747 (8)
H1	0.5772	0.4457	0.0671	0.090*
C2	0.6984 (4)	0.5621 (3)	0.0839 (3)	0.1018 (12)
H2	0.6887	0.5724	0.0263	0.122*
C3	0.7792 (4)	0.6224 (3)	0.1445 (3)	0.1074 (13)
H3	0.8253	0.6723	0.1280	0.129*
C4	0.7917 (3)	0.6089 (3)	0.2288 (3)	0.0909 (11)
H4	0.8454	0.6510	0.2696	0.109*
C5	0.7258 (2)	0.5336 (2)	0.25435 (19)	0.0663 (7)
H5	0.7351	0.5248	0.3121	0.080*
C6	0.6456 (2)	0.47105 (19)	0.19370 (16)	0.0548 (6)
C7	0.57234 (19)	0.3898 (2)	0.21839 (15)	0.0511 (6)
C8	0.60737 (18)	0.3091 (2)	0.27673 (14)	0.0466 (5)
C9	0.73116 (18)	0.27921 (18)	0.32782 (13)	0.0432 (5)
H9	0.7791	0.3442	0.3320	0.052*
C10	0.77602 (18)	0.19359 (19)	0.28023 (13)	0.0444 (5)

C11	0.8454 (2)	0.2243 (2)	0.23223 (16)	0.0542 (6)
H11	0.8655	0.2969	0.2306	0.065*
C12	0.8852 (2)	0.1489 (3)	0.18676 (17)	0.0687 (8)
H12	0.9314	0.1716	0.1547	0.082*
C13	0.8582 (2)	0.0407 (3)	0.18788 (17)	0.0673 (8)
C14	0.7875 (3)	0.0105 (2)	0.23479 (17)	0.0674 (7)
H14	0.7667	−0.0620	0.2356	0.081*
C15	0.7469 (2)	0.0853 (2)	0.28051 (16)	0.0582 (6)
H15	0.6996	0.0626	0.3118	0.070*
C16	0.74223 (19)	0.24382 (19)	0.41975 (14)	0.0470 (5)
H16	0.6991	0.1760	0.4166	0.056*
C17	0.8681 (2)	0.2242 (2)	0.47442 (14)	0.0546 (6)
C18	0.9536 (2)	0.2983 (3)	0.47948 (17)	0.0817 (10)
H18	0.9356	0.3627	0.4488	0.098*
C19	1.0676 (3)	0.2777 (4)	0.5303 (2)	0.1065 (14)
H19	1.1259	0.3280	0.5337	0.128*
C20	1.0928 (3)	0.1821 (4)	0.5755 (2)	0.1085 (14)
H20	1.1690	0.1669	0.6085	0.130*
C21	1.0084 (4)	0.1112 (4)	0.5723 (3)	0.1197 (15)
H21	1.0255	0.0481	0.6047	0.144*
C22	0.8967 (3)	0.1310 (3)	0.5213 (2)	0.0866 (10)
H22	0.8391	0.0801	0.5185	0.104*
C23	0.6893 (2)	0.3282 (3)	0.46202 (15)	0.0548 (6)
C24	0.5688 (3)	0.3495 (3)	0.5502 (2)	0.0914 (10)
H24A	0.5929	0.3296	0.6102	0.110*
H24B	0.5898	0.4247	0.5462	0.110*
C25	0.4454 (3)	0.3374 (3)	0.5139 (3)	0.1169 (14)
H25A	0.4205	0.3645	0.4564	0.175*
H25B	0.4078	0.3775	0.5473	0.175*
H25C	0.4253	0.2621	0.5136	0.175*
C26	0.9020 (3)	−0.0422 (3)	0.1379 (2)	0.1073 (13)
H26A	0.8593	−0.0354	0.0781	0.161*
H26B	0.8915	−0.1137	0.1571	0.161*
H26C	0.9831	−0.0299	0.1468	0.161*
N1	0.39102 (19)	0.3233 (3)	0.19430 (17)	0.0838 (8)
N2	0.45350 (19)	0.3936 (2)	0.17484 (14)	0.0701 (6)
O1	0.70126 (18)	0.42406 (18)	0.45645 (13)	0.0752 (5)
O2	0.62809 (16)	0.28144 (16)	0.50584 (12)	0.0692 (5)
Se1	0.48065 (2)	0.22922 (3)	0.27871 (2)	0.07445 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.090 (2)	0.0605 (18)	0.0701 (18)	0.0122 (16)	0.0208 (16)	0.0119 (14)
C2	0.136 (3)	0.083 (3)	0.098 (3)	0.019 (2)	0.053 (3)	0.029 (2)
C3	0.104 (3)	0.076 (3)	0.154 (4)	0.002 (2)	0.058 (3)	0.035 (3)
C4	0.071 (2)	0.059 (2)	0.131 (3)	−0.0017 (16)	0.017 (2)	0.007 (2)
C5	0.0551 (15)	0.0573 (17)	0.0774 (18)	0.0087 (13)	0.0085 (13)	0.0041 (14)

C6	0.0513 (13)	0.0466 (14)	0.0608 (15)	0.0148 (11)	0.0102 (11)	0.0049 (11)
C7	0.0396 (12)	0.0551 (15)	0.0512 (13)	0.0097 (10)	0.0045 (10)	−0.0050 (11)
C8	0.0366 (11)	0.0546 (14)	0.0452 (12)	0.0022 (10)	0.0083 (9)	−0.0033 (10)
C9	0.0352 (10)	0.0473 (13)	0.0442 (11)	0.0011 (9)	0.0085 (9)	0.0041 (10)
C10	0.0367 (11)	0.0522 (14)	0.0411 (11)	0.0048 (9)	0.0080 (9)	0.0061 (10)
C11	0.0448 (12)	0.0603 (15)	0.0583 (14)	0.0015 (11)	0.0176 (11)	0.0031 (12)
C12	0.0526 (15)	0.095 (2)	0.0645 (16)	0.0135 (15)	0.0268 (13)	0.0031 (15)
C13	0.0634 (16)	0.077 (2)	0.0576 (15)	0.0270 (15)	0.0138 (13)	0.0000 (14)
C14	0.0788 (18)	0.0554 (16)	0.0640 (16)	0.0120 (14)	0.0173 (15)	0.0007 (13)
C15	0.0626 (15)	0.0572 (16)	0.0564 (14)	0.0028 (12)	0.0215 (12)	0.0063 (12)
C16	0.0399 (11)	0.0549 (14)	0.0461 (12)	0.0030 (10)	0.0138 (9)	0.0046 (10)
C17	0.0457 (13)	0.0763 (17)	0.0405 (12)	0.0120 (12)	0.0120 (10)	0.0049 (12)
C18	0.0463 (15)	0.137 (3)	0.0567 (16)	−0.0064 (17)	0.0095 (12)	0.0272 (17)
C19	0.0470 (16)	0.210 (5)	0.0564 (18)	−0.013 (2)	0.0074 (14)	0.015 (2)
C20	0.060 (2)	0.183 (4)	0.066 (2)	0.043 (3)	−0.0019 (17)	−0.008 (3)
C21	0.101 (3)	0.109 (3)	0.108 (3)	0.041 (3)	−0.025 (2)	0.008 (2)
C22	0.078 (2)	0.075 (2)	0.083 (2)	0.0132 (17)	−0.0055 (16)	0.0092 (17)
C23	0.0440 (12)	0.0723 (19)	0.0446 (13)	0.0063 (12)	0.0093 (10)	0.0031 (12)
C24	0.076 (2)	0.126 (3)	0.085 (2)	0.001 (2)	0.0431 (17)	−0.025 (2)
C25	0.075 (2)	0.109 (3)	0.176 (4)	0.009 (2)	0.053 (3)	−0.033 (3)
C26	0.113 (3)	0.110 (3)	0.104 (3)	0.050 (2)	0.042 (2)	−0.015 (2)
N1	0.0359 (11)	0.112 (2)	0.0921 (18)	0.0028 (13)	0.0046 (12)	−0.0034 (16)
N2	0.0437 (12)	0.0825 (17)	0.0696 (14)	0.0147 (12)	−0.0020 (10)	0.0015 (12)
O1	0.0862 (14)	0.0675 (14)	0.0794 (13)	0.0092 (11)	0.0371 (11)	−0.0021 (10)
O2	0.0616 (11)	0.0898 (14)	0.0664 (11)	−0.0013 (10)	0.0349 (9)	−0.0087 (10)
Se1	0.04194 (15)	0.0938 (3)	0.0834 (2)	−0.01152 (14)	0.01441 (13)	0.00719 (16)

Geometric parameters (Å, º)

C1—C2	1.379 (5)	C15—H15	0.9300
C1—C6	1.379 (4)	C16—C23	1.508 (4)
C1—H1	0.9300	C16—C17	1.525 (3)
C2—C3	1.373 (6)	C16—H16	0.9800
C2—H2	0.9300	C17—C18	1.365 (4)
C3—C4	1.361 (5)	C17—C22	1.367 (4)
C3—H3	0.9300	C18—C19	1.392 (4)
C4—C5	1.379 (4)	C18—H18	0.9300
C4—H4	0.9300	C19—C20	1.376 (6)
C5—C6	1.385 (4)	C19—H19	0.9300
C5—H5	0.9300	C20—C21	1.336 (6)
C6—C7	1.482 (4)	C20—H20	0.9300
C7—C8	1.355 (3)	C21—C22	1.369 (5)
C7—N2	1.391 (3)	C21—H21	0.9300
C8—C9	1.514 (3)	C22—H22	0.9300
C8—Se1	1.837 (2)	C23—O1	1.198 (3)
C9—C10	1.518 (3)	C23—O2	1.325 (3)
C9—C16	1.544 (3)	C24—C25	1.432 (5)
C9—H9	0.9800	C24—O2	1.449 (3)

C10—C15	1.383 (3)	C24—H24A	0.9700
C10—C11	1.383 (3)	C24—H24B	0.9700
C11—C12	1.377 (4)	C25—H25A	0.9600
C11—H11	0.9300	C25—H25B	0.9600
C12—C13	1.376 (4)	C25—H25C	0.9600
C12—H12	0.9300	C26—H26A	0.9600
C13—C14	1.381 (4)	C26—H26B	0.9600
C13—C26	1.514 (4)	C26—H26C	0.9600
C14—C15	1.380 (4)	N1—N2	1.261 (3)
C14—H14	0.9300	N1—Se1	1.870 (3)

C2—C1—C6	120.1 (3)	C23—C16—C9	110.20 (19)
C2—C1—H1	119.9	C17—C16—C9	112.39 (18)
C6—C1—H1	119.9	C23—C16—H16	108.3
C3—C2—C1	120.2 (4)	C17—C16—H16	108.3
C3—C2—H2	119.9	C9—C16—H16	108.3
C1—C2—H2	119.9	C18—C17—C22	118.6 (3)
C4—C3—C2	119.9 (4)	C18—C17—C16	121.9 (2)
C4—C3—H3	120.0	C22—C17—C16	119.5 (2)
C2—C3—H3	120.0	C17—C18—C19	120.3 (3)
C3—C4—C5	120.7 (3)	C17—C18—H18	119.9
C3—C4—H4	119.7	C19—C18—H18	119.9
C5—C4—H4	119.7	C20—C19—C18	119.2 (4)
C4—C5—C6	119.7 (3)	C20—C19—H19	120.4
C4—C5—H5	120.1	C18—C19—H19	120.4
C6—C5—H5	120.1	C21—C20—C19	120.3 (3)
C1—C6—C5	119.3 (3)	C21—C20—H20	119.8
C1—C6—C7	119.2 (2)	C19—C20—H20	119.8
C5—C6—C7	121.5 (2)	C20—C21—C22	120.3 (4)
C8—C7—N2	115.4 (2)	C20—C21—H21	119.9
C8—C7—C6	127.8 (2)	C22—C21—H21	119.9
N2—C7—C6	116.7 (2)	C17—C22—C21	121.3 (4)
C7—C8—C9	127.1 (2)	C17—C22—H22	119.4
C7—C8—Se1	109.47 (16)	C21—C22—H22	119.4
C9—C8—Se1	123.15 (17)	O1—C23—O2	125.1 (2)
C8—C9—C10	109.78 (17)	O1—C23—C16	124.4 (2)
C8—C9—C16	111.95 (18)	O2—C23—C16	110.5 (2)
C10—C9—C16	112.37 (18)	C25—C24—O2	110.6 (3)
C8—C9—H9	107.5	C25—C24—H24A	109.5
C10—C9—H9	107.5	O2—C24—H24A	109.5
C16—C9—H9	107.5	C25—C24—H24B	109.5
C15—C10—C11	118.0 (2)	O2—C24—H24B	109.5
C15—C10—C9	122.4 (2)	H24A—C24—H24B	108.1
C11—C10—C9	119.5 (2)	C24—C25—H25A	109.5
C12—C11—C10	120.9 (3)	C24—C25—H25B	109.5
C12—C11—H11	119.5	H25A—C25—H25B	109.5
C10—C11—H11	119.5	C24—C25—H25C	109.5
C13—C12—C11	121.3 (3)	H25A—C25—H25C	109.5

C13—C12—H12	119.3	H25B—C25—H25C	109.5
C11—C12—H12	119.3	C13—C26—H26A	109.5
C12—C13—C14	117.7 (3)	C13—C26—H26B	109.5
C12—C13—C26	121.3 (3)	H26A—C26—H26B	109.5
C14—C13—C26	121.0 (3)	C13—C26—H26C	109.5
C15—C14—C13	121.5 (3)	H26A—C26—H26C	109.5
C15—C14—H14	119.2	H26B—C26—H26C	109.5
C13—C14—H14	119.2	N2—N1—Se1	111.30 (17)
C14—C15—C10	120.5 (2)	N1—N2—C7	117.0 (2)
C14—C15—H15	119.7	C23—O2—C24	118.8 (2)
C10—C15—H15	119.7	C8—Se1—N1	86.80 (11)
C23—C16—C17	109.34 (19)		

C6—C1—C2—C3	0.1 (5)	C11—C10—C15—C14	0.7 (3)
C1—C2—C3—C4	−1.4 (6)	C9—C10—C15—C14	178.5 (2)
C2—C3—C4—C5	1.4 (6)	C8—C9—C16—C23	−52.2 (3)
C3—C4—C5—C6	−0.2 (5)	C10—C9—C16—C23	−176.23 (19)
C2—C1—C6—C5	1.1 (4)	C8—C9—C16—C17	−174.4 (2)
C2—C1—C6—C7	179.6 (3)	C10—C9—C16—C17	61.6 (3)
C4—C5—C6—C1	−1.0 (4)	C23—C16—C17—C18	−72.9 (3)
C4—C5—C6—C7	−179.5 (2)	C9—C16—C17—C18	49.8 (3)
C1—C6—C7—C8	129.3 (3)	C23—C16—C17—C22	105.8 (3)
C5—C6—C7—C8	−52.2 (4)	C9—C16—C17—C22	−131.5 (3)
C1—C6—C7—N2	−48.3 (3)	C22—C17—C18—C19	1.1 (4)
C5—C6—C7—N2	130.1 (2)	C16—C17—C18—C19	179.8 (3)
N2—C7—C8—C9	174.4 (2)	C17—C18—C19—C20	−0.2 (5)
C6—C7—C8—C9	−3.3 (4)	C18—C19—C20—C21	−1.6 (6)
N2—C7—C8—Se1	−0.1 (3)	C19—C20—C21—C22	2.5 (7)
C6—C7—C8—Se1	−177.8 (2)	C18—C17—C22—C21	−0.2 (5)
C7—C8—C9—C10	−91.6 (3)	C16—C17—C22—C21	−178.9 (3)
Se1—C8—C9—C10	82.2 (2)	C20—C21—C22—C17	−1.6 (6)
C7—C8—C9—C16	142.9 (2)	C17—C16—C23—O1	82.0 (3)
Se1—C8—C9—C16	−43.3 (3)	C9—C16—C23—O1	−42.0 (3)
C8—C9—C10—C15	−78.9 (3)	C17—C16—C23—O2	−98.0 (2)
C16—C9—C10—C15	46.4 (3)	C9—C16—C23—O2	138.0 (2)
C8—C9—C10—C11	98.8 (2)	Se1—N1—N2—C7	−0.7 (3)
C16—C9—C10—C11	−135.9 (2)	C8—C7—N2—N1	0.6 (3)
C15—C10—C11—C12	−0.6 (3)	C6—C7—N2—N1	178.5 (2)
C9—C10—C11—C12	−178.5 (2)	O1—C23—O2—C24	0.9 (4)
C10—C11—C12—C13	−0.4 (4)	C16—C23—O2—C24	−179.1 (2)
C11—C12—C13—C14	1.4 (4)	C25—C24—O2—C23	114.7 (3)
C11—C12—C13—C26	−180.0 (3)	C7—C8—Se1—N1	−0.20 (19)
C12—C13—C14—C15	−1.3 (4)	C9—C8—Se1—N1	−175.0 (2)
C26—C13—C14—C15	−180.0 (3)	N2—N1—Se1—C8	0.5 (2)
C13—C14—C15—C10	0.3 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20···N1^{i}	0.93	2.61	3.522 (4)	165

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