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5-(2-Methyl-2-nitro-1-phenylpropyl)-4-phenyl-1,2,3-selenadiazole

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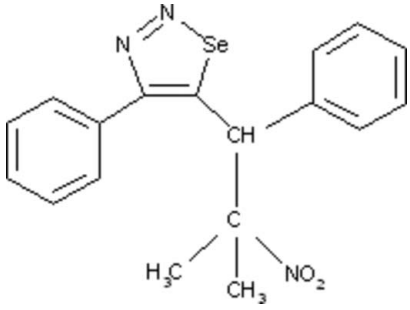
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.075; data-to-parameter ratio = 13.7.

In the title compound, $C_{18}H_{17}N_3O_2Se$, the selenadiazole ring makes dihedral angles of 37.71 (8) and 66.79 (6)° with the adjacent phenyl ring and the aromatic ring of the phenylpropyl group, respectively. The molecular structure is stabilized by weak intramolecular C—H···Se interactions and the crystal packing is stabilized by a weak C—H···π interaction.

Related literature

For related literature, see: Mellini & Merlino (1976*a*,*b*); Bertini *et al.* (1984); El-Kashef *et al.* (1986); El-Bahaie *et al.* (1990); Kuroda *et al.* (2001); Padmavathi *et al.* (2002); Saravanan *et al.* (2006); A similar compound with a chlorophenyl ring has been reported by Gunasekaran *et al.* (2007).



Experimental

Crystal data

$C_{18}H_{17}N_3O_2Se$
M_r = 386.31
Monoclinic, $P2_1/c$
a = 10.0178 (8) Å
b = 10.2084 (8) Å
c = 17.4139 (14) Å
β = 104.820 (1)°
V = 1721.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.20 mm^{-1}
T = 295 (2) K
0.20 × 0.18 × 0.14 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.656, T_{max} = 0.735
12015 measured reflections
3011 independent reflections
2648 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.075
S = 1.06
3011 reflections
219 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

*Cg*1 is the centroid of the selenadiazole ring.

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···Se1	0.93	2.84	3.534 (2)	133
C17—H17*B*···Se1	0.96	2.63	3.361 (3)	133
C5—H5···*Cg*1^{i}	0.93	2.76	3.6297 (3)	156

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2234).

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supplementary materials

Acta Cryst. (2007). E**63**, o4676 [**doi:10.1107/S1600536807057327**]

5-(2-Methyl-2-nitro-1-phenylpropyl)-4-phenyl-1,2,3-selenadiazole

A. Marx, V. Manivannan, S. Saravanan, S. Muthusubramanian and B. Sridhar

Comment

Selenium containing compounds like 1,2,3-selenadiazole possess various beneficial activities like antifungal (Kuroda *et al.*, 2001), antibacterial (El-Kashef *et al.*, 1986), antimicrobial (El-Bahaie *et al.*, 1990) and insecticidal (Padmavathi *et al.*, 2002) activities. As naturally occurring nitro compounds exhibit broad antibiotic activity and certain alkyl nitro compounds exhibit antitumor activity, it was decided to synthesize and structurally characterize a set of 1,2,3- selenadiazoles with nitro group in the side chain (Saravanan *et al.*, 2006).

The geometric parameters in the title compound, (I), agree with the reported values of similar structure (Mellini & Merlino, 1976*a*,b; Bertini *et al.*, 1984; Gunasekaran *et al.*, 2007). The C1—C6 phenyl ring makes a dihedral angle of 37.71 (8)° with the heterocyclic ring and the C13—C16 phenyl ring makes a dihedral angle of 66.79 (6)° with the heterocyclic ring (Fig. 1).

The details of the hydrogen bonding are given in Table 1. The molecular structure is stabilized by a weak intramolecular C—H···Se interaction and the crystal packing is stabilized by a weak C—H···π interaction involving the C7/C8/Se1/N2/N1 ring.

Experimental

A solution of 2-[4-methyl-4-nitro-1,3-diphenylpentylidene]-1-hydrazinecarboxamide (0.005 mol) and powdered selenium dioxide (0.05 mol) in dry tetrahydrofuran was gently heated on a water bath for 2 h. The selenium deposited on cooling was removed by filtration, and the filtrate was poured into crushed ice, extracted with chloroform, and purified by column chromatography using silica gel (60–120 mesh) with petroleum ether:ethyl acetate (97:3) as eluent to give the title compound, which was recrystallized from ethanol.

Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic C—H, C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for CH_3, and C—H = 0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) for tertiary CH.

Figures

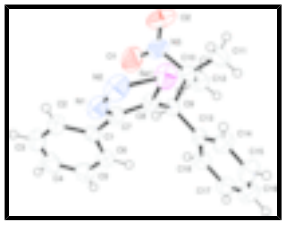


Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

5-(2-Methyl-2-nitro-1-phenylpropyl)-4-phenyl-1,2,3-selenadiazole

Crystal data

$C_{18}H_{17}N_3O_2Se$	$Z = 4$
$M_r = 386.31$	$F_{000} = 784$
Monoclinic, $P2_1/c$	$D_x = 1.490$ Mg m^{-3}
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.0178$ (8) Å	$\theta = 2.5$–26.5º
$b = 10.2084$ (8) Å	$\mu = 2.20$ mm^{-1}
$c = 17.4139$ (14) Å	$T = 295$ (2) K
$\beta = 104.820$ (1)º	Needles, colourless
$V = 1721.6$ (2) Å^3	0.20 × 0.18 × 0.14 mm

Data collection

Bruker APEXII CCD area-detector diffractometer	3011 independent reflections
Radiation source: fine-focus sealed tube	2648 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.025$
$T = 295$(2) K	$\theta_{max} = 25.0$º
ω and φ scan	$\theta_{min} = 2.1$º
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -11 \rightarrow 11$
$T_{min} = 0.656$, $T_{max} = 0.735$	$k = -12 \rightarrow 12$
12015 measured reflections	$l = -20 \rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.028$	H-atom parameters constrained
$wR(F^2) = 0.075$	$w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 0.596P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$

3011 reflections	$\Delta\rho_{max} = 0.45$ e Å^{-3}
219 parameters	$\Delta\rho_{min} = -0.28$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.66748 (18)	0.31725 (19)	0.28521 (11)	0.0402 (4)
C2	0.73047 (19)	0.2198 (2)	0.25334 (11)	0.0431 (4)
C3	0.8128 (2)	0.1080 (2)	0.29364 (13)	0.0460 (5)
C4	0.9297 (2)	0.0713 (2)	0.26935 (17)	0.0614 (6)
H4	0.9535	0.1174	0.2287	0.074*
C5	1.0099 (3)	−0.0320 (3)	0.3047 (2)	0.0748 (8)
H5	1.0877	−0.0551	0.2878	0.090*
C6	0.9766 (3)	−0.1009 (3)	0.3642 (2)	0.0776 (8)
H6	1.0323	−0.1698	0.3884	0.093*
C7	0.8601 (3)	−0.0683 (2)	0.38843 (19)	0.0726 (7)
H7	0.8364	−0.1161	0.4285	0.087*
C8	0.7786 (2)	0.0356 (2)	0.35307 (15)	0.0551 (5)
H8	0.6999	0.0570	0.3694	0.066*
C9	0.66122 (18)	0.32706 (18)	0.37080 (10)	0.0378 (4)
H9	0.7280	0.2624	0.3994	0.045*
C10	0.52177 (19)	0.28285 (18)	0.38264 (11)	0.0395 (4)
C11	0.3962 (2)	0.3206 (2)	0.33330 (13)	0.0556 (5)
H11	0.3946	0.3758	0.2906	0.067*
C12	0.2732 (2)	0.2775 (3)	0.34655 (15)	0.0657 (6)
H12	0.1899	0.3040	0.3127	0.079*
C13	0.2729 (2)	0.1960 (2)	0.40919 (14)	0.0606 (6)
H13	0.1900	0.1673	0.4180	0.073*
C14	0.3959 (2)	0.1575 (2)	0.45835 (13)	0.0548 (5)
H14	0.3965	0.1024	0.5010	0.066*
C15	0.5196 (2)	0.1996 (2)	0.44542 (11)	0.0455 (4)
H15	0.6024	0.1718	0.4792	0.055*
C16	0.7372 (3)	0.4458 (2)	0.50239 (14)	0.0654 (7)
H16A	0.7824	0.5232	0.5277	0.098*
H16B	0.7954	0.3711	0.5195	0.098*
H16C	0.6514	0.4341	0.5164	0.098*
C17	0.6152 (3)	0.5761 (2)	0.38362 (18)	0.0718 (7)
H17A	0.5244	0.5569	0.3893	0.108*
H17B	0.6106	0.5926	0.3287	0.108*
H17C	0.6509	0.6521	0.4146	0.108*
C18	0.7094 (2)	0.4603 (2)	0.41242 (12)	0.0471 (5)
N1	0.72242 (19)	0.2320 (2)	0.17298 (11)	0.0580 (5)
N2	0.6597 (2)	0.3306 (2)	0.13660 (11)	0.0672 (6)
N3	0.8516 (2)	0.4868 (2)	0.39698 (13)	0.0674 (6)
O1	0.8740 (3)	0.5919 (3)	0.37260 (19)	0.1272 (10)
O2	0.9345 (2)	0.4001 (2)	0.40993 (16)	0.0999 (7)

Se1	0.59391 (2)	0.43684 (3)	0.205995 (13)	0.06304 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0368 (9)	0.0485 (11)	0.0338 (9)	−0.0014 (8)	0.0062 (7)	0.0006 (8)
C2	0.0398 (10)	0.0528 (11)	0.0371 (10)	−0.0092 (8)	0.0106 (8)	−0.0110 (8)
C3	0.0443 (10)	0.0434 (11)	0.0523 (12)	−0.0078 (9)	0.0157 (9)	−0.0149 (9)
C4	0.0554 (13)	0.0611 (15)	0.0744 (16)	−0.0011 (11)	0.0288 (12)	−0.0077 (12)
C5	0.0578 (14)	0.0686 (16)	0.106 (2)	0.0093 (12)	0.0350 (15)	−0.0059 (16)
C6	0.0712 (17)	0.0532 (15)	0.108 (2)	0.0143 (12)	0.0221 (16)	−0.0011 (15)
C7	0.0861 (18)	0.0498 (14)	0.089 (2)	0.0021 (12)	0.0353 (16)	0.0072 (13)
C8	0.0534 (12)	0.0458 (12)	0.0711 (15)	−0.0022 (10)	0.0247 (11)	−0.0061 (11)
C9	0.0409 (9)	0.0401 (10)	0.0317 (9)	0.0051 (8)	0.0080 (7)	0.0007 (7)
C10	0.0448 (10)	0.0399 (10)	0.0342 (9)	0.0018 (8)	0.0109 (8)	−0.0031 (8)
C11	0.0487 (12)	0.0673 (14)	0.0493 (12)	0.0024 (10)	0.0098 (9)	0.0116 (11)
C12	0.0440 (12)	0.0875 (18)	0.0627 (15)	0.0022 (11)	0.0083 (10)	0.0027 (13)
C13	0.0543 (13)	0.0717 (15)	0.0606 (14)	−0.0155 (11)	0.0237 (11)	−0.0112 (12)
C14	0.0710 (14)	0.0537 (13)	0.0453 (12)	−0.0090 (11)	0.0250 (11)	−0.0019 (10)
C15	0.0541 (11)	0.0476 (11)	0.0353 (10)	0.0015 (9)	0.0124 (8)	0.0008 (8)
C16	0.0818 (17)	0.0696 (16)	0.0457 (13)	−0.0152 (12)	0.0176 (12)	−0.0183 (11)
C17	0.096 (2)	0.0455 (13)	0.0772 (18)	0.0073 (12)	0.0286 (15)	−0.0066 (12)
C18	0.0520 (11)	0.0475 (12)	0.0445 (11)	−0.0048 (9)	0.0176 (9)	−0.0068 (9)
N1	0.0585 (11)	0.0780 (13)	0.0391 (10)	−0.0126 (10)	0.0154 (8)	−0.0145 (9)
N2	0.0672 (12)	0.1000 (16)	0.0340 (9)	−0.0072 (12)	0.0121 (9)	−0.0023 (10)
N3	0.0674 (13)	0.0718 (14)	0.0678 (13)	−0.0237 (12)	0.0261 (11)	−0.0214 (11)
O1	0.130 (2)	0.0974 (17)	0.179 (3)	−0.0430 (15)	0.085 (2)	0.0092 (17)
O2	0.0529 (11)	0.1075 (16)	0.141 (2)	−0.0099 (11)	0.0285 (12)	−0.0342 (15)
Se1	0.06546 (17)	0.0811 (2)	0.04209 (15)	0.01614 (12)	0.01289 (11)	0.01866 (11)

Geometric parameters (Å, °)

C1—C2	1.369 (3)	C11—H11	0.9300
C1—C9	1.511 (2)	C12—C13	1.373 (3)
C1—Se1	1.8483 (18)	C12—H12	0.9300
C2—N1	1.387 (3)	C13—C14	1.366 (3)
C2—C3	1.477 (3)	C13—H13	0.9300
C3—C8	1.384 (3)	C14—C15	1.383 (3)
C3—C4	1.393 (3)	C14—H14	0.9300
C4—C5	1.372 (4)	C15—H15	0.9300
C4—H4	0.9300	C16—C18	1.527 (3)
C5—C6	1.363 (4)	C16—H16A	0.9600
C5—H5	0.9300	C16—H16B	0.9600
C6—C7	1.380 (4)	C16—H16C	0.9600
C6—H6	0.9300	C17—C18	1.516 (3)
C7—C8	1.383 (3)	C17—H17A	0.9600
C7—H7	0.9300	C17—H17B	0.9600
C8—H8	0.9300	C17—H17C	0.9600
C9—C10	1.531 (3)	C18—N3	1.540 (3)

C9—C18	1.559 (3)	N1—N2	1.267 (3)
C9—H9	0.9800	N2—Se1	1.865 (2)
C10—C11	1.384 (3)	N3—O2	1.195 (3)
C10—C15	1.389 (3)	N3—O1	1.197 (3)
C11—C12	1.382 (3)		
C2—C1—C9	125.99 (17)	C13—C12—C11	120.6 (2)
C2—C1—Se1	108.33 (14)	C13—C12—H12	119.7
C9—C1—Se1	125.67 (14)	C11—C12—H12	119.7
C1—C2—N1	115.48 (19)	C14—C13—C12	119.2 (2)
C1—C2—C3	128.94 (17)	C14—C13—H13	120.4
N1—C2—C3	115.47 (18)	C12—C13—H13	120.4
C8—C3—C4	118.1 (2)	C13—C14—C15	120.7 (2)
C8—C3—C2	123.56 (18)	C13—C14—H14	119.6
C4—C3—C2	118.3 (2)	C15—C14—H14	119.6
C5—C4—C3	120.8 (3)	C14—C15—C10	120.88 (19)
C5—C4—H4	119.6	C14—C15—H15	119.6
C3—C4—H4	119.6	C10—C15—H15	119.6
C6—C5—C4	120.5 (2)	C18—C16—H16A	109.5
C6—C5—H5	119.8	C18—C16—H16B	109.5
C4—C5—H5	119.8	H16A—C16—H16B	109.5
C5—C6—C7	120.0 (3)	C18—C16—H16C	109.5
C5—C6—H6	120.0	H16A—C16—H16C	109.5
C7—C6—H6	120.0	H16B—C16—H16C	109.5
C6—C7—C8	119.8 (3)	C18—C17—H17A	109.5
C6—C7—H7	120.1	C18—C17—H17B	109.5
C8—C7—H7	120.1	H17A—C17—H17B	109.5
C7—C8—C3	120.8 (2)	C18—C17—H17C	109.5
C7—C8—H8	119.6	H17A—C17—H17C	109.5
C3—C8—H8	119.6	H17B—C17—H17C	109.5
C1—C9—C10	112.50 (14)	C17—C18—C16	110.5 (2)
C1—C9—C18	115.50 (16)	C17—C18—N3	109.3 (2)
C10—C9—C18	112.28 (15)	C16—C18—N3	105.18 (18)
C1—C9—H9	105.1	C17—C18—C9	115.74 (18)
C10—C9—H9	105.1	C16—C18—C9	110.28 (17)
C18—C9—H9	105.1	N3—C18—C9	105.20 (16)
C11—C10—C15	117.65 (18)	N2—N1—C2	117.96 (19)
C11—C10—C9	123.35 (17)	N1—N2—Se1	110.50 (14)
C15—C10—C9	119.00 (16)	O2—N3—O1	123.2 (3)
C12—C11—C10	121.0 (2)	O2—N3—C18	117.8 (2)
C12—C11—H11	119.5	O1—N3—C18	119.0 (3)
C10—C11—H11	119.5	C1—Se1—N2	87.71 (9)
C9—C1—C2—N1	179.96 (17)	C9—C10—C11—C12	179.8 (2)
Se1—C1—C2—N1	−1.1 (2)	C10—C11—C12—C13	0.0 (4)
C9—C1—C2—C3	−4.1 (3)	C11—C12—C13—C14	−0.1 (4)
Se1—C1—C2—C3	174.85 (16)	C12—C13—C14—C15	−0.1 (4)
C1—C2—C3—C8	40.8 (3)	C13—C14—C15—C10	0.6 (3)
N1—C2—C3—C8	−143.3 (2)	C11—C10—C15—C14	−0.7 (3)
C1—C2—C3—C4	−140.7 (2)	C9—C10—C15—C14	179.88 (18)

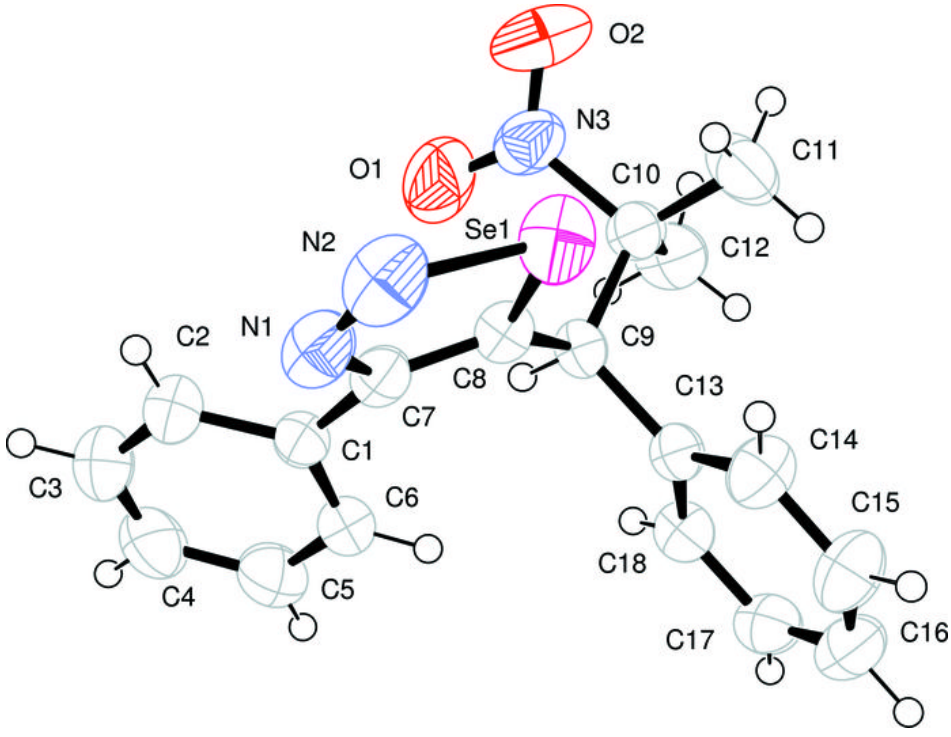
N1—C2—C3—C4	35.2 (3)	C1—C9—C18—C17	69.7 (2)
C8—C3—C4—C5	−1.4 (3)	C10—C9—C18—C17	−61.1 (2)
C2—C3—C4—C5	−179.9 (2)	C1—C9—C18—C16	−164.00 (18)
C3—C4—C5—C6	0.1 (4)	C10—C9—C18—C16	65.2 (2)
C4—C5—C6—C7	1.1 (5)	C1—C9—C18—N3	−51.1 (2)
C5—C6—C7—C8	−1.0 (4)	C10—C9—C18—N3	178.10 (16)
C6—C7—C8—C3	−0.3 (4)	C1—C2—N1—N2	0.5 (3)
C4—C3—C8—C7	1.4 (3)	C3—C2—N1—N2	−176.01 (18)
C2—C3—C8—C7	179.9 (2)	C2—N1—N2—Se1	0.4 (2)
C2—C1—C9—C10	−101.3 (2)	C17—C18—N3—O2	−173.6 (2)
Se1—C1—C9—C10	79.92 (19)	C16—C18—N3—O2	67.8 (3)
C2—C1—C9—C18	128.0 (2)	C9—C18—N3—O2	−48.7 (3)
Se1—C1—C9—C18	−50.8 (2)	C17—C18—N3—O1	6.2 (3)
C1—C9—C10—C11	−45.2 (3)	C16—C18—N3—O1	−112.4 (3)
C18—C9—C10—C11	87.1 (2)	C9—C18—N3—O1	131.1 (3)
C1—C9—C10—C15	134.18 (18)	C2—C1—Se1—N2	1.03 (14)
C18—C9—C10—C15	−93.5 (2)	C9—C1—Se1—N2	179.98 (16)
C15—C10—C11—C12	0.4 (3)	N1—N2—Se1—C1	−0.81 (16)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···Se1	0.93	2.84	3.534 (2)	133
C17—H17B···Se1	0.96	2.63	3.361 (3)	133
C5—H5···Cg1^{i}	0.93	2.76	3.6297 (3)	156

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

Fig. 1


O2
N3
O1
C10
C11
Se1
N2
C12
N1
C2
C9
C8
C13
C7
C14
C1
C3
C6
C15
C18
C4
C5
C17
C16