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1-{[3-(Thiophen-2-yl)-4,5-dihydro-1,2-oxazol-5-yl]-methyl}-2,3-dihydro-1*H*-indole-2,3-dione

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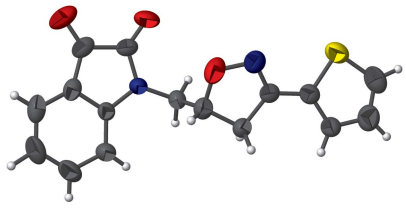
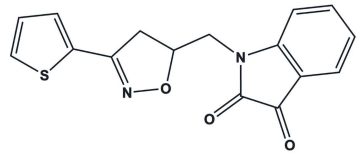
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{16}H_{12}N_2O_3S$, the indoline and thiophene rings are inclined to one another by 2.01 (2)°. The isoxazole ring adopts an envelope conformation, with the methine C atom as the flap, and its mean plane is inclined to the thiophene and indoline ring mean planes by 19.78 (14) and 20.83 (12)°, respectively. In the crystal, molecules are linked by C—H···O hydrogen bonds involving the same acceptor atom, forming chains propagating along [010]. The chains are linked by further C—H···O hydrogen bonds, forming slabs parallel to the ($\bar{1}$03) plane. The slabs are linked by offset π–π interactions [intercentroid distance = 3.792 (1) Å], forming a three-dimensional supramolecular structure.

3D view



Chemical scheme



Structure description

Isatin (indoline-2,3-dione) is a core constituent of many alkaloids and drugs (Aboul-Fadl *et al.*, 2010), as well as dyes, pesticides and analytical reagents. Literature surveys reveal that various derivatives of isatin possess diverse biological activities, such as antibacterial, antifungal, antiviral, anti-HIV (Bal *et al.*, 2005), anti-microbacterial, anticancer (Gürsoy & Karalı, 2003), anti-inflammatory (Sridhar & Ramesh, 2001) and anticonvulsant activities (Verma *et al.*, 2004). Continuing our research on the synthesis of new heterocyclic systems containing isatin and other moieties (Alsubari *et al.*, 2009; Bouhfid *et al.*, 2006), we report herein on the synthesis and crystal structure of the title compound, Fig. 1.

In the title compound, the indole ring system is almost planar as expected (r.m.s. deviation = 0.023 Å). The dihedral angle between this plane and that of the thiophene ring (r.m.s. deviation = 0.012 Å) is 2.01 (2)°. Puckering analysis of the isoxazole ring [parameters $Q(2)$ = 0.175 (2) Å and $\varphi(2)$ = 326.2 (8)°], indicates that it has an envelope

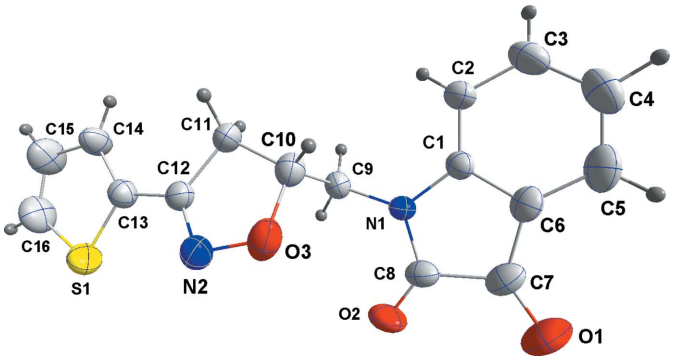


Figure 1
The molecular structure of the title compound, with the atom labelling and 40% probability displacement ellipsoids.

conformation with atom C10 as the flap. Its mean plane is inclined to the thiophene and indoline ring mean planes by 19.78 (14) and 20.83 (12)°, respectively.

In the crystal, the combination of C2—H2···O2^{i}, C9—H9*A*···O2^{i} and C16—H16···O1^{ii} hydrogen bonds (Table 1) forms stepped layers, or slabs two molecules thick, which are oriented parallel to ($\bar{1}$03); as shown in Fig. 2. These layers are associated through offset π-stacking interactions, involving inversion-related indole rings in adjacent layers, forming a supramolecular three-dimensional structure [$Cg\cdots Cg^{iii}$ = 3.792 (1) Å, *Cg* is the centroid of the N1/C1–C8 ring, interplanar distance = 3.479 (1) Å, slippage = 1.508 Å, symmetry code (iii): $-x+2, -y+1, -z+1$].

Synthesis and crystallization

To a solution of 0.4 g (2.18 mmol) of 1-allylindoline-2,3-dione and 0.5 g (4 mmol) of 2-thiophenecarboxaldehyde oxime in 15 ml of chloroform, were added 15 ml of bleach (24% weight) with a dropping funnel. The mixture was stirred for 4 h at 273 K. The solution was then concentrated to dryness under reduced pressure and the residue extracted with chloroform. The product isolated was chromatographed on a silica column (eluent: hexane/ethyl acetate 95:5 *v*/*v*). The solid obtained was crystallized from ethanol solution to give colourless rod-like crystals of the title compound.

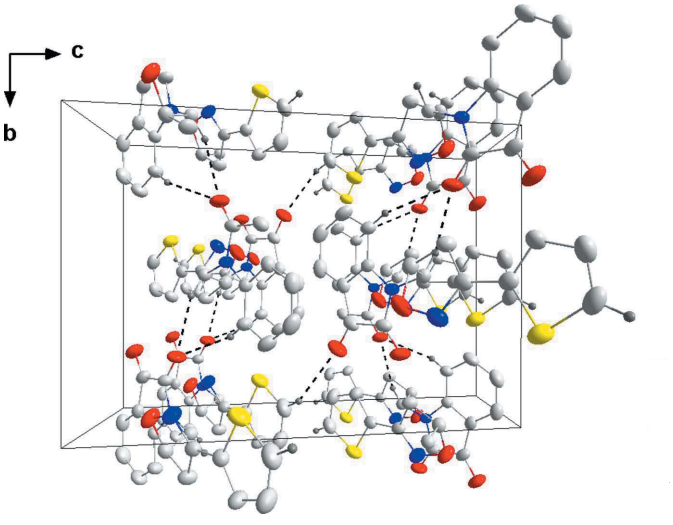


Figure 2
The partial view along the *a* axis of the crystal packing of the title compound. The hydrogen bonds are shown as dashed lines (see Table 1).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O2^{i}	0.88 (3)	2.60 (3)	3.455 (3)	162 (2)
C9—H9*A*···O2^{i}	0.98 (3)	2.39 (3)	3.297 (3)	153.7 (19)
C16—H16···O1^{ii}	0.93	2.49	3.212 (4)	134

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x-\frac{3}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{12}N_2O_3S$
M_r	312.34
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	298
a, *b*, *c* (Å)	7.3834 (2), 11.7331 (3), 16.9144 (4)
β (°)	101.731 (1)
V (Å^3)	1434.69 (6)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.14
Crystal size (mm)	0.24 × 0.19 × 0.14
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.64, 0.76
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10930, 2899, 2500
R_{int}	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.057, 0.166, 1.06
No. of reflections	2899
No. of parameters	235
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.80, −0.38

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170315 [https://doi.org/10.1107/S2414314617003157]

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Crystal data

$C_{16}H_{12}N_2O_3S$
M_r = 312.34
Monoclinic, $P2_1/n$
a = 7.3834 (2) Å
b = 11.7331 (3) Å
c = 16.9144 (4) Å
β = 101.731 (1)°
V = 1434.69 (6) Å^3
Z = 4
$F(000)$ = 648
D_x = 1.446 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 8282 reflections
θ = 3.8–74.3°
μ = 2.14 mm^{-1}
T = 298 K
Rod, colourless
0.24 × 0.19 × 0.14 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.64, T_{max} = 0.76
10930 measured reflections
2899 independent reflections
2500 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 74.7°, θ_{min} = 4.6°
h = −9→9
k = −14→14
l = −18→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.166
S = 1.06
2899 reflections
235 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.089P)^2 + 0.7078P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Special details

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

Refinement. 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 $F^2 > 2\text{sigma}(F^2)$ 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. The H-atoms of the thiophene moiety, although located in a difference map, did not refine satisfactorily and so were included as riding contributions in idealized positions.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	−0.04891 (11)	0.36107 (6)	0.11798 (5)	0.0697 (3)
O1	1.1460 (3)	0.26341 (19)	0.43119 (14)	0.0835 (7)
O2	0.8130 (3)	0.26371 (15)	0.30166 (14)	0.0718 (5)
O3	0.4468 (2)	0.41608 (18)	0.32154 (12)	0.0679 (6)
N1	0.8448 (2)	0.45816 (15)	0.31846 (11)	0.0434 (4)
N2	0.2829 (3)	0.39068 (19)	0.26398 (14)	0.0600 (6)
C1	0.9740 (3)	0.53126 (18)	0.36675 (12)	0.0410 (5)
C2	0.9783 (3)	0.6487 (2)	0.36514 (16)	0.0526 (6)
H2	0.900 (4)	0.691 (2)	0.3307 (18)	0.063 (8)*
C3	1.1224 (4)	0.7019 (3)	0.41754 (19)	0.0687 (8)
H3	1.130 (5)	0.778 (3)	0.415 (2)	0.081 (10)*
C4	1.2542 (4)	0.6412 (3)	0.47017 (19)	0.0729 (8)
H4	1.347 (5)	0.685 (3)	0.508 (2)	0.082 (10)*
C5	1.2494 (3)	0.5240 (3)	0.47092 (16)	0.0640 (7)
H5	1.332 (5)	0.486 (3)	0.506 (2)	0.083 (10)*
C6	1.1086 (3)	0.4687 (2)	0.41850 (13)	0.0486 (5)
C7	1.0666 (4)	0.3480 (2)	0.40177 (16)	0.0560 (6)
C8	0.8915 (3)	0.34648 (19)	0.33422 (15)	0.0509 (5)
C9	0.6847 (3)	0.4973 (2)	0.26000 (13)	0.0445 (5)
H9A	0.715 (3)	0.566 (2)	0.2327 (15)	0.048 (6)*
H9B	0.656 (4)	0.439 (2)	0.2200 (16)	0.053 (7)*
C10	0.5214 (3)	0.5228 (2)	0.29834 (16)	0.0525 (6)
H10	0.550 (4)	0.557 (3)	0.3435 (18)	0.062 (8)*
C11	0.3615 (3)	0.5784 (2)	0.24054 (18)	0.0553 (6)
H11A	0.299 (5)	0.641 (3)	0.267 (2)	0.102 (12)*
H11B	0.403 (4)	0.607 (3)	0.1921 (19)	0.071 (8)*
C12	0.2347 (3)	0.47894 (19)	0.22011 (14)	0.0464 (5)
C13	0.0679 (3)	0.4814 (2)	0.15739 (14)	0.0492 (5)
C14	−0.0204 (3)	0.5768 (2)	0.12228 (15)	0.0567 (6)
H14	0.0221	0.6506	0.1345	0.068*
C15	−0.1833 (5)	0.5507 (3)	0.06558 (19)	0.0782 (9)
H15	−0.2618	0.6058	0.0376	0.094*
C16	−0.2132 (5)	0.4392 (3)	0.05624 (18)	0.0768 (8)
H16	−0.3124	0.4078	0.0201	0.092*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0667 (5)	0.0567 (4)	0.0878 (5)	−0.0080 (3)	0.0209 (4)	−0.0166 (3)
O1	0.0917 (15)	0.0672 (12)	0.0930 (15)	0.0322 (11)	0.0222 (12)	0.0312 (11)
O2	0.0805 (13)	0.0373 (9)	0.0984 (14)	−0.0077 (9)	0.0201 (11)	−0.0075 (9)
O3	0.0485 (9)	0.0835 (13)	0.0735 (12)	0.0074 (9)	0.0166 (8)	0.0340 (10)
N1	0.0412 (9)	0.0336 (9)	0.0540 (10)	−0.0005 (7)	0.0063 (8)	−0.0014 (7)
N2	0.0500 (11)	0.0611 (12)	0.0718 (13)	−0.0004 (9)	0.0190 (10)	0.0190 (10)
C1	0.0357 (9)	0.0419 (11)	0.0455 (11)	−0.0003 (8)	0.0087 (8)	−0.0038 (8)
C2	0.0526 (13)	0.0418 (12)	0.0615 (14)	−0.0012 (10)	0.0069 (11)	−0.0051 (10)
C3	0.0675 (17)	0.0587 (17)	0.0792 (18)	−0.0155 (13)	0.0131 (14)	−0.0221 (14)
C4	0.0537 (15)	0.095 (2)	0.0673 (17)	−0.0160 (15)	0.0061 (13)	−0.0243 (16)
C5	0.0410 (12)	0.096 (2)	0.0536 (14)	0.0060 (13)	0.0068 (10)	0.0028 (13)
C6	0.0397 (10)	0.0608 (14)	0.0466 (11)	0.0073 (9)	0.0119 (9)	0.0049 (10)
C7	0.0562 (13)	0.0540 (13)	0.0617 (14)	0.0152 (11)	0.0213 (11)	0.0148 (11)
C8	0.0543 (13)	0.0379 (11)	0.0640 (14)	0.0028 (9)	0.0204 (11)	0.0035 (10)
C9	0.0407 (10)	0.0453 (11)	0.0463 (11)	−0.0025 (9)	0.0060 (9)	−0.0013 (9)
C10	0.0458 (12)	0.0581 (14)	0.0528 (13)	0.0034 (10)	0.0078 (10)	−0.0025 (11)
C11	0.0437 (11)	0.0466 (13)	0.0729 (16)	0.0028 (10)	0.0053 (11)	0.0018 (11)
C12	0.0435 (11)	0.0455 (11)	0.0539 (12)	0.0016 (9)	0.0186 (9)	0.0027 (9)
C13	0.0490 (12)	0.0504 (12)	0.0506 (12)	−0.0040 (10)	0.0159 (10)	−0.0014 (9)
C14	0.0562 (13)	0.0495 (13)	0.0605 (14)	−0.0050 (10)	0.0025 (11)	0.0108 (10)
C15	0.0731 (18)	0.089 (2)	0.0645 (17)	−0.0021 (16)	−0.0043 (14)	0.0148 (15)
C16	0.0726 (18)	0.094 (2)	0.0610 (16)	−0.0175 (17)	0.0073 (13)	−0.0166 (15)

Geometric parameters (Å, º)

S1—C16	1.699 (4)	C5—H5	0.88 (4)
S1—C13	1.717 (2)	C6—C7	1.465 (4)
O1—C7	1.207 (3)	C7—C8	1.542 (4)
O2—C8	1.205 (3)	C9—C10	1.510 (3)
O3—N2	1.422 (3)	C9—H9A	0.98 (3)
O3—C10	1.454 (3)	C9—H9B	0.96 (3)
N1—C8	1.367 (3)	C10—C11	1.519 (3)
N1—C1	1.413 (3)	C10—H10	0.85 (3)
N1—C9	1.453 (3)	C11—C12	1.493 (3)
N2—C12	1.282 (3)	C11—H11A	1.02 (4)
C1—C2	1.379 (3)	C11—H11B	0.99 (3)
C1—C6	1.393 (3)	C12—C13	1.453 (3)
C2—C3	1.387 (4)	C13—C14	1.369 (3)
C2—H2	0.88 (3)	C14—C15	1.411 (4)
C3—C4	1.376 (5)	C14—H14	0.9300
C3—H3	0.89 (4)	C15—C16	1.331 (5)
C4—C5	1.376 (5)	C15—H15	0.9300
C4—H4	0.98 (3)	C16—H16	0.9300
C5—C6	1.384 (4)		

C16—S1—C13	91.96 (14)	C10—C9—H9A	108.8 (14)
N2—O3—C10	108.19 (17)	N1—C9—H9B	106.8 (16)
C8—N1—C1	110.79 (18)	C10—C9—H9B	111.4 (15)
C8—N1—C9	125.00 (19)	H9A—C9—H9B	107 (2)
C1—N1—C9	124.21 (18)	O3—C10—C9	108.9 (2)
C12—N2—O3	109.0 (2)	O3—C10—C11	104.84 (19)
C2—C1—C6	121.5 (2)	C9—C10—C11	113.1 (2)
C2—C1—N1	127.7 (2)	O3—C10—H10	102 (2)
C6—C1—N1	110.8 (2)	C9—C10—H10	114 (2)
C1—C2—C3	117.0 (3)	C11—C10—H10	113 (2)
C1—C2—H2	123.7 (19)	C12—C11—C10	100.50 (19)
C3—C2—H2	119.1 (19)	C12—C11—H11A	110 (2)
C4—C3—C2	122.1 (3)	C10—C11—H11A	113 (2)
C4—C3—H3	121 (2)	C12—C11—H11B	111.0 (18)
C2—C3—H3	117 (2)	C10—C11—H11B	110.4 (18)
C5—C4—C3	120.4 (3)	H11A—C11—H11B	112 (3)
C5—C4—H4	122.0 (19)	N2—C12—C13	122.2 (2)
C3—C4—H4	117.5 (19)	N2—C12—C11	114.2 (2)
C4—C5—C6	118.7 (3)	C13—C12—C11	123.5 (2)
C4—C5—H5	120 (2)	C14—C13—C12	126.3 (2)
C6—C5—H5	121 (2)	C14—C13—S1	110.26 (19)
C5—C6—C1	120.2 (2)	C12—C13—S1	123.45 (18)
C5—C6—C7	132.8 (2)	C13—C14—C15	112.5 (3)
C1—C6—C7	107.0 (2)	C13—C14—H14	123.7
O1—C7—C6	130.5 (3)	C15—C14—H14	123.7
O1—C7—C8	124.1 (3)	C16—C15—C14	113.0 (3)
C6—C7—C8	105.47 (18)	C16—C15—H15	123.5
O2—C8—N1	127.2 (2)	C14—C15—H15	123.5
O2—C8—C7	126.9 (2)	C15—C16—S1	112.2 (2)
N1—C8—C7	105.9 (2)	C15—C16—H16	123.9
N1—C9—C10	112.35 (19)	S1—C16—H16	123.9
N1—C9—H9A	110.3 (14)		

C10—O3—N2—C12	−12.4 (3)	O1—C7—C8—N1	179.6 (2)
C8—N1—C1—C2	176.5 (2)	C6—C7—C8—N1	−1.1 (2)
C9—N1—C1—C2	−3.3 (3)	C8—N1—C9—C10	96.1 (3)
C8—N1—C1—C6	−2.0 (2)	C1—N1—C9—C10	−84.1 (3)
C9—N1—C1—C6	178.19 (19)	N2—O3—C10—C9	−103.2 (2)
C6—C1—C2—C3	−0.2 (4)	N2—O3—C10—C11	18.1 (3)
N1—C1—C2—C3	−178.6 (2)	N1—C9—C10—O3	−71.4 (2)
C1—C2—C3—C4	−1.2 (4)	N1—C9—C10—C11	172.41 (19)
C2—C3—C4—C5	1.7 (5)	O3—C10—C11—C12	−16.3 (2)
C3—C4—C5—C6	−0.7 (4)	C9—C10—C11—C12	102.3 (2)
C4—C5—C6—C1	−0.6 (4)	O3—N2—C12—C13	−177.69 (19)
C4—C5—C6—C7	177.5 (3)	O3—N2—C12—C11	0.9 (3)
C2—C1—C6—C5	1.1 (3)	C10—C11—C12—N2	10.0 (3)
N1—C1—C6—C5	179.7 (2)	C10—C11—C12—C13	−171.4 (2)
C2—C1—C6—C7	−177.5 (2)	N2—C12—C13—C14	161.9 (2)

N1—C1—C6—C7	1.2 (2)	C11—C12—C13—C14	−16.6 (4)
C5—C6—C7—O1	1.0 (5)	N2—C12—C13—S1	−16.9 (3)
C1—C6—C7—O1	179.2 (3)	C11—C12—C13—S1	164.62 (19)
C5—C6—C7—C8	−178.3 (2)	C16—S1—C13—C14	−0.3 (2)
C1—C6—C7—C8	−0.1 (2)	C16—S1—C13—C12	178.6 (2)
C1—N1—C8—O2	−177.7 (2)	C12—C13—C14—C15	−177.5 (2)
C9—N1—C8—O2	2.1 (4)	S1—C13—C14—C15	1.4 (3)
C1—N1—C8—C7	1.8 (2)	C13—C14—C15—C16	−2.1 (4)
C9—N1—C8—C7	−178.35 (18)	C14—C15—C16—S1	1.9 (4)
O1—C7—C8—O2	−0.9 (4)	C13—S1—C16—C15	−0.9 (3)
C6—C7—C8—O2	178.4 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O2^{i}	0.88 (3)	2.60 (3)	3.455 (3)	162 (2)
C9—H9*A*···O2^{i}	0.98 (3)	2.39 (3)	3.297 (3)	153.7 (19)
C16—H16···O1^{ii}	0.93	2.49	3.212 (4)	134

Symmetry codes: (i) −*x*+3/2, *y*+1/2, −*z*+1/2; (ii) *x*−3/2, −*y*+1/2, *z*−1/2.