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2-[3-(4-Chlorophenyl)-5-(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazol-1-yl]-8*H*-indeno[1,2-*d*]thiazole

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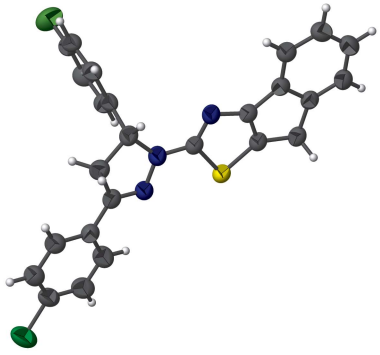
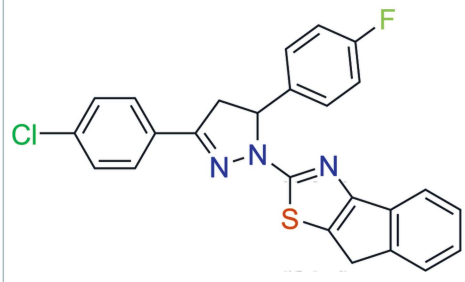
Structural data: full structural data are available from iucrdata.iucr.org

The title molecule, $C_{25}H_{17}ClFN_3S$, contains indenothiazolyl (*A*), pyrazolyl (*B*), fluorophenyl (*C*) and chlorophenyl (*D*) groups. The dihedral angles between the ring planes *A*/*B*, *B*/C and *B*/*D* are 14.2 (1), 83.0 (1) and 6.5 (2)°, respectively. In the crystal, pairs of molecules related by inversion symmetry are linked by pairwise weak C—H···N interactions, forming dimers. These dimers interact through π–π contacts between the thiazolyl units [centroid-to-centroid distance = 3.826 (1) Å], forming chains along [010].

3D view



Chemical scheme



Structure description

Indeno[1,2-*d*]thiazoles act as histone deacetylase inhibitors (Zhou *et al.*, 2013; Chordia *et al.*, 2005). Thiazoles and pyrazoles have various biological activities (Chhabria *et al.*, 2016; Faria *et al.*, 2017). As part of our studies in these areas we now report the synthesis and structure of the title compound.

The asymmetric unit consists of one molecule of the title compound. The molecule contains an indenothiazolyl ring system (*A*) and pyrazolyl (*B*), fluorophenyl (*C*) and chlorophenyl (*D*) rings (Fig. 1). The twist angles between the planes through neighbouring ring pairs *A*/*B*, *B*/*C* and *B*/*D* are 14.2 (1)°, 83.0 (1)° and 6.5 (2)°, respectively. In the crystal, pairs of molecules related by inversion symmetry are linked by C—H···N interactions, forming dimers in the crystal structure (Table 1, Fig. 2). Neighbouring dimers interact through π–π contacts involving the thiazolyl fragments with centroid-to-centroid distances of 3.826 (1) Å, forming chains along [010].

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···N1^{i}	0.93	2.59	3.392 (3)	145

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

Synthesis and crystallization

The title compound was synthesized from the condensation reaction between 3-(4-chlorophenyl)-5-(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazole-1-carbothioamide (0.67 g, 2.0 mmol) and 2-bromo-2,3-dihydro-1*H*-inden-1-one (1.10 g, 2.0 mmol) in anhydrous ethanol (20 ml) under reflux for 2 h. The solid obtained was recrystallized from dimethylformamide solution to give colourless crystals (72%), m.p. 510–511 K.

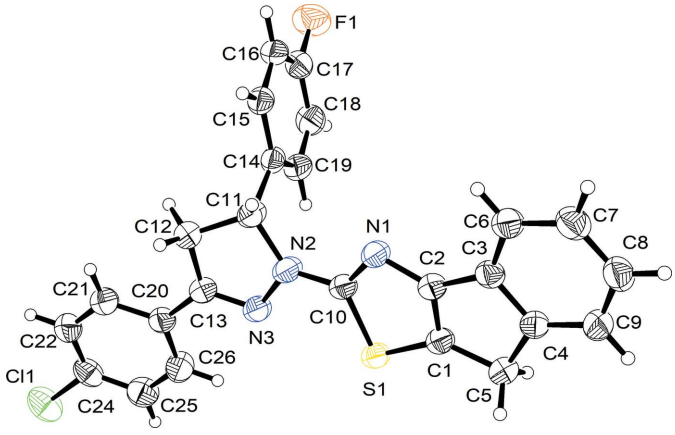


Figure 1
The molecular structure of the title compound showing 50% probability ellipsoids.

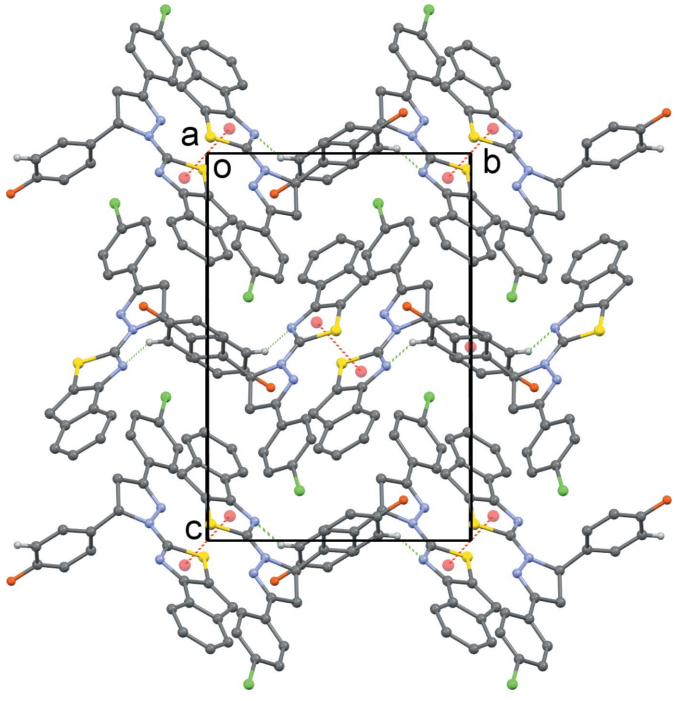


Figure 2
The crystal packing viewed along the *a* axis showing intermolecular contacts as dotted lines (C—H···N in green and π–π in red) with some hydrogen atoms omitted for clarity.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{25}H_{17}ClFN_3S$
M_r	445.92
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	11.6975 (6), 11.0671 (5), 16.5395 (10)
β (°)	100.303 (6)
V (Å^3)	2106.6 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.31
Crystal size (mm)	0.44 × 0.32 × 0.06
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.989, 0.998
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21492, 5397, 3547
R_{int}	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.703
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.129, 1.03
No. of reflections	5397
No. of parameters	280
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.22

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2019). **4**, x190218 [https://doi.org/10.1107/S2414314619002189]

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Crystal data

$C_{25}H_{17}ClFN_3S$
M_r = 445.92
Monoclinic, $P2_1/c$
a = 11.6975 (6) Å
b = 11.0671 (5) Å
c = 16.5395 (10) Å
β = 100.303 (6)°
V = 2106.6 (2) Å^3
Z = 4
$F(000)$ = 920
D_x = 1.406 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5333 reflections
θ = 4.0–27.3°
μ = 0.31 mm^{-1}
T = 296 K
Plate, colourless
0.44 × 0.32 × 0.06 mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas diffractometer
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2015)
T_{min} = 0.989, T_{max} = 0.998
21492 measured reflections
5397 independent reflections
3547 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 30.0°, θ_{min} = 3.4°
h = −15→15
k = −15→13
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.129
S = 1.03
5397 reflections
280 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 0.7878P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 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. All hydrogen atoms were placed in calculated positions and refined using a riding model. Bond distances for methine and aromatic C—H H atoms were set to 0.98 Å and 0.93 Å respectively. Bond distances for methylene C—H H atoms were set to 0.97 Å and all U_{iso}(H) set to 1.2 times U_{eq}(C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.36830 (18)	−0.00576 (17)	−0.10974 (13)	0.0483 (5)
C2	0.44396 (17)	0.08820 (17)	−0.10383 (13)	0.0462 (5)
C3	0.52516 (17)	0.06919 (17)	−0.15981 (12)	0.0464 (5)
C4	0.49318 (18)	−0.03929 (17)	−0.20216 (13)	0.0475 (5)
C5	0.3909 (2)	−0.09670 (18)	−0.17192 (14)	0.0538 (5)
H5A	0.324551	−0.105536	−0.215951	0.065*
H5B	0.411204	−0.174911	−0.146943	0.065*
C6	0.61892 (19)	0.13560 (19)	−0.17651 (14)	0.0544 (5)
H6	0.641714	0.206470	−0.147914	0.065*
C7	0.6778 (2)	0.0942 (2)	−0.23659 (15)	0.0624 (6)
H7	0.740834	0.137899	−0.248192	0.075*
C8	0.6448 (2)	−0.0103 (2)	−0.27944 (15)	0.0624 (6)
H8	0.684815	−0.035674	−0.320197	0.075*
C9	0.5523 (2)	−0.0782 (2)	−0.26226 (14)	0.0575 (6)
H9	0.530384	−0.149161	−0.291019	0.069*
C10	0.34436 (18)	0.15028 (16)	−0.01316 (13)	0.0471 (5)
C11	0.35404 (19)	0.33553 (17)	0.07738 (13)	0.0514 (5)
H11	0.439164	0.333925	0.086955	0.062*
C12	0.3099 (2)	0.33867 (18)	0.15953 (13)	0.0540 (5)
H12A	0.371666	0.320498	0.205330	0.065*
H12B	0.276437	0.416657	0.168531	0.065*
C13	0.21881 (18)	0.24094 (17)	0.14765 (13)	0.0497 (5)
C14	0.30859 (17)	0.44092 (17)	0.02312 (12)	0.0448 (4)
C15	0.37269 (18)	0.54709 (18)	0.02780 (13)	0.0483 (5)
H15	0.446141	0.549470	0.060477	0.058*
C16	0.32965 (19)	0.64896 (18)	−0.01498 (14)	0.0530 (5)
H16	0.373157	0.719698	−0.011724	0.064*
C17	0.2220 (2)	0.6434 (2)	−0.06206 (14)	0.0569 (6)
C18	0.1550 (2)	0.5415 (2)	−0.06839 (15)	0.0623 (6)
H18	0.081432	0.540603	−0.100926	0.075*
C19	0.19912 (19)	0.4400 (2)	−0.02540 (14)	0.0553 (5)
H19	0.154650	0.369904	−0.029061	0.066*
C20	0.13608 (18)	0.21879 (18)	0.20216 (13)	0.0495 (5)
C21	0.1378 (2)	0.2885 (2)	0.27216 (14)	0.0600 (6)
H21	0.193419	0.348873	0.284704	0.072*
C22	0.0585 (2)	0.2697 (2)	0.32356 (15)	0.0647 (6)
H22	0.059898	0.317708	0.369871	0.078*
C24	−0.0221 (2)	0.1798 (2)	0.30554 (15)	0.0591 (6)
C25	−0.0244 (2)	0.1081 (2)	0.23778 (17)	0.0673 (6)
H25	−0.078825	0.046278	0.226694	0.081*
C26	0.0535 (2)	0.1274 (2)	0.18630 (15)	0.0632 (6)

H26	0.051152	0.078706	0.140185	0.076*
N1	0.43084 (15)	0.17969 (14)	−0.04911 (11)	0.0488 (4)
N2	0.30655 (17)	0.21900 (15)	0.04455 (12)	0.0582 (5)
N3	0.22147 (16)	0.17424 (15)	0.08447 (12)	0.0529 (4)
F1	0.17949 (14)	0.74318 (13)	−0.10484 (10)	0.0883 (5)
Cl1	−0.12023 (6)	0.15339 (7)	0.37082 (5)	0.0860 (2)
S1	0.27382 (5)	0.01232 (4)	−0.04205 (3)	0.05072 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0528 (12)	0.0401 (10)	0.0530 (12)	0.0004 (9)	0.0120 (10)	−0.0012 (9)
C2	0.0492 (11)	0.0405 (10)	0.0490 (11)	0.0013 (8)	0.0090 (9)	0.0003 (9)
C3	0.0492 (11)	0.0431 (10)	0.0466 (11)	0.0056 (9)	0.0080 (9)	0.0056 (9)
C4	0.0545 (12)	0.0413 (10)	0.0464 (11)	0.0058 (9)	0.0084 (9)	0.0033 (9)
C5	0.0631 (13)	0.0428 (11)	0.0560 (13)	0.0009 (10)	0.0123 (11)	−0.0032 (9)
C6	0.0576 (13)	0.0480 (11)	0.0594 (14)	−0.0001 (10)	0.0154 (11)	0.0005 (10)
C7	0.0642 (14)	0.0611 (14)	0.0668 (15)	0.0035 (11)	0.0247 (12)	0.0086 (12)
C8	0.0743 (16)	0.0621 (14)	0.0560 (14)	0.0138 (12)	0.0260 (12)	0.0073 (11)
C9	0.0729 (15)	0.0490 (12)	0.0520 (13)	0.0080 (11)	0.0153 (12)	−0.0003 (10)
C10	0.0531 (12)	0.0372 (9)	0.0520 (12)	−0.0001 (8)	0.0122 (10)	−0.0003 (9)
C11	0.0544 (12)	0.0423 (10)	0.0591 (13)	−0.0048 (9)	0.0149 (10)	−0.0069 (9)
C12	0.0653 (14)	0.0468 (11)	0.0499 (12)	−0.0032 (10)	0.0106 (11)	−0.0019 (9)
C13	0.0553 (12)	0.0419 (10)	0.0520 (12)	0.0014 (9)	0.0103 (10)	−0.0012 (9)
C14	0.0474 (11)	0.0453 (10)	0.0441 (11)	−0.0066 (8)	0.0148 (9)	−0.0082 (8)
C15	0.0460 (11)	0.0515 (11)	0.0489 (12)	−0.0086 (9)	0.0128 (9)	−0.0069 (9)
C16	0.0599 (13)	0.0466 (11)	0.0557 (13)	−0.0113 (10)	0.0191 (11)	−0.0031 (10)
C17	0.0667 (14)	0.0527 (12)	0.0525 (13)	0.0027 (11)	0.0141 (11)	0.0022 (10)
C18	0.0561 (13)	0.0701 (15)	0.0568 (14)	−0.0075 (11)	−0.0007 (11)	−0.0016 (12)
C19	0.0555 (12)	0.0529 (12)	0.0574 (13)	−0.0152 (10)	0.0097 (11)	−0.0070 (10)
C20	0.0552 (12)	0.0435 (10)	0.0503 (12)	0.0047 (9)	0.0108 (10)	0.0026 (9)
C21	0.0714 (15)	0.0521 (12)	0.0591 (14)	−0.0044 (11)	0.0186 (12)	−0.0020 (11)
C22	0.0825 (17)	0.0596 (14)	0.0559 (14)	0.0024 (12)	0.0231 (13)	−0.0005 (11)
C24	0.0531 (13)	0.0668 (14)	0.0605 (14)	0.0118 (11)	0.0187 (11)	0.0170 (12)
C25	0.0587 (14)	0.0705 (15)	0.0743 (17)	−0.0080 (12)	0.0163 (13)	0.0031 (13)
C26	0.0623 (14)	0.0668 (14)	0.0622 (15)	−0.0082 (11)	0.0164 (12)	−0.0100 (12)
N1	0.0522 (10)	0.0406 (8)	0.0554 (10)	−0.0033 (7)	0.0143 (8)	−0.0059 (7)
N2	0.0699 (12)	0.0414 (9)	0.0705 (12)	−0.0104 (8)	0.0324 (10)	−0.0115 (8)
N3	0.0598 (11)	0.0432 (9)	0.0601 (11)	−0.0049 (8)	0.0224 (9)	−0.0049 (8)
F1	0.0987 (11)	0.0689 (9)	0.0919 (12)	0.0080 (8)	0.0023 (9)	0.0216 (8)
Cl1	0.0753 (4)	0.1069 (6)	0.0848 (5)	0.0073 (4)	0.0388 (4)	0.0210 (4)
S1	0.0565 (3)	0.0401 (3)	0.0580 (3)	−0.0045 (2)	0.0169 (3)	−0.0028 (2)

Geometric parameters (Å, º)

C1—C2	1.358 (3)	C12—H12B	0.9700
C1—C5	1.496 (3)	C13—N3	1.284 (3)
C1—S1	1.720 (2)	C13—C20	1.457 (3)

C2—N1	1.385 (3)	C14—C19	1.384 (3)
C2—C3	1.455 (3)	C14—C15	1.389 (3)
C3—C6	1.388 (3)	C15—C16	1.378 (3)
C3—C4	1.406 (3)	C15—H15	0.9300
C4—C9	1.377 (3)	C16—C17	1.359 (3)
C4—C5	1.516 (3)	C16—H16	0.9300
C5—H5A	0.9700	C17—F1	1.357 (3)
C5—H5B	0.9700	C17—C18	1.366 (3)
C6—C7	1.384 (3)	C18—C19	1.379 (3)
C6—H6	0.9300	C18—H18	0.9300
C7—C8	1.375 (3)	C19—H19	0.9300
C7—H7	0.9300	C20—C21	1.388 (3)
C8—C9	1.389 (3)	C20—C26	1.391 (3)
C8—H8	0.9300	C21—C22	1.382 (3)
C9—H9	0.9300	C21—H21	0.9300
C10—N1	1.303 (3)	C22—C24	1.367 (3)
C10—N2	1.355 (3)	C22—H22	0.9300
C10—S1	1.7605 (19)	C24—C25	1.369 (3)
C11—N2	1.469 (2)	C24—Cl1	1.735 (2)
C11—C14	1.509 (3)	C25—C26	1.371 (3)
C11—C12	1.538 (3)	C25—H25	0.9300
C11—H11	0.9800	C26—H26	0.9300
C12—C13	1.506 (3)	N2—N3	1.381 (2)
C12—H12A	0.9700		

C2—C1—C5	111.81 (19)	N3—C13—C20	121.49 (19)
C2—C1—S1	110.52 (15)	N3—C13—C12	113.55 (19)
C5—C1—S1	137.66 (16)	C20—C13—C12	124.95 (18)
C1—C2—N1	117.39 (19)	C19—C14—C15	118.22 (19)
C1—C2—C3	109.55 (18)	C19—C14—C11	122.01 (18)
N1—C2—C3	133.06 (18)	C15—C14—C11	119.43 (18)
C6—C3—C4	120.1 (2)	C16—C15—C14	121.32 (19)
C6—C3—C2	132.74 (19)	C16—C15—H15	119.3
C4—C3—C2	107.13 (17)	C14—C15—H15	119.3
C9—C4—C3	120.2 (2)	C17—C16—C15	118.24 (19)
C9—C4—C5	129.37 (19)	C17—C16—H16	120.9
C3—C4—C5	110.41 (18)	C15—C16—H16	120.9
C1—C5—C4	101.07 (17)	F1—C17—C16	118.5 (2)
C1—C5—H5A	111.6	F1—C17—C18	118.7 (2)
C4—C5—H5A	111.6	C16—C17—C18	122.8 (2)
C1—C5—H5B	111.6	C17—C18—C19	118.4 (2)
C4—C5—H5B	111.6	C17—C18—H18	120.8
H5A—C5—H5B	109.4	C19—C18—H18	120.8
C7—C6—C3	118.7 (2)	C18—C19—C14	121.0 (2)
C7—C6—H6	120.7	C18—C19—H19	119.5
C3—C6—H6	120.7	C14—C19—H19	119.5
C8—C7—C6	121.2 (2)	C21—C20—C26	117.9 (2)
C8—C7—H7	119.4	C21—C20—C13	120.70 (19)

C6—C7—H7	119.4	C26—C20—C13	121.4 (2)
C7—C8—C9	120.5 (2)	C22—C21—C20	121.2 (2)
C7—C8—H8	119.8	C22—C21—H21	119.4
C9—C8—H8	119.8	C20—C21—H21	119.4
C4—C9—C8	119.3 (2)	C24—C22—C21	119.2 (2)
C4—C9—H9	120.4	C24—C22—H22	120.4
C8—C9—H9	120.4	C21—C22—H22	120.4
N1—C10—N2	123.99 (18)	C22—C24—C25	120.8 (2)
N1—C10—S1	117.21 (15)	C22—C24—Cl1	119.6 (2)
N2—C10—S1	118.80 (16)	C25—C24—Cl1	119.6 (2)
N2—C11—C14	112.88 (18)	C24—C25—C26	120.0 (2)
N2—C11—C12	100.47 (16)	C24—C25—H25	120.0
C14—C11—C12	111.69 (17)	C26—C25—H25	120.0
N2—C11—H11	110.5	C25—C26—C20	120.8 (2)
C14—C11—H11	110.5	C25—C26—H26	119.6
C12—C11—H11	110.5	C20—C26—H26	119.6
C13—C12—C11	102.13 (16)	C10—N1—C2	107.54 (16)
C13—C12—H12A	111.3	C10—N2—N3	119.31 (16)
C11—C12—H12A	111.3	C10—N2—C11	127.12 (18)
C13—C12—H12B	111.3	N3—N2—C11	113.29 (17)
C11—C12—H12B	111.3	C13—N3—N2	107.89 (17)
H12A—C12—H12B	109.2	C1—S1—C10	87.31 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···N1^{i}	0.93	2.59	3.392 (3)	145

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