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4-(Benzofuran-2-yl)-2-[3-(4-chlorophenyl)-5-(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazol-1-yl]thiazole

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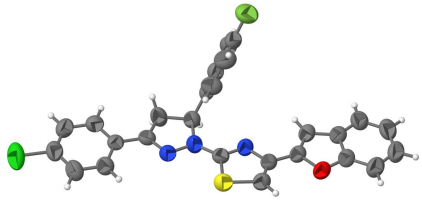
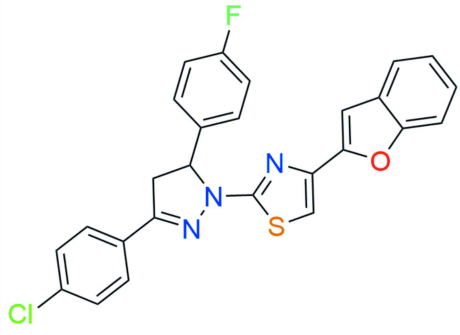
The molecule of the title compound, $C_{26}H_{17}ClFN_3OS$, comprises benzofuranyl (A), thiazolyl (B), pyrazolyl (C), chlorophenyl (D) and fluorophenyl (E) ring systems. Rings A–D are almost coplanar, as indicated by the twist angles between the ring pairs A/B, B/C and C/D of 7.6 (1), 4.7 (1) and 6.9 (2)°, respectively. Ring E is twisted by 73.2 (1)° from the plane through ring C. In the crystal, pairwise C—H···F interactions link the molecules into inversion dimers. Aromatic π–π interactions are also observed between rings A and E and between rings B and C for neighbouring pairs of molecules related by inversion symmetry. Taken together, the weak interactions generate [010] chains.

3D view



Chemical scheme



Structure description

Compounds containing a benzofuran moiety are present in many important natural products and drugs (Naik *et al.*, 2015). In addition, thiazoles and pyrazoles are an essential core scaffold in many natural products and have various biological activities (Chhabria *et al.*, 2016; Faria *et al.*, 2017). Therefore, the synthesis, characterization and applications of compounds containing such heterocycles are of continued interest and we describe here the synthesis and structure of the title compound.

The molecule of the title compound comprises benzofuranyl (A), thiazolyl (B), pyrazolyl (C), chlorophenyl (D) and fluorophenyl (E) ring systems (Fig. 1). Rings A–D are almost coplanar, as indicated by the twist angles between the ring pairs A/B, B/C and C/D of 7.6 (1), 4.7 (1) and 6.9 (2)°, respectively. Ring E is twisted by 73.2 (1)° from the plane through ring C. In the arbitrarily-chosen asymmetric unit, the stereogenic centre C12 has an *S* configuration, but crystal symmetry generates a racemic mixture.

In the crystal, pairwise C—H···F interactions link molecules into inversion dimers (Table 1). Aromatic π–π interactions are also observed between rings A and E [centroid–centroid separation = 3.755 (2) Å] and between rings B and C [3.796 (2) Å] for neighbouring pairs of molecules related by inversion symmetry; this results in each pair of molecules being linked by four π–π interactions (Fig. 2). The combination of C—H···F and π–π interactions generates [010] chains.

Synthesis and crystallization

The title compound was synthesized from the condensation of molar equivalents of 3-(4-chlorophenyl)-5-(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazole-1-carbothioamide with 1-(benzofuran-2-yl)-2-bromoethanone in anhydrous ethanol under reflux for 2 h. The crude product was recrystallized from dimethylformamide solution to give colourless needles (yield 74%, m.p. 234–236 °C).

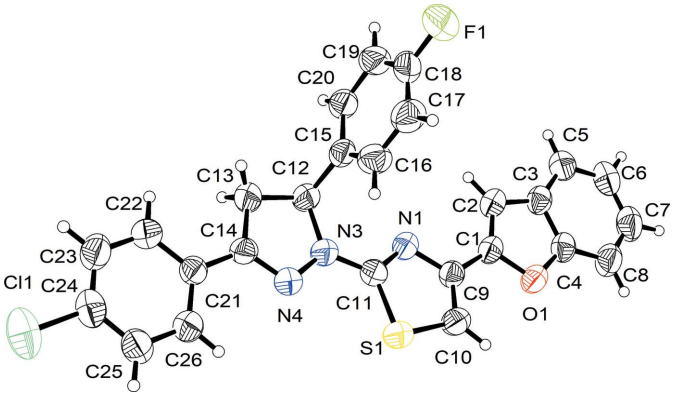


Figure 1
The molecular structure of the title compound showing 50% probability displacement ellipsoids.

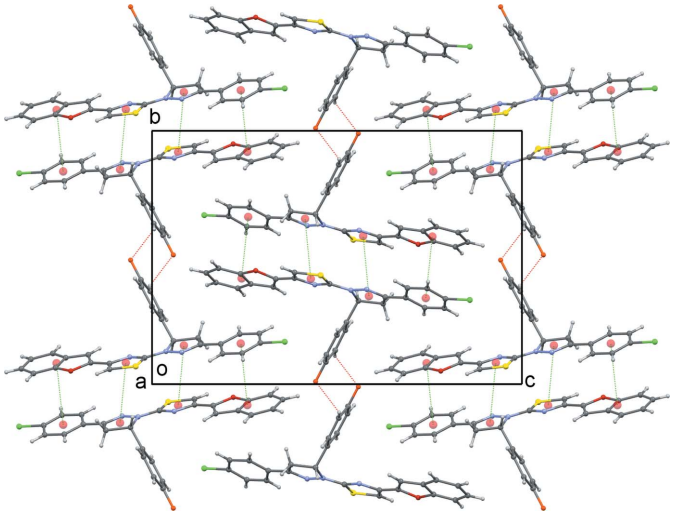


Figure 2
A view of the crystal structure down the *a* axis, showing π–π contacts as green dotted lines and C—H···F contacts in red.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19···F1^{i}	0.93	2.58	3.254 (5)	130

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{26}H_{17}ClFN_3OS$
M_r	473.93
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, *b*, *c* (Å)	6.6631 (6), 15.2297 (17), 22.431 (3)
β (°)	96.390 (9)
V (Å^3)	2262.1 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.29
Crystal size (mm)	0.46 × 0.19 × 0.11
Data collection	
Diffractometer	Rigaku OD SuperNova Dual source diffractometer with an Atlas detector
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.990, 0.997
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10799, 4617, 2323
R_{int}	0.042
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.060, 0.171, 1.03
No. of reflections	4617
No. of parameters	298
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.21

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

Refinement

All H atoms were placed in calculated positions and refined using a riding model. Bond lengths were set at 0.98, 0.97 and 0.93 Å for methine, methylene and aromatic C—H H atoms, respectively, with their U_{iso}(H) values set at 1.2 times the U_{eq} of the atom to which they are bonded. Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2019). **4**, x190359 [https://doi.org/10.1107/S2414314619003596]

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4-(Benzofuran-2-yl)-2-[3-(4-chlorophenyl)-5-(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazol-1-yl]thiazole

Crystal data

$C_{26}H_{17}ClFN_3OS$
M_r = 473.93
Monoclinic, $P2_1/c$
a = 6.6631 (6) Å
b = 15.2297 (17) Å
c = 22.431 (3) Å
β = 96.390 (9)°
V = 2262.1 (4) Å^3
Z = 4
$F(000)$ = 976
D_x = 1.392 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1999 reflections
θ = 3.7–23.3°
μ = 0.29 mm^{-1}
T = 296 K
Needle, colourless
0.46 × 0.19 × 0.11 mm

Data collection

Rigaku OD SuperNova Dual source diffractometer with an Atlas detector
ω scans
Absorption correction: gaussian (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.990, T_{max} = 0.997
10799 measured reflections
4617 independent reflections
2323 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 26.4°, θ_{min} = 3.4°
h = −6→8
k = −19→17
l = −28→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.171
S = 1.03
4617 reflections
298 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0542P)^2 + 0.6825P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.0420 (5)	0.9153 (2)	0.16557 (14)	0.0617 (8)
C2	−0.2264 (5)	0.8840 (2)	0.17209 (15)	0.0666 (9)
H2	−0.315276	0.858931	0.141930	0.080*
C3	−0.2636 (5)	0.8956 (2)	0.23330 (15)	0.0659 (9)
C4	−0.0873 (5)	0.9353 (2)	0.26072 (16)	0.0669 (9)
C5	−0.4193 (6)	0.8785 (3)	0.26796 (18)	0.0805 (11)
H5	−0.538290	0.852152	0.251208	0.097*
C6	−0.3937 (7)	0.9014 (3)	0.32729 (19)	0.0923 (12)
H6	−0.497815	0.891053	0.350794	0.111*
C7	−0.2172 (8)	0.9393 (3)	0.35304 (18)	0.0948 (13)
H7	−0.204363	0.952927	0.393693	0.114*
C8	−0.0587 (7)	0.9576 (3)	0.32022 (18)	0.0898 (12)
H8	0.060249	0.983506	0.337468	0.108*
C9	0.0725 (5)	0.9187 (2)	0.11473 (14)	0.0591 (8)
C10	0.2685 (5)	0.9408 (2)	0.11469 (16)	0.0712 (10)
H10	0.351786	0.959633	0.148300	0.085*
C11	0.1001 (5)	0.8959 (2)	0.01989 (16)	0.0637 (8)
C12	−0.1510 (5)	0.8293 (2)	−0.05800 (15)	0.0661 (9)
H12	−0.261981	0.869744	−0.052668	0.079*
C13	−0.1304 (5)	0.8178 (3)	−0.12471 (15)	0.0810 (11)
H13A	−0.154473	0.757287	−0.137032	0.097*
H13B	−0.224552	0.855387	−0.148931	0.097*
C14	0.0830 (5)	0.8439 (2)	−0.13025 (15)	0.0601 (8)
C15	−0.1805 (5)	0.7438 (2)	−0.02572 (14)	0.0602 (8)
C16	−0.0221 (6)	0.6941 (3)	0.00002 (18)	0.0819 (11)
H16	0.109071	0.713957	−0.001787	0.098*
C17	−0.0516 (6)	0.6161 (3)	0.02832 (19)	0.0900 (12)
H17	0.057272	0.583478	0.045913	0.108*
C18	−0.2429 (8)	0.5880 (3)	0.02992 (16)	0.0842 (12)
C19	−0.4061 (6)	0.6335 (3)	0.00476 (17)	0.0840 (12)
H19	−0.536128	0.611895	0.005850	0.101*
C20	−0.3735 (5)	0.7132 (3)	−0.02265 (15)	0.0706 (10)
H20	−0.483302	0.746331	−0.039096	0.085*
C21	0.1776 (5)	0.8416 (2)	−0.18589 (14)	0.0599 (8)
C22	0.0785 (6)	0.8020 (2)	−0.23703 (17)	0.0777 (10)
H22	−0.047482	0.776451	−0.235296	0.093*
C23	0.1650 (7)	0.8002 (3)	−0.29021 (18)	0.0883 (12)
H23	0.097113	0.774069	−0.324130	0.106*
C24	0.3519 (6)	0.8371 (3)	−0.29268 (17)	0.0790 (11)
C25	0.4505 (5)	0.8776 (3)	−0.24365 (18)	0.0794 (11)
H25	0.575572	0.903742	−0.245998	0.095*
C26	0.3637 (5)	0.8797 (2)	−0.19036 (16)	0.0706 (9)
H26	0.431759	0.907147	−0.157005	0.085*
N1	−0.0258 (4)	0.89273 (19)	0.06012 (12)	0.0645 (7)
N3	0.0437 (4)	0.8709 (2)	−0.03768 (13)	0.0748 (8)

N4	0.1770 (4)	0.87408 (18)	−0.08051 (12)	0.0629 (7)
O1	0.0500 (3)	0.94806 (16)	0.21956 (10)	0.0709 (6)
Cl1	0.4626 (2)	0.83256 (9)	−0.35884 (5)	0.1214 (5)
F1	−0.2761 (5)	0.51028 (17)	0.05775 (12)	0.1259 (10)
S1	0.34414 (13)	0.92974 (7)	0.04410 (4)	0.0766 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.063 (2)	0.063 (2)	0.056 (2)	0.0041 (17)	−0.0049 (16)	−0.0023 (16)
C2	0.066 (2)	0.071 (2)	0.060 (2)	0.0049 (18)	−0.0033 (17)	−0.0044 (17)
C3	0.071 (2)	0.062 (2)	0.062 (2)	0.0090 (18)	−0.0027 (18)	0.0024 (17)
C4	0.075 (2)	0.065 (2)	0.059 (2)	0.0109 (18)	−0.0007 (18)	0.0038 (17)
C5	0.085 (3)	0.084 (3)	0.072 (3)	0.000 (2)	0.008 (2)	0.009 (2)
C6	0.115 (3)	0.093 (3)	0.071 (3)	0.009 (3)	0.019 (3)	0.016 (2)
C7	0.132 (4)	0.093 (3)	0.058 (2)	0.006 (3)	0.009 (3)	0.002 (2)
C8	0.110 (3)	0.093 (3)	0.063 (3)	−0.003 (3)	−0.006 (2)	−0.007 (2)
C9	0.0597 (18)	0.059 (2)	0.057 (2)	0.0007 (16)	0.0008 (16)	0.0016 (16)
C10	0.068 (2)	0.077 (2)	0.067 (2)	−0.0116 (19)	0.0042 (17)	−0.0081 (18)
C11	0.070 (2)	0.058 (2)	0.063 (2)	−0.0065 (17)	0.0039 (18)	0.0037 (17)
C12	0.0570 (18)	0.077 (2)	0.063 (2)	−0.0064 (18)	0.0009 (16)	−0.0006 (18)
C13	0.072 (2)	0.109 (3)	0.061 (2)	−0.021 (2)	0.0003 (18)	0.009 (2)
C14	0.0591 (18)	0.056 (2)	0.063 (2)	−0.0051 (16)	−0.0002 (16)	0.0059 (16)
C15	0.0571 (18)	0.072 (2)	0.0513 (19)	−0.0030 (18)	0.0052 (15)	−0.0078 (16)
C16	0.067 (2)	0.081 (3)	0.096 (3)	−0.007 (2)	0.001 (2)	0.005 (2)
C17	0.090 (3)	0.078 (3)	0.098 (3)	0.000 (2)	−0.010 (2)	0.002 (2)
C18	0.122 (4)	0.073 (3)	0.057 (2)	−0.016 (3)	0.004 (2)	0.0010 (19)
C19	0.082 (3)	0.098 (3)	0.075 (3)	−0.027 (2)	0.023 (2)	−0.009 (2)
C20	0.061 (2)	0.086 (3)	0.065 (2)	−0.005 (2)	0.0091 (17)	−0.0046 (19)
C21	0.068 (2)	0.0521 (19)	0.058 (2)	−0.0010 (16)	0.0029 (16)	0.0048 (16)
C22	0.088 (3)	0.073 (2)	0.071 (3)	−0.016 (2)	0.004 (2)	0.000 (2)
C23	0.116 (3)	0.083 (3)	0.064 (3)	−0.006 (3)	0.002 (2)	−0.006 (2)
C24	0.099 (3)	0.075 (3)	0.064 (2)	0.013 (2)	0.016 (2)	0.008 (2)
C25	0.071 (2)	0.096 (3)	0.072 (3)	0.003 (2)	0.012 (2)	0.013 (2)
C26	0.068 (2)	0.077 (2)	0.067 (2)	−0.0017 (19)	0.0035 (18)	0.0026 (18)
N1	0.0649 (16)	0.0714 (19)	0.0562 (17)	−0.0042 (14)	0.0018 (14)	−0.0032 (14)
N3	0.0708 (18)	0.095 (2)	0.0586 (18)	−0.0241 (16)	0.0089 (15)	−0.0044 (16)
N4	0.0627 (16)	0.0638 (18)	0.0622 (18)	−0.0054 (14)	0.0064 (14)	−0.0006 (14)
O1	0.0718 (14)	0.0755 (16)	0.0627 (15)	−0.0045 (12)	−0.0045 (12)	−0.0076 (12)
Cl1	0.1498 (11)	0.1418 (12)	0.0796 (8)	0.0282 (9)	0.0433 (7)	0.0075 (7)
F1	0.176 (3)	0.0949 (19)	0.105 (2)	−0.0308 (18)	0.0060 (17)	0.0190 (15)
S1	0.0685 (6)	0.0863 (7)	0.0745 (6)	−0.0181 (5)	0.0061 (5)	−0.0031 (5)

Geometric parameters (Å, º)

C1—C2	1.341 (4)	C13—H13A	0.9700
C1—O1	1.388 (4)	C13—H13B	0.9700
C1—C9	1.442 (4)	C14—N4	1.301 (4)

C2—C3	1.433 (4)	C14—C21	1.460 (4)
C2—H2	0.9300	C15—C16	1.372 (5)
C3—C5	1.389 (5)	C15—C20	1.377 (4)
C3—C4	1.401 (5)	C16—C17	1.372 (5)
C4—C8	1.370 (5)	C16—H16	0.9300
C4—O1	1.384 (4)	C17—C18	1.349 (5)
C5—C6	1.368 (5)	C17—H17	0.9300
C5—H5	0.9300	C18—C19	1.358 (5)
C6—C7	1.378 (6)	C18—F1	1.367 (4)
C6—H6	0.9300	C19—C20	1.389 (5)
C7—C8	1.381 (6)	C19—H19	0.9300
C7—H7	0.9300	C20—H20	0.9300
C8—H8	0.9300	C21—C26	1.383 (4)
C9—C10	1.350 (4)	C21—C22	1.396 (5)
C9—N1	1.381 (4)	C22—C23	1.382 (5)
C10—S1	1.722 (4)	C22—H22	0.9300
C10—H10	0.9300	C23—C24	1.373 (5)
C11—N1	1.300 (4)	C23—H23	0.9300
C11—N3	1.359 (4)	C24—C25	1.365 (5)
C11—S1	1.734 (3)	C24—Cl1	1.731 (4)
C12—N3	1.470 (4)	C25—C26	1.385 (5)
C12—C15	1.513 (5)	C25—H25	0.9300
C12—C13	1.528 (5)	C26—H26	0.9300
C12—H12	0.9800	N3—N4	1.380 (3)
C13—C14	1.495 (4)		

C2—C1—O1	110.7 (3)	N4—C14—C13	113.2 (3)
C2—C1—C9	132.1 (3)	C21—C14—C13	124.7 (3)
O1—C1—C9	117.1 (3)	C16—C15—C20	118.1 (3)
C1—C2—C3	108.6 (3)	C16—C15—C12	122.7 (3)
C1—C2—H2	125.7	C20—C15—C12	119.1 (3)
C3—C2—H2	125.7	C17—C16—C15	121.9 (4)
C5—C3—C4	118.5 (3)	C17—C16—H16	119.0
C5—C3—C2	137.1 (4)	C15—C16—H16	119.0
C4—C3—C2	104.4 (3)	C18—C17—C16	118.1 (4)
C8—C4—O1	125.8 (4)	C18—C17—H17	120.9
C8—C4—C3	123.6 (4)	C16—C17—H17	120.9
O1—C4—C3	110.6 (3)	C17—C18—C19	122.8 (4)
C6—C5—C3	118.5 (4)	C17—C18—F1	119.2 (4)
C6—C5—H5	120.7	C19—C18—F1	118.0 (4)
C3—C5—H5	120.7	C18—C19—C20	118.3 (4)
C5—C6—C7	121.5 (4)	C18—C19—H19	120.9
C5—C6—H6	119.3	C20—C19—H19	120.9
C7—C6—H6	119.3	C15—C20—C19	120.7 (4)
C6—C7—C8	121.9 (4)	C15—C20—H20	119.7
C6—C7—H7	119.0	C19—C20—H20	119.7
C8—C7—H7	119.0	C26—C21—C22	117.9 (3)
C4—C8—C7	115.9 (4)	C26—C21—C14	121.9 (3)

C4—C8—H8	122.0	C22—C21—C14	120.2 (3)
C7—C8—H8	122.0	C23—C22—C21	120.9 (3)
C10—C9—N1	115.8 (3)	C23—C22—H22	119.5
C10—C9—C1	127.4 (3)	C21—C22—H22	119.5
N1—C9—C1	116.8 (3)	C24—C23—C22	119.6 (4)
C9—C10—S1	111.0 (3)	C24—C23—H23	120.2
C9—C10—H10	124.5	C22—C23—H23	120.2
S1—C10—H10	124.5	C25—C24—C23	120.7 (3)
N1—C11—N3	121.2 (3)	C25—C24—Cl1	119.7 (3)
N1—C11—S1	116.7 (3)	C23—C24—Cl1	119.6 (3)
N3—C11—S1	122.1 (3)	C24—C25—C26	119.7 (4)
N3—C12—C15	112.3 (3)	C24—C25—H25	120.1
N3—C12—C13	100.4 (3)	C26—C25—H25	120.1
C15—C12—C13	113.6 (3)	C21—C26—C25	121.2 (3)
N3—C12—H12	110.1	C21—C26—H26	119.4
C15—C12—H12	110.1	C25—C26—H26	119.4
C13—C12—H12	110.1	C11—N1—C9	109.0 (3)
C14—C13—C12	103.9 (3)	C11—N3—N4	121.3 (3)
C14—C13—H13A	111.0	C11—N3—C12	123.9 (3)
C12—C13—H13A	111.0	N4—N3—C12	114.4 (3)
C14—C13—H13B	111.0	C14—N4—N3	107.4 (3)
C12—C13—H13B	111.0	C4—O1—C1	105.7 (3)
H13A—C13—H13B	109.0	C10—S1—C11	87.54 (17)
N4—C14—C21	122.0 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19···F1^{i}	0.93	2.58	3.254 (5)	130

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