

S-[2-(2,2-Dimethylpropanamido)-3-(trifluoromethyl)phenyl] *N,N*-diisopropylthiocarbamate

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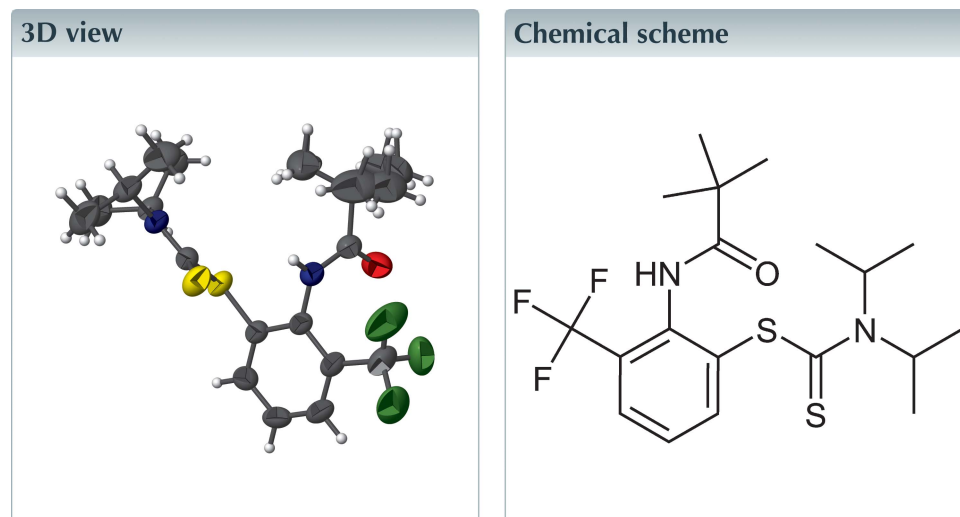
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Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, C₁₉H₂₇F₃N₂OS₂, the dihedral angle between the benzene ring and dithiocarbamate group is 67.00 (9)° and a weak intramolecular N—H···S interaction generates a *S*(7) ring. The *tert*-butyl group is disordered over two orientations in a 0.628 (14):0.372 (14) ratio. In the crystal, inversion dimers linked by pairs of weak C—H···O interactions generate *R*₂²(20) loops and the aromatic rings of neighbouring pairs of molecules are involved in very weak π – π stacking interactions [centroid–centroid separation = 4.0042 (13) Å].



Structure description

Various *N*-(substituted phenyl)pivalamides can be substituted efficiently in reactions with lithium reagents followed by reaction with electrophiles (*e.g.*: Smith *et al.*, 2015; Smith *et al.*, 2012). Recently, the X-ray crystal structure of 4-(pivaloylamino)pyridin-3-yl *N,N*-diisopropylthiocarbamate has been published (El-Hiti *et al.*, 2014). We now describe the synthesis and structure of the title compound (Fig. 1).

An intramolecular N1—H1···S2 contact is observed (Table 1). The crystal packing is shown in Fig. 2 and features inversion dimers linked by weak C—H···O interactions and very weak aromatic π – π stacking interactions [centroid–centroid separation = 4.0042 (13) Å].

Synthesis and crystallization

N-(2-(trifluoromethyl)phenyl)pivalamide and *n*-butyllithium (two equivalents) in anhydrous tetrahydrofuran at 0°C was reacted with tetraisopropylthiuram disulfide (one

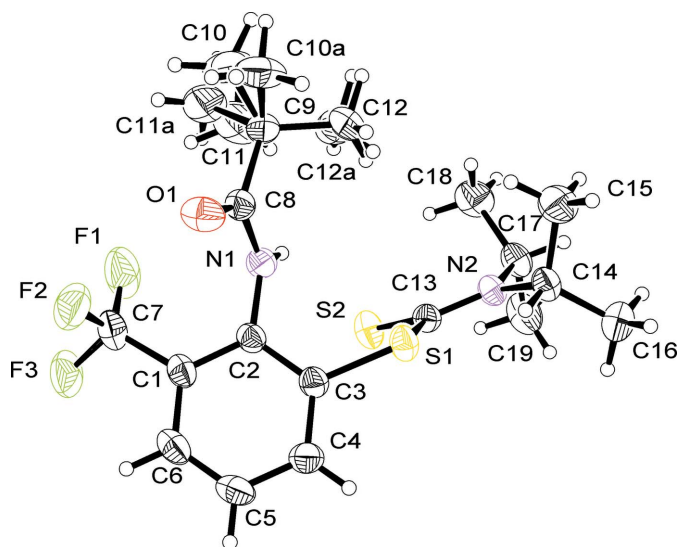


Figure 1
The molecular structure, with displacement ellipsoids at the 50% probability level, showing both orientations of the disordered *tert*-butyl group.

equivalent). Crystallization of the crude product using ethyl acetate as solvent gave colourless blocks, m.p. 129–131°C.

The NMR spectrum indicates that the two *iso*-propyl groups are different, possibly due to restricted rotation about the N–C bond (Chatgililoglu & Asmus, 1990). The NMR assignments are based on predicted chemical shifts and coupling patterns and have not been rigorously confirmed. ¹H NMR (500 MHz, CDCl₃): δ 7.84 (*d*, *J* = 7.8 Hz, 1 H, H-6), 7.74 (*d*, *J* = 7.8 Hz, 1 H, H-4), 7.72 (*br s*, *exch.*, 1 H, NH), 7.48 (*app. t*, *J* =

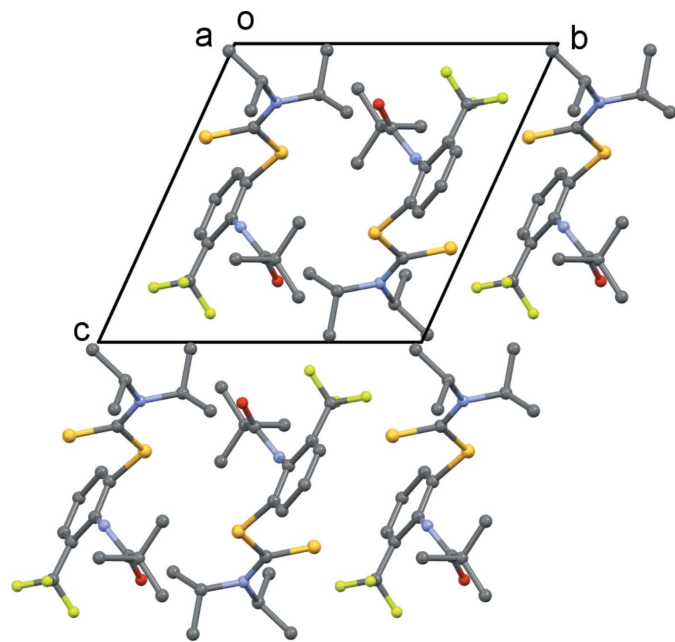


Figure 2
Crystal packing, viewed down [100]. Hydrogen atoms have been omitted for clarity.

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

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
N1–H1···S2	0.86	2.65	3.2576 (18)	129
C14–H14···O1 ⁱ	0.98	2.35	3.097 (4)	132

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

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₉ H ₂₇ F ₃ N ₂ OS ₂
<i>M_r</i>	420.54
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	10.0633 (3), 11.5253 (4), 11.8648 (3)
α , β , γ (°)	103.597 (2), 112.018 (3), 109.899 (3)
<i>V</i> (Å ³)	1090.81 (6)
<i>Z</i>	2
Radiation type	Cu <i>K</i> α
μ (mm ⁻¹)	2.53
Crystal size (mm)	0.36 × 0.21 × 0.20
Data collection	
Diffractometer	Agilent SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (<i>CrysAlis PRO</i> ; Agilent, 2014)
<i>T_{min}</i> , <i>T_{max}</i>	0.874, 0.917
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	17158, 4349, 3933
<i>R_{int}</i>	0.022
(sin θ / λ) _{max} (Å ⁻¹)	0.623
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.048, 0.135, 1.08
No. of reflections	4349
No. of parameters	282
No. of restraints	72
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³)	0.70, -0.52

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXS2013* (Sheldrick, 2008), *SHELXL2013* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

7.8 Hz, 1 H, H-5), 4.99, 4.07 [2 *br*, 2 H, 2 CH(CH₃)₂], 1.66, 1.41 [2 *br*, 12 H, 2 CH(CH₃)₂], 1.31 [*s*, 9 H, C(CH₃)₃]; ¹³C NMR (125 MHz, CDCl₃): δ 192.4 (C=S), 177.8 (C=O), 140.6 (C-6), 140.5 (C-1), 133.6 (*m*, C-2), 130.4 (*q*, *J* = 30.1 Hz, C-3), 129.2 (*q*, *J* = 5.0 Hz, C-4), 128.1 (C-5), 123.2 (*q*, *J* = 274.0 Hz, CF₃), 56.5, 52.7 [2 CH(CH₃)₂], 39.1 [C(CH₃)₃], 27.4 [C(CH₃)₃], 20.2, 19.6 [2 CH(CH₃)₂]; EI-MS: *m/z* (%) = 420 (*M*⁺, 12), 259 (31), 244 (72), 219 (23), 144 (80), 102 (100), 100 (41), 57 (26); HRMS (EI): calculated for C₁₉H₂₇F₃N₂OS₂ (*MH*⁺): 420.1517; found: 420.1512.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The *tert*-butyl group is disordered and was modelled with two components with occupancies of 0.628 (14)/0.372 (14).

Funding information

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full crystallographic data

IUCrData (2018). 3, x180029 [https://doi.org/10.1107/S2414314618000299]

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S-[2-(2,2-Dimethylpropanamido)-3-(trifluoromethyl)phenyl] *N,N*-diisopropyl-dithiocarbamate

Crystal data

$C_{19}H_{27}F_3N_2OS_2$	$Z = 2$
$M_r = 420.54$	$F(000) = 444$
Triclinic, $P\bar{1}$	$D_x = 1.280 \text{ Mg m}^{-3}$
$a = 10.0633 (3) \text{ \AA}$	Cu $K\alpha$ radiation, $\lambda = 1.54184 \text{ \AA}$
$b = 11.5253 (4) \text{ \AA}$	Cell parameters from 12098 reflections
$c = 11.8648 (3) \text{ \AA}$	$\theta = 4.4\text{--}74.0^\circ$
$\alpha = 103.597 (2)^\circ$	$\mu = 2.53 \text{ mm}^{-1}$
$\beta = 112.018 (3)^\circ$	$T = 296 \text{ K}$
$\gamma = 109.899 (3)^\circ$	Block, colourless
$V = 1090.81 (6) \text{ \AA}^3$	$0.36 \times 0.21 \times 0.20 \text{ mm}$

Data collection

Agilent SuperNova, Dual, Cu at zero, Atlas diffractometer	4349 independent reflections
ω scans	3933 reflections with $I > 2\sigma(I)$
Absorption correction: gaussian (CrysAlis PRO; Agilent, 2014)	$R_{\text{int}} = 0.022$
$T_{\text{min}} = 0.874$, $T_{\text{max}} = 0.917$	$\theta_{\text{max}} = 74.0^\circ$, $\theta_{\text{min}} = 4.4^\circ$
17158 measured reflections	$h = -12 \rightarrow 12$
	$k = -13 \rightarrow 14$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.048$	$w = 1/[\sigma^2(F_o^2) + (0.0682P)^2 + 0.462P]$
$wR(F^2) = 0.135$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{\text{max}} < 0.001$
4349 reflections	$\Delta\rho_{\text{max}} = 0.70 \text{ e \AA}^{-3}$
282 parameters	$\Delta\rho_{\text{min}} = -0.52 \text{ e \AA}^{-3}$
72 restraints	

Special details

Experimental. CrysAlisPro, Agilent Technologies, Version 1.171.37.33 (release 27-03-2014 CrysAlis171 .NET) (compiled Mar 27 2014, 17:12:48) numerical absorption correction based on gaussian integration over a multifaceted crystal model empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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. Methyl C—H bonds were fixed at 0.96 Å, with displacement parameters 1.5 times $U_{eq}(C)$, and were allowed to spin about the C—C bond. The N—H bond was fixed at 0.86 Å and aromatic C—H distances were set to 0.93 Å and their $U(iso)$ set to 1.2 times the U_{eq} for the atoms to which they are bonded.

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

	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}	Occ. (<1)
C1	0.5618 (2)	0.1992 (2)	0.6694 (2)	0.0492 (5)	
C2	0.4617 (2)	0.23679 (19)	0.58578 (18)	0.0436 (4)	
C3	0.4637 (2)	0.2317 (2)	0.46719 (19)	0.0458 (4)	
C4	0.5665 (3)	0.1937 (2)	0.4360 (2)	0.0550 (5)	
H4	0.5669	0.1905	0.3570	0.066*	
C5	0.6685 (3)	0.1604 (2)	0.5223 (2)	0.0613 (6)	
H5	0.7390	0.1365	0.5022	0.074*	
C6	0.6659 (3)	0.1627 (2)	0.6372 (2)	0.0584 (5)	
H6	0.7342	0.1396	0.6945	0.070*	
C7	0.5636 (3)	0.1943 (3)	0.7954 (3)	0.0671 (6)	
C8	0.4096 (2)	0.3958 (2)	0.7162 (2)	0.0482 (4)	
C9	0.2774 (3)	0.4292 (3)	0.7235 (2)	0.0596 (6)	
C10	0.3551 (12)	0.5554 (10)	0.8486 (7)	0.121 (3)	0.628 (14)
H10A	0.3875	0.5347	0.9252	0.181*	0.628 (14)
H10B	0.2782	0.5882	0.8444	0.181*	0.628 (14)
H10C	0.4491	0.6239	0.8561	0.181*	0.628 (14)
C11	0.1496 (12)	0.3079 (9)	0.7222 (14)	0.115 (3)	0.628 (14)
H11A	0.2034	0.2724	0.7790	0.172*	0.628 (14)
H11B	0.0788	0.2386	0.6326	0.172*	0.628 (14)
H11C	0.0867	0.3369	0.7542	0.172*	0.628 (14)
C12	0.1958 (10)	0.4518 (9)	0.5999 (6)	0.080 (2)	0.628 (14)
H12A	0.1168	0.4785	0.6048	0.121*	0.628 (14)
H12B	0.1424	0.3692	0.5214	0.121*	0.628 (14)
H12C	0.2765	0.5219	0.5954	0.121*	0.628 (14)
C10A	0.3656 (18)	0.5855 (7)	0.8072 (15)	0.095 (4)	0.372 (14)
H10D	0.3964	0.6315	0.7563	0.143*	0.372 (14)
H10E	0.4612	0.6105	0.8883	0.143*	0.372 (14)
H10F	0.2935	0.6107	0.8285	0.143*	0.372 (14)
C11A	0.2190 (19)	0.3623 (14)	0.8041 (16)	0.093 (3)	0.372 (14)
H11D	0.1357	0.3818	0.8098	0.140*	0.372 (14)
H11E	0.3089	0.3970	0.8924	0.140*	0.372 (14)
H11F	0.1757	0.2660	0.7609	0.140*	0.372 (14)
C12A	0.1355 (17)	0.391 (2)	0.5898 (8)	0.113 (5)	0.372 (14)
H12D	0.0662	0.2941	0.5481	0.169*	0.372 (14)
H12E	0.1759	0.4174	0.5335	0.169*	0.372 (14)
H12F	0.0746	0.4357	0.6030	0.169*	0.372 (14)

C13	0.1484 (2)	0.1780 (2)	0.28142 (18)	0.0441 (4)
C14	0.1219 (3)	0.3324 (2)	0.1703 (2)	0.0508 (5)
H14	0.2404	0.3683	0.2152	0.061*
C15	0.0900 (4)	0.4433 (3)	0.2300 (3)	0.0743 (7)
H15A	-0.0252	0.4126	0.1868	0.111*
H15B	0.1432	0.5219	0.2176	0.111*
H15C	0.1316	0.4660	0.3239	0.111*
C16	0.0630 (4)	0.2946 (3)	0.0227 (3)	0.0744 (7)
H16A	0.0758	0.2179	-0.0136	0.112*
H16B	0.1258	0.3700	0.0111	0.112*
H16C	-0.0499	0.2718	-0.0229	0.112*
C17	-0.1287 (2)	0.1370 (2)	0.1281 (2)	0.0564 (5)
H17	-0.1658	0.1857	0.0767	0.068*
C18	-0.1937 (3)	0.1447 (3)	0.2245 (3)	0.0773 (7)
H18A	-0.1688	0.0922	0.2731	0.116*
H18B	-0.3096	0.1093	0.1754	0.116*
H18C	-0.1438	0.2376	0.2859	0.116*
C19	-0.2022 (3)	-0.0068 (3)	0.0255 (3)	0.0786 (8)
H19A	-0.1534	-0.0057	-0.0302	0.118*
H19B	-0.3176	-0.0423	-0.0287	0.118*
H19C	-0.1821	-0.0630	0.0708	0.118*
N1	0.3565 (2)	0.27758 (18)	0.61456 (16)	0.0489 (4)
H1	0.2532	0.2247	0.5651	0.059*
N2	0.05355 (19)	0.21183 (17)	0.19727 (16)	0.0458 (4)
O1	0.55330 (19)	0.46862 (17)	0.79613 (18)	0.0683 (5)
F1	0.4313 (3)	0.1794 (3)	0.8007 (2)	0.1186 (8)
F2	0.6854 (3)	0.30527 (19)	0.90418 (15)	0.0974 (6)
F3	0.5919 (3)	0.09416 (18)	0.81723 (17)	0.0949 (6)
S1	0.36197 (6)	0.29820 (5)	0.36548 (5)	0.05110 (16)
S2	0.08666 (7)	0.04280 (5)	0.31403 (6)	0.05922 (18)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0437 (10)	0.0475 (10)	0.0471 (10)	0.0224 (8)	0.0137 (8)	0.0191 (8)
C2	0.0377 (9)	0.0446 (10)	0.0429 (9)	0.0205 (8)	0.0156 (7)	0.0158 (8)
C3	0.0396 (9)	0.0498 (10)	0.0429 (9)	0.0220 (8)	0.0163 (8)	0.0175 (8)
C4	0.0504 (11)	0.0603 (12)	0.0523 (11)	0.0289 (10)	0.0254 (9)	0.0168 (9)
C5	0.0500 (11)	0.0609 (13)	0.0695 (14)	0.0345 (10)	0.0259 (11)	0.0162 (11)
C6	0.0469 (11)	0.0541 (12)	0.0616 (13)	0.0289 (10)	0.0135 (10)	0.0201 (10)
C7	0.0670 (15)	0.0782 (16)	0.0636 (14)	0.0414 (13)	0.0255 (12)	0.0422 (13)
C8	0.0490 (11)	0.0556 (11)	0.0501 (10)	0.0288 (9)	0.0276 (9)	0.0268 (9)
C9	0.0616 (13)	0.0820 (16)	0.0579 (12)	0.0466 (12)	0.0374 (11)	0.0327 (12)
C10	0.105 (5)	0.167 (6)	0.072 (4)	0.092 (5)	0.033 (3)	-0.001 (4)
C11	0.101 (5)	0.152 (6)	0.173 (8)	0.079 (5)	0.107 (6)	0.099 (6)
C12	0.085 (4)	0.118 (5)	0.081 (3)	0.080 (4)	0.045 (3)	0.052 (3)
C10A	0.108 (6)	0.100 (6)	0.122 (8)	0.071 (5)	0.080 (7)	0.042 (5)
C11A	0.100 (7)	0.132 (7)	0.119 (7)	0.073 (5)	0.089 (6)	0.077 (6)

C12A	0.095 (8)	0.183 (12)	0.078 (6)	0.093 (8)	0.045 (5)	0.038 (7)
C13	0.0421 (9)	0.0462 (10)	0.0400 (9)	0.0224 (8)	0.0174 (8)	0.0148 (8)
C14	0.0446 (10)	0.0562 (11)	0.0546 (11)	0.0258 (9)	0.0217 (9)	0.0297 (9)
C15	0.0895 (19)	0.0542 (13)	0.0849 (18)	0.0357 (13)	0.0461 (16)	0.0308 (13)
C16	0.0861 (18)	0.0880 (18)	0.0624 (14)	0.0449 (16)	0.0399 (14)	0.0415 (14)
C17	0.0386 (10)	0.0569 (12)	0.0615 (12)	0.0209 (9)	0.0148 (9)	0.0256 (10)
C18	0.0533 (13)	0.0873 (19)	0.099 (2)	0.0336 (13)	0.0424 (14)	0.0440 (16)
C19	0.0589 (14)	0.0589 (14)	0.0694 (16)	0.0187 (12)	0.0026 (12)	0.0150 (12)
N1	0.0385 (8)	0.0600 (10)	0.0445 (8)	0.0250 (7)	0.0181 (7)	0.0179 (7)
N2	0.0384 (8)	0.0483 (9)	0.0467 (8)	0.0215 (7)	0.0163 (7)	0.0203 (7)
O1	0.0495 (9)	0.0578 (9)	0.0769 (11)	0.0219 (7)	0.0263 (8)	0.0105 (8)
F1	0.1074 (14)	0.208 (2)	0.1278 (16)	0.0988 (16)	0.0815 (13)	0.1291 (18)
F2	0.1329 (16)	0.0901 (12)	0.0533 (8)	0.0560 (12)	0.0331 (10)	0.0231 (8)
F3	0.1371 (16)	0.0857 (11)	0.0758 (10)	0.0685 (11)	0.0409 (10)	0.0520 (9)
S1	0.0404 (3)	0.0597 (3)	0.0505 (3)	0.0226 (2)	0.0177 (2)	0.0290 (2)
S2	0.0527 (3)	0.0490 (3)	0.0594 (3)	0.0190 (2)	0.0150 (2)	0.0265 (2)

Geometric parameters (Å, °)

C1—C2	1.392 (3)	C10A—H10D	0.9600
C1—C6	1.394 (3)	C10A—H10E	0.9600
C1—C7	1.503 (3)	C10A—H10F	0.9600
C2—C3	1.402 (3)	C11A—H11D	0.9600
C2—N1	1.411 (3)	C11A—H11E	0.9600
C3—C4	1.385 (3)	C11A—H11F	0.9600
C3—S1	1.770 (2)	C12A—H12D	0.9600
C4—C5	1.384 (3)	C12A—H12E	0.9600
C4—H4	0.9300	C12A—H12F	0.9600
C5—C6	1.368 (4)	C13—N2	1.335 (2)
C5—H5	0.9300	C13—S2	1.664 (2)
C6—H6	0.9300	C13—S1	1.803 (2)
C7—F1	1.310 (3)	C14—N2	1.493 (3)
C7—F2	1.332 (3)	C14—C15	1.504 (4)
C7—F3	1.337 (3)	C14—C16	1.515 (3)
C8—O1	1.211 (3)	C14—H14	0.9800
C8—N1	1.359 (3)	C15—H15A	0.9600
C8—C9	1.532 (3)	C15—H15B	0.9600
C9—C10	1.507 (6)	C15—H15C	0.9600
C9—C12A	1.513 (7)	C16—H16A	0.9600
C9—C11A	1.520 (7)	C16—H16B	0.9600
C9—C12	1.522 (5)	C16—H16C	0.9600
C9—C11	1.536 (6)	C17—N2	1.498 (2)
C9—C10A	1.558 (7)	C17—C18	1.515 (4)
C10—H10A	0.9600	C17—C19	1.522 (4)
C10—H10B	0.9600	C17—H17	0.9800
C10—H10C	0.9600	C18—H18A	0.9600
C11—H11A	0.9600	C18—H18B	0.9600
C11—H11B	0.9600	C18—H18C	0.9600

C11—H11C	0.9600	C19—H19A	0.9600
C12—H12A	0.9600	C19—H19B	0.9600
C12—H12B	0.9600	C19—H19C	0.9600
C12—H12C	0.9600	N1—H1	0.8600
C2—C1—C6	120.0 (2)	H10D—C10A—H10F	109.5
C2—C1—C7	123.1 (2)	H10E—C10A—H10F	109.5
C6—C1—C7	116.90 (19)	C9—C11A—H11D	109.5
C1—C2—C3	118.57 (18)	C9—C11A—H11E	109.5
C1—C2—N1	122.61 (18)	H11D—C11A—H11E	109.5
C3—C2—N1	118.80 (17)	C9—C11A—H11F	109.5
C4—C3—C2	120.60 (19)	H11D—C11A—H11F	109.5
C4—C3—S1	116.70 (16)	H11E—C11A—H11F	109.5
C2—C3—S1	121.95 (15)	C9—C12A—H12D	109.5
C5—C4—C3	119.9 (2)	C9—C12A—H12E	109.5
C5—C4—H4	120.0	H12D—C12A—H12E	109.5
C3—C4—H4	120.0	C9—C12A—H12F	109.5
C6—C5—C4	120.1 (2)	H12D—C12A—H12F	109.5
C6—C5—H5	120.0	H12E—C12A—H12F	109.5
C4—C5—H5	120.0	N2—C13—S2	126.48 (15)
C5—C6—C1	120.7 (2)	N2—C13—S1	113.18 (14)
C5—C6—H6	119.6	S2—C13—S1	120.33 (11)
C1—C6—H6	119.6	N2—C14—C15	111.50 (19)
F1—C7—F2	105.7 (3)	N2—C14—C16	112.07 (19)
F1—C7—F3	107.3 (2)	C15—C14—C16	112.0 (2)
F2—C7—F3	103.7 (2)	N2—C14—H14	107.0
F1—C7—C1	115.9 (2)	C15—C14—H14	107.0
F2—C7—C1	112.5 (2)	C16—C14—H14	107.0
F3—C7—C1	110.9 (2)	C14—C15—H15A	109.5
O1—C8—N1	121.13 (19)	C14—C15—H15B	109.5
O1—C8—C9	122.8 (2)	H15A—C15—H15B	109.5
N1—C8—C9	116.04 (18)	C14—C15—H15C	109.5
C12A—C9—C11A	111.0 (6)	H15A—C15—H15C	109.5
C10—C9—C12	110.6 (5)	H15B—C15—H15C	109.5
C10—C9—C8	109.1 (4)	C14—C16—H16A	109.5
C12A—C9—C8	115.1 (6)	C14—C16—H16B	109.5
C11A—C9—C8	108.0 (5)	H16A—C16—H16B	109.5
C12—C9—C8	107.8 (3)	C14—C16—H16C	109.5
C10—C9—C11	111.3 (4)	H16A—C16—H16C	109.5
C12—C9—C11	108.8 (4)	H16B—C16—H16C	109.5
C8—C9—C11	109.1 (3)	N2—C17—C18	112.87 (19)
C12A—C9—C10A	109.8 (6)	N2—C17—C19	113.3 (2)
C11A—C9—C10A	107.0 (5)	C18—C17—C19	113.3 (2)
C8—C9—C10A	105.5 (6)	N2—C17—H17	105.5
C9—C10—H10A	109.5	C18—C17—H17	105.5
C9—C10—H10B	109.5	C19—C17—H17	105.5
H10A—C10—H10B	109.5	C17—C18—H18A	109.5
C9—C10—H10C	109.5	C17—C18—H18B	109.5

H10A—C10—H10C	109.5	H18A—C18—H18B	109.5
H10B—C10—H10C	109.5	C17—C18—H18C	109.5
C9—C11—H11A	109.5	H18A—C18—H18C	109.5
C9—C11—H11B	109.5	H18B—C18—H18C	109.5
H11A—C11—H11B	109.5	C17—C19—H19A	109.5
C9—C11—H11C	109.5	C17—C19—H19B	109.5
H11A—C11—H11C	109.5	H19A—C19—H19B	109.5
H11B—C11—H11C	109.5	C17—C19—H19C	109.5
C9—C12—H12A	109.5	H19A—C19—H19C	109.5
C9—C12—H12B	109.5	H19B—C19—H19C	109.5
H12A—C12—H12B	109.5	C8—N1—C2	123.57 (17)
C9—C12—H12C	109.5	C8—N1—H1	118.2
H12A—C12—H12C	109.5	C2—N1—H1	118.2
H12B—C12—H12C	109.5	C13—N2—C14	122.25 (16)
C9—C10A—H10D	109.5	C13—N2—C17	123.01 (17)
C9—C10A—H10E	109.5	C14—N2—C17	114.67 (16)
H10D—C10A—H10E	109.5	C3—S1—C13	105.47 (9)
C9—C10A—H10F	109.5		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1...S2	0.86	2.65	3.2576 (18)	129
C14—H14...O1 ⁱ	0.98	2.35	3.097 (4)	132

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