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Diethyl 5,5′-thiobis[2-amino-4-(4-fluorophenyl)-1-phenyl-1*H*-pyrrole-3-carboxylate]

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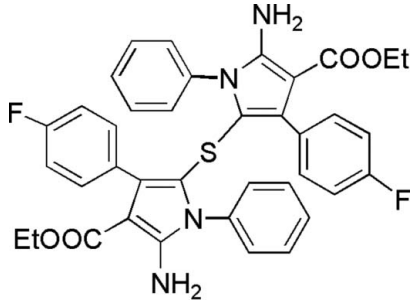
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.047; wR factor = 0.135; data-to-parameter ratio = 12.2.

In the title compound, $C_{38}H_{32}F_2N_4O_4S$, the ethyl chain of the ethoxycarbonyl group displays rotational disorder with site occupancy factors *ca* 0.6 and 0.4. The S atom lies on a twofold rotation axis. There are both inter- and intramolecular hydrogen bonds in the crystal structure. An intramolecular N—H···O hydrogen bond forms a six-membered ring, while an intermolecular N—H···F hydrogen bond results in a chain.

Related literature

For related literature, see: Yin & Pidgeon (1997); Herradura *et al.* (2000); Baumgarten & Tyutyulkov (1998); Barton & Ollis (1979).



Experimental

Crystal data

$C_{38}H_{32}F_2N_4O_4S$
M_r = 678.74
Monoclinic, $C2/c$
a = 12.158 (3) Å
b = 19.160 (4) Å
c = 14.958 (3) Å
β = 106.944 (4)°
V = 3333.0 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.16 mm^{-1}
T = 294 (2) K
0.20 × 0.18 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.970, T_{max} = 0.973
8487 measured reflections
2942 independent reflections
1645 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.135
S = 1.08
2942 reflections
241 parameters
31 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···F1^{ii}	0.90	2.49	3.181 (3)	134
N2—H2B···O1	0.90	2.23	2.825 (3)	124

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2503).

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supporting information

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S1. Comment

Organic sulfides represent important building blocks in organic and medicinal chemistry (Barton *et al.*, 1979) due to their diverse biological and pharmacological properties (Herradura *et al.*, 2000). Because of their synthetic and biological potential, considerable interest has been focused on the synthesis of organic sulfides (Yin *et al.*, 1997). In addition, polysubstituted pyrroles are molecular frameworks having immense importance in material science (Baumgarten *et al.*, 1998). In order to develop new biological activities, we synthesized the title compound, (I) (Fig.1), the structure of which is reported here.

The title compound adopts a V conformation, which contains two parts which are same to each other, and each part comprises three rings, two phenyl rings and one pyrrole ring. In each part, the two phenyl rings are not conjugated with the pyrrole ring, with the dihedral angle of 49.07° and 73.04°, respectively.

All the bond lengths and angles (Table 1) in the title compound are within the normal range. The bond lengths of C7—C8 (1.356 Å) and C9—C10 (1.380 Å) in the pyrrole ring is obviously shorter than C—C (1.52 Å) but are close to normal C?C (1.32 Å), it is indicated that they are both C?C. The bond length of C7—C10 (1.454 Å) is between C—C and C?C.

X-ray analysis reveals that there exists both intermolecular hydrogen and intromolecular hydrogen bonds in the crystal structure (Fig. 2). The intromolecular N2—H2B···O1 hydrogen bond forms a six-membered ring, while the intermolecular N2—H2A···F1 hydrogen bond makes the molecule extended in line.

S2. Experimental

A mixture of 2-(4-fluorophenyl)-2-oxo-*N*-phenylethanethioamide (3 mmol, 0.819 g), ethyl 2-cyanoacetate (3 mmol, 0.339 g), 10% NaOH solution (0.5 ml), and 15 ml e thanol in a 25 ml flask was stirred for 3 h at room temperature (monitored by TLC). The yellow solid was got by filtering. And then the solid was added to a stirred solution of acetic acid (1 ml) in ethanol (15 ml) at 313 K under MW for 30 min. After cooling to room temperature, the solid product was then got by filtering. The pure product was purified by recrystallization from ethanol (m.p. 498 K).

S3. Refinement

All H atoms were placed in calculated positions, with C—H distances in the range 0.93 - 0.97 Å, and N—H = 0.90 Å and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C,*N*). The ethyl chain of the ethoxycarbonyl group displays rotational disorder. The site-occupation factors of the disordered atoms C12, C13 and C12′, C13′ refined to 0.588 (14) and 0.412 (146), respectively.

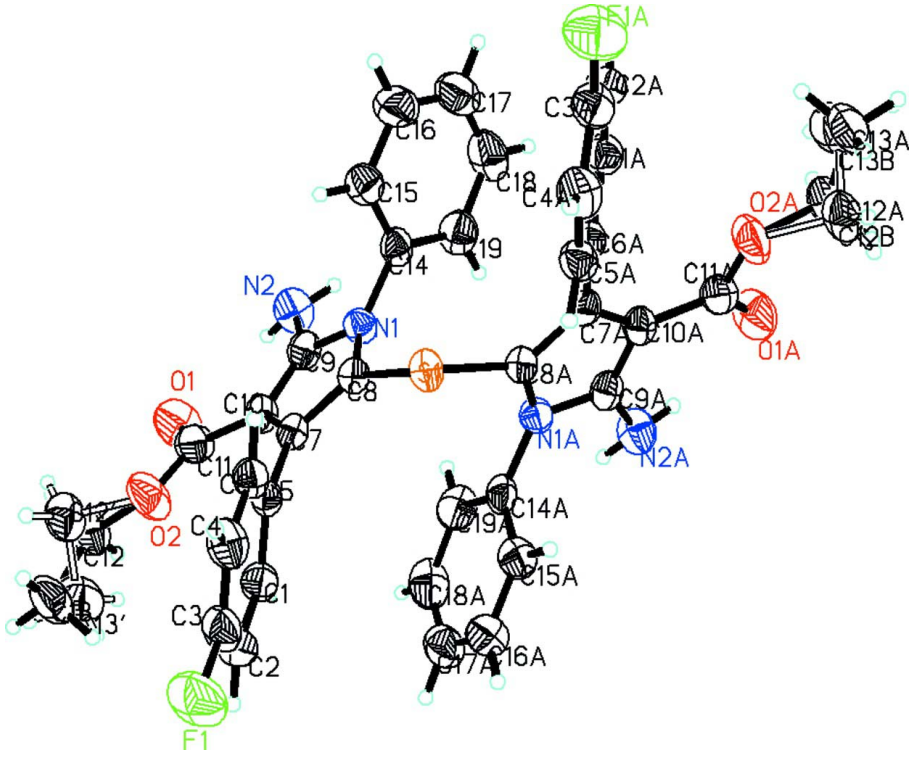

Figure 1

View of the title compound with 35% probability ellipsoid. Both disordered components are shown.

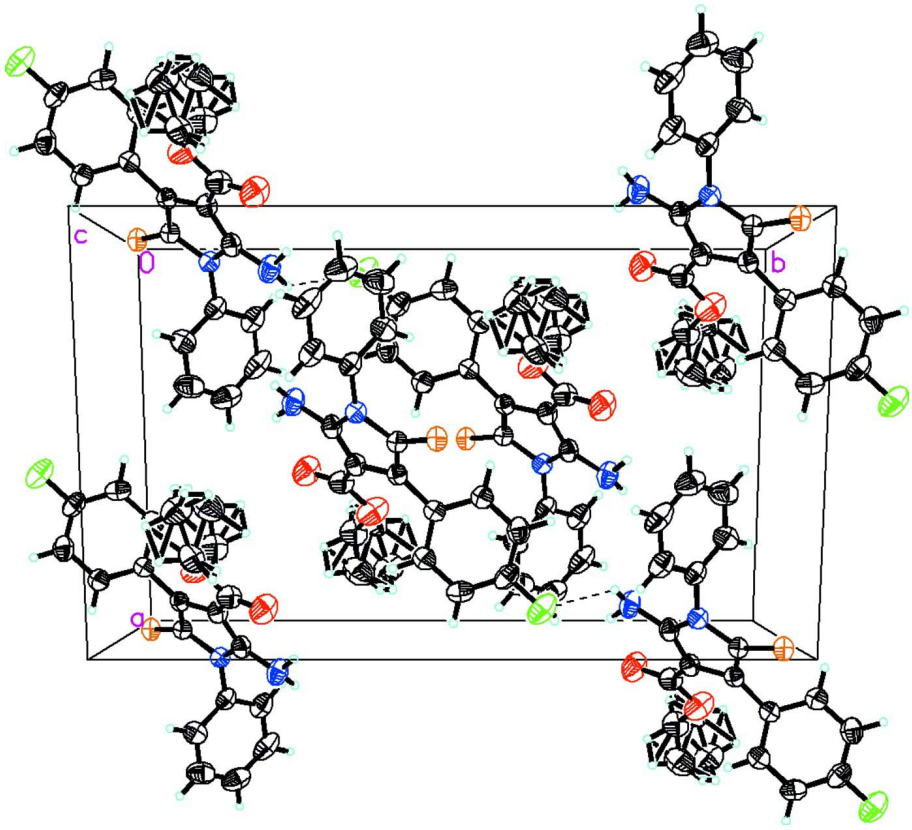

Figure 2

The packing of the title compound viewed along the *c* axis. Hydrogen bonds are shown as dashed lines.

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$c = 14.958$ (3) Å
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$V = 3333.0$ (13) Å^3
$Z = 4$
$F(000) = 1416$
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Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1735 reflections
$\theta = 2.6$–21.3°
$\mu = 0.16$ mm^{-1}
$T = 294$ K
Prism, yellow
0.20 × 0.18 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.970$, $T_{max} = 0.973$
8487 measured reflections
2942 independent reflections
1645 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -14 \rightarrow 8$
$k = -22 \rightarrow 21$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.135$
$S = 1.08$
2942 reflections
241 parameters
31 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.060P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.0000	0.02157 (5)	0.2500	0.0518 (3)	
F1	0.41195 (19)	−0.13211 (10)	0.15342 (15)	0.1094 (7)	
O1	0.0803 (2)	0.21900 (12)	−0.06429 (16)	0.0943 (8)	
O2	0.1802 (2)	0.11943 (13)	−0.04003 (15)	0.0918 (8)	
N1	−0.0635 (2)	0.13810 (11)	0.13685 (14)	0.0495 (6)	
N2	−0.0895 (2)	0.23284 (12)	0.02943 (17)	0.0715 (8)	
H2A	−0.1284	0.2575	0.0614	0.086*	
H2B	−0.0521	0.2595	−0.0014	0.086*	
C1	0.2891 (3)	0.04044 (15)	0.13523 (18)	0.0581 (8)	
H1	0.3128	0.0867	0.1378	0.070*	
C2	0.3696 (3)	−0.01205 (18)	0.14655 (19)	0.0669 (9)	
H2	0.4470	−0.0017	0.1566	0.080*	
C3	0.3327 (3)	−0.08003 (18)	0.1426 (2)	0.0680 (9)	
C4	0.2211 (3)	−0.09736 (16)	0.1275 (2)	0.0687 (9)	
H4	0.1986	−0.1439	0.1249	0.082*	
C5	0.1410 (3)	−0.04417 (14)	0.11607 (17)	0.0555 (8)	
H5	0.0638	−0.0554	0.1055	0.067*	
C6	0.1734 (2)	0.02548 (14)	0.12005 (16)	0.0458 (7)	
C7	0.0855 (2)	0.07966 (13)	0.11175 (17)	0.0460 (7)	
C8	0.0077 (2)	0.07882 (13)	0.16089 (17)	0.0455 (7)	
C9	−0.0292 (3)	0.17553 (14)	0.07162 (18)	0.0532 (8)	
C10	0.0626 (3)	0.14193 (14)	0.05373 (18)	0.0518 (7)	
C11	0.1072 (3)	0.16536 (19)	−0.0206 (2)	0.0672 (9)	
C12	0.2371 (9)	0.1505 (5)	−0.1060 (7)	0.079 (3)	0.588 (14)
H12A	0.2721	0.1950	−0.0832	0.094*	0.588 (14)

H12B	0.1829	0.1570	−0.1674	0.094*	0.588 (14)
C13	0.3270 (9)	0.0970 (6)	−0.1087 (6)	0.095 (3)	0.588 (14)
H13A	0.3698	0.1129	−0.1496	0.142*	0.588 (14)
H13B	0.2903	0.0535	−0.1312	0.142*	0.588 (14)
H13C	0.3783	0.0907	−0.0469	0.142*	0.588 (14)
C12′	0.2111 (9)	0.1190 (9)	−0.1291 (6)	0.080 (4)	0.412 (14)
H12C	0.1642	0.1513	−0.1743	0.095*	0.412 (14)
H12D	0.2047	0.0727	−0.1563	0.095*	0.412 (14)
C13′	0.3355 (12)	0.1429 (10)	−0.0939 (9)	0.113 (5)	0.412 (14)
H13D	0.3671	0.1462	−0.1456	0.170*	0.412 (14)
H13E	0.3791	0.1099	−0.0493	0.170*	0.412 (14)
H13F	0.3388	0.1878	−0.0648	0.170*	0.412 (14)
C14	−0.1757 (3)	0.14464 (15)	0.14982 (18)	0.0524 (7)	
C15	−0.2597 (3)	0.09787 (17)	0.1047 (2)	0.0688 (9)	
H15	−0.2425	0.0621	0.0690	0.083*	
C16	−0.3690 (3)	0.1044 (2)	0.1128 (2)	0.0853 (11)	
H16	−0.4256	0.0726	0.0827	0.102*	
C17	−0.3948 (4)	0.1564 (3)	0.1640 (3)	0.0874 (12)	
H17	−0.4694	0.1605	0.1682	0.105*	
C18	−0.3129 (4)	0.2029 (2)	0.2097 (3)	0.0886 (12)	
H18	−0.3316	0.2384	0.2452	0.106*	
C19	−0.2004 (3)	0.19735 (16)	0.2033 (2)	0.0741 (10)	
H19	−0.1438	0.2287	0.2345	0.089*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0657 (8)	0.0467 (6)	0.0470 (6)	0.000	0.0226 (5)	0.000
F1	0.1062 (17)	0.0986 (14)	0.1301 (17)	0.0439 (14)	0.0450 (15)	0.0001 (13)
O1	0.110 (2)	0.0893 (16)	0.0968 (17)	0.0169 (15)	0.0499 (16)	0.0455 (14)
O2	0.0972 (19)	0.1199 (19)	0.0773 (15)	0.0303 (16)	0.0551 (15)	0.0414 (14)
N1	0.0517 (15)	0.0512 (13)	0.0475 (13)	0.0019 (12)	0.0175 (12)	0.0028 (11)
N2	0.091 (2)	0.0552 (15)	0.0735 (16)	0.0113 (15)	0.0327 (16)	0.0166 (13)
C1	0.059 (2)	0.0615 (18)	0.0543 (18)	−0.0052 (18)	0.0178 (16)	−0.0033 (14)
C2	0.052 (2)	0.089 (2)	0.061 (2)	0.005 (2)	0.0178 (17)	0.0000 (18)
C3	0.076 (3)	0.070 (2)	0.061 (2)	0.026 (2)	0.0260 (19)	−0.0023 (17)
C4	0.085 (3)	0.0581 (19)	0.068 (2)	0.000 (2)	0.031 (2)	−0.0103 (16)
C5	0.059 (2)	0.0592 (19)	0.0512 (17)	−0.0006 (17)	0.0206 (15)	−0.0082 (14)
C6	0.0503 (18)	0.0531 (17)	0.0353 (14)	−0.0031 (15)	0.0147 (13)	−0.0013 (12)
C7	0.0507 (18)	0.0471 (16)	0.0380 (14)	−0.0035 (14)	0.0094 (13)	−0.0042 (12)
C8	0.0503 (18)	0.0468 (15)	0.0399 (15)	0.0003 (14)	0.0139 (14)	−0.0007 (12)
C9	0.066 (2)	0.0473 (16)	0.0453 (16)	−0.0019 (16)	0.0141 (16)	0.0030 (13)
C10	0.061 (2)	0.0505 (16)	0.0451 (16)	−0.0028 (15)	0.0181 (15)	0.0061 (13)
C11	0.063 (2)	0.078 (2)	0.062 (2)	−0.0014 (19)	0.0203 (18)	0.0137 (18)
C12	0.086 (6)	0.093 (6)	0.068 (5)	−0.005 (5)	0.039 (4)	0.013 (4)
C13	0.098 (6)	0.118 (6)	0.089 (5)	0.016 (5)	0.059 (4)	0.013 (4)
C12′	0.097 (7)	0.081 (7)	0.073 (6)	−0.022 (6)	0.044 (5)	0.008 (5)
C13′	0.101 (8)	0.126 (9)	0.121 (8)	−0.026 (7)	0.046 (6)	−0.009 (7)

C14	0.063 (2)	0.0549 (17)	0.0414 (15)	0.0123 (16)	0.0187 (15)	0.0105 (14)
C15	0.070 (2)	0.078 (2)	0.062 (2)	−0.007 (2)	0.0243 (19)	0.0014 (17)
C16	0.068 (3)	0.110 (3)	0.079 (3)	−0.006 (2)	0.025 (2)	0.015 (2)
C17	0.072 (3)	0.114 (3)	0.083 (3)	0.023 (3)	0.032 (2)	0.036 (2)
C18	0.105 (3)	0.091 (3)	0.080 (3)	0.050 (3)	0.043 (3)	0.019 (2)
C19	0.084 (3)	0.072 (2)	0.065 (2)	0.022 (2)	0.020 (2)	−0.0003 (17)

Geometric parameters (Å, º)

S1—C8	1.750 (2)	C9—C10	1.380 (4)
S1—C8^{i}	1.750 (2)	C10—C11	1.443 (4)
F1—C3	1.363 (3)	C12—C13	1.507 (8)
O1—C11	1.211 (3)	C12—H12A	0.9700
O2—C11	1.341 (4)	C12—H12B	0.9700
O2—C12	1.484 (6)	C13—H13A	0.9600
O2—C12′	1.485 (8)	C13—H13B	0.9600
N1—C9	1.370 (3)	C13—H13C	0.9600
N1—C8	1.409 (3)	C12′—C13′	1.520 (9)
N1—C14	1.438 (3)	C12′—H12C	0.9700
N2—C9	1.368 (3)	C12′—H12D	0.9700
N2—H2A	0.8989	C13′—H13D	0.9600
N2—H2B	0.8954	C13′—H13E	0.9600
C1—C2	1.379 (4)	C13′—H13F	0.9600
C1—C6	1.388 (4)	C14—C19	1.375 (4)
C1—H1	0.9300	C14—C15	1.378 (4)
C2—C3	1.373 (4)	C15—C16	1.375 (4)
C2—H2	0.9300	C15—H15	0.9300
C3—C4	1.350 (4)	C16—C17	1.349 (5)
C4—C5	1.385 (4)	C16—H16	0.9300
C4—H4	0.9300	C17—C18	1.363 (5)
C5—C6	1.388 (4)	C17—H17	0.9300
C5—H5	0.9300	C18—C19	1.403 (5)
C6—C7	1.469 (4)	C18—H18	0.9300
C7—C8	1.356 (3)	C19—H19	0.9300
C7—C10	1.454 (3)		

C8—S1—C8^{i}	102.35 (16)	O2—C12—C13	103.1 (6)
C11—O2—C12	110.3 (4)	O2—C12—H12A	111.1
C11—O2—C12′	123.7 (6)	C13—C12—H12A	111.1
C12—O2—C12′	28.1 (4)	O2—C12—H12B	111.1
C9—N1—C8	108.2 (2)	C13—C12—H12B	111.1
C9—N1—C14	123.2 (2)	H12A—C12—H12B	109.1
C8—N1—C14	124.8 (2)	C12—C13—H13A	109.5
C9—N2—H2A	118.1	C12—C13—H13B	109.5
C9—N2—H2B	114.3	H13A—C13—H13B	109.5
H2A—N2—H2B	113.4	C12—C13—H13C	109.5
C2—C1—C6	121.2 (3)	H13A—C13—H13C	109.5
C2—C1—H1	119.4	H13B—C13—H13C	109.5

C6—C1—H1	119.4	O2—C12′—C13′	100.0 (9)
C3—C2—C1	118.4 (3)	O2—C12′—H12C	111.8
C3—C2—H2	120.8	C13′—C12′—H12C	111.8
C1—C2—H2	120.8	O2—C12′—H12D	111.8
C4—C3—F1	118.7 (3)	C13′—C12′—H12D	111.8
C4—C3—C2	122.7 (3)	H12C—C12′—H12D	109.5
F1—C3—C2	118.6 (3)	C12′—C13′—H13D	109.5
C3—C4—C5	118.4 (3)	C12′—C13′—H13E	109.5
C3—C4—H4	120.8	H13D—C13′—H13E	109.5
C5—C4—H4	120.8	C12′—C13′—H13F	109.5
C4—C5—C6	121.4 (3)	H13D—C13′—H13F	109.5
C4—C5—H5	119.3	H13E—C13′—H13F	109.5
C6—C5—H5	119.3	C19—C14—C15	120.4 (3)
C1—C6—C5	117.9 (3)	C19—C14—N1	121.3 (3)
C1—C6—C7	123.1 (2)	C15—C14—N1	118.3 (3)
C5—C6—C7	119.0 (3)	C16—C15—C14	119.7 (3)
C8—C7—C10	106.9 (2)	C16—C15—H15	120.1
C8—C7—C6	123.4 (2)	C14—C15—H15	120.1
C10—C7—C6	129.6 (2)	C17—C16—C15	120.5 (4)
C7—C8—N1	109.0 (2)	C17—C16—H16	119.7
C7—C8—S1	128.4 (2)	C15—C16—H16	119.7
N1—C8—S1	122.32 (19)	C16—C17—C18	120.7 (4)
N2—C9—N1	121.0 (3)	C16—C17—H17	119.6
N2—C9—C10	129.8 (3)	C18—C17—H17	119.6
N1—C9—C10	109.0 (2)	C17—C18—C19	120.0 (3)
C9—C10—C11	120.7 (3)	C17—C18—H18	120.0
C9—C10—C7	107.0 (2)	C19—C18—H18	120.0
C11—C10—C7	131.7 (3)	C14—C19—C18	118.6 (3)
O1—C11—O2	122.2 (3)	C14—C19—H19	120.7
O1—C11—C10	125.2 (3)	C18—C19—H19	120.7
O2—C11—C10	112.6 (3)		

C6—C1—C2—C3	−0.1 (4)	N2—C9—C10—C7	−173.8 (3)
C1—C2—C3—C4	0.4 (5)	N1—C9—C10—C7	0.2 (3)
C1—C2—C3—F1	179.8 (3)	C8—C7—C10—C9	0.0 (3)
F1—C3—C4—C5	−179.6 (2)	C6—C7—C10—C9	180.0 (3)
C2—C3—C4—C5	−0.3 (5)	C8—C7—C10—C11	−171.0 (3)
C3—C4—C5—C6	−0.2 (4)	C6—C7—C10—C11	9.0 (5)
C2—C1—C6—C5	−0.4 (4)	C12—O2—C11—O1	11.3 (7)
C2—C1—C6—C7	177.2 (2)	C12′—O2—C11—O1	−16.7 (7)
C4—C5—C6—C1	0.5 (4)	C12—O2—C11—C10	−171.2 (6)
C4—C5—C6—C7	−177.2 (2)	C12′—O2—C11—C10	160.8 (6)
C1—C6—C7—C8	−129.7 (3)	C9—C10—C11—O1	9.6 (5)
C5—C6—C7—C8	47.9 (3)	C7—C10—C11—O1	179.6 (3)
C1—C6—C7—C10	50.3 (4)	C9—C10—C11—O2	−167.8 (3)
C5—C6—C7—C10	−132.1 (3)	C7—C10—C11—O2	2.2 (5)
C10—C7—C8—N1	−0.2 (3)	C11—O2—C12—C13	171.9 (9)
C6—C7—C8—N1	179.8 (2)	C12′—O2—C12—C13	−63.9 (13)

C10—C7—C8—S1	−173.5 (2)	C11—O2—C12′—C13′	110.4 (13)
C6—C7—C8—S1	6.5 (4)	C12—O2—C12′—C13′	41.5 (12)
C9—N1—C8—C7	0.4 (3)	C9—N1—C14—C19	−82.7 (3)
C14—N1—C8—C7	159.1 (2)	C8—N1—C14—C19	121.7 (3)
C9—N1—C8—S1	174.16 (19)	C9—N1—C14—C15	95.3 (3)
C14—N1—C8—S1	−27.2 (3)	C8—N1—C14—C15	−60.3 (3)
C8^{i}—S1—C8—C7	128.1 (3)	C19—C14—C15—C16	0.5 (4)
C8^{i}—S1—C8—N1	−44.36 (16)	N1—C14—C15—C16	−177.5 (3)
C8—N1—C9—N2	174.3 (2)	C14—C15—C16—C17	0.4 (5)
C14—N1—C9—N2	15.2 (4)	C15—C16—C17—C18	−0.8 (5)
C8—N1—C9—C10	−0.4 (3)	C16—C17—C18—C19	0.4 (5)
C14—N1—C9—C10	−159.5 (2)	C15—C14—C19—C18	−0.9 (4)
N2—C9—C10—C11	−1.6 (5)	N1—C14—C19—C18	177.0 (3)
N1—C9—C10—C11	172.5 (2)	C17—C18—C19—C14	0.4 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···F1^{ii}	0.90	2.49	3.181 (3)	134
N2—H2*B*···O1	0.90	2.23	2.825 (3)	124

Symmetry code: (ii) *x*−1/2, *y*+1/2, *z*.