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# Methyl 4-(4-fluorophenyl)-6-isopropyl-2-(methylsulfonyl)pyrimidine-5-carboxylate

**Wei He,[a] Hong-Shun Sun,[a] Chun-Xiang Ji,[a] Dong-Ling Yang[b] and Cheng Guo[a]***

[a]Department of Applied Chemistry, College of Science, Nanjing University of Technolgy, Xinmofan Road No. 5, Nanjing 210009, People's Republic of China, and [b]Nanjing Frochem Tech. Co. Ltd, Xinmofan Road No. 36, Nanjing 210009, People's Republic of China
Correspondence e-mail: guocheng@njut.edu.cn

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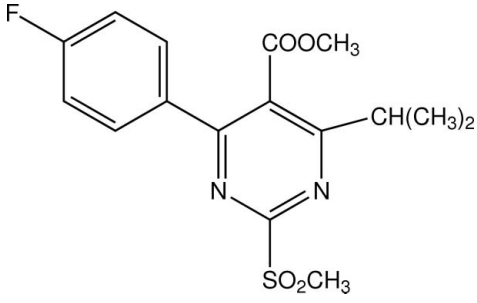
Key indicators: single-crystal X-ray study; $T$ = 294 K; mean $\sigma$(C–C) = 0.008 Å; $R$ factor = 0.079; $wR$ factor = 0.207; data-to-parameter ratio = 15.9.

The asymmetric unit of the title compound, $C_{16}H_{17}FN_2O_4S$, contains three independent molecules, in which the pyrimidine and benzene rings are oriented at dihedral angles of 41.72 (3)°, 26.21 (3)° and 36.49 (3)°. Intramolecular C—H···O hydrogen bonds result in the formation of two six- and one seven-membered non-planar rings, which have have twist conformations. In the crystal structure, intermolecular C—H···O hydrogen bonds link the molecules.

## Related literature

For related literature, see: Gompper *et al.* (1997); Laufer & Wagner (2002). For bond-length data, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{16}H_{17}FN_2O_4S$ $M_r$ = 352.39
Monoclinic, $P2_1/c$
$a$ = 28.875 (6) Å
$b$ = 9.887 (2) Å
$c$ = 18.400 (4) Å
$\beta$ = 98.09 (3)°
$V$ = 5200.7 (18) Å$^3$
$Z$ = 12
Mo $K\alpha$ radiation
$\mu$ = 0.22 mm$^{-1}$
$T$ = 294 (2) K
0.40 × 0.20 × 0.20 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.918, $T_{max}$ = 0.958
10466 measured reflections
10124 independent reflections
4777 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.066
3 standard reflections
frequency: 120 min
intensity decay: none

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.206
$S$ = 1.03
10124 reflections
637 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.58 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C3—H3$B$···O1 | 0.98 | 2.54 | 3.089 (7) | 115 |
| C17—H17$C$···F1 | 0.96 | 2.51 | 3.191 (8) | 128 |
| C19—H19$A$···O6 | 0.98 | 2.55 | 3.224 (7) | 126 |
| C28—H28$A$···O6 | 0.93 | 2.56 | 3.378 (6) | 147 |
| C8—H8$B$···O3$^{i}$ | 0.96 | 2.48 | 3.373 (6) | 155 |
| C35—H35$A$···O12$^{ii}$ | 0.98 | 2.57 | 3.484 (6) | 154 |
| C42—H42$A$···O9$^{iii}$ | 0.96 | 2.43 | 3.229 (6) | 141 |
| C48—H48$A$···O12$^{iv}$ | 0.93 | 2.42 | 3.224 (6) | 146 |

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2457).

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# supporting information

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# Methyl 4-(4-fluorophenyl)-6-isopropyl-2-(methylsulfonyl)pyrimidine-5-carboxylate

**Wei He, Hong-Shun Sun, Chun-Xiang Ji, Dong-Ling Yang and Cheng Guo**

## S1. Comment

Some derivatives of pyrimidine are important chemical materials. We report herein the crystal structure of the title compound, (I).

The asymmetric unit of the title compound, (I), (Fig. 1) contains three independent molecules. Rings A (N1/N2/C4-C7), B (C11-C16), C (N3/N4/C20-C23), D (C27-C32), E (N5/N6/C36-C9) and F (C43-C48) are, of course, planar, and the dihedral angles between them are A/B = 41.72 (3)°, B/C = 26.21 (3)° and D/E = 36.49 (3)°. The intramolecular C-H···O hydrogen bonds (Table 1) result in the formation of two six- and one seven-membered non-planar rings: G (O1/C3-C5/C9/H3B), H (O6/C19-C21/C25/H19A) and I (O6/C21/C22/C25/C27/C28/H28A). They adopt twisted conformations, having total puckering amplitudes, $Q_T$, of 0.788 (3) Å, 1.806 (3) Å and 1.290 (3) Å, respectively.

In the crystal structure, intermolecular C-H···O hydrogen bonds (Table 1) link the molecules (Fig. 2), in which they may be effective in the stabilization of the structure.

## S2. Experimental

For the preparation of the title compound, methyl4-(4-fluorophenyl)-6-isopropyl -2-(methylthio)pyrimidine-5-carboxylate (100 g, 312.50 mmol), ammonium molybdate tetrahydrate (4.95 g, 4.00 mmol) and sulfuric acid (0.32 g, 3.26 mmol) were added to methanol (1000 ml) in a round bottom flask, and then stirred for 1 h at 303 K. $H_2O_2$ (106.2 ml) was added dropwise in 30 min, and stirred for 2 h. The mixture was stirred for 5 h, by increasing the temperatue to 323 K. After completion of the reaction, the mixture was cooled to 273 K and stirred for 1 h. It was filtered, washed with water, and then dried (yield; 88%). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

## S3. Refinement

H atoms were positioned geometrically, with C-H = 0.93, 0.98 and 0.96 Å for aromatic, methine and methyl H, respectively, and constrained to ride on their parent atoms with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

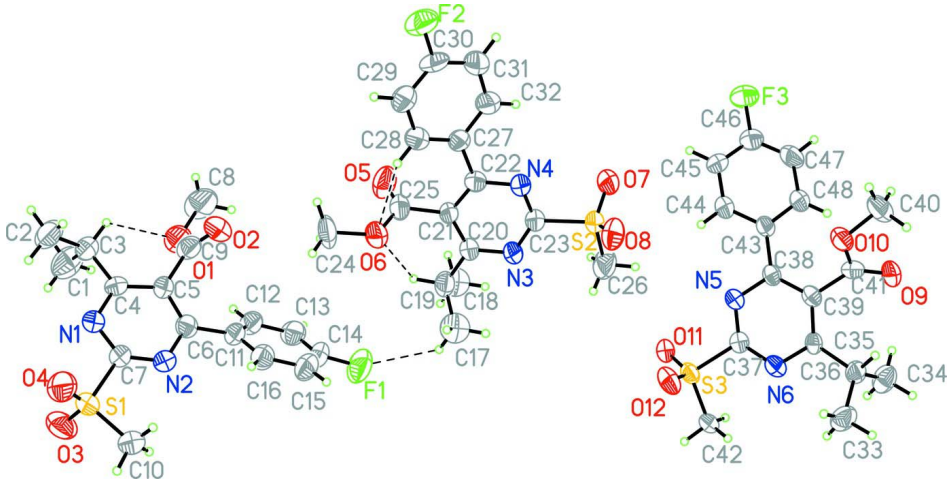


**Figure 1**

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines.

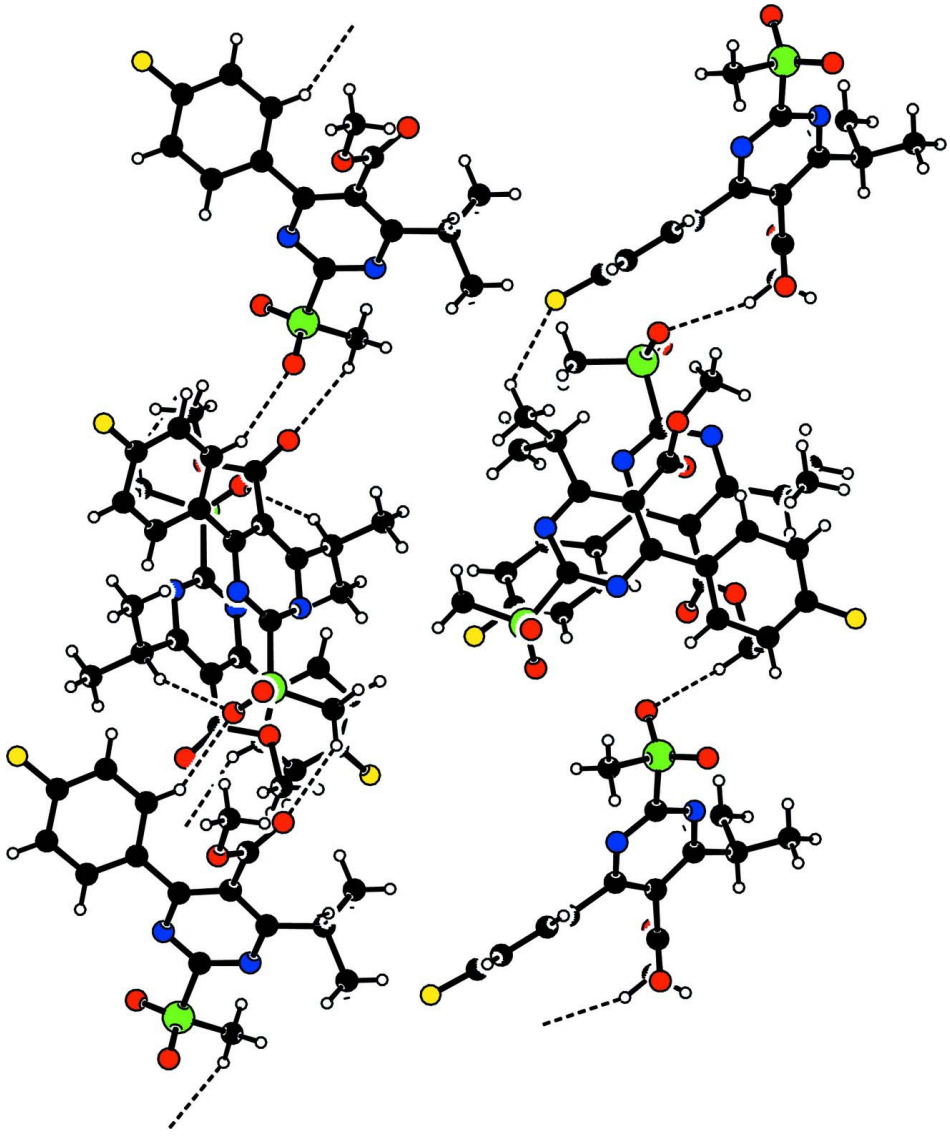

**Figure 2**

A partial packing diagram of (I). Hydrogen bonds are shown as dashed lines.

**Methyl 4-(4-fluorophenyl)-6-isopropyl-2-(methylsulfonyl)pyrimidine-5-carboxylate**

*Crystal data*

$C_{16}H_{17}FN_2O_4S$
$M_r = 352.39$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 28.875\ (6)$ Å
$b = 9.887\ (2)$ Å
$c = 18.400\ (4)$ Å
$\beta = 98.09\ (3)°$
$V = 5200.7\ (18)$ Å$^3$
$Z = 12$
$F(000) = 2208$
$D_x = 1.350$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9–12°$
$\mu = 0.22$ mm$^{-1}$
$T = 294$ K
Block, colorless
0.40 × 0.20 × 0.20 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.918, $T_{max}$ = 0.958
10466 measured reflections
10124 independent reflections
4777 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.066
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 1.4°
$h$ = −34→34
$k$ = 0→11
$l$ = 0→22
3 standard reflections every 120 min
intensity decay: none

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.206
$S$ = 1.03
10124 reflections
637 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.080P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.42 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.58 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 $F^2 > 2\text{sigma}(F^2)$ 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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.14585 (5) | 0.53855 (18) | 0.81769 (7) | 0.0619 (4) |
| O1 | 0.06944 (14) | 0.1784 (4) | 0.5211 (2) | 0.0781 (12) |
| O2 | 0.08271 (14) | 0.3803 (5) | 0.4713 (2) | 0.0777 (13) |
| O3 | 0.15061 (15) | 0.4344 (5) | 0.8708 (2) | 0.0881 (14) |
| O4 | 0.11470 (14) | 0.6475 (4) | 0.8258 (2) | 0.0848 (13) |
| N1 | 0.08452 (15) | 0.4164 (4) | 0.7203 (2) | 0.0531 (11) |
| N2 | 0.15938 (14) | 0.4561 (5) | 0.6845 (2) | 0.0538 (11) |
| F1 | 0.29201 (13) | 0.3184 (4) | 0.4561 (2) | 0.1078 (14) |
| C1 | 0.0211 (2) | 0.1644 (6) | 0.6804 (4) | 0.096 (2) |
| H1B | 0.0424 | 0.1062 | 0.6596 | 0.144* |
| H1C | −0.0097 | 0.1262 | 0.6722 | 0.144* |
| H1D | 0.0310 | 0.1735 | 0.7322 | 0.144* |
| C2 | −0.0138 (2) | 0.3993 (7) | 0.6734 (4) | 0.084 (2) |
| H2B | −0.0142 | 0.4842 | 0.6479 | 0.125* |
| H2C | −0.0043 | 0.4138 | 0.7249 | 0.125* |
| H2D | −0.0445 | 0.3602 | 0.6657 | 0.125* |

| | | | | |
|---|---|---|---|---|
| C3 | 0.02057 (18) | 0.3038 (5) | 0.6440 (3) | 0.0578 (14) |
| H3B | 0.0105 | 0.2918 | 0.5913 | 0.069* |
| C4 | 0.06945 (16) | 0.3576 (5) | 0.6538 (3) | 0.0466 (12) |
| C5 | 0.09929 (17) | 0.3535 (5) | 0.6005 (3) | 0.0455 (12) |
| C6 | 0.14539 (18) | 0.3964 (5) | 0.6189 (3) | 0.0463 (12) |
| C7 | 0.12823 (17) | 0.4613 (5) | 0.7291 (3) | 0.0484 (13) |
| C8 | 0.0534 (2) | 0.1242 (8) | 0.4483 (4) | 0.109 (3) |
| H8A | 0.0455 | 0.0305 | 0.4523 | 0.164* |
| H8B | 0.0779 | 0.1330 | 0.4182 | 0.164* |
| H8C | 0.0264 | 0.1734 | 0.4265 | 0.164* |
| C9 | 0.08202 (18) | 0.3085 (6) | 0.5234 (3) | 0.0559 (14) |
| C10 | 0.20124 (19) | 0.6025 (7) | 0.8115 (3) | 0.0742 (18) |
| H10A | 0.2133 | 0.6466 | 0.8567 | 0.111* |
| H10B | 0.1993 | 0.6664 | 0.7719 | 0.111* |
| H10C | 0.2217 | 0.5297 | 0.8025 | 0.111* |
| C11 | 0.18219 (17) | 0.3796 (5) | 0.5712 (3) | 0.0474 (13) |
| C12 | 0.18688 (19) | 0.2589 (6) | 0.5343 (3) | 0.0569 (14) |
| H12A | 0.1652 | 0.1901 | 0.5365 | 0.068* |
| C13 | 0.22339 (19) | 0.2399 (6) | 0.4946 (3) | 0.0616 (15) |
| H13A | 0.2263 | 0.1598 | 0.4691 | 0.074* |
| C14 | 0.2548 (2) | 0.3406 (7) | 0.4936 (3) | 0.0682 (17) |
| C15 | 0.2519 (2) | 0.4624 (7) | 0.5281 (3) | 0.0737 (18) |
| H15A | 0.2736 | 0.5306 | 0.5245 | 0.088* |
| C16 | 0.21536 (19) | 0.4801 (6) | 0.5686 (3) | 0.0577 (14) |
| H16A | 0.2131 | 0.5602 | 0.5943 | 0.069* |
| S2 | 0.30615 (5) | 0.60184 (15) | 0.02405 (7) | 0.0538 (4) |
| O5 | 0.14659 (15) | 0.3704 (4) | 0.2138 (2) | 0.0810 (13) |
| O6 | 0.18226 (13) | 0.5146 (4) | 0.29765 (19) | 0.0654 (11) |
| O7 | 0.28275 (14) | 0.5614 (5) | −0.04534 (19) | 0.0805 (13) |
| O8 | 0.32002 (14) | 0.7407 (4) | 0.0338 (2) | 0.0748 (12) |
| N3 | 0.28601 (14) | 0.4816 (4) | 0.1474 (2) | 0.0481 (10) |
| N4 | 0.22682 (15) | 0.6175 (4) | 0.0759 (2) | 0.0514 (11) |
| F2 | 0.02822 (11) | 0.8653 (4) | 0.0472 (2) | 0.0861 (11) |
| C17 | 0.3160 (2) | 0.4249 (7) | 0.3020 (4) | 0.088 |
| H17A | 0.3074 | 0.5104 | 0.3210 | 0.132* |
| H17B | 0.3400 | 0.4383 | 0.2716 | 0.132* |
| H17C | 0.3274 | 0.3660 | 0.3420 | 0.132* |
| C18 | 0.2865 (2) | 0.2228 (6) | 0.2288 (4) | 0.086 |
| H18A | 0.2589 | 0.1828 | 0.2020 | 0.128* |
| H18B | 0.2982 | 0.1656 | 0.2694 | 0.128* |
| H18C | 0.3099 | 0.2329 | 0.1970 | 0.128* |
| C19 | 0.27420 (19) | 0.3627 (6) | 0.2577 (3) | 0.0592 (15) |
| H19A | 0.2498 | 0.3512 | 0.2892 | 0.071* |
| C20 | 0.25592 (17) | 0.4539 (5) | 0.1949 (3) | 0.0474 (12) |
| C21 | 0.20956 (17) | 0.5053 (5) | 0.1837 (3) | 0.0440 (12) |
| C22 | 0.19646 (17) | 0.5897 (5) | 0.1238 (3) | 0.0446 (12) |
| C23 | 0.26833 (18) | 0.5614 (5) | 0.0913 (3) | 0.0515 (13) |
| C24 | 0.1506 (2) | 0.4707 (7) | 0.3498 (3) | 0.094 (2) |

| | | | | |
|---|---|---|---|---|
| H24A | 0.1581 | 0.5191 | 0.3952 | 0.141* |
| H24B | 0.1544 | 0.3754 | 0.3588 | 0.141* |
| H24C | 0.1188 | 0.4891 | 0.3293 | 0.141* |
| C25 | 0.1753 (2) | 0.4533 (6) | 0.2322 (3) | 0.0517 (13) |
| C26 | 0.3550 (2) | 0.4989 (7) | 0.0467 (4) | 0.088 (2) |
| H26A | 0.3768 | 0.5148 | 0.0128 | 0.132* |
| H26B | 0.3455 | 0.4057 | 0.0440 | 0.132* |
| H26C | 0.3695 | 0.5194 | 0.0956 | 0.132* |
| C27 | 0.15002 (17) | 0.6563 (5) | 0.1054 (3) | 0.0460 (12) |
| C28 | 0.12203 (18) | 0.6904 (5) | 0.1578 (3) | 0.0545 (14) |
| H28A | 0.1313 | 0.6676 | 0.2067 | 0.065* |
| C29 | 0.08071 (19) | 0.7578 (6) | 0.1378 (3) | 0.0629 (16) |
| H29A | 0.0614 | 0.7781 | 0.1727 | 0.075* |
| C30 | 0.06822 (19) | 0.7948 (6) | 0.0661 (3) | 0.0653 (16) |
| C31 | 0.0941 (2) | 0.7609 (7) | 0.0118 (3) | 0.0755 (19) |
| H31A | 0.0842 | 0.7836 | −0.0370 | 0.091* |
| C32 | 0.13540 (19) | 0.6920 (6) | 0.0324 (3) | 0.0663 (16) |
| H32A | 0.1539 | 0.6687 | −0.0032 | 0.080* |
| S3 | 0.49545 (4) | 0.64141 (12) | 0.08480 (6) | 0.0412 (3) |
| O9 | 0.51612 (12) | 0.9595 (4) | −0.23235 (17) | 0.0565 (9) |
| O10 | 0.44927 (12) | 1.0270 (3) | −0.19608 (17) | 0.0496 (9) |
| O11 | 0.47036 (11) | 0.5155 (3) | 0.07353 (16) | 0.0494 (9) |
| O12 | 0.47873 (13) | 0.7416 (3) | 0.13142 (17) | 0.0572 (10) |
| N5 | 0.45677 (13) | 0.7060 (4) | −0.04859 (19) | 0.0377 (9) |
| N6 | 0.53247 (14) | 0.7946 (4) | −0.0098 (2) | 0.0429 (10) |
| F3 | 0.29254 (12) | 0.6619 (4) | −0.30536 (18) | 0.1047 (14) |
| C33 | 0.59905 (19) | 0.9978 (6) | −0.0043 (3) | 0.0654 (16) |
| H33A | 0.5771 | 1.0440 | 0.0214 | 0.098* |
| H33B | 0.6241 | 1.0580 | −0.0112 | 0.098* |
| H33C | 0.6114 | 0.9208 | 0.0238 | 0.098* |
| C34 | 0.60853 (18) | 0.8738 (5) | −0.1197 (3) | 0.0620 (15) |
| H34A | 0.5927 | 0.8462 | −0.1667 | 0.093* |
| H34B | 0.6198 | 0.7954 | −0.0919 | 0.093* |
| H34C | 0.6344 | 0.9313 | −0.1264 | 0.093* |
| C35 | 0.57467 (17) | 0.9510 (5) | −0.0785 (3) | 0.0437 (12) |
| H35A | 0.5648 | 1.0320 | −0.1073 | 0.052* |
| C36 | 0.53143 (15) | 0.8689 (4) | −0.0722 (2) | 0.0335 (10) |
| C37 | 0.49502 (16) | 0.7209 (4) | −0.0025 (2) | 0.0320 (10) |
| C38 | 0.45494 (16) | 0.7761 (4) | −0.1125 (2) | 0.0346 (10) |
| C39 | 0.49147 (16) | 0.8610 (4) | −0.1245 (2) | 0.0343 (10) |
| C40 | 0.4413 (2) | 1.1136 (5) | −0.2599 (3) | 0.0640 (16) |
| H40A | 0.4129 | 1.1637 | −0.2592 | 0.096* |
| H40B | 0.4387 | 1.0593 | −0.3036 | 0.096* |
| H40C | 0.4670 | 1.1753 | −0.2593 | 0.096* |
| C41 | 0.48822 (16) | 0.9515 (5) | −0.1902 (3) | 0.0397 (11) |
| C42 | 0.55448 (16) | 0.6089 (5) | 0.1152 (2) | 0.0459 (12) |
| H42A | 0.5576 | 0.5657 | 0.1623 | 0.069* |
| H42B | 0.5715 | 0.6926 | 0.1192 | 0.069* |

| | | | | |
|---|---|---|---|---|
| H42C | 0.5668 | 0.5507 | 0.0808 | 0.069* |
| C43 | 0.41179 (16) | 0.7494 (4) | −0.1652 (2) | 0.0372 (11) |
| C44 | 0.37025 (18) | 0.7269 (5) | −0.1387 (3) | 0.0524 (13) |
| H44A | 0.3693 | 0.7319 | −0.0885 | 0.063* |
| C45 | 0.33026 (18) | 0.6972 (6) | −0.1854 (3) | 0.0682 (17) |
| H45A | 0.3022 | 0.6821 | −0.1674 | 0.082* |
| C46 | 0.3326 (2) | 0.6902 (6) | −0.2588 (3) | 0.0651 (16) |
| C47 | 0.3727 (2) | 0.7107 (6) | −0.2877 (3) | 0.0601 (15) |
| H47A | 0.3730 | 0.7049 | −0.3380 | 0.072* |
| C48 | 0.41319 (18) | 0.7402 (5) | −0.2408 (2) | 0.0467 (12) |
| H48A | 0.4411 | 0.7539 | −0.2594 | 0.056* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0506 (9) | 0.0947 (11) | 0.0395 (8) | −0.0079 (9) | 0.0030 (6) | −0.0031 (8) |
| O1 | 0.070 (3) | 0.091 (3) | 0.073 (3) | −0.008 (2) | 0.011 (2) | −0.030 (2) |
| O2 | 0.076 (3) | 0.106 (3) | 0.049 (2) | 0.006 (2) | 0.001 (2) | 0.003 (2) |
| O3 | 0.095 (3) | 0.112 (3) | 0.052 (2) | −0.013 (3) | −0.004 (2) | 0.020 (3) |
| O4 | 0.066 (3) | 0.111 (3) | 0.079 (3) | 0.016 (3) | 0.014 (2) | −0.035 (3) |
| N1 | 0.043 (3) | 0.073 (3) | 0.042 (2) | 0.002 (2) | 0.005 (2) | 0.002 (2) |
| N2 | 0.040 (2) | 0.075 (3) | 0.046 (3) | −0.002 (2) | 0.004 (2) | 0.000 (2) |
| F1 | 0.071 (3) | 0.155 (4) | 0.108 (3) | −0.005 (2) | 0.047 (2) | −0.024 (3) |
| C1 | 0.074 (5) | 0.082 (5) | 0.134 (7) | −0.021 (4) | 0.020 (4) | 0.014 (5) |
| C2 | 0.047 (4) | 0.109 (5) | 0.097 (5) | −0.007 (4) | 0.015 (3) | −0.023 (4) |
| C3 | 0.044 (3) | 0.072 (4) | 0.058 (3) | −0.001 (3) | 0.009 (3) | −0.005 (3) |
| C4 | 0.035 (3) | 0.056 (3) | 0.046 (3) | −0.005 (2) | −0.002 (2) | −0.003 (3) |
| C5 | 0.040 (3) | 0.055 (3) | 0.043 (3) | 0.004 (2) | 0.010 (2) | 0.000 (3) |
| C6 | 0.049 (3) | 0.044 (3) | 0.046 (3) | −0.005 (2) | 0.008 (2) | 0.004 (2) |
| C7 | 0.039 (3) | 0.061 (3) | 0.045 (3) | 0.000 (3) | 0.006 (2) | 0.002 (3) |
| C8 | 0.079 (5) | 0.137 (7) | 0.111 (6) | −0.019 (5) | 0.009 (4) | −0.071 (5) |
| C9 | 0.041 (3) | 0.063 (4) | 0.063 (4) | 0.003 (3) | 0.007 (3) | −0.013 (3) |
| C10 | 0.050 (4) | 0.112 (5) | 0.059 (4) | −0.014 (4) | 0.001 (3) | −0.008 (4) |
| C11 | 0.037 (3) | 0.058 (3) | 0.049 (3) | 0.004 (3) | 0.010 (2) | 0.003 (3) |
| C12 | 0.044 (3) | 0.066 (4) | 0.061 (4) | 0.004 (3) | 0.009 (3) | 0.005 (3) |
| C13 | 0.054 (4) | 0.068 (4) | 0.063 (4) | 0.013 (3) | 0.009 (3) | −0.008 (3) |
| C14 | 0.045 (3) | 0.102 (5) | 0.062 (4) | −0.008 (3) | 0.021 (3) | −0.006 (4) |
| C15 | 0.055 (4) | 0.096 (5) | 0.073 (4) | −0.026 (4) | 0.018 (3) | −0.006 (4) |
| C16 | 0.054 (4) | 0.062 (3) | 0.058 (4) | −0.006 (3) | 0.012 (3) | −0.003 (3) |
| S2 | 0.0423 (8) | 0.0774 (10) | 0.0432 (8) | −0.0012 (7) | 0.0115 (6) | 0.0141 (7) |
| O5 | 0.074 (3) | 0.084 (3) | 0.092 (3) | −0.028 (3) | 0.034 (2) | −0.005 (3) |
| O6 | 0.063 (3) | 0.089 (3) | 0.047 (2) | 0.007 (2) | 0.0173 (19) | −0.002 (2) |
| O7 | 0.066 (3) | 0.135 (4) | 0.042 (2) | −0.025 (3) | 0.0103 (19) | 0.003 (2) |
| O8 | 0.074 (3) | 0.073 (3) | 0.082 (3) | −0.016 (2) | 0.029 (2) | 0.013 (2) |
| N3 | 0.048 (3) | 0.056 (3) | 0.042 (2) | −0.001 (2) | 0.009 (2) | 0.014 (2) |
| N4 | 0.042 (3) | 0.070 (3) | 0.042 (2) | 0.000 (2) | 0.009 (2) | 0.011 (2) |
| F2 | 0.049 (2) | 0.103 (3) | 0.103 (3) | 0.0164 (19) | 0.0001 (18) | 0.012 (2) |
| C17 | 0.088 | 0.088 | 0.088 | 0.000 | 0.012 | 0.000 |

| | | | | | | |
|---|---|---|---|---|---|---|
| C18 | 0.086 | 0.086 | 0.086 | 0.000 | 0.012 | 0.000 |
| C19 | 0.050 (3) | 0.074 (4) | 0.057 (3) | 0.005 (3) | 0.021 (3) | 0.010 (3) |
| C20 | 0.045 (3) | 0.056 (3) | 0.041 (3) | −0.004 (3) | 0.009 (2) | 0.006 (3) |
| C21 | 0.043 (3) | 0.055 (3) | 0.035 (3) | −0.008 (2) | 0.009 (2) | 0.000 (2) |
| C22 | 0.043 (3) | 0.049 (3) | 0.041 (3) | −0.003 (2) | 0.003 (2) | −0.001 (2) |
| C23 | 0.044 (3) | 0.072 (4) | 0.040 (3) | −0.007 (3) | 0.009 (2) | 0.002 (3) |
| C24 | 0.087 (5) | 0.145 (6) | 0.061 (4) | 0.019 (5) | 0.045 (4) | 0.030 (4) |
| C25 | 0.056 (4) | 0.053 (3) | 0.050 (3) | 0.005 (3) | 0.020 (3) | 0.008 (3) |
| C26 | 0.057 (4) | 0.119 (6) | 0.094 (5) | 0.026 (4) | 0.033 (4) | 0.032 (4) |
| C27 | 0.038 (3) | 0.055 (3) | 0.045 (3) | 0.007 (2) | 0.007 (2) | −0.001 (3) |
| C28 | 0.051 (3) | 0.064 (4) | 0.047 (3) | 0.003 (3) | 0.003 (3) | 0.000 (3) |
| C29 | 0.049 (4) | 0.075 (4) | 0.067 (4) | 0.011 (3) | 0.016 (3) | −0.003 (3) |
| C30 | 0.033 (3) | 0.083 (4) | 0.076 (4) | 0.013 (3) | −0.008 (3) | 0.008 (4) |
| C31 | 0.055 (4) | 0.113 (5) | 0.059 (4) | 0.022 (4) | 0.009 (3) | 0.025 (4) |
| C32 | 0.047 (3) | 0.099 (5) | 0.052 (4) | 0.012 (3) | 0.005 (3) | 0.002 (3) |
| S3 | 0.0468 (7) | 0.0510 (7) | 0.0270 (6) | 0.0044 (6) | 0.0087 (5) | 0.0025 (6) |
| O9 | 0.057 (2) | 0.079 (2) | 0.038 (2) | −0.002 (2) | 0.0198 (18) | 0.0074 (19) |
| O10 | 0.057 (2) | 0.054 (2) | 0.0382 (19) | 0.0029 (18) | 0.0064 (16) | 0.0090 (17) |
| O11 | 0.050 (2) | 0.060 (2) | 0.041 (2) | −0.0063 (17) | 0.0139 (16) | 0.0081 (17) |
| O12 | 0.076 (3) | 0.061 (2) | 0.0372 (19) | 0.015 (2) | 0.0180 (18) | 0.0050 (18) |
| N5 | 0.043 (2) | 0.040 (2) | 0.030 (2) | 0.0006 (18) | 0.0060 (17) | 0.0033 (17) |
| N6 | 0.053 (2) | 0.041 (2) | 0.035 (2) | 0.0003 (19) | 0.0030 (18) | 0.0041 (18) |
| F3 | 0.067 (2) | 0.172 (4) | 0.066 (2) | −0.050 (3) | −0.0211 (19) | 0.012 (2) |
| C33 | 0.056 (4) | 0.080 (4) | 0.061 (4) | −0.024 (3) | 0.010 (3) | −0.023 (3) |
| C34 | 0.054 (3) | 0.068 (4) | 0.069 (4) | −0.007 (3) | 0.026 (3) | −0.017 (3) |
| C35 | 0.050 (3) | 0.041 (3) | 0.041 (3) | −0.013 (2) | 0.007 (2) | −0.003 (2) |
| C36 | 0.039 (2) | 0.032 (2) | 0.032 (2) | −0.001 (2) | 0.0138 (19) | −0.002 (2) |
| C37 | 0.039 (3) | 0.022 (2) | 0.037 (2) | 0.0067 (19) | 0.011 (2) | −0.0030 (19) |
| C38 | 0.041 (3) | 0.035 (2) | 0.030 (2) | 0.003 (2) | 0.011 (2) | −0.002 (2) |
| C39 | 0.044 (3) | 0.031 (2) | 0.028 (2) | 0.006 (2) | 0.0080 (19) | −0.0020 (19) |
| C40 | 0.082 (4) | 0.060 (4) | 0.047 (3) | 0.001 (3) | 0.002 (3) | 0.017 (3) |
| C41 | 0.035 (3) | 0.044 (3) | 0.038 (3) | 0.003 (2) | −0.003 (2) | −0.004 (2) |
| C42 | 0.044 (3) | 0.060 (3) | 0.032 (3) | −0.001 (3) | 0.001 (2) | 0.010 (2) |
| C43 | 0.044 (3) | 0.036 (3) | 0.032 (2) | −0.003 (2) | 0.006 (2) | 0.004 (2) |
| C44 | 0.050 (3) | 0.073 (4) | 0.034 (3) | −0.008 (3) | 0.010 (2) | 0.005 (3) |
| C45 | 0.036 (3) | 0.119 (5) | 0.048 (3) | −0.019 (3) | −0.002 (3) | 0.011 (3) |
| C46 | 0.053 (4) | 0.087 (4) | 0.051 (4) | −0.022 (3) | −0.006 (3) | 0.006 (3) |
| C47 | 0.070 (4) | 0.074 (4) | 0.033 (3) | −0.008 (3) | −0.001 (3) | 0.000 (3) |
| C48 | 0.049 (3) | 0.059 (3) | 0.033 (3) | −0.003 (3) | 0.009 (2) | −0.001 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—O3 | 1.412 (4) | C19—H19A | 0.9800 |
| S1—O4 | 1.425 (4) | C20—C21 | 1.420 (7) |
| S1—C7 | 1.807 (5) | C21—C22 | 1.391 (6) |
| S1—C10 | 1.738 (6) | C21—C25 | 1.513 (7) |
| O1—C8 | 1.456 (7) | C22—C27 | 1.490 (6) |
| O1—C9 | 1.335 (6) | C24—H24A | 0.9600 |

| | | | |
|---|---|---|---|
| O2—C9 | 1.195 (6) | C24—H24B | 0.9600 |
| N1—C4 | 1.369 (6) | C24—H24C | 0.9600 |
| N1—C7 | 1.326 (6) | C26—H26A | 0.9600 |
| N2—C6 | 1.353 (6) | C26—H26B | 0.9600 |
| N2—C7 | 1.301 (6) | C26—H26C | 0.9600 |
| F1—C14 | 1.374 (6) | C27—C28 | 1.384 (6) |
| C1—C3 | 1.530 (8) | C27—C32 | 1.395 (7) |
| C1—H1B | 0.9600 | C28—C29 | 1.371 (7) |
| C1—H1C | 0.9600 | C28—H28A | 0.9300 |
| C1—H1D | 0.9600 | C29—C30 | 1.367 (7) |
| C2—C3 | 1.523 (7) | C29—H29A | 0.9300 |
| C2—H2B | 0.9600 | C30—C31 | 1.371 (8) |
| C2—H2C | 0.9600 | C31—C32 | 1.380 (7) |
| C2—H2D | 0.9600 | C31—H31A | 0.9300 |
| C3—C4 | 1.495 (7) | C32—H32A | 0.9300 |
| C3—H3B | 0.9800 | S3—O11 | 1.440 (3) |
| C4—C5 | 1.395 (6) | S3—O12 | 1.438 (3) |
| C5—C6 | 1.393 (6) | S3—C37 | 1.786 (4) |
| C5—C9 | 1.503 (7) | S3—C42 | 1.747 (5) |
| C6—C11 | 1.480 (6) | O9—C41 | 1.198 (5) |
| C8—H8A | 0.9600 | O10—C40 | 1.446 (5) |
| C8—H8B | 0.9600 | O10—C41 | 1.341 (5) |
| C8—H8C | 0.9600 | N5—C37 | 1.303 (5) |
| C10—H10A | 0.9600 | N5—C38 | 1.360 (5) |
| C10—H10B | 0.9600 | N6—C36 | 1.360 (5) |
| C10—H10C | 0.9600 | N6—C37 | 1.326 (5) |
| C11—C12 | 1.388 (7) | F3—C46 | 1.369 (6) |
| C11—C16 | 1.386 (7) | C33—C35 | 1.517 (6) |
| C12—C13 | 1.378 (7) | C33—H33A | 0.9600 |
| C12—H12A | 0.9300 | C33—H33B | 0.9600 |
| C13—C14 | 1.349 (8) | C33—H33C | 0.9600 |
| C13—H13A | 0.9300 | C34—C35 | 1.523 (6) |
| C14—C15 | 1.369 (8) | C34—H34A | 0.9600 |
| C15—C16 | 1.385 (7) | C34—H34B | 0.9600 |
| C15—H15A | 0.9300 | C34—H34C | 0.9600 |
| C16—H16A | 0.9300 | C35—C36 | 1.508 (6) |
| S2—O7 | 1.416 (4) | C35—H35A | 0.9800 |
| S2—O8 | 1.435 (4) | C36—C39 | 1.397 (6) |
| S2—C23 | 1.807 (5) | C38—C39 | 1.390 (6) |
| S2—C26 | 1.742 (6) | C38—C43 | 1.491 (6) |
| O5—C25 | 1.180 (6) | C39—C41 | 1.496 (6) |
| O6—C24 | 1.481 (6) | C40—H40A | 0.9600 |
| O6—C25 | 1.338 (6) | C40—H40B | 0.9600 |
| N3—C20 | 1.346 (6) | C40—H40C | 0.9600 |
| N3—C23 | 1.341 (6) | C42—H42A | 0.9600 |
| N4—C22 | 1.356 (6) | C42—H42B | 0.9600 |
| N4—C23 | 1.315 (6) | C42—H42C | 0.9600 |
| F2—C30 | 1.352 (6) | C43—C44 | 1.375 (6) |

| | | | |
|---|---|---|---|
| C17—C19 | 1.490 (8) | C43—C48 | 1.401 (6) |
| C17—H17A | 0.9600 | C44—C45 | 1.370 (7) |
| C17—H17B | 0.9600 | C44—H44A | 0.9300 |
| C17—H17C | 0.9600 | C45—C46 | 1.363 (7) |
| C18—C19 | 1.541 (8) | C45—H45A | 0.9300 |
| C18—H18A | 0.9600 | C46—C47 | 1.355 (7) |
| C18—H18B | 0.9600 | C47—C48 | 1.382 (7) |
| C18—H18C | 0.9600 | C47—H47A | 0.9300 |
| C19—C20 | 1.501 (7) | C48—H48A | 0.9300 |
| | | | |
| O3—S1—O4 | 118.7 (3) | N4—C23—N3 | 130.6 (4) |
| O3—S1—C7 | 107.6 (3) | N4—C23—S2 | 112.3 (4) |
| O3—S1—C10 | 108.0 (3) | N3—C23—S2 | 117.1 (4) |
| O4—S1—C7 | 108.2 (2) | O6—C24—H24A | 109.5 |
| O4—S1—C10 | 109.4 (3) | O6—C24—H24B | 109.5 |
| C10—S1—C7 | 103.9 (3) | H24A—C24—H24B | 109.5 |
| C9—O1—C8 | 115.7 (5) | O6—C24—H24C | 109.5 |
| C7—N1—C4 | 115.4 (4) | H24A—C24—H24C | 109.5 |
| C7—N2—C6 | 115.7 (4) | H24B—C24—H24C | 109.5 |
| C3—C1—H1B | 109.5 | O5—C25—O6 | 125.7 (5) |
| C3—C1—H1C | 109.5 | O5—C25—C21 | 124.0 (5) |
| H1B—C1—H1C | 109.5 | O6—C25—C21 | 110.4 (5) |
| C3—C1—H1D | 109.5 | S2—C26—H26A | 109.5 |
| H1B—C1—H1D | 109.5 | S2—C26—H26B | 109.5 |
| H1C—C1—H1D | 109.5 | H26A—C26—H26B | 109.5 |
| C3—C2—H2B | 109.5 | S2—C26—H26C | 109.5 |
| C3—C2—H2C | 109.5 | H26A—C26—H26C | 109.5 |
| H2B—C2—H2C | 109.5 | H26B—C26—H26C | 109.5 |
| C3—C2—H2D | 109.5 | C28—C27—C32 | 118.8 (5) |
| H2B—C2—H2D | 109.5 | C28—C27—C22 | 123.0 (5) |
| H2C—C2—H2D | 109.5 | C32—C27—C22 | 118.1 (4) |
| C4—C3—C2 | 112.8 (5) | C29—C28—C27 | 120.2 (5) |
| C4—C3—C1 | 108.4 (5) | C29—C28—H28A | 119.9 |
| C2—C3—C1 | 111.8 (5) | C27—C28—H28A | 119.9 |
| C4—C3—H3B | 107.9 | C30—C29—C28 | 119.3 (5) |
| C2—C3—H3B | 107.9 | C30—C29—H29A | 120.3 |
| C1—C3—H3B | 107.9 | C28—C29—H29A | 120.3 |
| N1—C4—C5 | 119.4 (4) | F2—C30—C29 | 119.1 (5) |
| N1—C4—C3 | 115.8 (4) | F2—C30—C31 | 118.1 (5) |
| C5—C4—C3 | 124.8 (5) | C29—C30—C31 | 122.8 (5) |
| C6—C5—C4 | 118.9 (5) | C30—C31—C32 | 117.3 (6) |
| C6—C5—C9 | 119.9 (4) | C30—C31—H31A | 121.3 |
| C4—C5—C9 | 121.1 (5) | C32—C31—H31A | 121.3 |
| N2—C6—C5 | 120.4 (4) | C31—C32—C27 | 121.5 (5) |
| N2—C6—C11 | 115.4 (4) | C31—C32—H32A | 119.3 |
| C5—C6—C11 | 124.2 (5) | C27—C32—H32A | 119.3 |
| N2—C7—N1 | 129.8 (5) | O11—S3—C37 | 108.1 (2) |
| N2—C7—S1 | 117.0 (4) | O11—S3—C42 | 109.6 (2) |

| | | | |
|---|---|---|---|
| N1—C7—S1 | 113.2 (4) | O12—S3—O11 | 118.5 (2) |
| O1—C8—H8A | 109.5 | O12—S3—C37 | 105.83 (19) |
| O1—C8—H8B | 109.5 | O12—S3—C42 | 109.3 (2) |
| H8A—C8—H8B | 109.5 | C42—S3—C37 | 104.6 (2) |
| O1—C8—H8C | 109.5 | C41—O10—C40 | 115.5 (4) |
| H8A—C8—H8C | 109.5 | C37—N5—C38 | 115.6 (4) |
| H8B—C8—H8C | 109.5 | C37—N6—C36 | 117.4 (4) |
| O2—C9—O1 | 125.6 (6) | C35—C33—H33A | 109.5 |
| O2—C9—C5 | 122.7 (5) | C35—C33—H33B | 109.5 |
| O1—C9—C5 | 111.6 (5) | H33A—C33—H33B | 109.5 |
| S1—C10—H10A | 109.5 | C35—C33—H33C | 109.5 |
| S1—C10—H10B | 109.5 | H33A—C33—H33C | 109.5 |
| H10A—C10—H10B | 109.5 | H33B—C33—H33C | 109.5 |
| S1—C10—H10C | 109.5 | C35—C34—H34A | 109.5 |
| H10A—C10—H10C | 109.5 | C35—C34—H34B | 109.5 |
| H10B—C10—H10C | 109.5 | H34A—C34—H34B | 109.5 |
| C16—C11—C12 | 118.9 (5) | C35—C34—H34C | 109.5 |
| C16—C11—C6 | 119.8 (5) | H34A—C34—H34C | 109.5 |
| C12—C11—C6 | 120.9 (5) | H34B—C34—H34C | 109.5 |
| C13—C12—C11 | 120.7 (5) | C36—C35—C33 | 112.3 (4) |
| C13—C12—H12A | 119.6 | C36—C35—C34 | 111.4 (4) |
| C11—C12—H12A | 119.6 | C33—C35—C34 | 110.6 (4) |
| C14—C13—C12 | 118.2 (5) | C36—C35—H35A | 107.4 |
| C14—C13—H13A | 120.9 | C33—C35—H35A | 107.4 |
| C12—C13—H13A | 120.9 | C34—C35—H35A | 107.4 |
| C13—C14—C15 | 123.9 (5) | N6—C36—C39 | 118.0 (4) |
| C13—C14—F1 | 117.6 (6) | N6—C36—C35 | 115.9 (4) |
| C15—C14—F1 | 118.5 (6) | C39—C36—C35 | 126.1 (4) |
| C14—C15—C16 | 117.5 (5) | N5—C37—N6 | 128.6 (4) |
| C14—C15—H15A | 121.3 | N5—C37—S3 | 115.7 (3) |
| C16—C15—H15A | 121.3 | N6—C37—S3 | 115.5 (3) |
| C15—C16—C11 | 120.7 (5) | N5—C38—C39 | 120.5 (4) |
| C15—C16—H16A | 119.7 | N5—C38—C43 | 113.5 (4) |
| C11—C16—H16A | 119.7 | C39—C38—C43 | 126.0 (4) |
| O7—S2—O8 | 118.2 (3) | C38—C39—C36 | 119.7 (4) |
| O7—S2—C23 | 107.3 (2) | C38—C39—C41 | 121.8 (4) |
| O7—S2—C26 | 108.5 (3) | C36—C39—C41 | 118.4 (4) |
| O8—S2—C23 | 108.1 (2) | O10—C40—H40A | 109.5 |
| O8—S2—C26 | 109.1 (3) | O10—C40—H40B | 109.5 |
| C26—S2—C23 | 104.7 (3) | H40A—C40—H40B | 109.5 |
| C25—O6—C24 | 114.9 (5) | O10—C40—H40C | 109.5 |
| C23—N3—C20 | 114.2 (4) | H40A—C40—H40C | 109.5 |
| C23—N4—C22 | 115.3 (4) | H40B—C40—H40C | 109.5 |
| C19—C17—H17A | 109.5 | O9—C41—O10 | 122.9 (4) |
| C19—C17—H17B | 109.5 | O9—C41—C39 | 126.2 (4) |
| H17A—C17—H17B | 109.5 | O10—C41—C39 | 110.8 (4) |
| C19—C17—H17C | 109.5 | S3—C42—H42A | 109.5 |
| H17A—C17—H17C | 109.5 | S3—C42—H42B | 109.5 |

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| H17B—C17—H17C | 109.5 | H42A—C42—H42B | 109.5 |
| C19—C18—H18A | 109.5 | S3—C42—H42C | 109.5 |
| C19—C18—H18B | 109.5 | H42A—C42—H42C | 109.5 |
| H18A—C18—H18B | 109.5 | H42B—C42—H42C | 109.5 |
| C19—C18—H18C | 109.5 | C44—C43—C48 | 119.4 (4) |
| H18A—C18—H18C | 109.5 | C44—C43—C38 | 119.3 (4) |
| H18B—C18—H18C | 109.5 | C48—C43—C38 | 121.3 (4) |
| C17—C19—C20 | 110.0 (5) | C45—C44—C43 | 120.9 (5) |
| C17—C19—C18 | 110.6 (5) | C45—C44—H44A | 119.6 |
| C20—C19—C18 | 110.3 (5) | C43—C44—H44A | 119.6 |
| C17—C19—H19A | 108.6 | C46—C45—C44 | 118.4 (5) |
| C20—C19—H19A | 108.6 | C46—C45—H45A | 120.8 |
| C18—C19—H19A | 108.6 | C44—C45—H45A | 120.8 |
| N3—C20—C21 | 121.0 (4) | C47—C46—C45 | 123.1 (5) |
| N3—C20—C19 | 115.7 (4) | C47—C46—F3 | 118.6 (5) |
| C21—C20—C19 | 123.3 (4) | C45—C46—F3 | 118.4 (5) |
| C22—C21—C20 | 118.4 (4) | C46—C47—C48 | 118.8 (5) |
| C22—C21—C25 | 122.9 (5) | C46—C47—H47A | 120.6 |
| C20—C21—C25 | 118.3 (4) | C48—C47—H47A | 120.6 |
| N4—C22—C21 | 120.5 (5) | C47—C48—C43 | 119.5 (5) |
| N4—C22—C27 | 113.9 (4) | C47—C48—H48A | 120.2 |
| C21—C22—C27 | 125.6 (4) | C43—C48—H48A | 120.2 |

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| O3—S1—C7—N1 | 71.3 (4) | C19—C20—C21—C25 | −7.2 (7) |
| O3—S1—C7—N2 | −107.9 (4) | C20—C21—C22—N4 | 2.5 (7) |
| O4—S1—C7—N1 | −58.1 (5) | C25—C21—C22—N4 | −170.3 (5) |
| O4—S1—C7—N2 | 122.7 (4) | C20—C21—C22—C27 | −177.7 (5) |
| C10—S1—C7—N1 | −174.3 (4) | C25—C21—C22—C27 | 9.5 (8) |
| C10—S1—C7—N2 | 6.5 (5) | C22—C21—C25—O5 | 72.0 (7) |
| C8—O1—C9—O2 | −2.9 (8) | C20—C21—C25—O5 | −100.8 (7) |
| C8—O1—C9—C5 | −178.3 (5) | C22—C21—C25—O6 | −107.9 (5) |
| C7—N1—C4—C5 | −2.5 (7) | C20—C21—C25—O6 | 79.3 (6) |
| C7—N1—C4—C3 | 178.7 (5) | N4—C22—C27—C28 | −152.0 (5) |
| C4—N1—C7—N2 | −1.2 (8) | C21—C22—C27—C28 | 28.2 (8) |
| C4—N1—C7—S1 | 179.7 (3) | N4—C22—C27—C32 | 24.6 (7) |
| C7—N2—C6—C5 | 4.4 (7) | C21—C22—C27—C32 | −155.2 (5) |
| C7—N2—C6—C11 | −174.7 (4) | C32—C27—C28—C29 | 0.1 (8) |
| C6—N2—C7—N1 | 0.3 (8) | C22—C27—C28—C29 | 176.7 (5) |
| C6—N2—C7—S1 | 179.3 (4) | C27—C28—C29—C30 | −2.2 (9) |
| C2—C3—C4—N1 | 42.9 (7) | C28—C29—C30—F2 | −177.7 (5) |
| C1—C3—C4—N1 | −81.4 (6) | C28—C29—C30—C31 | 3.7 (10) |
| C2—C3—C4—C5 | −135.9 (6) | F2—C30—C31—C32 | 178.4 (5) |
| C1—C3—C4—C5 | 99.8 (6) | C29—C30—C31—C32 | −3.0 (10) |
| N1—C4—C5—C6 | 6.8 (7) | C30—C31—C32—C27 | 0.8 (10) |
| C3—C4—C5—C6 | −174.4 (5) | C28—C27—C32—C31 | 0.5 (9) |
| N1—C4—C5—C9 | −171.1 (5) | C22—C27—C32—C31 | −176.2 (5) |
| C3—C4—C5—C9 | 7.7 (8) | O11—S3—C37—N5 | 36.4 (4) |
| C4—C5—C6—N2 | −7.9 (7) | O11—S3—C37—N6 | −147.9 (3) |

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| C9—C5—C6—N2 | 170.0 (5) | O12—S3—C37—N5 | −91.5 (4) |
| C4—C5—C6—C11 | 171.1 (5) | O12—S3—C37—N6 | 84.2 (4) |
| C9—C5—C6—C11 | −11.0 (8) | C42—S3—C37—N5 | 153.1 (3) |
| C6—C5—C9—O2 | −58.8 (7) | C42—S3—C37—N6 | −31.2 (4) |
| C4—C5—C9—O2 | 119.1 (6) | C40—O10—C41—O9 | 3.8 (7) |
| C6—C5—C9—O1 | 116.8 (5) | C40—O10—C41—C39 | −177.0 (4) |
| C4—C5—C9—O1 | −65.3 (6) | C38—N5—C37—S3 | 174.5 (3) |
| N2—C6—C11—C16 | −38.1 (7) | C38—N5—C37—N6 | −0.5 (7) |
| C5—C6—C11—C16 | 142.9 (5) | C37—N5—C38—C39 | −2.3 (6) |
| N2—C6—C11—C12 | 135.4 (5) | C37—N5—C38—C43 | 176.5 (4) |
| C5—C6—C11—C12 | −43.6 (7) | C37—N6—C36—C39 | −0.9 (6) |
| C16—C11—C12—C13 | −1.3 (8) | C37—N6—C36—C35 | −179.9 (4) |
| C6—C11—C12—C13 | −174.9 (5) | C36—N6—C37—S3 | −172.9 (3) |
| C11—C12—C13—C14 | 1.3 (8) | C36—N6—C37—N5 | 2.1 (7) |
| C12—C13—C14—C15 | −2.0 (9) | C33—C35—C36—N6 | −31.2 (6) |
| C12—C13—C14—F1 | 177.6 (5) | C34—C35—C36—N6 | 93.5 (5) |
| C13—C14—C15—C16 | 2.7 (10) | C33—C35—C36—C39 | 150.0 (5) |
| F1—C14—C15—C16 | −176.9 (5) | C34—C35—C36—C39 | −85.4 (6) |
| C14—C15—C16—C11 | −2.6 (9) | N6—C36—C39—C38 | −1.6 (6) |
| C12—C11—C16—C15 | 2.0 (8) | C35—C36—C39—C38 | 177.2 (4) |
| C6—C11—C16—C15 | 175.6 (5) | N6—C36—C39—C41 | 174.6 (4) |
| O7—S2—C23—N3 | 123.8 (4) | C35—C36—C39—C41 | −6.6 (6) |
| O7—S2—C23—N4 | −56.0 (5) | N5—C38—C39—C36 | 3.3 (6) |
| O8—S2—C23—N3 | −107.6 (4) | C43—C38—C39—C36 | −175.4 (4) |
| O8—S2—C23—N4 | 72.5 (4) | N5—C38—C39—C41 | −172.8 (4) |
| C26—S2—C23—N3 | 8.6 (5) | C43—C38—C39—C41 | 8.5 (7) |
| C26—S2—C23—N4 | −171.3 (4) | C38—C39—C41—O9 | −128.5 (5) |
| C24—O6—C25—O5 | 0.4 (8) | C36—C39—C41—O9 | 55.4 (6) |
| C24—O6—C25—C21 | −179.7 (4) | C38—C39—C41—O10 | 52.3 (5) |
| C23—N3—C20—C19 | 178.9 (4) | C36—C39—C41—O10 | −123.8 (4) |
| C23—N3—C20—C21 | 0.9 (7) | N5—C38—C43—C44 | 35.1 (6) |
| C20—N3—C23—S2 | −179.1 (4) | C39—C38—C43—C44 | −146.2 (5) |
| C20—N3—C23—N4 | 0.7 (8) | N5—C38—C43—C48 | −141.8 (4) |
| C23—N4—C22—C21 | −1.1 (7) | C39—C38—C43—C48 | 37.0 (7) |
| C23—N4—C22—C27 | 179.1 (4) | C48—C43—C44—C45 | −0.7 (8) |
| C22—N4—C23—S2 | 179.2 (3) | C38—C43—C44—C45 | −177.6 (5) |
| C22—N4—C23—N3 | −0.7 (8) | C44—C43—C48—C47 | 0.9 (7) |
| C17—C19—C20—N3 | 59.9 (6) | C38—C43—C48—C47 | 177.8 (4) |
| C18—C19—C20—N3 | −62.3 (6) | C43—C44—C45—C46 | 0.1 (9) |
| C17—C19—C20—C21 | −122.1 (5) | C44—C45—C46—C47 | 0.4 (10) |
| C18—C19—C20—C21 | 115.6 (6) | C44—C45—C46—F3 | −179.3 (5) |
| N3—C20—C21—C22 | −2.5 (7) | C45—C46—C47—C48 | −0.1 (9) |
| C19—C20—C21—C22 | 179.7 (5) | F3—C46—C47—C48 | 179.6 (5) |
| N3—C20—C21—C25 | 170.7 (5) | C46—C47—C48—C43 | −0.5 (8) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C3—H3*B*···O1 | 0.98 | 2.54 | 3.089 (7) | 115 |
| C17—H17*C*···F1 | 0.96 | 2.51 | 3.191 (8) | 128 |
| C19—H19*A*···O6 | 0.98 | 2.55 | 3.224 (7) | 126 |
| C28—H28*A*···O6 | 0.93 | 2.56 | 3.378 (6) | 147 |
| C8—H8*B*···O3$^{i}$ | 0.96 | 2.48 | 3.373 (6) | 155 |
| C35—H35*A*···O12$^{ii}$ | 0.98 | 2.57 | 3.484 (6) | 154 |
| C42—H42*A*···O9$^{iii}$ | 0.96 | 2.43 | 3.229 (6) | 141 |
| C48—H48*A*···O12$^{iv}$ | 0.93 | 2.42 | 3.224 (6) | 146 |

Symmetry codes: (i) $x$, $-y+1/2$, $z-1/2$; (ii) $-x+1$, $-y+2$, $-z$; (iii) $x$, $-y+3/2$, $z+1/2$; (iv) $x$, $-y+3/2$, $z-1/2$.