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# 4-(3,7-Dimethyl-4-oxo-4,5-dihydro-isoxazolo[4,5-*d*]pyridazin-5-yl)benzene-sulfonamide

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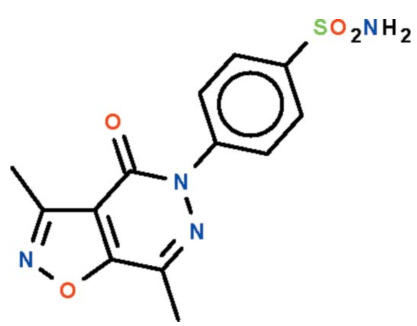
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.033; $wR$ factor = 0.096; data-to-parameter ratio = 9.1.

The nine-membered fused-ring system of the title pyridazine derivative, $C_{13}H_{12}N_4O_4S$, is approximately planar (r.m.s. deviation 0.027 Å), and the benzene ring of the phenyl-sulfamide substituent is aligned at 43.5 (1)° to the fused-ring system. The amine group of the sulfonamide substituent forms an N—H···O hydrogen bond to the ketonic O atom of two neigboring molecules to generate a chain running along the *c* axis.

## Related literature

For a related structure, see: Abdel-Aziz *et al.* (2010). For the biological activity of the class of pyridazines, see: Faid-Allah *et al.* (2011); Makki & Faid-Allah (1996).




## Experimental

*Crystal data*

$C_{13}H_{12}N_4O_4S$
$M_r$ = 320.33
Orthorhombic, *Fdd*2
$a$ = 18.0113 (4) Å
$b$ = 35.5302 (11) Å
$c$ = 8.2900 (2) Å
$V$ = 5305.1 (2) Å$^3$
$Z$ = 16
Cu $K\alpha$ radiation
$\mu$ = 2.43 mm$^{-1}$
$T$ = 100 K
0.30 × 0.20 × 0.05 mm

*Data collection*

Agilent Technologies SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010) $T_{min}$ = 0.529, $T_{max}$ = 0.888
7699 measured reflections
1886 independent reflections
1870 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.096
$S$ = 1.08
1886 reflections
207 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 e Å$^{-3}$
Absolute structure: Flack (1983), 441 Friedel pairs
Flack parameter: 0.026 (18)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N4—H1···O2$^{i}$ | 0.95 (3) | 2.09 (4) | 3.012 (3) | 163 (3) |
| N4—H2···O2$^{ii}$ | 0.85 (5) | 2.11 (5) | 2.933 (3) | 162 (4) |

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank King Abdulaziz University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5287).

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supporting information

*Acta Cryst.* (2011). E**67**, o2466 [doi:10.1107/S1600536811034325]

# 4-(3,7-Dimethyl-4-oxo-4,5-dihydroisoxazolo[4,5-*d*]pyridazin-5-yl)benzene-sulfonamide

**Abdullah M. Asiri, Hassan M. Faidallah, Abdulrahman O. Al-Youbi, Abdullah.Y. Obaid and Seik Weng Ng**

### S1. Comment

We have reported the synthesis of some pyridazines, which exhibit biological activity (Faid-Allah *et al.*, 2011; Makki & Faid-Allah, 1996). There are few crystal structure reports of such systems; recently, we reported the crystal structure of 3-methyl-2-(4-methyl)-2*H*-pyrazolo[3,4-*d*]pyridazin-5-ium thiocyanate, a salt (Abdel-Aziz *et al.*, 2010).

The nine-membered fused-ring system of $C_{13}H_{12}N_4O_4S$ (Scheme I), is planar and the benzene ring of the phenyl-sufamido substitutent is aligned at 43.5 (1) ° (Fig. 1). The amino group the substitutent forms a hydrogen bond to the ketonic O atom of two neigboring molecules to generate a chain running along the *c*-axis of the orthorhombic unit cell (Table 1).

### S2. Experimental

A solution of ethyl 5-acetyl-3-methylisoxazole-4-carboxylate (0.39 g, 0.002 mol) in ethanol (25 ml) was refluxed with *p*-sulfonamidophenyl hydrazine hydrochloride (0.49 g, 0.002 mol) for 2 h. The pyridazine which separated after concentration of the reaction mixture was filtered off, washed with ethanol and recrystallized from the same solvent to give long thin prisms in 90% yield, m.p. 488 K.

### S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H 0.95 to 0.98 Å, $U_{iso}$(H) 1.2 to 1.5$U_{eq}$(C)] and were included in the refinement in the riding model approximation.

The amino H-atoms were located in a difference Fourier map, and were refined freely.

The Flack (Flack, 1983) parameter was refined from 441 Friedel pairs.

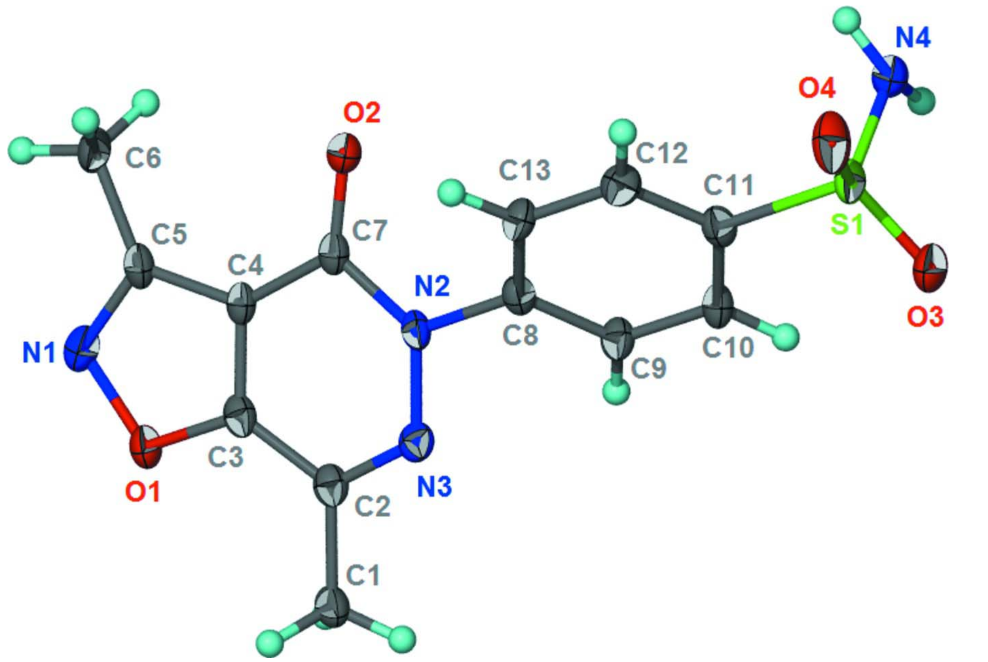


**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of $C_{13}H_{12}N_4O_4S$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

### 4-(3,7-Dimethyl-4-oxo-4,5- dihydroisoxazolo[4,5-*d*]pyridazin-5-yl)benzenesulfonamide

*Crystal data*

$C_{13}H_{12}N_4O_4S$
$M_r$ = 320.33
Orthorhombic, *Fdd*2
Hall symbol: F 2 -2d
*a* = 18.0113 (4) Å
*b* = 35.5302 (11) Å
*c* = 8.2900 (2) Å
*V* = 5305.1 (2) Å$^3$
*Z* = 16
*F*(000) = 2656
$D_x$ = 1.604 Mg m$^{-3}$
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 5872 reflections
*θ* = 4.9–74.4°
*μ* = 2.43 mm$^{-1}$
*T* = 100 K
Plate, colorless
0.30 × 0.20 × 0.05 mm

*Data collection*

Agilent Technologies SuperNova Dual diffractometer with Atlas detector
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm$^{-1}$
*ω* scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min}$ = 0.529, $T_{max}$ = 0.888
7699 measured reflections
1886 independent reflections
1870 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032
$\theta_{max}$ = 74.5°, $\theta_{min}$ = 5.0°
*h* = −42→44
*k* = −22→22
*l* = −10→7

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.096$
$S = 1.08$
1886 reflections
207 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0772P)^2 + 4.3892P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å$^{-3}$
$\Delta\rho_{min} = -0.35$ e Å$^{-3}$
Absolute structure: Flack (1983), 441 Friedel pairs
Absolute structure parameter: 0.026 (18)

*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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.12413 (3) | 0.212823 (15) | 0.43880 (7) | 0.01769 (17) |
| O1 | 0.21513 (9) | 0.37146 (4) | −0.5296 (2) | 0.0193 (4) |
| O2 | 0.05983 (9) | 0.28881 (4) | −0.2671 (2) | 0.0188 (4) |
| O3 | 0.17529 (10) | 0.22599 (5) | 0.5595 (2) | 0.0235 (4) |
| N4 | 0.04217 (11) | 0.22369 (5) | 0.5034 (3) | 0.0213 (4) |
| N1 | 0.14841 (11) | 0.36838 (5) | −0.6234 (3) | 0.0200 (4) |
| N2 | 0.17467 (10) | 0.30278 (5) | −0.1592 (3) | 0.0154 (4) |
| N3 | 0.24011 (10) | 0.32316 (5) | −0.1526 (3) | 0.0163 (4) |
| O4 | 0.12339 (11) | 0.17367 (5) | 0.3966 (3) | 0.0277 (5) |
| C1 | 0.32798 (13) | 0.36781 (6) | −0.2608 (3) | 0.0204 (5) |
| H1A | 0.3547 | 0.3612 | −0.1618 | 0.031* |
| H1B | 0.3168 | 0.3948 | −0.2603 | 0.031* |
| H1C | 0.3589 | 0.3618 | −0.3546 | 0.031* |
| C2 | 0.25679 (12) | 0.34585 (6) | −0.2694 (3) | 0.0170 (5) |
| C3 | 0.20621 (12) | 0.34980 (6) | −0.3997 (3) | 0.0169 (5) |
| C4 | 0.13880 (13) | 0.33186 (6) | −0.4030 (3) | 0.0156 (5) |
| C5 | 0.10469 (13) | 0.34528 (6) | −0.5465 (3) | 0.0177 (5) |
| C6 | 0.02971 (13) | 0.33542 (7) | −0.6145 (3) | 0.0213 (5) |
| H6A | 0.0218 | 0.3492 | −0.7153 | 0.032* |
| H6B | −0.0090 | 0.3423 | −0.5367 | 0.032* |
| H6C | 0.0275 | 0.3083 | −0.6357 | 0.032* |
| C7 | 0.11926 (12) | 0.30620 (6) | −0.2766 (3) | 0.0155 (5) |
| C8 | 0.16360 (12) | 0.28011 (6) | −0.0177 (3) | 0.0159 (5) |
| C9 | 0.18337 (13) | 0.29491 (6) | 0.1314 (3) | 0.0175 (5) |
| H9 | 0.2040 | 0.3195 | 0.1383 | 0.021* |
| C10 | 0.17290 (12) | 0.27382 (6) | 0.2696 (3) | 0.0175 (5) |
| H10 | 0.1876 | 0.2835 | 0.3715 | 0.021* |

| | | | | |
|---|---|---|---|---|
| C11 | 0.14063 (12) | 0.23826 (6) | 0.2583 (3) | 0.0171 (5) |
| C12 | 0.12297 (12) | 0.22293 (7) | 0.1099 (4) | 0.0189 (5) |
| H12 | 0.1026 | 0.1983 | 0.1037 | 0.023* |
| C13 | 0.13496 (12) | 0.24347 (6) | −0.0300 (3) | 0.0174 (5) |
| H13 | 0.1240 | 0.2329 | −0.1325 | 0.021* |
| H1 | 0.0433 (17) | 0.2472 (9) | 0.559 (4) | 0.025 (8)* |
| H2 | 0.008 (2) | 0.2165 (10) | 0.439 (6) | 0.043 (10)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0235 (3) | 0.0179 (3) | 0.0117 (3) | −0.00015 (18) | −0.0010 (2) | 0.0027 (2) |
| O1 | 0.0226 (8) | 0.0227 (7) | 0.0124 (9) | −0.0015 (6) | 0.0005 (7) | 0.0035 (7) |
| O2 | 0.0198 (8) | 0.0231 (7) | 0.0135 (9) | −0.0028 (5) | −0.0009 (7) | 0.0002 (7) |
| O3 | 0.0273 (9) | 0.0289 (8) | 0.0143 (10) | −0.0008 (7) | −0.0034 (8) | 0.0049 (7) |
| N4 | 0.0219 (10) | 0.0270 (10) | 0.0150 (11) | −0.0041 (8) | −0.0011 (9) | 0.0002 (9) |
| N1 | 0.0230 (9) | 0.0225 (9) | 0.0145 (11) | 0.0025 (7) | −0.0033 (9) | 0.0000 (8) |
| N2 | 0.0190 (8) | 0.0174 (8) | 0.0098 (10) | −0.0005 (7) | 0.0018 (8) | 0.0000 (8) |
| N3 | 0.0183 (9) | 0.0169 (7) | 0.0136 (10) | 0.0005 (7) | 0.0002 (8) | −0.0033 (8) |
| O4 | 0.0464 (11) | 0.0194 (8) | 0.0172 (11) | 0.0006 (7) | −0.0003 (8) | 0.0042 (8) |
| C1 | 0.0236 (10) | 0.0242 (10) | 0.0134 (13) | −0.0058 (8) | 0.0020 (11) | −0.0016 (9) |
| C2 | 0.0208 (10) | 0.0163 (8) | 0.0139 (12) | 0.0009 (8) | 0.0016 (10) | −0.0015 (8) |
| C3 | 0.0219 (10) | 0.0166 (9) | 0.0123 (12) | 0.0003 (8) | 0.0025 (10) | −0.0015 (9) |
| C4 | 0.0201 (10) | 0.0171 (9) | 0.0096 (12) | 0.0017 (8) | 0.0007 (9) | −0.0015 (9) |
| C5 | 0.0220 (10) | 0.0202 (9) | 0.0107 (12) | 0.0031 (8) | 0.0020 (10) | 0.0003 (9) |
| C6 | 0.0220 (11) | 0.0291 (11) | 0.0128 (12) | 0.0017 (8) | −0.0028 (10) | 0.0024 (10) |
| C7 | 0.0195 (10) | 0.0164 (9) | 0.0107 (13) | 0.0032 (7) | 0.0005 (9) | −0.0007 (9) |
| C8 | 0.0170 (9) | 0.0176 (9) | 0.0130 (13) | 0.0022 (7) | 0.0013 (10) | 0.0015 (9) |
| C9 | 0.0220 (10) | 0.0176 (10) | 0.0127 (12) | −0.0001 (8) | 0.0001 (10) | −0.0016 (9) |
| C10 | 0.0223 (10) | 0.0195 (10) | 0.0107 (11) | 0.0017 (8) | 0.0003 (10) | −0.0007 (9) |
| C11 | 0.0179 (9) | 0.0186 (10) | 0.0147 (13) | 0.0027 (8) | 0.0016 (10) | 0.0030 (10) |
| C12 | 0.0210 (11) | 0.0171 (9) | 0.0186 (14) | 0.0000 (8) | −0.0009 (10) | −0.0022 (10) |
| C13 | 0.0212 (10) | 0.0189 (10) | 0.0122 (13) | 0.0004 (8) | −0.0022 (9) | −0.0023 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—O4 | 1.4345 (19) | C2—C3 | 1.420 (3) |
| S1—O3 | 1.4385 (19) | C3—C4 | 1.372 (3) |
| S1—N4 | 1.617 (2) | C4—C5 | 1.422 (4) |
| S1—C11 | 1.773 (3) | C4—C7 | 1.433 (3) |
| O1—C3 | 1.333 (3) | C5—C6 | 1.505 (3) |
| O1—N1 | 1.435 (3) | C6—H6A | 0.9800 |
| O2—C7 | 1.238 (3) | C6—H6B | 0.9800 |
| N4—H1 | 0.95 (3) | C6—H6C | 0.9800 |
| N4—H2 | 0.85 (5) | C8—C9 | 1.389 (4) |
| N1—C5 | 1.304 (3) | C8—C13 | 1.404 (3) |
| N2—N3 | 1.384 (3) | C9—C10 | 1.382 (3) |
| N2—C7 | 1.399 (3) | C9—H9 | 0.9500 |

| | | | |
|---|---|---|---|
| N2—C8 | 1.437 (3) | C10—C11 | 1.394 (3) |
| N3—C2 | 1.296 (3) | C10—H10 | 0.9500 |
| C1—C2 | 1.502 (3) | C11—C12 | 1.383 (4) |
| C1—H1A | 0.9800 | C12—C13 | 1.387 (4) |
| C1—H1B | 0.9800 | C12—H12 | 0.9500 |
| C1—H1C | 0.9800 | C13—H13 | 0.9500 |

| | | | |
|---|---|---|---|
| O4—S1—O3 | 119.41 (11) | N1—C5—C4 | 111.0 (2) |
| O4—S1—N4 | 107.69 (11) | N1—C5—C6 | 120.4 (2) |
| O3—S1—N4 | 106.07 (12) | C4—C5—C6 | 128.5 (2) |
| O4—S1—C11 | 106.85 (12) | C5—C6—H6A | 109.5 |
| O3—S1—C11 | 108.30 (11) | C5—C6—H6B | 109.5 |
| N4—S1—C11 | 108.10 (11) | H6A—C6—H6B | 109.5 |
| C3—O1—N1 | 107.01 (16) | C5—C6—H6C | 109.5 |
| S1—N4—H1 | 110.4 (18) | H6A—C6—H6C | 109.5 |
| S1—N4—H2 | 112 (3) | H6B—C6—H6C | 109.5 |
| H1—N4—H2 | 125 (3) | O2—C7—N2 | 121.9 (2) |
| C5—N1—O1 | 106.8 (2) | O2—C7—C4 | 125.2 (2) |
| N3—N2—C7 | 126.1 (2) | N2—C7—C4 | 112.9 (2) |
| N3—N2—C8 | 112.27 (18) | C9—C8—C13 | 120.6 (2) |
| C7—N2—C8 | 121.16 (18) | C9—C8—N2 | 118.59 (18) |
| C2—N3—N2 | 119.6 (2) | C13—C8—N2 | 120.8 (2) |
| C2—C1—H1A | 109.5 | C10—C9—C8 | 119.8 (2) |
| C2—C1—H1B | 109.5 | C10—C9—H9 | 120.1 |
| H1A—C1—H1B | 109.5 | C8—C9—H9 | 120.1 |
| C2—C1—H1C | 109.5 | C9—C10—C11 | 119.5 (2) |
| H1A—C1—H1C | 109.5 | C9—C10—H10 | 120.2 |
| H1B—C1—H1C | 109.5 | C11—C10—H10 | 120.2 |
| N3—C2—C3 | 118.8 (2) | C12—C11—C10 | 120.8 (2) |
| N3—C2—C1 | 119.0 (2) | C12—C11—S1 | 120.77 (17) |
| C3—C2—C1 | 122.2 (2) | C10—C11—S1 | 118.4 (2) |
| O1—C3—C4 | 111.0 (2) | C11—C12—C13 | 120.0 (2) |
| O1—C3—C2 | 126.5 (2) | C11—C12—H12 | 120.0 |
| C4—C3—C2 | 122.5 (2) | C13—C12—H12 | 120.0 |
| C3—C4—C5 | 104.1 (2) | C12—C13—C8 | 119.0 (2) |
| C3—C4—C7 | 119.9 (2) | C12—C13—H13 | 120.5 |
| C5—C4—C7 | 136.0 (2) | C8—C13—H13 | 120.5 |

| | | | |
|---|---|---|---|
| C3—O1—N1—C5 | −0.6 (2) | C3—C4—C7—O2 | 179.4 (2) |
| C7—N2—N3—C2 | −5.6 (3) | C5—C4—C7—O2 | −1.1 (4) |
| C8—N2—N3—C2 | −177.91 (19) | C3—C4—C7—N2 | 0.3 (3) |
| N2—N3—C2—C3 | 1.5 (3) | C5—C4—C7—N2 | 179.9 (2) |
| N2—N3—C2—C1 | 179.99 (19) | N3—N2—C8—C9 | 38.9 (3) |
| N1—O1—C3—C4 | 1.5 (2) | C7—N2—C8—C9 | −133.9 (2) |
| N1—O1—C3—C2 | −176.5 (2) | N3—N2—C8—C13 | −139.7 (2) |
| N3—C2—C3—O1 | −179.1 (2) | C7—N2—C8—C13 | 47.5 (3) |
| C1—C2—C3—O1 | 2.4 (4) | C13—C8—C9—C10 | −1.8 (3) |
| N3—C2—C3—C4 | 3.2 (3) | N2—C8—C9—C10 | 179.60 (19) |

| | | | |
|---|---|---|---|
| C1—C2—C3—C4 | −175.3 (2) | C8—C9—C10—C11 | −1.8 (3) |
| O1—C3—C4—C5 | −1.7 (2) | C9—C10—C11—C12 | 3.8 (3) |
| C2—C3—C4—C5 | 176.3 (2) | C9—C10—C11—S1 | −177.18 (17) |
| O1—C3—C4—C7 | 177.95 (19) | O4—S1—C11—C12 | 24.3 (2) |
| C2—C3—C4—C7 | −4.0 (3) | O3—S1—C11—C12 | 154.11 (18) |
| O1—N1—C5—C4 | −0.5 (3) | N4—S1—C11—C12 | −91.4 (2) |
| O1—N1—C5—C6 | −179.15 (19) | O4—S1—C11—C10 | −154.73 (18) |
| C3—C4—C5—N1 | 1.3 (3) | O3—S1—C11—C10 | −24.9 (2) |
| C7—C4—C5—N1 | −178.2 (2) | N4—S1—C11—C10 | 89.6 (2) |
| C3—C4—C5—C6 | 179.9 (2) | C10—C11—C12—C13 | −2.2 (3) |
| C7—C4—C5—C6 | 0.3 (4) | S1—C11—C12—C13 | 178.81 (17) |
| N3—N2—C7—O2 | −174.6 (2) | C11—C12—C13—C8 | −1.4 (3) |
| C8—N2—C7—O2 | −2.9 (3) | C9—C8—C13—C12 | 3.4 (3) |
| N3—N2—C7—C4 | 4.5 (3) | N2—C8—C13—C12 | −178.04 (19) |
| C8—N2—C7—C4 | 176.19 (19) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N4—H1···O2$^{i}$ | 0.95 (3) | 2.09 (4) | 3.012 (3) | 163 (3) |
| N4—H2···O2$^{ii}$ | 0.85 (5) | 2.11 (5) | 2.933 (3) | 162 (4) |

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