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# A second triclinic polymorph of azimsulfuron

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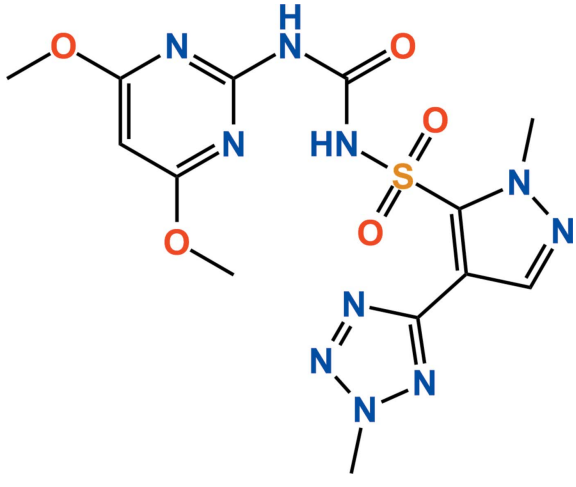
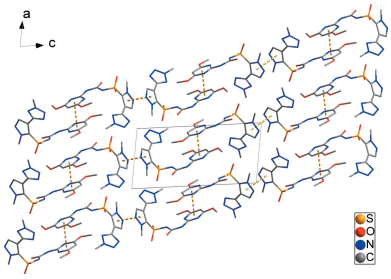
The title compound, $C_{13}H_{16}N_{10}O_5S$ (systematic name: 1-(4,6-dimethoxypyrimidin-2-yl)-3-{[1-methyl-4-(2-methyl-2*H*-tetrazol-5-yl)pyrazol-5-yl]sulfonyl}urea), is a second triclinic polymorph of this crystal [for the other, see: Jeon *et al.*, (2015). *Acta Cryst.* E**71**, o470–o471]. There are two molecules, *A* and *B*, in the asymmetric unit; the dihedral angles between the pyrazole ring and the tetrazole and dimethoxypyrimidine ring planes are 72.84 (10) and 37.24 (14)°, respectively (molecule *A*) and 84.38 (9) and 26.09 (15)°, respectively (molecule *B*). Each molecule features an intramolecular N—H···N hydrogen bond. In the crystal, aromatic $\pi$–$\pi$ stacking interactions [centroid–centroid separations = 3.9871 (16), 3.4487 (14) and 3.5455 (16) Å] link the molecules into [001] chains. In addition, N—H···N, N—H···O, C—H···O and C—H···N hydrogen bonds occur, forming a three-dimensional architecture. We propose that the dimorphism results from differences in conformations and packing owing to different intermolecular interactions, especially aromatic $\pi$–$\pi$ stacking.

## 1. Chemical context

Sulfonylurea herbicides are well known as being highly beneficial for controlling undesirable vegetation in agronomically desirable crops including corn and cereals such as wheat and barley. Azimsulfuron is a recently introduced highly selective sulfonylurea herbicide (Valle *et al.*, 2006) and has been found to be particularly useful as a post-emergent herbicide for weed control in rice paddies and suppression of barnyard grass in rice (Venkatesh *et al.*, 2016). The crystal structure of azimsulfuron (dimorph I) has already been reported in our previous study (Jeon *et al.*, 2015). We now report the crystal structure of a second triclinic polymorph, grown under different conditions, as observed for other systems (Schmidt & Jansen, 2012; Ebenezer & Muthiah, 2010).

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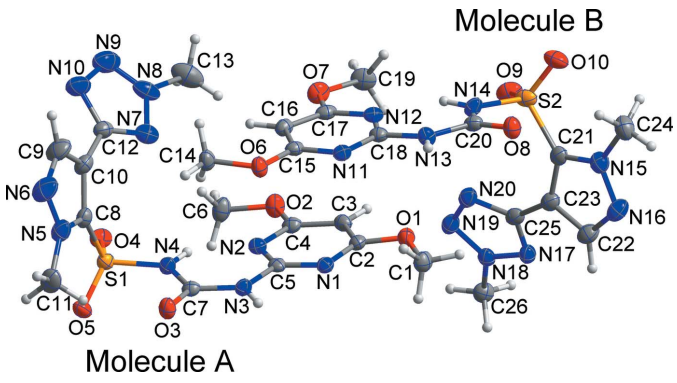


**Figure 1**
The asymmetric unit of the title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3*N*···N11$^{i}$ | 0.88 | 2.65 | 3.494 (3) | 162 |
| N4—H4*N*···N2 | 0.88 | 1.89 | 2.611 (3) | 138 |
| N13—H13*N*···O3$^{i}$ | 0.88 | 2.04 | 2.844 (2) | 151 |
| N14—H14*N*···N12 | 0.88 | 1.95 | 2.636 (3) | 134 |
| C1—H1*C*···O8$^{ii}$ | 0.98 | 2.58 | 3.559 (3) | 178 |
| C11—H11*B*···O3 | 0.98 | 2.38 | 3.236 (3) | 146 |
| C11—H11*B*···O8$^{i}$ | 0.98 | 2.57 | 3.278 (3) | 129 |
| C11—H11*C*···N10$^{iii}$ | 0.98 | 2.58 | 3.290 (4) | 130 |
| C13—H13*A*···O9$^{iv}$ | 0.98 | 2.40 | 3.374 (4) | 175 |
| C14—H14*A*···O5$^{v}$ | 0.98 | 2.39 | 3.335 (3) | 162 |
| C22—H22···N17$^{vi}$ | 0.95 | 2.57 | 3.435 (3) | 152 |
| C24—H24*B*···O8 | 0.98 | 2.33 | 3.080 (3) | 133 |
| C26—H26*B*···N16$^{vi}$ | 0.98 | 2.52 | 3.376 (3) | 146 |

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

## 2. Structural commentary

The asymmetric unit of the new dimorph II (Fig. 1), consists of two independent molecules, *A* and *B*, which are curved and form a 'boxing glove' shape around the pyrazole ring. The dihedral angles between the pyrazole ring and the tetrazole and dimethoxypyrimidine ring planes are 72.84 (10) and 37.24 (14)°, respectively, in molecule *A* and 84.38 (9) and 26.09 (15)°, respectively, in molecule *B*. All bond lengths and bond angles are normal and comparable to those observed in similar crystal structures (Chopra *et al.*, 2004; Kwon *et al.*, 2015). Each molecule features an intramolecular N—H···N hydrogen bond (Table 1), which closes an *S*(6) ring.

## 3. Supramolecular features

In the crystal, aromatic $\pi$–$\pi$ stacking interactions, $Cg1\cdots Cg1^{iii}$ = 3.9817 (16), $Cg3\cdots Cg6^{vii}$ = 3.4487 (14) and $Cg4\cdots Cg4^{viii}$ = 3.5455 (16) Å occur [*Cg*1, *Cg*3, *Cg*4 and *Cg*6 are the centroids of the N5/N6/C8–C10, N1/N2/C2–C5, N15/N16/C21–C23 and N11/N12/C15–C18 rings, respectively; symmetry codes: (vii) $x, y, z$, (viii) $-x+2, -y, -z+2$]. Together, these link adjacent molecules, forming chains propagating along the *c* axis. (Fig. 2). In addition, there are N—H···N, N—H···O, C—H···O and C—H···N hydrogen bonds in dimorph II (Table 1), which generate a three-dimensional architecture.

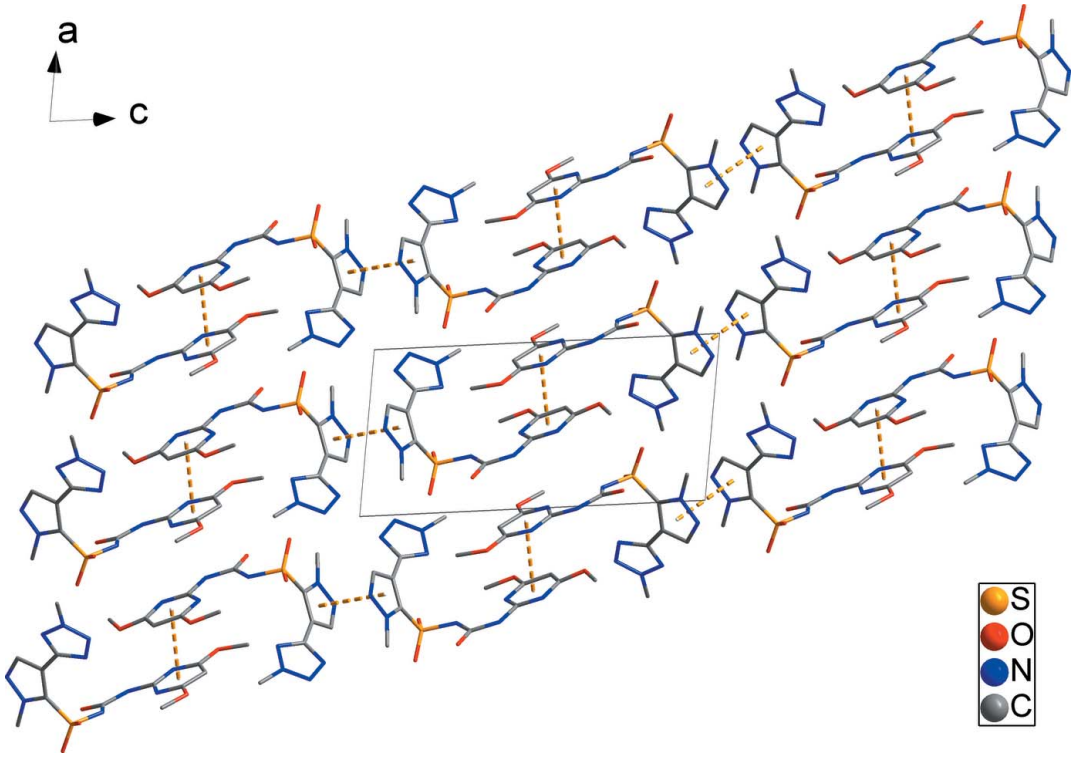


**Figure 2**
The crystal packing, viewed along the *b* axis. H atoms have been omitted for clarity.

The previous dimorph has only one $\pi$–$\pi$ interaction between the tetrazole rings of neighboring molecules, while the present dimorph has three $\pi$–$\pi$ interactions between dimethoxypyrimidine rings in the asymmetric unit, and between the pyrazole rings of neighboring *A* or *B* molecules.

## 4. Synthesis and crystallization

In the previous report, crystals were obtained by using $CH_3CN$ solvent, whereas colourless needles of the title polymorph were prepared by slow evaporation of a methanol solution.

## 5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were positioned geometrically and refined using a riding model with $d$(N—H) = 0.88 Å, $U_{iso}$ = 1.2$U_{eq}$(C) for N—H groups, $d$(C—H) = 0.88 Å, $U_{iso}$ = 1.2$U_{eq}$(C) for C$sp^2$—H and $d$(C—H) = 0.98 Å, $U_{iso}$ = 1.5$U_{eq}$(C) for methyl groups.

## Acknowledgements

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**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{13}H_{16}N_{10}O_5S$ |
| $M_r$ | 424.42 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 173 |
| $a$, $b$, $c$ (Å) | 7.6451 (2), 15.1102 (4), 17.0314 (5) |
| $\alpha$, $\beta$, $\gamma$ (°) | 67.1562 (18), 80.5936 (17), 84.0996 (17) |
| $V$ (Å$^3$) | 1787.08 (9) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.24 |
| Crystal size (mm) | 0.30 × 0.04 × 0.04 |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2014) |
| $T_{min}$, $T_{max}$ | 0.686, 0.746 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 25718, 6265, 4741 |
| $R_{int}$ | 0.060 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.595 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.045, 0.114, 1.07 |
| No. of reflections | 6265 |
| No. of parameters | 531 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.38, −0.39 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2010) and *publCIF* (Westrip, 2010).

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# supporting information

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## A second triclinic polymorph of azimsulfuron

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### Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

**1-(4,6-Dimethoxypyrimidin-2-yl)-3-{[1-methyl-4-(2-methyl-2*H*-tetrazol-5-yl)pyrazol-5-yl]sulfonyl}urea**

*Crystal data*

$C_{13}H_{16}N_{10}O_5S$
$M_r = 424.42$
Triclinic, $P\overline{1}$
$a = 7.6451$ (2) Å
$b = 15.1102$ (4) Å
$c = 17.0314$ (5) Å
$\alpha = 67.1562$ (18)°
$\beta = 80.5936$ (17)°
$\gamma = 84.0996$ (17)°
$V = 1787.08$ (9) Å$^3$
$Z = 4$
$F(000) = 880$
$D_x = 1.577$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3336 reflections
$\theta = 2.3$–$24.2°$
$\mu = 0.24$ mm$^{-1}$
$T = 173$ K
Needle, colourless
0.30 × 0.04 × 0.04 mm

*Data collection*

Bruker APEXII CCD diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
$T_{min} = 0.686$, $T_{max} = 0.746$
25718 measured reflections
6265 independent reflections
4741 reflections with $I > 2\sigma(I)$
$R_{int} = 0.060$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.5°$
$h = -8 \rightarrow 9$
$k = -17 \rightarrow 17$
$l = -20 \rightarrow 20$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.114$
$S = 1.07$
6265 reflections
531 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0457P)^2 + 0.2151P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.38$ e Å$^{-3}$
$\Delta\rho_{min} = -0.39$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.29659 (8) | 0.39202 (4) | 0.20930 (4) | 0.02210 (17) |
| S2 | 1.16721 (9) | 0.10185 (4) | 0.78289 (4) | 0.02695 (18) |
| O1 | 0.6095 (2) | 0.23247 (11) | 0.66818 (10) | 0.0267 (4) |
| O2 | 0.5902 (2) | 0.10067 (11) | 0.46454 (10) | 0.0295 (4) |
| O3 | 0.2038 (2) | 0.50940 (11) | 0.31822 (10) | 0.0260 (4) |
| O4 | 0.3602 (2) | 0.30534 (11) | 0.19780 (11) | 0.0288 (4) |
| O5 | 0.1186 (2) | 0.42651 (12) | 0.19829 (11) | 0.0294 (4) |
| O6 | 0.7598 (2) | 0.48627 (11) | 0.37801 (10) | 0.0260 (4) |
| O7 | 1.0204 (2) | 0.17015 (12) | 0.45730 (11) | 0.0315 (4) |
| O8 | 1.0811 (2) | 0.30423 (11) | 0.75749 (11) | 0.0285 (4) |
| O9 | 1.1625 (2) | 0.01909 (11) | 0.76253 (12) | 0.0346 (5) |
| O10 | 1.3265 (2) | 0.12288 (12) | 0.80359 (12) | 0.0360 (5) |
| N1 | 0.4586 (3) | 0.31656 (13) | 0.55273 (12) | 0.0217 (5) |
| N2 | 0.4580 (3) | 0.25049 (13) | 0.44580 (12) | 0.0214 (5) |
| N3 | 0.3252 (3) | 0.40128 (13) | 0.43281 (12) | 0.0210 (5) |
| H3N | 0.2896 | 0.4405 | 0.4598 | 0.025* |
| N4 | 0.3313 (3) | 0.37078 (13) | 0.30805 (12) | 0.0212 (5) |
| H4N | 0.3867 | 0.3161 | 0.3356 | 0.025* |
| N5 | 0.3879 (3) | 0.57663 (15) | 0.10476 (13) | 0.0327 (6) |
| N6 | 0.5224 (4) | 0.62778 (16) | 0.05092 (15) | 0.0458 (7) |
| N7 | 0.7561 (3) | 0.31962 (15) | 0.20532 (14) | 0.0311 (5) |
| N8 | 0.8972 (3) | 0.26823 (15) | 0.18460 (16) | 0.0357 (6) |
| N9 | 0.9657 (4) | 0.3035 (2) | 0.10352 (18) | 0.0519 (7) |
| N10 | 0.8695 (3) | 0.3815 (2) | 0.06687 (16) | 0.0466 (7) |
| N11 | 0.8673 (3) | 0.41362 (13) | 0.50271 (12) | 0.0219 (5) |
| N12 | 1.0024 (3) | 0.25495 (13) | 0.54475 (12) | 0.0215 (5) |
| N13 | 0.9852 (3) | 0.34673 (13) | 0.62868 (12) | 0.0218 (5) |
| H13N | 0.9551 | 0.4035 | 0.6311 | 0.026* |
| N14 | 1.1044 (3) | 0.19100 (13) | 0.69852 (12) | 0.0242 (5) |
| H14N | 1.0987 | 0.1805 | 0.6517 | 0.029* |
| N15 | 1.0132 (3) | 0.13158 (14) | 0.92857 (13) | 0.0293 (5) |
| N16 | 0.8644 (3) | 0.11937 (15) | 0.98511 (14) | 0.0350 (6) |
| N17 | 0.6174 (3) | −0.04932 (14) | 0.89155 (12) | 0.0247 (5) |
| N18 | 0.5689 (3) | −0.07811 (14) | 0.83420 (13) | 0.0241 (5) |
| N19 | 0.6566 (3) | −0.03852 (15) | 0.75612 (13) | 0.0298 (5) |
| N20 | 0.7690 (3) | 0.01978 (15) | 0.76081 (13) | 0.0295 (5) |
| C1 | 0.5501 (4) | 0.30726 (18) | 0.70047 (16) | 0.0298 (6) |
| H1A | 0.5859 | 0.3696 | 0.6566 | 0.045* |
| H1B | 0.6036 | 0.2952 | 0.7524 | 0.045* |

| | | | | |
|---|---|---|---|---|
| H1C | 0.4206 | 0.3078 | 0.7143 | 0.045* |
| C2 | 0.5514 (3) | 0.23781 (16) | 0.59675 (15) | 0.0218 (6) |
| C3 | 0.5963 (3) | 0.16081 (16) | 0.57120 (15) | 0.0229 (6) |
| H3 | 0.6570 | 0.1042 | 0.6051 | 0.028* |
| C4 | 0.5473 (3) | 0.17177 (16) | 0.49379 (15) | 0.0224 (6) |
| C5 | 0.4184 (3) | 0.31774 (16) | 0.47966 (15) | 0.0200 (5) |
| C6 | 0.5328 (4) | 0.11182 (18) | 0.38456 (16) | 0.0336 (7) |
| H6A | 0.4032 | 0.1201 | 0.3896 | 0.050* |
| H6B | 0.5705 | 0.0545 | 0.3715 | 0.050* |
| H6C | 0.5858 | 0.1684 | 0.3383 | 0.050* |
| C7 | 0.2806 (3) | 0.43161 (16) | 0.35078 (15) | 0.0200 (5) |
| C8 | 0.4391 (4) | 0.48225 (17) | 0.14203 (15) | 0.0241 (6) |
| C9 | 0.6598 (4) | 0.5660 (2) | 0.05491 (18) | 0.0427 (8) |
| H9 | 0.7736 | 0.5832 | 0.0230 | 0.051* |
| C10 | 0.6187 (4) | 0.47261 (18) | 0.11140 (15) | 0.0281 (6) |
| C11 | 0.2159 (4) | 0.62701 (19) | 0.11317 (18) | 0.0393 (8) |
| H11A | 0.2286 | 0.6964 | 0.0824 | 0.059* |
| H11B | 0.1741 | 0.6133 | 0.1741 | 0.059* |
| H11C | 0.1298 | 0.6050 | 0.0887 | 0.059* |
| C12 | 0.7435 (3) | 0.38992 (18) | 0.12941 (16) | 0.0272 (6) |
| C13 | 0.9717 (4) | 0.1819 (2) | 0.2470 (2) | 0.0522 (9) |
| H13A | 0.9361 | 0.1250 | 0.2404 | 0.078* |
| H13B | 0.9277 | 0.1791 | 0.3053 | 0.078* |
| H13C | 1.1015 | 0.1837 | 0.2374 | 0.078* |
| C14 | 0.7391 (4) | 0.49082 (18) | 0.29395 (15) | 0.0278 (6) |
| H14A | 0.8562 | 0.4869 | 0.2617 | 0.042* |
| H14B | 0.6774 | 0.5516 | 0.2631 | 0.042* |
| H14C | 0.6697 | 0.4370 | 0.2998 | 0.042* |
| C15 | 0.8417 (3) | 0.40702 (16) | 0.42896 (15) | 0.0217 (6) |
| C16 | 0.8940 (3) | 0.32688 (17) | 0.40905 (16) | 0.0239 (6) |
| H16 | 0.8781 | 0.3240 | 0.3560 | 0.029* |
| C17 | 0.9710 (3) | 0.25142 (17) | 0.47177 (16) | 0.0233 (6) |
| C18 | 0.9502 (3) | 0.33713 (16) | 0.55572 (15) | 0.0211 (6) |
| C19 | 1.0937 (4) | 0.09138 (17) | 0.52594 (18) | 0.0334 (7) |
| H19A | 1.1971 | 0.1126 | 0.5401 | 0.050* |
| H19B | 1.1298 | 0.0376 | 0.5074 | 0.050* |
| H19C | 1.0038 | 0.0706 | 0.5768 | 0.050* |
| C20 | 1.0601 (3) | 0.28177 (16) | 0.69881 (16) | 0.0221 (6) |
| C21 | 0.9977 (3) | 0.09825 (16) | 0.86629 (15) | 0.0249 (6) |
| C22 | 0.7537 (4) | 0.07751 (18) | 0.95834 (16) | 0.0313 (7) |
| H22 | 0.6371 | 0.0604 | 0.9865 | 0.038* |
| C23 | 0.8294 (4) | 0.06179 (17) | 0.88397 (16) | 0.0259 (6) |
| C24 | 1.1580 (4) | 0.17922 (19) | 0.94119 (18) | 0.0367 (7) |
| H24A | 1.1204 | 0.1980 | 0.9906 | 0.055* |
| H24B | 1.1880 | 0.2365 | 0.8895 | 0.055* |
| H24C | 1.2623 | 0.1349 | 0.9519 | 0.055* |
| C25 | 0.7428 (3) | 0.01230 (16) | 0.84415 (15) | 0.0246 (6) |
| C26 | 0.4366 (4) | −0.14953 (17) | 0.85757 (17) | 0.0297 (6) |

| | | | | |
|---|---|---|---|---|
| H26A | 0.4199 | −0.1609 | 0.8065 | 0.044* |
| H26B | 0.3240 | −0.1263 | 0.8811 | 0.044* |
| H26C | 0.4767 | −0.2097 | 0.9009 | 0.044* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0221 (4) | 0.0230 (3) | 0.0234 (3) | 0.0007 (3) | −0.0029 (3) | −0.0116 (3) |
| S2 | 0.0239 (4) | 0.0192 (3) | 0.0317 (4) | 0.0031 (3) | −0.0010 (3) | −0.0051 (3) |
| O1 | 0.0284 (11) | 0.0289 (9) | 0.0222 (9) | 0.0028 (8) | −0.0049 (8) | −0.0096 (8) |
| O2 | 0.0415 (12) | 0.0205 (9) | 0.0287 (10) | 0.0040 (8) | −0.0094 (9) | −0.0113 (8) |
| O3 | 0.0347 (11) | 0.0193 (9) | 0.0233 (9) | 0.0069 (8) | −0.0078 (8) | −0.0077 (7) |
| O4 | 0.0290 (11) | 0.0271 (9) | 0.0368 (10) | −0.0005 (8) | −0.0028 (8) | −0.0199 (8) |
| O5 | 0.0214 (11) | 0.0373 (10) | 0.0323 (10) | 0.0059 (8) | −0.0076 (8) | −0.0165 (8) |
| O6 | 0.0316 (11) | 0.0263 (9) | 0.0235 (9) | 0.0038 (8) | −0.0092 (8) | −0.0121 (7) |
| O7 | 0.0377 (12) | 0.0265 (9) | 0.0370 (11) | 0.0034 (8) | −0.0042 (9) | −0.0208 (8) |
| O8 | 0.0362 (12) | 0.0238 (9) | 0.0264 (10) | 0.0031 (8) | −0.0085 (8) | −0.0099 (8) |
| O9 | 0.0368 (12) | 0.0196 (9) | 0.0421 (11) | 0.0040 (8) | 0.0031 (9) | −0.0105 (8) |
| O10 | 0.0221 (11) | 0.0329 (10) | 0.0472 (12) | 0.0008 (8) | −0.0071 (9) | −0.0086 (9) |
| N1 | 0.0205 (12) | 0.0218 (10) | 0.0205 (11) | −0.0026 (9) | −0.0011 (9) | −0.0058 (9) |
| N2 | 0.0213 (12) | 0.0178 (10) | 0.0232 (11) | 0.0003 (8) | −0.0016 (9) | −0.0066 (9) |
| N3 | 0.0238 (12) | 0.0198 (10) | 0.0197 (11) | 0.0026 (8) | −0.0019 (9) | −0.0093 (8) |
| N4 | 0.0246 (13) | 0.0171 (10) | 0.0196 (10) | 0.0053 (8) | −0.0032 (9) | −0.0057 (8) |
| N5 | 0.0399 (15) | 0.0255 (11) | 0.0251 (12) | 0.0036 (10) | −0.0017 (11) | −0.0037 (10) |
| N6 | 0.0538 (19) | 0.0303 (13) | 0.0362 (14) | −0.0034 (12) | 0.0064 (13) | 0.0013 (11) |
| N7 | 0.0271 (14) | 0.0277 (12) | 0.0424 (14) | −0.0009 (10) | −0.0050 (11) | −0.0173 (11) |
| N8 | 0.0252 (14) | 0.0316 (12) | 0.0614 (17) | 0.0047 (10) | −0.0119 (12) | −0.0288 (12) |
| N9 | 0.0380 (17) | 0.0719 (19) | 0.0605 (19) | 0.0015 (14) | −0.0009 (14) | −0.0443 (16) |
| N10 | 0.0320 (16) | 0.0691 (18) | 0.0476 (16) | 0.0033 (13) | 0.0005 (12) | −0.0354 (14) |
| N11 | 0.0210 (12) | 0.0222 (10) | 0.0233 (11) | −0.0020 (9) | −0.0005 (9) | −0.0102 (9) |
| N12 | 0.0188 (12) | 0.0194 (10) | 0.0277 (12) | −0.0023 (8) | 0.0000 (9) | −0.0112 (9) |
| N13 | 0.0262 (13) | 0.0164 (10) | 0.0257 (11) | 0.0031 (8) | −0.0074 (9) | −0.0105 (9) |
| N14 | 0.0302 (13) | 0.0196 (10) | 0.0196 (11) | 0.0033 (9) | 0.0006 (9) | −0.0066 (9) |
| N15 | 0.0332 (15) | 0.0229 (11) | 0.0283 (12) | −0.0032 (9) | −0.0063 (10) | −0.0046 (9) |
| N16 | 0.0431 (16) | 0.0301 (12) | 0.0271 (12) | −0.0043 (11) | 0.0035 (11) | −0.0083 (10) |
| N17 | 0.0276 (13) | 0.0261 (11) | 0.0213 (11) | 0.0023 (9) | −0.0047 (9) | −0.0103 (9) |
| N18 | 0.0244 (13) | 0.0236 (11) | 0.0244 (12) | 0.0058 (9) | −0.0062 (10) | −0.0097 (9) |
| N19 | 0.0337 (15) | 0.0309 (12) | 0.0215 (12) | 0.0039 (10) | −0.0019 (10) | −0.0085 (10) |
| N20 | 0.0323 (14) | 0.0287 (12) | 0.0223 (12) | 0.0013 (10) | −0.0022 (10) | −0.0055 (9) |
| C1 | 0.0329 (17) | 0.0333 (14) | 0.0283 (14) | −0.0024 (12) | −0.0032 (12) | −0.0171 (12) |
| C2 | 0.0183 (14) | 0.0257 (13) | 0.0189 (13) | −0.0025 (10) | 0.0006 (10) | −0.0064 (10) |
| C3 | 0.0201 (15) | 0.0198 (12) | 0.0239 (13) | 0.0000 (10) | −0.0025 (11) | −0.0033 (10) |
| C4 | 0.0208 (15) | 0.0191 (12) | 0.0242 (13) | −0.0038 (10) | 0.0013 (11) | −0.0057 (10) |
| C5 | 0.0153 (14) | 0.0200 (12) | 0.0221 (13) | −0.0055 (10) | 0.0001 (10) | −0.0049 (10) |
| C6 | 0.048 (2) | 0.0288 (14) | 0.0254 (14) | 0.0016 (13) | −0.0055 (13) | −0.0130 (12) |
| C7 | 0.0187 (14) | 0.0172 (12) | 0.0224 (13) | −0.0037 (10) | 0.0002 (10) | −0.0061 (10) |
| C8 | 0.0308 (16) | 0.0236 (13) | 0.0180 (13) | −0.0003 (11) | −0.0026 (11) | −0.0086 (10) |
| C9 | 0.045 (2) | 0.0371 (16) | 0.0341 (17) | −0.0085 (14) | 0.0087 (14) | −0.0040 (13) |

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|---|---|---|---|---|---|---|
| C10 | 0.0319 (17) | 0.0302 (14) | 0.0207 (13) | −0.0044 (12) | 0.0026 (12) | −0.0098 (11) |
| C11 | 0.047 (2) | 0.0314 (15) | 0.0322 (16) | 0.0151 (13) | −0.0080 (14) | −0.0075 (13) |
| C12 | 0.0226 (16) | 0.0330 (14) | 0.0294 (15) | −0.0038 (11) | 0.0002 (12) | −0.0164 (12) |
| C13 | 0.042 (2) | 0.0348 (16) | 0.085 (3) | 0.0064 (14) | −0.0173 (18) | −0.0268 (17) |
| C14 | 0.0323 (17) | 0.0321 (14) | 0.0224 (14) | 0.0030 (12) | −0.0082 (12) | −0.0133 (11) |
| C15 | 0.0157 (14) | 0.0254 (13) | 0.0256 (14) | −0.0040 (10) | 0.0009 (11) | −0.0119 (11) |
| C16 | 0.0229 (15) | 0.0280 (13) | 0.0238 (13) | −0.0051 (11) | 0.0001 (11) | −0.0133 (11) |
| C17 | 0.0185 (15) | 0.0240 (13) | 0.0304 (14) | −0.0047 (10) | 0.0028 (11) | −0.0151 (11) |
| C18 | 0.0177 (14) | 0.0198 (12) | 0.0241 (13) | −0.0023 (10) | 0.0003 (11) | −0.0074 (10) |
| C19 | 0.0363 (18) | 0.0193 (13) | 0.0460 (17) | 0.0026 (11) | −0.0045 (14) | −0.0150 (12) |
| C20 | 0.0192 (15) | 0.0191 (12) | 0.0249 (14) | −0.0002 (10) | 0.0002 (11) | −0.0063 (11) |
| C21 | 0.0276 (16) | 0.0201 (12) | 0.0225 (13) | 0.0031 (11) | −0.0040 (11) | −0.0040 (10) |
| C22 | 0.0332 (18) | 0.0277 (14) | 0.0291 (15) | −0.0044 (12) | 0.0031 (13) | −0.0085 (12) |
| C23 | 0.0269 (16) | 0.0213 (12) | 0.0249 (14) | 0.0015 (11) | −0.0010 (11) | −0.0053 (11) |
| C24 | 0.0420 (19) | 0.0344 (15) | 0.0341 (16) | −0.0048 (13) | −0.0132 (14) | −0.0096 (13) |
| C25 | 0.0243 (16) | 0.0198 (12) | 0.0245 (14) | 0.0037 (11) | −0.0008 (11) | −0.0050 (11) |
| C26 | 0.0312 (17) | 0.0281 (14) | 0.0329 (15) | −0.0003 (12) | −0.0039 (12) | −0.0154 (12) |

*Geometric parameters (Å, º)*

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|---|---|---|---|
| S1—O5 | 1.4212 (18) | N15—C21 | 1.364 (3) |
| S1—O4 | 1.4238 (16) | N15—C24 | 1.467 (4) |
| S1—N4 | 1.647 (2) | N16—C22 | 1.336 (4) |
| S1—C8 | 1.745 (3) | N17—N18 | 1.327 (3) |
| S2—O10 | 1.420 (2) | N17—C25 | 1.336 (3) |
| S2—O9 | 1.4267 (18) | N18—N19 | 1.323 (3) |
| S2—N14 | 1.6431 (19) | N18—C26 | 1.451 (3) |
| S2—C21 | 1.747 (3) | N19—N20 | 1.324 (3) |
| O1—C2 | 1.333 (3) | N20—C25 | 1.362 (3) |
| O1—C1 | 1.443 (3) | C1—H1A | 0.9800 |
| O2—C4 | 1.342 (3) | C1—H1B | 0.9800 |
| O2—C6 | 1.441 (3) | C1—H1C | 0.9800 |
| O3—C7 | 1.222 (3) | C2—C3 | 1.387 (3) |
| O6—C15 | 1.340 (3) | C3—C4 | 1.373 (3) |
| O6—C14 | 1.440 (3) | C3—H3 | 0.9500 |
| O7—C17 | 1.349 (3) | C6—H6A | 0.9800 |
| O7—C19 | 1.447 (3) | C6—H6B | 0.9800 |
| O8—C20 | 1.211 (3) | C6—H6C | 0.9800 |
| N1—C5 | 1.323 (3) | C8—C10 | 1.400 (4) |
| N1—C2 | 1.338 (3) | C9—C10 | 1.398 (4) |
| N2—C5 | 1.338 (3) | C9—H9 | 0.9500 |
| N2—C4 | 1.345 (3) | C10—C12 | 1.455 (3) |
| N3—C7 | 1.380 (3) | C11—H11A | 0.9800 |
| N3—C5 | 1.399 (3) | C11—H11B | 0.9800 |
| N3—H3N | 0.8800 | C11—H11C | 0.9800 |
| N4—C7 | 1.370 (3) | C13—H13A | 0.9800 |
| N4—H4N | 0.8800 | C13—H13B | 0.9800 |
| N5—N6 | 1.341 (3) | C13—H13C | 0.9800 |

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| N5—C8 | 1.361 (3) | C14—H14A | 0.9800 |
| N5—C11 | 1.465 (3) | C14—H14B | 0.9800 |
| N6—C9 | 1.324 (4) | C14—H14C | 0.9800 |
| N7—C12 | 1.328 (3) | C15—C16 | 1.384 (3) |
| N7—N8 | 1.344 (3) | C16—C17 | 1.382 (3) |
| N8—N9 | 1.310 (3) | C16—H16 | 0.9500 |
| N8—C13 | 1.458 (4) | C19—H19A | 0.9800 |
| N9—N10 | 1.312 (3) | C19—H19B | 0.9800 |
| N10—C12 | 1.350 (3) | C19—H19C | 0.9800 |
| N11—C18 | 1.333 (3) | C21—C23 | 1.393 (4) |
| N11—C15 | 1.345 (3) | C22—C23 | 1.400 (3) |
| N12—C17 | 1.326 (3) | C22—H22 | 0.9500 |
| N12—C18 | 1.338 (3) | C23—C25 | 1.449 (4) |
| N13—C18 | 1.376 (3) | C24—H24A | 0.9800 |
| N13—C20 | 1.384 (3) | C24—H24B | 0.9800 |
| N13—H13N | 0.8800 | C24—H24C | 0.9800 |
| N14—C20 | 1.380 (3) | C26—H26A | 0.9800 |
| N14—H14N | 0.8800 | C26—H26B | 0.9800 |
| N15—N16 | 1.343 (3) | C26—H26C | 0.9800 |

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|---|---|---|---|
| O5—S1—O4 | 120.08 (11) | O3—C7—N3 | 121.2 (2) |
| O5—S1—N4 | 110.06 (10) | N4—C7—N3 | 116.2 (2) |
| O4—S1—N4 | 103.25 (10) | N5—C8—C10 | 107.4 (2) |
| O5—S1—C8 | 108.81 (11) | N5—C8—S1 | 124.3 (2) |
| O4—S1—C8 | 107.74 (11) | C10—C8—S1 | 128.17 (18) |
| N4—S1—C8 | 105.99 (11) | N6—C9—C10 | 112.4 (3) |
| O10—S2—O9 | 119.77 (11) | N6—C9—H9 | 123.8 |
| O10—S2—N14 | 110.51 (11) | C10—C9—H9 | 123.8 |
| O9—S2—N14 | 103.83 (11) | C9—C10—C8 | 103.2 (2) |
| O10—S2—C21 | 108.05 (13) | C9—C10—C12 | 124.8 (3) |
| O9—S2—C21 | 109.42 (12) | C8—C10—C12 | 132.0 (2) |
| N14—S2—C21 | 104.16 (11) | N5—C11—H11A | 109.5 |
| C2—O1—C1 | 117.82 (19) | N5—C11—H11B | 109.5 |
| C4—O2—C6 | 117.94 (19) | H11A—C11—H11B | 109.5 |
| C15—O6—C14 | 117.12 (18) | N5—C11—H11C | 109.5 |
| C17—O7—C19 | 116.6 (2) | H11A—C11—H11C | 109.5 |
| C5—N1—C2 | 114.6 (2) | H11B—C11—H11C | 109.5 |
| C5—N2—C4 | 114.8 (2) | N7—C12—N10 | 112.7 (2) |
| C7—N3—C5 | 129.9 (2) | N7—C12—C10 | 126.6 (2) |
| C7—N3—H3N | 115.0 | N10—C12—C10 | 120.5 (2) |
| C5—N3—H3N | 115.0 | N8—C13—H13A | 109.5 |
| C7—N4—S1 | 125.14 (16) | N8—C13—H13B | 109.5 |
| C7—N4—H4N | 117.4 | H13A—C13—H13B | 109.5 |
| S1—N4—H4N | 117.4 | N8—C13—H13C | 109.5 |
| N6—N5—C8 | 111.0 (2) | H13A—C13—H13C | 109.5 |
| N6—N5—C11 | 118.1 (2) | H13B—C13—H13C | 109.5 |
| C8—N5—C11 | 130.9 (2) | O6—C14—H14A | 109.5 |
| C9—N6—N5 | 105.9 (2) | O6—C14—H14B | 109.5 |

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| C12—N7—N8 | 100.5 (2) | H14A—C14—H14B | 109.5 |
| N9—N8—N7 | 114.3 (2) | O6—C14—H14C | 109.5 |
| N9—N8—C13 | 122.4 (2) | H14A—C14—H14C | 109.5 |
| N7—N8—C13 | 123.2 (2) | H14B—C14—H14C | 109.5 |
| N8—N9—N10 | 106.2 (2) | O6—C15—N11 | 112.2 (2) |
| N9—N10—C12 | 106.2 (2) | O6—C15—C16 | 124.5 (2) |
| C18—N11—C15 | 115.0 (2) | N11—C15—C16 | 123.3 (2) |
| C17—N12—C18 | 115.4 (2) | C17—C16—C15 | 115.3 (2) |
| C18—N13—C20 | 130.6 (2) | C17—C16—H16 | 122.3 |
| C18—N13—H13N | 114.7 | C15—C16—H16 | 122.3 |
| C20—N13—H13N | 114.7 | N12—C17—O7 | 118.0 (2) |
| C20—N14—S2 | 122.10 (18) | N12—C17—C16 | 123.7 (2) |
| C20—N14—H14N | 119.0 | O7—C17—C16 | 118.3 (2) |
| S2—N14—H14N | 119.0 | N11—C18—N12 | 127.2 (2) |
| N16—N15—C21 | 111.3 (2) | N11—C18—N13 | 114.6 (2) |
| N16—N15—C24 | 117.3 (2) | N12—C18—N13 | 118.2 (2) |
| C21—N15—C24 | 131.4 (2) | O7—C19—H19A | 109.5 |
| C22—N16—N15 | 105.5 (2) | O7—C19—H19B | 109.5 |
| N18—N17—C25 | 102.1 (2) | H19A—C19—H19B | 109.5 |
| N19—N18—N17 | 113.8 (2) | O7—C19—H19C | 109.5 |
| N19—N18—C26 | 124.1 (2) | H19A—C19—H19C | 109.5 |
| N17—N18—C26 | 122.0 (2) | H19B—C19—H19C | 109.5 |
| N18—N19—N20 | 106.5 (2) | O8—C20—N14 | 122.8 (2) |
| N19—N20—C25 | 105.9 (2) | O8—C20—N13 | 120.8 (2) |
| O1—C1—H1A | 109.5 | N14—C20—N13 | 116.4 (2) |
| O1—C1—H1B | 109.5 | N15—C21—C23 | 107.4 (2) |
| H1A—C1—H1B | 109.5 | N15—C21—S2 | 123.5 (2) |
| O1—C1—H1C | 109.5 | C23—C21—S2 | 129.0 (2) |
| H1A—C1—H1C | 109.5 | N16—C22—C23 | 112.2 (3) |
| H1B—C1—H1C | 109.5 | N16—C22—H22 | 123.9 |
| O1—C2—N1 | 119.3 (2) | C23—C22—H22 | 123.9 |
| O1—C2—C3 | 117.0 (2) | C21—C23—C22 | 103.6 (2) |
| N1—C2—C3 | 123.7 (2) | C21—C23—C25 | 132.5 (2) |
| C4—C3—C2 | 115.6 (2) | C22—C23—C25 | 123.8 (2) |
| C4—C3—H3 | 122.2 | N15—C24—H24A | 109.5 |
| C2—C3—H3 | 122.2 | N15—C24—H24B | 109.5 |
| O2—C4—N2 | 118.3 (2) | H24A—C24—H24B | 109.5 |
| O2—C4—C3 | 118.6 (2) | N15—C24—H24C | 109.5 |
| N2—C4—C3 | 123.1 (2) | H24A—C24—H24C | 109.5 |
| N1—C5—N2 | 128.1 (2) | H24B—C24—H24C | 109.5 |
| N1—C5—N3 | 114.3 (2) | N17—C25—N20 | 111.8 (2) |
| N2—C5—N3 | 117.5 (2) | N17—C25—C23 | 119.4 (2) |
| O2—C6—H6A | 109.5 | N20—C25—C23 | 128.8 (2) |
| O2—C6—H6B | 109.5 | N18—C26—H26A | 109.5 |
| H6A—C6—H6B | 109.5 | N18—C26—H26B | 109.5 |
| O2—C6—H6C | 109.5 | H26A—C26—H26B | 109.5 |
| H6A—C6—H6C | 109.5 | N18—C26—H26C | 109.5 |
| H6B—C6—H6C | 109.5 | H26A—C26—H26C | 109.5 |

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| O3—C7—N4 | 122.6 (2) | H26B—C26—H26C | 109.5 |
| | | | |
| O5—S1—N4—C7 | −46.2 (2) | N5—C8—C10—C12 | 179.0 (3) |
| O4—S1—N4—C7 | −175.6 (2) | S1—C8—C10—C12 | −5.2 (5) |
| C8—S1—N4—C7 | 71.3 (2) | N8—N7—C12—N10 | −0.2 (3) |
| C8—N5—N6—C9 | −0.8 (3) | N8—N7—C12—C10 | −176.4 (3) |
| C11—N5—N6—C9 | −179.6 (3) | N9—N10—C12—N7 | 0.2 (3) |
| C12—N7—N8—N9 | 0.2 (3) | N9—N10—C12—C10 | 176.7 (3) |
| C12—N7—N8—C13 | 178.5 (3) | C9—C10—C12—N7 | 140.6 (3) |
| N7—N8—N9—N10 | −0.1 (3) | C8—C10—C12—N7 | −39.5 (5) |
| C13—N8—N9—N10 | −178.4 (3) | C9—C10—C12—N10 | −35.4 (4) |
| N8—N9—N10—C12 | −0.1 (3) | C8—C10—C12—N10 | 144.6 (3) |
| O10—S2—N14—C20 | −62.4 (2) | C14—O6—C15—N11 | 174.7 (2) |
| O9—S2—N14—C20 | 167.96 (19) | C14—O6—C15—C16 | −5.5 (3) |
| C21—S2—N14—C20 | 53.4 (2) | C18—N11—C15—O6 | −179.3 (2) |
| C21—N15—N16—C22 | 0.2 (3) | C18—N11—C15—C16 | 0.9 (3) |
| C24—N15—N16—C22 | 178.3 (2) | O6—C15—C16—C17 | −177.9 (2) |
| C25—N17—N18—N19 | 0.3 (2) | N11—C15—C16—C17 | 1.9 (4) |
| C25—N17—N18—C26 | 177.8 (2) | C18—N12—C17—O7 | −179.8 (2) |
| N17—N18—N19—N20 | −0.2 (3) | C18—N12—C17—C16 | 1.6 (3) |
| C26—N18—N19—N20 | −177.7 (2) | C19—O7—C17—N12 | 3.8 (3) |
| N18—N19—N20—C25 | 0.0 (2) | C19—O7—C17—C16 | −177.5 (2) |
| C1—O1—C2—N1 | 7.6 (3) | C15—C16—C17—N12 | −3.2 (4) |
| C1—O1—C2—C3 | −174.1 (2) | C15—C16—C17—O7 | 178.2 (2) |
| C5—N1—C2—O1 | 175.3 (2) | C15—N11—C18—N12 | −2.9 (4) |
| C5—N1—C2—C3 | −2.9 (3) | C15—N11—C18—N13 | 176.3 (2) |
| O1—C2—C3—C4 | −174.8 (2) | C17—N12—C18—N11 | 1.7 (4) |
| N1—C2—C3—C4 | 3.4 (4) | C17—N12—C18—N13 | −177.5 (2) |
| C6—O2—C4—N2 | −1.9 (3) | C20—N13—C18—N11 | 176.5 (2) |
| C6—O2—C4—C3 | 178.0 (2) | C20—N13—C18—N12 | −4.2 (4) |
| C5—N2—C4—O2 | 179.3 (2) | S2—N14—C20—O8 | 7.5 (3) |
| C5—N2—C4—C3 | −0.6 (3) | S2—N14—C20—N13 | −171.02 (17) |
| C2—C3—C4—O2 | 178.6 (2) | C18—N13—C20—O8 | 179.7 (2) |
| C2—C3—C4—N2 | −1.5 (4) | C18—N13—C20—N14 | −1.8 (4) |
| C2—N1—C5—N2 | 0.5 (4) | N16—N15—C21—C23 | −0.4 (3) |
| C2—N1—C5—N3 | −178.47 (19) | C24—N15—C21—C23 | −178.2 (2) |
| C4—N2—C5—N1 | 1.2 (4) | N16—N15—C21—S2 | −179.42 (17) |
| C4—N2—C5—N3 | −179.9 (2) | C24—N15—C21—S2 | 2.8 (4) |
| C7—N3—C5—N1 | 171.6 (2) | O10—S2—C21—N15 | 13.3 (2) |
| C7—N3—C5—N2 | −7.5 (4) | O9—S2—C21—N15 | 145.26 (19) |
| S1—N4—C7—O3 | −0.4 (4) | N14—S2—C21—N15 | −104.2 (2) |
| S1—N4—C7—N3 | −178.80 (17) | O10—S2—C21—C23 | −165.5 (2) |
| C5—N3—C7—O3 | −177.1 (2) | O9—S2—C21—C23 | −33.5 (3) |
| C5—N3—C7—N4 | 1.4 (4) | N14—S2—C21—C23 | 77.0 (2) |
| N6—N5—C8—C10 | 1.2 (3) | N15—N16—C22—C23 | 0.1 (3) |
| C11—N5—C8—C10 | 179.8 (3) | N15—C21—C23—C22 | 0.4 (3) |
| N6—N5—C8—S1 | −174.8 (2) | S2—C21—C23—C22 | 179.38 (19) |
| C11—N5—C8—S1 | 3.8 (4) | N15—C21—C23—C25 | −175.6 (2) |

| | | | |
|---|---|---|---|
| O5—S1—C8—N5 | 16.9 (3) | S2—C21—C23—C25 | 3.4 (4) |
| O4—S1—C8—N5 | 148.5 (2) | N16—C22—C23—C21 | −0.3 (3) |
| N4—S1—C8—N5 | −101.5 (2) | N16—C22—C23—C25 | 176.1 (2) |
| O5—S1—C8—C10 | −158.3 (2) | N18—N17—C25—N20 | −0.2 (3) |
| O4—S1—C8—C10 | −26.6 (3) | N18—N17—C25—C23 | 179.0 (2) |
| N4—S1—C8—C10 | 83.4 (3) | N19—N20—C25—N17 | 0.1 (3) |
| N5—N6—C9—C10 | 0.1 (3) | N19—N20—C25—C23 | −179.0 (2) |
| N6—C9—C10—C8 | 0.5 (3) | C21—C23—C25—N17 | 151.6 (3) |
| N6—C9—C10—C12 | −179.5 (3) | C22—C23—C25—N17 | −23.7 (4) |
| N5—C8—C10—C9 | −1.0 (3) | C21—C23—C25—N20 | −29.3 (4) |
| S1—C8—C10—C9 | 174.8 (2) | C22—C23—C25—N20 | 155.4 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3*N*···N11$^{i}$ | 0.88 | 2.65 | 3.494 (3) | 162 |
| N4—H4*N*···N2 | 0.88 | 1.89 | 2.611 (3) | 138 |
| N13—H13*N*···O3$^{i}$ | 0.88 | 2.04 | 2.844 (2) | 151 |
| N14—H14*N*···N12 | 0.88 | 1.95 | 2.636 (3) | 134 |
| C1—H1*C*···O8$^{ii}$ | 0.98 | 2.58 | 3.559 (3) | 178 |
| C11—H11*B*···O3 | 0.98 | 2.38 | 3.236 (3) | 146 |
| C11—H11*B*···O8$^{i}$ | 0.98 | 2.57 | 3.278 (3) | 129 |
| C11—H11*C*···N10$^{iii}$ | 0.98 | 2.58 | 3.290 (4) | 130 |
| C13—H13*A*···O9$^{iv}$ | 0.98 | 2.40 | 3.374 (4) | 175 |
| C14—H14*A*···O5$^{v}$ | 0.98 | 2.39 | 3.335 (3) | 162 |
| C22—H22···N17$^{vi}$ | 0.95 | 2.57 | 3.435 (3) | 152 |
| C24—H24*B*···O8 | 0.98 | 2.33 | 3.080 (3) | 133 |
| C26—H26*B*···N16$^{vi}$ | 0.98 | 2.52 | 3.376 (3) | 146 |

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*−1, *y*, *z*; (iii) −*x*+1, −*y*+1, −*z*; (iv) −*x*+2, −*y*, −*z*+1; (v) *x*+1, *y*, *z*; (vi) −*x*+1, −*y*, −*z*+2.