Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 4-[(4-Methoxybenzylidene)amino]-benzenesulfonamide

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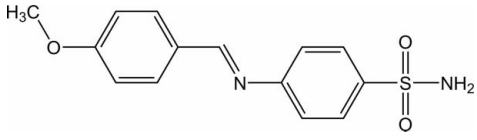
Received 18 April 2012; accepted 26 April 2012

Key indicators: single-crystal X-ray study; $T$ = 200 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.035; $wR$ factor = 0.095; data-to-parameter ratio = 18.6.

The title Schiff base compound, $C_{14}H_{14}N_2O_3S$, is non-planar, with a dihedral angle of 24.16 (7)° between the benzene rings. In the crystal, N—H···O and N—H···N hydrogen bonds link the molecules into a layer parallel to (011). Intra- and interlayer C—H···O interactions and $\pi$–$\pi$ interactions [centroid–centroid distances = 3.8900 (9) and 3.9355 (8) Å] are also present.

## Related literature

For general background to the applications of sulfanilamide Schiff bases, see: Gupta *et al.* (2003); Khalil *et al.* (2009); Nagpal & Singh (2004); Sharaby (2007); Wu *et al.* (2004).



## Experimental

### Crystal data

$C_{14}H_{14}N_2O_3S$
$M_r$ = 290.33
Monoclinic, $P2_1/c$
$a$ = 16.3315 (5) Å
$b$ = 11.1597 (3) Å
$c$ = 7.6876 (3) Å
$\beta$ = 100.661 (1)°
$V$ = 1376.92 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.24 mm$^{-1}$
$T$ = 200 K
0.60 × 0.33 × 0.12 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.90, $T_{max}$ = 0.97
10501 measured reflections
3383 independent reflections
2821 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.017

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.095
$S$ = 1.08
3383 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

The authors thank the Department of Chemistry and Govan Mbeki Research and Development Centre (GMRDC), University of Fort Hare, for their support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2541).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, o1599 [doi:10.1107/S1600536812018818]

## 4-[(4-Methoxybenzylidene)amino]benzenesulfonamide

**Omoruyi G. Idemudia, Alexander P. Sadimenko, Anthony J. Afolayan and Eric C. Hosten**

### Comment

Biological applications of sulfa compounds either alone or as metal complexes are well known (Gupta *et al.*, 2003; Nagpal & Singh, 2004). Their chelating powers towards metal ions tend to increase on forming a Schiff base by way of reaction with a carbonyl (Khalil *et al.*, 2009; Sharaby, 2007; Wu *et al.*, 2004). Herein, we report a new sulfanilamide Schiff base (Fig. 1), as part of our look at developing better chelating ligands from biologically active amine compounds.

The least-squares planes through the phenyl rings of the benzenesulfonamide and methoxybenzaldehyde groups have a dihedral angle of 24.16 (7)°. In the crystal, the molecules are stacked along the *c* axis and linked by N—H···O and N—H···N hydrogen bonds (Table 1 and Fig. 2) into a layer parallel to (0 1 1) (Fig. 3). The least-squares planes through adjacent two methoxybenzaldehyde phenyl rings (C11–C16) are almost parallel with a dihedral angle of 3.97° and a centroid-to-centroid distance of 3.8900 (9) Å. The centroid-to-centroid distance between adjacent two benzenesulfonamide phenyl rings (C21–C26) is 3.9355 (8) Å. C22—H22···$\pi$ interaction occurs with the adjacent C21–C26 ring (H···*Cg* distance = 2.81 Å). Intra- and interlayer C—H···O interactions are also observed.

### Experimental

A mixture of (4-aminobenzenesulfonamide)sulfadiazine and 4-methoxybenzaldehyde (anisaldehyde) (molar ratio 1:1) in methanol was refluxed for 15 h. The resultant pale yellow precipitate was isolated by filtration and recrystalized from methanol. Yield 68% and melting point 199–201°C. Single crystals suitable for X-ray analysis were obtained from methanol by slow evaporation at room temperature.

### Refinement

C-bound H atoms were placed in calculated positions and refined as riding atoms, with C—H = 0.95 (CH), 0.98 ($CH_3$) Å and with $U_{iso}$(H) = 1.2(1.5 for methyl)$U_{eq}$(C). N-bound H atoms were located on a difference Fourier map and refined as riding with $U_{iso}$(H) = 1.2$U_{eq}$(N).

### Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

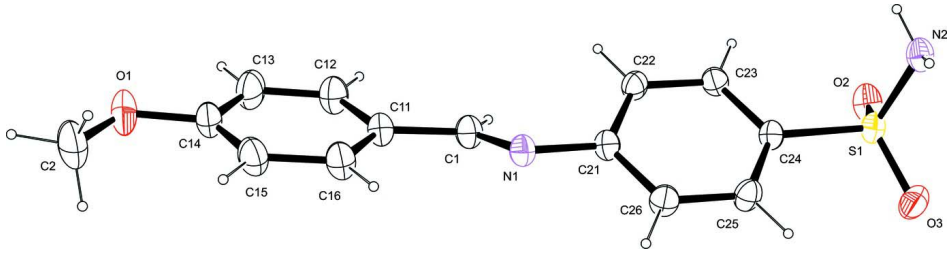


**Figure 1**

The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

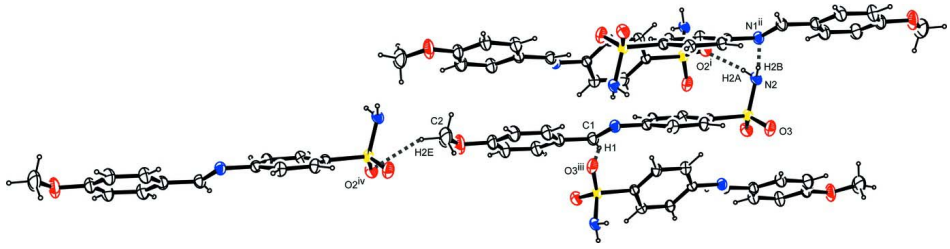


**Figure 2**

Hydrogen bonds in the title compound. [Symmetry codes: (i) *x*, -*y*+3/2, *z*-1/2; (ii) -*x*+1, -*y*+2, -*z*+1; (iii) -*x*+1, *y*-1/2, -*z*+3/2; (iv) *x*-1, *y*, *z*-1.]

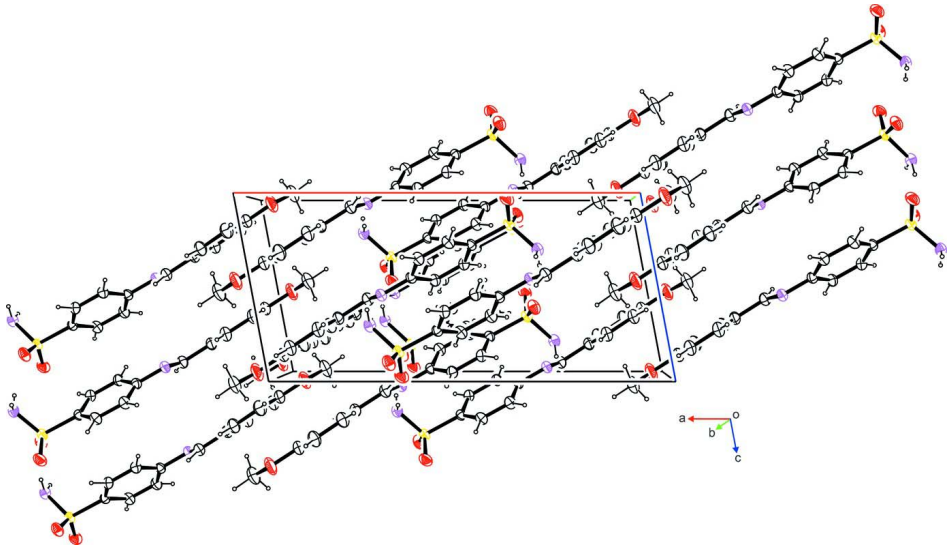


**Figure 3**

Crystal packing of the title compound viewed along [0 1 0].

### 4-[(4-Methoxybenzylidene)amino]benzenesulfonamide

*Crystal data*

$C_{14}H_{14}N_2O_3S$
$M_r$ = 290.33
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 16.3315 (5) Å
$b$ = 11.1597 (3) Å
$c$ = 7.6876 (3) Å
$\beta$ = 100.661 (1)°
$V$ = 1376.92 (8) Å$^3$
$Z$ = 4
$F$(000) = 608
$D_x$ = 1.401 Mg m$^{-3}$

Melting point: 473.15 K
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 118 reflections
$\theta$ = 3.1–29.3°
$\mu$ = 0.24 mm$^{-1}$
$T$ = 200 K
Platelet, yellow
0.60 × 0.33 × 0.12 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.90, $T_{max}$ = 0.97
10501 measured reflections
3383 independent reflections
2821 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.017
$\theta_{max}$ = 28.3°, $\theta_{min}$ = 2.2°
$h$ = −21→21
$k$ = −14→14
$l$ = −10→8

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.095
$S$ = 1.08
3383 reflections
182 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 0.7392P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 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)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.663198 (19) | 0.87003 (3) | 0.83688 (5) | 0.02211 (10) |
| O1 | −0.04751 (7) | 0.67929 (13) | 0.0325 (2) | 0.0479 (4) |
| O2 | 0.68589 (6) | 0.74895 (9) | 0.88958 (16) | 0.0306 (3) |
| O3 | 0.66935 (7) | 0.96150 (10) | 0.96956 (16) | 0.0333 (3) |
| N1 | 0.31032 (7) | 0.85378 (10) | 0.45630 (17) | 0.0231 (2) |
| N2 | 0.72148 (7) | 0.90797 (11) | 0.69963 (17) | 0.0248 (3) |
| H2A | 0.719 | 0.8559 | 0.6172 | 0.03* |
| H2B | 0.7141 | 0.9792 | 0.6628 | 0.03* |
| C1 | 0.27140 (8) | 0.75396 (13) | 0.4333 (2) | 0.0250 (3) |
| H1 | 0.2986 | 0.6843 | 0.4867 | 0.03* |
| C2 | −0.10221 (11) | 0.7766 (2) | −0.0293 (3) | 0.0553 (6) |
| H2C | −0.0756 | 0.8292 | −0.1044 | 0.083* |

| | | | | |
|---|---|---|---|---|
| H2D | −0.1142 | 0.8221 | 0.0721 | 0.083* |
| H2E | −0.1543 | 0.7451 | −0.0979 | 0.083* |
| C11 | 0.18743 (8) | 0.74102 (13) | 0.3295 (2) | 0.0257 (3) |
| C12 | 0.15750 (9) | 0.62521 (14) | 0.2867 (2) | 0.0319 (3) |
| H12 | 0.1914 | 0.558 | 0.3275 | 0.038* |
| C13 | 0.07929 (10) | 0.60763 (15) | 0.1859 (2) | 0.0365 (4) |
| H13 | 0.0598 | 0.5287 | 0.1558 | 0.044* |
| C14 | 0.02902 (9) | 0.70602 (16) | 0.1285 (2) | 0.0335 (4) |
| C15 | 0.05726 (9) | 0.82138 (15) | 0.1709 (2) | 0.0344 (4) |
| H15 | 0.0228 | 0.8884 | 0.1321 | 0.041* |
| C16 | 0.13644 (9) | 0.83808 (14) | 0.2707 (2) | 0.0310 (3) |
| H16 | 0.1561 | 0.9171 | 0.2993 | 0.037* |
| C21 | 0.39382 (8) | 0.85383 (12) | 0.55004 (19) | 0.0206 (3) |
| C22 | 0.44881 (8) | 0.75989 (12) | 0.5357 (2) | 0.0225 (3) |
| H22 | 0.43 | 0.6923 | 0.4643 | 0.027* |
| C23 | 0.53057 (8) | 0.76496 (12) | 0.6253 (2) | 0.0223 (3) |
| H23 | 0.5675 | 0.7002 | 0.6176 | 0.027* |
| C24 | 0.55836 (8) | 0.86504 (11) | 0.72618 (19) | 0.0199 (3) |
| C25 | 0.50485 (9) | 0.96019 (12) | 0.7391 (2) | 0.0244 (3) |
| H25 | 0.5244 | 1.0287 | 0.8077 | 0.029* |
| C26 | 0.42248 (8) | 0.95441 (12) | 0.6508 (2) | 0.0246 (3) |
| H26 | 0.3857 | 1.0192 | 0.6592 | 0.03* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.01897 (16) | 0.02111 (17) | 0.02420 (19) | −0.00156 (11) | −0.00138 (12) | 0.00123 (13) |
| O1 | 0.0217 (5) | 0.0634 (9) | 0.0533 (9) | −0.0056 (5) | −0.0072 (5) | −0.0087 (7) |
| O2 | 0.0250 (5) | 0.0263 (5) | 0.0377 (7) | 0.0009 (4) | −0.0015 (4) | 0.0113 (5) |
| O3 | 0.0301 (5) | 0.0363 (6) | 0.0304 (6) | −0.0027 (4) | −0.0023 (4) | −0.0097 (5) |
| N1 | 0.0194 (5) | 0.0234 (6) | 0.0252 (6) | 0.0002 (4) | 0.0007 (4) | 0.0015 (5) |
| N2 | 0.0224 (5) | 0.0197 (5) | 0.0314 (7) | −0.0027 (4) | 0.0029 (5) | 0.0025 (5) |
| C1 | 0.0216 (6) | 0.0235 (6) | 0.0284 (8) | −0.0005 (5) | 0.0010 (5) | 0.0029 (5) |
| C2 | 0.0239 (8) | 0.0838 (16) | 0.0532 (13) | 0.0076 (9) | −0.0063 (8) | −0.0003 (12) |
| C11 | 0.0198 (6) | 0.0279 (7) | 0.0282 (8) | −0.0023 (5) | 0.0013 (5) | 0.0010 (6) |
| C12 | 0.0263 (7) | 0.0282 (7) | 0.0391 (9) | −0.0030 (6) | 0.0005 (6) | 0.0016 (7) |
| C13 | 0.0282 (7) | 0.0346 (8) | 0.0440 (10) | −0.0092 (6) | −0.0002 (7) | −0.0053 (7) |
| C14 | 0.0188 (6) | 0.0477 (9) | 0.0323 (9) | −0.0032 (6) | 0.0005 (6) | −0.0036 (7) |
| C15 | 0.0226 (7) | 0.0388 (9) | 0.0398 (10) | 0.0041 (6) | 0.0008 (6) | 0.0013 (7) |
| C16 | 0.0234 (7) | 0.0292 (7) | 0.0388 (9) | −0.0004 (6) | 0.0014 (6) | 0.0009 (7) |
| C21 | 0.0191 (6) | 0.0199 (6) | 0.0217 (7) | −0.0003 (5) | 0.0013 (5) | 0.0036 (5) |
| C22 | 0.0218 (6) | 0.0191 (6) | 0.0259 (7) | −0.0024 (5) | 0.0026 (5) | −0.0029 (5) |
| C23 | 0.0202 (6) | 0.0193 (6) | 0.0274 (7) | 0.0002 (5) | 0.0045 (5) | −0.0008 (5) |
| C24 | 0.0183 (5) | 0.0192 (6) | 0.0213 (7) | −0.0016 (4) | 0.0014 (5) | 0.0022 (5) |
| C25 | 0.0254 (6) | 0.0176 (6) | 0.0281 (7) | −0.0009 (5) | 0.0000 (5) | −0.0023 (5) |
| C26 | 0.0238 (6) | 0.0190 (6) | 0.0297 (8) | 0.0026 (5) | 0.0015 (5) | −0.0011 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—O3 | 1.4333 (11) | C12—H12 | 0.95 |
| S1—O2 | 1.4393 (10) | C13—C14 | 1.393 (2) |
| S1—N2 | 1.6032 (13) | C13—H13 | 0.95 |
| S1—C24 | 1.7663 (13) | C14—C15 | 1.386 (2) |
| O1—C14 | 1.3617 (17) | C15—C16 | 1.389 (2) |
| O1—C2 | 1.430 (2) | C15—H15 | 0.95 |
| N1—C1 | 1.2786 (18) | C16—H16 | 0.95 |
| N1—C21 | 1.4196 (16) | C21—C26 | 1.3945 (19) |
| N2—H2A | 0.8551 | C21—C22 | 1.3978 (18) |
| N2—H2B | 0.8452 | C22—C23 | 1.3856 (18) |
| C1—C11 | 1.4607 (18) | C22—H22 | 0.95 |
| C1—H1 | 0.95 | C23—C24 | 1.3875 (19) |
| C2—H2C | 0.98 | C23—H23 | 0.95 |
| C2—H2D | 0.98 | C24—C25 | 1.3904 (18) |
| C2—H2E | 0.98 | C25—C26 | 1.3916 (19) |
| C11—C16 | 1.390 (2) | C25—H25 | 0.95 |
| C11—C12 | 1.399 (2) | C26—H26 | 0.95 |
| C12—C13 | 1.380 (2) | | |

| | | | |
|---|---|---|---|
| O3—S1—O2 | 119.20 (7) | C14—C13—H13 | 120.1 |
| O3—S1—N2 | 107.96 (7) | O1—C14—C15 | 124.27 (15) |
| O2—S1—N2 | 106.25 (7) | O1—C14—C13 | 115.28 (15) |
| O3—S1—C24 | 107.42 (6) | C15—C14—C13 | 120.44 (14) |
| O2—S1—C24 | 106.39 (6) | C14—C15—C16 | 119.35 (15) |
| N2—S1—C24 | 109.38 (6) | C14—C15—H15 | 120.3 |
| C14—O1—C2 | 117.90 (15) | C16—C15—H15 | 120.3 |
| C1—N1—C21 | 118.48 (12) | C15—C16—C11 | 121.04 (15) |
| S1—N2—H2A | 110.9 | C15—C16—H16 | 119.5 |
| S1—N2—H2B | 113.8 | C11—C16—H16 | 119.5 |
| H2A—N2—H2B | 114.0 | C26—C21—C22 | 119.53 (12) |
| N1—C1—C11 | 123.66 (13) | C26—C21—N1 | 118.32 (12) |
| N1—C1—H1 | 118.2 | C22—C21—N1 | 122.04 (12) |
| C11—C1—H1 | 118.2 | C23—C22—C21 | 120.29 (12) |
| O1—C2—H2C | 109.5 | C23—C22—H22 | 119.9 |
| O1—C2—H2D | 109.5 | C21—C22—H22 | 119.9 |
| H2C—C2—H2D | 109.5 | C22—C23—C24 | 119.74 (12) |
| O1—C2—H2E | 109.5 | C22—C23—H23 | 120.1 |
| H2C—C2—H2E | 109.5 | C24—C23—H23 | 120.1 |
| H2D—C2—H2E | 109.5 | C23—C24—C25 | 120.64 (12) |
| C16—C11—C12 | 118.77 (13) | C23—C24—S1 | 118.85 (10) |
| C16—C11—C1 | 123.09 (13) | C25—C24—S1 | 120.51 (10) |
| C12—C11—C1 | 118.13 (13) | C24—C25—C26 | 119.57 (13) |
| C13—C12—C11 | 120.67 (14) | C24—C25—H25 | 120.2 |
| C13—C12—H12 | 119.7 | C26—C25—H25 | 120.2 |
| C11—C12—H12 | 119.7 | C25—C26—C21 | 120.19 (12) |
| C12—C13—C14 | 119.73 (15) | C25—C26—H26 | 119.9 |
| C12—C13—H13 | 120.1 | C21—C26—H26 | 119.9 |

| | | | |
|---|---|---|---|
| C21—N1—C1—C11 | −175.87 (13) | C26—C21—C22—C23 | 1.9 (2) |
| N1—C1—C11—C16 | −11.2 (2) | N1—C21—C22—C23 | 178.05 (13) |
| N1—C1—C11—C12 | 168.42 (16) | C21—C22—C23—C24 | −1.5 (2) |
| C16—C11—C12—C13 | 0.9 (3) | C22—C23—C24—C25 | 0.3 (2) |
| C1—C11—C12—C13 | −178.67 (16) | C22—C23—C24—S1 | −179.27 (11) |
| C11—C12—C13—C14 | −1.1 (3) | O3—S1—C24—C23 | −163.03 (12) |
| C2—O1—C14—C15 | 0.3 (3) | O2—S1—C24—C23 | −34.34 (13) |
| C2—O1—C14—C13 | 179.64 (17) | N2—S1—C24—C23 | 80.04 (12) |
| C12—C13—C14—O1 | −178.90 (16) | O3—S1—C24—C25 | 17.41 (14) |
| C12—C13—C14—C15 | 0.4 (3) | O2—S1—C24—C25 | 146.11 (12) |
| O1—C14—C15—C16 | 179.57 (16) | N2—S1—C24—C25 | −99.52 (13) |
| C13—C14—C15—C16 | 0.3 (3) | C23—C24—C25—C26 | 0.5 (2) |
| C14—C15—C16—C11 | −0.4 (3) | S1—C24—C25—C26 | 180.00 (11) |
| C12—C11—C16—C15 | −0.2 (2) | C24—C25—C26—C21 | 0.0 (2) |
| C1—C11—C16—C15 | 179.39 (15) | C22—C21—C26—C25 | −1.2 (2) |
| C1—N1—C21—C26 | −148.41 (14) | N1—C21—C26—C25 | −177.44 (13) |
| C1—N1—C21—C22 | 35.4 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*A*···O2$^{i}$ | 0.86 | 2.09 | 2.9280 (17) | 166 |
| N2—H2*B*···N1$^{ii}$ | 0.85 | 2.08 | 2.9233 (17) | 173 |
| C1—H1···O3$^{iii}$ | 0.95 | 2.55 | 3.4466 (18) | 157 |
| C2—H2*E*···O2$^{iv}$ | 0.98 | 2.59 | 3.415 (2) | 141 |

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