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N-(2,5-Dimethoxyphenyl)-4-nitrobenzenesulfonamide

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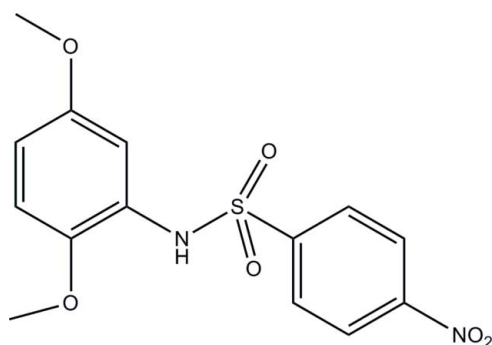
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 Key indicators: single-crystal X-ray study; $T = 292$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.040; wR factor = 0.121; data-to-parameter ratio = 13.4.

The title compound, $\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}_6\text{S}$, is an intermediate for the synthesis of β -3-adrenergic receptor agonists. The two methoxy groups are approximately coplanar with the attached benzene ring [$\text{C}-\text{O}-\text{C}-\text{C} = -2.7$ (4) and 9.4 (4) $^\circ$]. The dihedral angle between the two aromatic rings is 67.16 (12) $^\circ$. An intramolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bond is observed. In the crystal, molecules are linked into chains along the c axis by $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For biological activity of β -3-adrenergic receptors, see: Bardou *et al.* (1998); Hu *et al.* (2001); Klaus *et al.* (2001); Margareto *et al.* (2001); Ok *et al.* (2000); Parmee *et al.* (1998, 2000); Tonello *et al.* (1998); Weber *et al.* (1998).



Experimental

Crystal data

 $\text{C}_{14}\text{H}_{14}\text{N}_2\text{O}_6\text{S}$
 $M_r = 338.33$
 Orthorhombic, $Pbca$
 $a = 14.532$ (4) Å
 $b = 12.375$ (4) Å
 $c = 17.311$ (4) Å

 $V = 3113.2$ (14) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.24$ mm⁻¹
 $T = 292$ K
 $0.48 \times 0.44 \times 0.42$ mm

Data collection

 Enraf-Nonius CAD-4 diffractometer
 Absorption correction: for a sphere (*WinGX*; Farrugia, 1999)
 $T_{\min} = 0.893$, $T_{\max} = 0.906$
 4003 measured reflections

 2877 independent reflections
 1790 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.004$
 3 standard reflections every 200 reflections
 intensity decay: 0.9%

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.121$
 $S = 1.06$
 2877 reflections
 214 parameters

 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.20$ e Å⁻³
 $\Delta\rho_{\min} = -0.32$ e Å⁻³

Table 1

 Hydrogen-bond geometry (Å, $^\circ$).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|----------|-------------|-------------|---------------|
| $\text{N1}-\text{H1N}\cdots\text{O2}$ | 0.78 (3) | 2.20 (3) | 2.607 (3) | 113 (2) |
| $\text{C8}-\text{H8C}\cdots\text{O4}^i$ | 0.96 | 2.55 | 3.414 (4) | 150 |

 Symmetry code: (i) $x, -y + \frac{3}{2}, z - \frac{1}{2}$.

Data collection: *DIFRAC* (Gabe & White, 1993); cell refinement: *DIFRAC*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); 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: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2846).

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supporting information

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N*-(2,5-Dimethoxyphenyl)-4-nitrobenzenesulfonamide*Guo-Yao Zhang, Shan Qian, Xiao-Cen Li and Yong Wu****S1. Comment**

The beta 3-adrenergic receptor has been shown to mediate various pharmacological and physiological effects such as lipolysis in white adipocyte tissue, thermogenesis in brown adipocyte tissue (Tonello *et al.*, 1998; Ok *et al.*, 2000; Parmee *et al.*, 1998, 2000) and relaxation of urinary bladder detrusor tissue (Hu *et al.*, 2001; Parmee *et al.*, 1998; Weber *et al.*, 1998). Consequently, several pharmaceutical firms, including ourselves, are engaged in developing potent and selective beta 3-adrenergic receptor agonists for the treatment of obesity, type II diabetes, and frequent urination (Margareto *et al.*, 2001; Bardou *et al.*, 1998; Klaus *et al.*, 2001). In our synthetic work of beta 3-adrenergic receptor agonists, we obtained the title compound. Its crystal structure is reported here.

The two methoxy groups are approximately coplanar with the attached benzene ring [$C7-O1-C3-C4 = -2.7 (4)^\circ$ and $C8-O2-C6-C5 = 9.4 (4)^\circ$]. The nitro group is coplanar with the C9-C14 benzene ring. The dihedral angle between the two aromatic rings is $67.16 (12)^\circ$. An intramolecular N—H \cdots O hydrogen bond is observed.

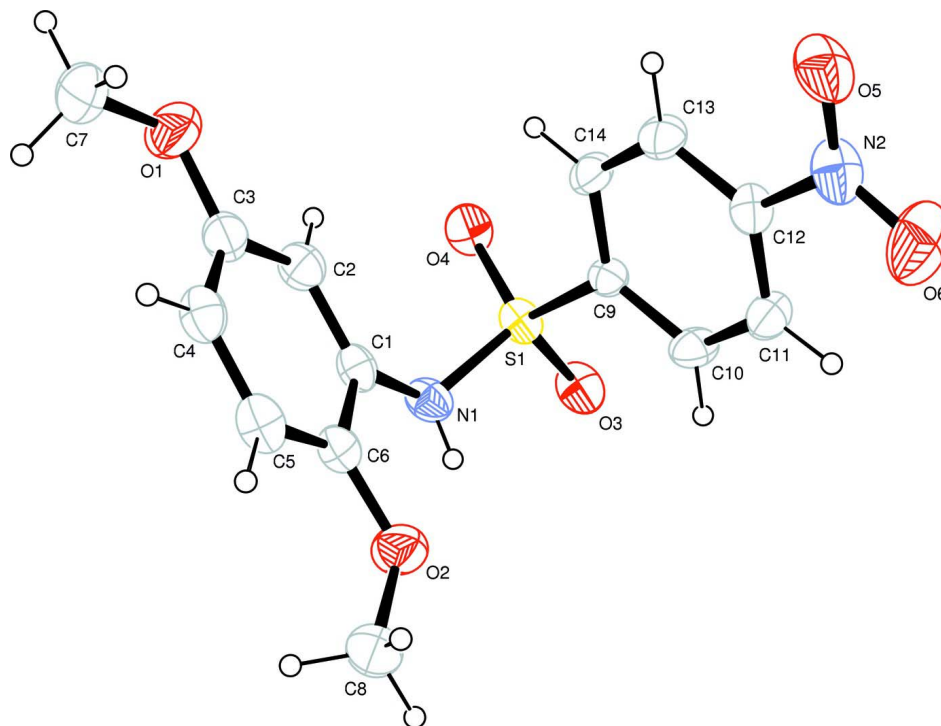
The crystal packing of the title compound shows that the molecules are linked by C—H \cdots O hydrogen bonds (Table 1) to form chains along the *c* axis.

S2. Experimental

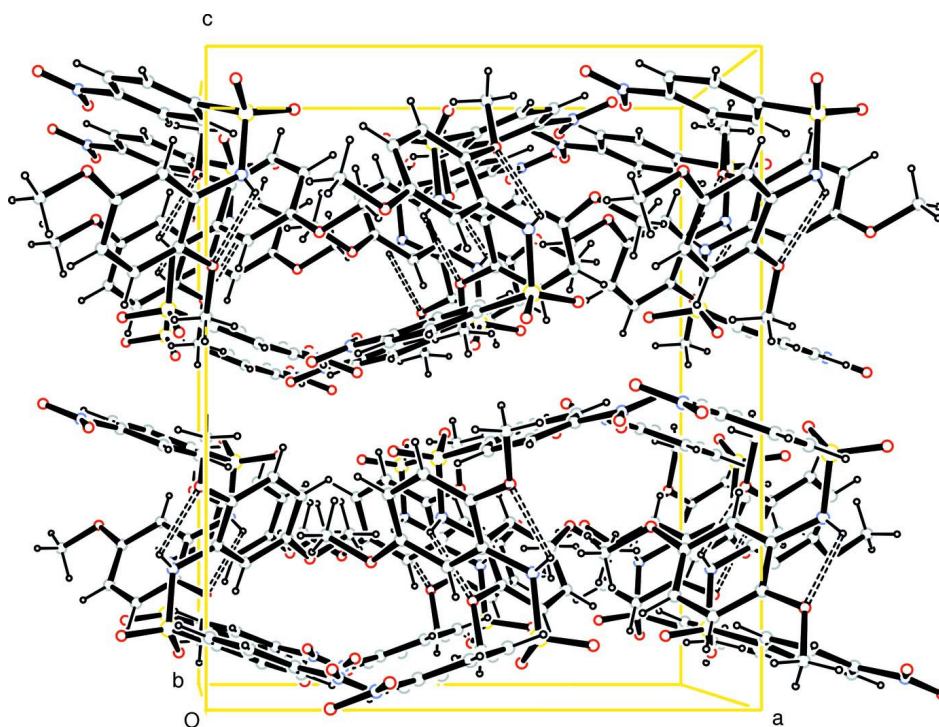
2,5-Dimethoxybenzenamine (10 mmol) and excess pyridine were dissolved in dichloromethane (20 ml) and a solution of 4-nitrobenzene-1-sulfonyl chloride (13 mmol) in dichloromethane (20 ml) was added dropwise with vigorous stirring at 273 K. After 1 h, the reaction was quenched by addition of water and the oil was washed with diluted HCl. The organic layer separated was evaporated to give the crude product, which was recrystallized from n-hexane -dichloromethane (5:1). Colourless crystals suitable for X-ray analysis were obtained by slow evaporation in n-hexane-dichloromethane at room temperature.

S3. Refinement

Atom H1N was located in a difference map and was refined freely. All other H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined using a riding model, with $U_{iso}(H) = 1.2-1.5U_{eq}(C)$.

**Figure 1**

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

**Figure 2**

A packing diagram for the title compound.

N*-(2,5-Dimethoxyphenyl)-4-nitrobenzenesulfonamideCrystal data*C₁₄H₁₄N₂O₆S $M_r = 338.33$ Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

 $a = 14.532$ (4) Å $b = 12.375$ (4) Å $c = 17.311$ (4) Å $V = 3113.2$ (14) Å³ $Z = 8$ $F(000) = 1408$ $D_x = 1.444$ Mg m⁻³Mo *K*α radiation, $\lambda = 0.71073$ Å

Cell parameters from 32 reflections

 $\theta = 4.3$ – 7.5° $\mu = 0.24$ mm⁻¹ $T = 292$ K

Block, colourless

 $0.48 \times 0.44 \times 0.42$ mm*Data collection*

Enraf–Nonius CAD-4

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 $\omega/2\theta$ scans

Absorption correction: for a sphere

(WinGX; Farrugia, 1999)

 $T_{\min} = 0.893$, $T_{\max} = 0.906$

4003 measured reflections

2877 independent reflections

1790 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.004$ $\theta_{\max} = 25.4^\circ$, $\theta_{\min} = 2.4^\circ$ $h = -17 \rightarrow 10$ $k = -2 \rightarrow 14$ $l = -11 \rightarrow 20$

3 standard reflections every 200 reflections

intensity decay: 0.9%

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.040$ $wR(F^2) = 0.121$ $S = 1.06$

2877 reflections

214 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

 $w = 1/[\sigma^2(F_o^2) + (0.0632P)^2 + 0.3387P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.20$ e Å⁻³ $\Delta\rho_{\min} = -0.32$ 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)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|-------------|--------------|----------------------------------|
| S1 | 0.06666 (4) | 0.69183 (6) | 0.38224 (3) | 0.0473 (2) |
| N1 | 0.05816 (14) | 0.7151 (2) | 0.28983 (13) | 0.0530 (6) |
| H1N | 0.0834 (18) | 0.669 (2) | 0.2672 (16) | 0.057 (10)* |
| N2 | -0.23262 (16) | 0.3748 (2) | 0.44664 (14) | 0.0662 (7) |

| | | | | |
|-----|---------------|--------------|--------------|-------------|
| O1 | -0.20633 (15) | 0.94720 (18) | 0.27633 (11) | 0.0854 (7) |
| O2 | 0.00947 (13) | 0.61834 (17) | 0.16246 (10) | 0.0731 (6) |
| O3 | 0.15329 (11) | 0.63919 (17) | 0.39190 (10) | 0.0624 (5) |
| O4 | 0.04683 (13) | 0.78981 (14) | 0.42213 (10) | 0.0615 (5) |
| O5 | -0.30528 (13) | 0.40717 (19) | 0.47199 (13) | 0.0831 (7) |
| O6 | -0.21642 (16) | 0.28124 (19) | 0.43150 (18) | 0.1057 (9) |
| C1 | -0.02551 (15) | 0.7501 (2) | 0.25371 (14) | 0.0452 (6) |
| C2 | -0.07889 (17) | 0.8326 (2) | 0.28188 (15) | 0.0549 (7) |
| H2 | -0.0618 | 0.8681 | 0.3270 | 0.066* |
| C3 | -0.15884 (18) | 0.8634 (2) | 0.24300 (15) | 0.0569 (7) |
| C4 | -0.18336 (17) | 0.8124 (2) | 0.17588 (15) | 0.0562 (7) |
| H4 | -0.2366 | 0.8329 | 0.1499 | 0.067* |
| C5 | -0.12900 (19) | 0.7305 (2) | 0.14695 (15) | 0.0576 (7) |
| H5 | -0.1456 | 0.6966 | 0.1011 | 0.069* |
| C6 | -0.04991 (17) | 0.6982 (2) | 0.18527 (14) | 0.0495 (6) |
| C7 | -0.2851 (2) | 0.9874 (3) | 0.23675 (18) | 0.0916 (11) |
| H7A | -0.2688 | 1.0047 | 0.1844 | 0.137* |
| H7B | -0.3071 | 1.0512 | 0.2623 | 0.137* |
| H7C | -0.3325 | 0.9334 | 0.2368 | 0.137* |
| C8 | -0.0013 (2) | 0.5726 (3) | 0.08822 (16) | 0.0856 (11) |
| H8A | -0.0571 | 0.5312 | 0.0866 | 0.128* |
| H8B | 0.0501 | 0.5263 | 0.0772 | 0.128* |
| H8C | -0.0041 | 0.6292 | 0.0504 | 0.128* |
| C9 | -0.02178 (15) | 0.59843 (19) | 0.40462 (12) | 0.0392 (5) |
| C10 | -0.00660 (16) | 0.4902 (2) | 0.39088 (14) | 0.0518 (6) |
| H10 | 0.0498 | 0.4670 | 0.3716 | 0.062* |
| C11 | -0.07563 (18) | 0.4167 (2) | 0.40591 (15) | 0.0542 (7) |
| H11 | -0.0664 | 0.3432 | 0.3978 | 0.065* |
| C12 | -0.15815 (16) | 0.4544 (2) | 0.43310 (14) | 0.0474 (6) |
| C13 | -0.17421 (17) | 0.5610 (2) | 0.44706 (15) | 0.0536 (7) |
| H13 | -0.2310 | 0.5838 | 0.4657 | 0.064* |
| C14 | -0.10508 (15) | 0.6342 (2) | 0.43313 (15) | 0.0494 (6) |
| H14 | -0.1144 | 0.7073 | 0.4428 | 0.059* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|-------------|-------------|-------------|--------------|--------------|--------------|
| S1 | 0.0389 (3) | 0.0590 (4) | 0.0440 (3) | -0.0088 (3) | -0.0050 (3) | 0.0049 (3) |
| N1 | 0.0418 (12) | 0.0706 (17) | 0.0467 (12) | -0.0002 (12) | 0.0015 (9) | 0.0032 (12) |
| N2 | 0.0512 (15) | 0.0693 (18) | 0.0780 (16) | -0.0135 (13) | -0.0120 (12) | 0.0180 (14) |
| O1 | 0.0911 (14) | 0.0898 (16) | 0.0751 (13) | 0.0359 (14) | -0.0083 (11) | -0.0015 (12) |
| O2 | 0.0859 (14) | 0.0786 (14) | 0.0547 (12) | 0.0178 (12) | -0.0074 (10) | -0.0102 (11) |
| O3 | 0.0344 (9) | 0.0884 (14) | 0.0645 (11) | -0.0040 (9) | -0.0062 (8) | 0.0152 (10) |
| O4 | 0.0738 (12) | 0.0565 (11) | 0.0541 (11) | -0.0146 (10) | -0.0101 (9) | -0.0053 (10) |
| O5 | 0.0478 (11) | 0.0999 (18) | 0.1017 (16) | -0.0122 (12) | 0.0057 (11) | 0.0330 (14) |
| O6 | 0.0880 (17) | 0.0563 (15) | 0.173 (3) | -0.0261 (13) | -0.0048 (17) | 0.0040 (16) |
| C1 | 0.0409 (12) | 0.0526 (14) | 0.0422 (12) | -0.0101 (13) | -0.0033 (11) | 0.0099 (13) |
| C2 | 0.0566 (15) | 0.0624 (18) | 0.0458 (13) | -0.0020 (14) | -0.0048 (12) | 0.0002 (13) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C3 | 0.0563 (15) | 0.0618 (17) | 0.0525 (15) | 0.0030 (14) | 0.0020 (12) | 0.0101 (14) |
| C4 | 0.0475 (14) | 0.0632 (18) | 0.0577 (15) | -0.0060 (14) | -0.0077 (12) | 0.0131 (15) |
| C5 | 0.0602 (17) | 0.0620 (18) | 0.0505 (15) | -0.0190 (15) | -0.0130 (12) | 0.0054 (14) |
| C6 | 0.0533 (14) | 0.0506 (15) | 0.0446 (13) | -0.0061 (13) | 0.0019 (11) | 0.0057 (13) |
| C7 | 0.082 (2) | 0.105 (3) | 0.088 (2) | 0.036 (2) | 0.0062 (18) | 0.030 (2) |
| C8 | 0.128 (3) | 0.078 (2) | 0.0505 (17) | 0.016 (2) | -0.0012 (17) | -0.0066 (17) |
| C9 | 0.0350 (12) | 0.0436 (13) | 0.0389 (12) | 0.0026 (11) | -0.0008 (9) | 0.0004 (11) |
| C10 | 0.0390 (12) | 0.0553 (16) | 0.0612 (16) | 0.0061 (12) | 0.0085 (11) | -0.0058 (13) |
| C11 | 0.0547 (15) | 0.0425 (14) | 0.0653 (16) | 0.0039 (13) | 0.0012 (12) | -0.0019 (13) |
| C12 | 0.0391 (13) | 0.0484 (15) | 0.0548 (14) | -0.0044 (12) | -0.0053 (11) | 0.0091 (12) |
| C13 | 0.0360 (13) | 0.0545 (16) | 0.0703 (17) | 0.0073 (12) | 0.0093 (12) | 0.0041 (14) |
| C14 | 0.0427 (13) | 0.0409 (14) | 0.0646 (15) | 0.0075 (12) | 0.0074 (12) | 0.0013 (13) |

Geometric parameters (Å, °)

| | | | |
|-----------|-------------|------------|-----------|
| S1—O4 | 1.4249 (19) | C4—H4 | 0.93 |
| S1—O3 | 1.4273 (18) | C5—C6 | 1.386 (3) |
| S1—N1 | 1.630 (2) | C5—H5 | 0.93 |
| S1—C9 | 1.771 (2) | C7—H7A | 0.96 |
| N1—C1 | 1.434 (3) | C7—H7B | 0.96 |
| N1—H1N | 0.78 (3) | C7—H7C | 0.96 |
| N2—O6 | 1.210 (3) | C8—H8A | 0.96 |
| N2—O5 | 1.212 (3) | C8—H8B | 0.96 |
| N2—C12 | 1.482 (3) | C8—H8C | 0.96 |
| O1—C3 | 1.373 (3) | C9—C10 | 1.378 (4) |
| O1—C7 | 1.424 (3) | C9—C14 | 1.380 (3) |
| O2—C6 | 1.370 (3) | C10—C11 | 1.379 (3) |
| O2—C8 | 1.413 (3) | C10—H10 | 0.93 |
| C1—C2 | 1.372 (3) | C11—C12 | 1.371 (3) |
| C1—C6 | 1.393 (3) | C11—H11 | 0.93 |
| C2—C3 | 1.396 (3) | C12—C13 | 1.360 (3) |
| C2—H2 | 0.93 | C13—C14 | 1.374 (3) |
| C3—C4 | 1.370 (4) | C13—H13 | 0.93 |
| C4—C5 | 1.379 (4) | C14—H14 | 0.93 |
| O4—S1—O3 | 120.67 (12) | C5—C6—C1 | 119.0 (2) |
| O4—S1—N1 | 108.06 (13) | O1—C7—H7A | 109.5 |
| O3—S1—N1 | 105.22 (11) | O1—C7—H7B | 109.5 |
| O4—S1—C9 | 107.61 (11) | H7A—C7—H7B | 109.5 |
| O3—S1—C9 | 108.45 (11) | O1—C7—H7C | 109.5 |
| N1—S1—C9 | 105.95 (11) | H7A—C7—H7C | 109.5 |
| C1—N1—S1 | 123.06 (17) | H7B—C7—H7C | 109.5 |
| C1—N1—H1N | 114 (2) | O2—C8—H8A | 109.5 |
| S1—N1—H1N | 109 (2) | O2—C8—H8B | 109.5 |
| O6—N2—O5 | 124.4 (3) | H8A—C8—H8B | 109.5 |
| O6—N2—C12 | 117.4 (3) | O2—C8—H8C | 109.5 |
| O5—N2—C12 | 118.3 (3) | H8A—C8—H8C | 109.5 |
| C3—O1—C7 | 117.8 (2) | H8B—C8—H8C | 109.5 |

| | | | |
|-------------|------------|-----------------|--------------|
| C6—O2—C8 | 118.8 (2) | C10—C9—C14 | 120.9 (2) |
| C2—C1—C6 | 120.1 (2) | C10—C9—S1 | 118.70 (18) |
| C2—C1—N1 | 123.3 (2) | C14—C9—S1 | 120.34 (19) |
| C6—C1—N1 | 116.6 (2) | C9—C10—C11 | 119.5 (2) |
| C1—C2—C3 | 120.2 (2) | C9—C10—H10 | 120.3 |
| C1—C2—H2 | 119.9 | C11—C10—H10 | 120.3 |
| C3—C2—H2 | 119.9 | C12—C11—C10 | 118.4 (2) |
| C4—C3—O1 | 125.0 (2) | C12—C11—H11 | 120.8 |
| C4—C3—C2 | 120.0 (3) | C10—C11—H11 | 120.8 |
| O1—C3—C2 | 115.0 (2) | C13—C12—C11 | 122.8 (2) |
| C3—C4—C5 | 119.9 (2) | C13—C12—N2 | 119.4 (2) |
| C3—C4—H4 | 120.1 | C11—C12—N2 | 117.8 (2) |
| C5—C4—H4 | 120.1 | C12—C13—C14 | 118.9 (2) |
| C4—C5—C6 | 120.9 (2) | C12—C13—H13 | 120.6 |
| C4—C5—H5 | 119.6 | C14—C13—H13 | 120.6 |
| C6—C5—H5 | 119.6 | C13—C14—C9 | 119.5 (2) |
| O2—C6—C5 | 126.3 (2) | C13—C14—H14 | 120.3 |
| O2—C6—C1 | 114.7 (2) | C9—C14—H14 | 120.3 |
| | | | |
| O4—S1—N1—C1 | -61.0 (2) | N1—C1—C6—C5 | -178.5 (2) |
| O3—S1—N1—C1 | 168.9 (2) | O4—S1—C9—C10 | -162.61 (19) |
| C9—S1—N1—C1 | 54.1 (2) | O3—S1—C9—C10 | -30.5 (2) |
| S1—N1—C1—C2 | 47.4 (3) | N1—S1—C9—C10 | 82.0 (2) |
| S1—N1—C1—C6 | -134.8 (2) | O4—S1—C9—C14 | 19.3 (2) |
| C6—C1—C2—C3 | 1.3 (4) | O3—S1—C9—C14 | 151.32 (19) |
| N1—C1—C2—C3 | 179.0 (2) | N1—S1—C9—C14 | -96.1 (2) |
| C7—O1—C3—C4 | -2.7 (4) | C14—C9—C10—C11 | -0.1 (4) |
| C7—O1—C3—C2 | 175.8 (3) | S1—C9—C10—C11 | -178.18 (19) |
| C1—C2—C3—C4 | -1.0 (4) | C9—C10—C11—C12 | 1.0 (4) |
| C1—C2—C3—O1 | -179.7 (2) | C10—C11—C12—C13 | -1.1 (4) |
| O1—C3—C4—C5 | 178.6 (2) | C10—C11—C12—N2 | 178.1 (2) |
| C2—C3—C4—C5 | 0.1 (4) | O6—N2—C12—C13 | 178.0 (3) |
| C3—C4—C5—C6 | 0.6 (4) | O5—N2—C12—C13 | -2.0 (4) |
| C8—O2—C6—C5 | 9.4 (4) | O6—N2—C12—C11 | -1.3 (4) |
| C8—O2—C6—C1 | -170.3 (2) | O5—N2—C12—C11 | 178.7 (2) |
| C4—C5—C6—O2 | -180.0 (2) | C11—C12—C13—C14 | 0.2 (4) |
| C4—C5—C6—C1 | -0.3 (4) | N2—C12—C13—C14 | -179.0 (2) |
| C2—C1—C6—O2 | 179.1 (2) | C12—C13—C14—C9 | 0.7 (4) |
| N1—C1—C6—O2 | 1.2 (3) | C10—C9—C14—C13 | -0.8 (4) |
| C2—C1—C6—C5 | -0.7 (4) | S1—C9—C14—C13 | 177.25 (19) |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------------------------|----------|-------------|-------------|---------------|
| N1—H1N \cdots O2 | 0.78 (3) | 2.20 (3) | 2.607 (3) | 113 (2) |
| C8—H8C \cdots O4 ⁱ | 0.96 | 2.55 | 3.414 (4) | 150 |

Symmetry code: (i) $x, -y+3/2, z-1/2$.