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[(1S,2S)-2-aminocyclohexyl]-2,4,6-trimethylbenzenesulfonamide

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Crystal structure of \(N-[(1S,2S)-2\text{-aminocyclohexyl}]\)-2,4,6-trimethylbenzenesulfonamide

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The title compound, \(C_{15}H_{24}N_{2}O_{2}S\), was synthesized via a substitution reaction between the enantiopure \((1S,2S)-(+)-1,2\text{-diaminocyclohexane}\) and \(2,4,6\text{-trimethylbenzene-1-sulfonyl chloride}\). The cyclohexyl and phenyl substituents are oriented gauche around the sulfonamide S–N bond. In the crystal, molecules are linked via N–H···N hydrogen bonds, forming chains propagating along [100].

1. Chemical context

Many sulfonamides have been reported as anticancer, anti-inflammatory, and antiviral agents (Navia, 2000; Yan \textit{et al.}, 2006; Palakurthy & Mandal, 2011). The use of sulfonamides as catalysts in asymmetric synthesis has also been reported (Lao \textit{et al.}, 2009; Feng \textit{et al.}, 2010; Jin \textit{et al.}, 2010). Through explicit hydrogen-bonding interactions with specific functional groups, the electrophilicity and stereoselectivity of a given substrate is enhanced.

Conjugate addition reactions of aldehydes and ketones to nitroalkenes, catalyzed by chiral primary amines, have been reported (Huang & Jacobsen, 2006; Rabalakos & Wulff, 2008; Lao \textit{et al.}, 2009; Sun \textit{et al.}, 2012; Zhou \textit{et al.}, 2014; Ruiz-Olalla \textit{et al.}, 2015; Yang \textit{et al.}, 2015). The catalytic activity of chiral primary amine organocatalysts with particular emphasis on the role of the N–H acidity and hydrogen bonding has also been investigated (Lao \textit{et al.}, 2009). Although the N–H acidity and hydrogen-bonding modes could have an effect on the catalytic activity of the organocatalysts, the nature of the substrate and reaction conditions could be more important. Asymmetric conjugate addition reactions of aldehydes to nitroalkenes have also been reported as a convenient synthesis of \(\gamma\)-amino acids (Horne & Gellman, 2008; Wiesner \textit{et al.}, 2008; Chi \textit{et al.}, 2008).

In line with our research interest in the synthesis of heterogeneous foldamers (Hayen \textit{et al.}, 2004), we synthesized the title compound as a chiral organocatalyst for conjugate addition. This conjugate addition was then applied for the
synthesis of \(\gamma\)-amino acids, which have been shown to be interesting foldamer building blocks (Horne & Gellman, 2008). Therefore, as the title compound is of interest in our ongoing effort on foldamer design and synthesis, we report here on the synthesis and crystal structure of this chiral sulfonamide.

2. Structural commentary

The asymmetric part of the unit cell is shown in Fig. 1 along with the atom-numbering scheme. The absolute stereochemistry of this chiral sulfonamide was confirmed by a Flack parameter of 0.00 (2) (Parsons et al., 2013). The cyclohexyl (C1–C6) and benzene (C7–C12) substituents are oriented gauche around the sulfonamide S–N bond, with a C1–N1–S1–C7 torsion angle of 70.4 (2)°. A weak intramolecular interaction is present between the amine H2A atom and the sp²-hybridized sulfonamide N1 atom (Table 1).

As described in the Database survey section below, the structure of a racemic crystal of this compound has been reported (FA VHEP; Balsells, et al., 1998). In this crystal, there are two crystallographically unique molecules of the sulfonamide compound in the asymmetric unit. Here, the cyclohexyl and benzene substituents are oriented gauche around the S–N bond with torsion angles of 86.8 (8)° and 69.1 (7)°. While we expected that there would be an intramolecular hydrogen bond in this crystal, in the model deposited in the CSD there are no intramolecular hydrogen bonds present between the amine N–H group and the sulfonamide N atom.

3. Supramolecular features

Molecules of the title compound are held together in the solid state by intermolecular hydrogen-bonding interactions between the donor sulfonamide N1–H1 and the acceptor amine N2 atoms (Table 1 and Fig. 2). These hydrogen bonds arrange molecules into supramolecular chains that are oriented along the [100] axis (Fig. 2). Weaker N2–H2B···O1(1 + x, y, z) interactions with an H2B···O1(1 + x, y, z) distance of 2.72 Å between the donor amine N2–H2B and the acceptor sulfonamide O1 atoms can also be noticed within this chain.

As for the racemic crystal FAVHEP, in the model deposited in the CSD there is one intramolecular hydrogen bond present between a donor sulfonamide N1–H1 and a nearby amine

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### Table 1

Hydrogen-bond geometry (Å, °).

| D—H—A | D—H | H···A | D···A | D—H···A |
|--------|------|-------|-------|---------|
| N2—H2A···N1 | 0.89 (3) | 2.43 (3) | 2.877 (3) | 111 (2) |
| N1—H1···N2' | 0.79 (3) | 2.14 (3) | 2.921 (3) | 170 (3) |

Symmetry code: (i) \(x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1\).
acceptor N atom \([D \cdots H = 0.860 (7) \AA; H \cdots A = 2.160 (8) \AA; D \cdots A = 3.011 (8) \AA; D - H \cdots A = 169.9 (5)^\circ]\).

4. Database survey

The Cambridge Structural Database (CSD, Version 5.36, May 2015; Groom & Allen, 2014) contains 35 sulfonamides bearing a mesitylene group on the S atom. Of these, there are four structures where the substituent bonded to the sulfonamide N atom is an aliphatic six-membered ring. In structures RAWMAF (Hou et al., 2012) and ZIQPAS (Wu et al., 2014), the aminocyclohexane substituent is part of a larger fused-ring system. Interestingly, there are two structures with 1,2-diaminocyclohexane rings as the amide substituent. In structure AVEHPEP (Balsells et al., 1998) is the same as the title compound, but is present as a racemic mixture that crystallized in the space group \(PT\).

5. Synthesis and crystallization

To a stirred solution of (1S,2S)-(+) or 1,2-diaminocyclohexane (0.77 g, 6.74 mmol) in 5 ml of CH\(_2\)Cl\(_2\) at 273 K was added a solution of 2,4,6-trimethylbenzene-1-sulfonyl chloride (0.44 g, 2.01 mmol) in 5 ml CH\(_2\)Cl\(_2\). After the addition was complete (20 min), the mixture was allowed to warm to room temperature and stirred overnight. The reaction mixture was washed with H\(_2\)O (3 × 25 ml) and the aqueous layer was back-extracted with CH\(_2\)Cl\(_2\) (20 ml). The combined organic extracts were dried over Na\(_2\)SO\(_4\) and the solvent was removed under reduced pressure. The residue was purified by column chromatography over silica gel (CH\(_2\)Cl\(_2\)/EtOAc 1:1 \(v/v\)) to afford a pale-yellow–white solid (yield: 0.46 g, 78%). Part of the purified product was redissolved in CH\(_2\)Cl\(_2\) and after slow evaporation for several days, white large chunky crystals (stained yellow) were formed that were suitable for analysis by X-ray diffraction (m.p. 406–407 K).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The positions of all non-polar H atoms were calculated geometrically and refined to ride on their parent atoms, with \(U_{iso}(H) = 1.2U_{eq}(C)\) for methine, methylene and aryl groups, and \(U_{iso}(H) = 1.5U_{eq}(C)\) for methyl groups. H atoms bonded directly to N atoms (H1, H2A and H2B) were located in difference-Fourier maps and refined isotropically.

Acknowledgements

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Table 2

| Crystal data |
|-------------|
| Chemical formula | \(\text{C}_2\text{H}_2\text{Na}_2\text{O}_2\text{S}\) |
| \(M_r\) | 296.42 |
| Crystal system, space group | Orthorhombic, \(P2_12_12_1\) |
| Temperature (K) | 173 |
| \(a\), \(b\), \(c\) (\(\AA\)) | 6.5215 (4), 10.0202 (6), 23.3660 (15) |
| \(V\) (\(\AA^3\)) | 1526.89 (16) |
| \(Z\) | 4 |
| Radiant type | Mo K\(\alpha\) |
| \(\mu\) (\(\text{mm}^{-1}\)) | 0.22 |
| Crystal size (mm) | 0.37 × 0.20 × 0.15 |

Data collection

| Diffractioneter |
|----------------|
| Bruker APEXI CCD |
| \(T_{\text{min}}, T_{\text{max}}\) | 0.706, 0.745 |
| No. of measured, independent and observed \([I > 2\sigma(I)]\) reflections | 25587, 2799, 2667 |
| \(R_{\text{int}}\) | 0.034 |
| (\(\sin \theta/\lambda\))\(_{\text{max}}\) (\(\AA^{-1}\)) | 0.602 |

Refinement

\(R[F^2 > 2\sigma(F^2)], wR(F^2), S\) | 0.029, 0.071, 1.06 |
| No. of reflections | 2799 |
| No. of parameters | 196 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| \(\Delta \rho_{\text{max}}, \Delta \rho_{\text{min}}\) (e \(\AA^{-3}\)) | 0.19, –0.21 |
| Absolute structure | Flack parameter x determined using 1098 quotients \([|F^2|-(|F^2|)]/[|F^2|+(|F^2|)]\) (Parsons et al., 2013) |
| Absolute structure parameter | 0.00 (2) |

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supporting information

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Crystal structure of N-[(1S,2S)-2-aminocyclohexyl]-2,4,6-trimethylbenzene-sulfonamide

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Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov et al., 2009; Bourhis et al., 2015); software used to prepare material for publication: *CrystalMaker* (Palmer, 2007).

**N-[(1S,2S)-2-Aminocyclohexyl]-2,4,6-trimethylbenzenesulfonamide**

Crystal data

\[C_{15}H_{24}N_2O_2S\]

Mr = 296.42

Orthorhombic, \(P2_12_12_1\)

\(a = 6.5215 (4)\) Å

\(b = 10.0202 (6)\) Å

\(c = 23.3660 (15)\) Å

\(V = 1526.89 (16)\) Å³

\(Z = 4\)

\(F(000) = 640\)

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: sealed tube

Graphite monochromator

Detector resolution: 8 pixels mm⁻¹

\(\varphi\) and \(\omega\) scans

Absorption correction: multi-scan

\(\text{SADABS};\) Bruker, 2014

\(T_{\text{min}} = 0.706, T_{\text{max}} = 0.745\)

Refinement

Refinement on \(F^2\)

Least-squares matrix: full

\(R[F^2 > 2\sigma(F^2)] = 0.029\)

\(wR(F^2) = 0.071\)

\(S = 1.06\)

25587 measured reflections

2799 independent reflections

2667 reflections with \(I > 2\sigma(I)\)

\(R_{\text{int}} = 0.034\)

\(\theta_{\text{max}} = 25.4^\circ, \theta_{\text{min}} = 1.7^\circ\)

\(h = -7\rightarrow 7\)

\(k = -12\rightarrow 12\)

\(l = -28\rightarrow 28\)

H atoms treated by a mixture of independent and constrained refinement

\[
\begin{align*}
\omega & = 1/\left[\sigma^2(Fo^2) + (0.0313P)^2 + 0.5049P\right] \\
& \quad \text{where } P = (Fo^2 + 2Fe^2)/3 \\
\Delta\sigma & < 0.001 \\
\Delta\rho_{\text{max}} & = 0.19 \text{ e Å}^{-3} \\
\Delta\rho_{\text{min}} & = -0.21 \text{ e Å}^{-3}
\end{align*}
\]

\(D_x = 1.289\) Mg m⁻³

Mo Kα radiation, \(\lambda = 0.71073\) Å

Cell parameters from 9968 reflections

Block, colourless

\(0.37 \times 0.20 \times 0.15\) mm

\(T = 173\) K

0.37 × 0.20 × 0.15 mm
Absolute structure: Flack parameter $x$
determined using 1098 quotients 
$[(I')-(I)]/[(I')+(I)]$ (Parsons et al., 2013)
Absolute structure parameter: 0.00 (2)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

|     | x     | y     | z     | $U_{iso}$/$U_{eq}$ |
|-----|-------|-------|-------|-------------------|
| S1  | 0.39425 (9) | 0.81200 (6) | 0.62892 (2) | 0.03018 (16) |
| O1  | 0.2464 (3) | 0.72704 (19) | 0.65596 (8) | 0.0412 (4) |
| O2  | 0.3238 (3) | 0.93797 (17) | 0.60697 (8) | 0.0408 (5) |
| N1  | 0.5015 (3) | 0.7361 (2) | 0.57616 (9) | 0.0297 (5) |
| N2  | 0.9140 (3) | 0.6769 (2) | 0.54061 (8) | 0.0287 (4) |
| C1  | 0.5776 (3) | 0.5984 (2) | 0.58084 (9) | 0.0238 (5) |
| H1A | 0.6425 | 0.5872 | 0.6193 | 0.029* |
| C2  | 0.7442 (3) | 0.5816 (2) | 0.53502 (9) | 0.0234 (5) |
| H2  | 0.6780 | 0.5986 | 0.4971 | 0.028* |
| C3  | 0.8271 (3) | 0.4398 (2) | 0.53360 (10) | 0.0273 (5) |
| H3A | 0.9052 | 0.4225 | 0.5692 | 0.033* |
| H3B | 0.9228 | 0.4306 | 0.5009 | 0.033* |
| C4  | 0.6574 (4) | 0.3363 (2) | 0.52793 (10) | 0.0308 (5) |
| H4A | 0.7174 | 0.2457 | 0.5300 | 0.037* |
| H4B | 0.5902 | 0.3460 | 0.4902 | 0.037* |
| C5  | 0.4980 (4) | 0.3528 (2) | 0.57518 (11) | 0.0314 (5) |
| H5A | 0.3864 | 0.2871 | 0.5696 | 0.038* |
| H5B | 0.5624 | 0.3353 | 0.6128 | 0.038* |
| C6  | 0.4094 (4) | 0.4934 (2) | 0.57442 (10) | 0.0300 (5) |
| H6A | 0.3095 | 0.5031 | 0.6061 | 0.036* |
| H6B | 0.3356 | 0.5080 | 0.5379 | 0.036* |
| C7  | 0.5988 (4) | 0.8413 (2) | 0.67770 (9) | 0.0252 (5) |
| C8  | 0.7523 (4) | 0.9336 (2) | 0.66163 (9) | 0.0270 (5) |
| C9  | 0.9071 (4) | 0.9619 (2) | 0.69984 (10) | 0.0321 (5) |
| H9  | 1.0119 | 1.0225 | 0.6887 | 0.039* |
| C10 | 0.9154 (4) | 0.9054 (2) | 0.75383 (10) | 0.0340 (6) |
| C11 | 0.7662 (4) | 0.8131 (3) | 0.76822 (10) | 0.0346 (5) |
| H11 | 0.7724 | 0.7723 | 0.8049 | 0.042* |
| C12 | 0.6078 (4) | 0.7775 (2) | 0.73148 (9) | 0.0291 (5) |
| C13 | 0.7568 (5) | 1.0087 (2) | 0.60541 (10) | 0.0384 (6) |
| H13A | 0.7084 | 0.9502 | 0.5746 | 0.058* |
| H13B | 0.8974 | 1.0373 | 0.5972 | 0.058* |
| H13C | 0.6675 | 1.0871 | 0.6080 | 0.058* |
| C14 | 1.0799 (5) | 0.9459 (3) | 0.79566 (13) | 0.0532 (8) |
| H14A | 1.2117 | 0.9523 | 0.7757 | 0.080* |
| Atomic displacement parameters (Å²) |
|------------------------------------|
| $U_1^{11}$ | $U_2^{12}$ | $U_3^{13}$ | $U_1^{12}$ | $U_2^{13}$ | $U_3^{13}$ |
| S1 | 0.0271 (3) | 0.0327 (3) | 0.0307 (3) | 0.0072 (3) | 0.0005 (3) | −0.0065 (2) |
| O1 | 0.0275 (8) | 0.0496 (11) | 0.0465 (10) | −0.0037 (8) | 0.0092 (8) | −0.0111 (8) |
| O2 | 0.0427 (10) | 0.0387 (10) | 0.0410 (10) | 0.0196 (8) | −0.0057 (8) | −0.0067 (8) |
| N1 | 0.0371 (11) | 0.0293 (11) | 0.0228 (10) | 0.0109 (9) | −0.0014 (9) | −0.0010 (9) |
| N2 | 0.0283 (10) | 0.0250 (10) | 0.0329 (10) | −0.0021 (9) | 0.0002 (9) | −0.0004 (9) |
| C1 | 0.0239 (11) | 0.0250 (11) | 0.0225 (10) | 0.0044 (9) | −0.0012 (9) | −0.0009 (9) |
| C2 | 0.0228 (10) | 0.0238 (11) | 0.0236 (10) | 0.0009 (9) | 0.0001 (9) | 0.0016 (9) |
| C3 | 0.0261 (11) | 0.0259 (12) | 0.0300 (12) | 0.0053 (10) | 0.0036 (9) | 0.0003 (9) |
| C4 | 0.0357 (13) | 0.0241 (11) | 0.0326 (12) | 0.0008 (10) | 0.0001 (10) | −0.0010 (9) |
| C5 | 0.0315 (13) | 0.0313 (13) | 0.0315 (12) | −0.0059 (10) | 0.0014 (10) | 0.0010 (10) |
| C6 | 0.0229 (11) | 0.0359 (12) | 0.0312 (11) | −0.0006 (11) | 0.0032 (11) | −0.0033 (10) |
| C7 | 0.0278 (11) | 0.0242 (10) | 0.0235 (10) | 0.0038 (10) | 0.0040 (10) | −0.0040 (8) |
| C8 | 0.0327 (12) | 0.0217 (11) | 0.0267 (11) | 0.0030 (10) | 0.0081 (10) | −0.0020 (9) |
| C9 | 0.0291 (12) | 0.0290 (12) | 0.0382 (13) | −0.0015 (11) | 0.0069 (12) | −0.0045 (10) |
| C10 | 0.0319 (13) | 0.0361 (13) | 0.0340 (13) | 0.0076 (11) | −0.0008 (11) | −0.0102 (10) |
| C11 | 0.0465 (14) | 0.0342 (12) | 0.0232 (11) | 0.0075 (13) | 0.0014 (11) | 0.0010 (10) |
| C12 | 0.0367 (12) | 0.0247 (11) | 0.0259 (11) | 0.0018 (11) | 0.0062 (11) | −0.0010 (9) |
| C13 | 0.0536 (16) | 0.0285 (12) | 0.0331 (13) | −0.0021 (12) | 0.0098 (13) | 0.0058 (11) |
| C14 | 0.0455 (18) | 0.0629 (19) | 0.0512 (17) | 0.0037 (16) | −0.0124 (16) | −0.0140 (15) |
| C15 | 0.0569 (18) | 0.0351 (14) | 0.0401 (14) | −0.0079 (13) | 0.0094 (13) | 0.0066 (12) |

Geometric parameters (Å, °)

| S1—O1 | 1.4330 (19) | C6—H6A | 0.9900 |
| S1—O2 | 1.4379 (18) | C6—H6B | 0.9900 |
| S1—N1 | 1.609 (2) | C7—C8 | 1.414 (3) |
| S1—C7 | 1.779 (2) | C7—C12 | 1.411 (3) |
| N1—C1 | 1.470 (3) | C8—C9 | 1.377 (3) |
| N1—H1 | 0.79 (3) | C8—C13 | 1.514 (3) |
| N2—C2 | 1.469 (3) | C9—H9 | 0.9500 |
| N2—H2A | 0.89 (3) | C9—C10 | 1.384 (3) |
| N2—H2B | 0.93 (3) | C10—C11 | 1.384 (4) |
| C1—H1A | 1.0000 | C10—C14 | 1.507 (4) |
| C1—C2 | 1.535 (3) | C11—H11 | 0.9500 |
| C1—C6 | 1.527 (3) | C11—C12 | 1.390 (4) |
| Bond          | Distance (Å) |
|---------------|--------------|
| C2—H2        | 1.0000       |
| C2—C3        | 1.521 (3)    |
| C3—H3A       | 0.9900       |
| C3—H3B       | 0.9900       |
| C3—C4        | 1.522 (3)    |
| C4—H4A       | 0.9900       |
| C4—H4B       | 0.9900       |
| C4—C5        | 1.525 (3)    |
| C5—H5A       | 0.9900       |
| C5—H5B       | 0.9900       |
| C5—C6        | 1.523 (3)    |

| Bond          | Distance (Å) |
|---------------|--------------|
| O1—S1—O2     | 117.62 (12)  |
| O1—S1—N1     | 110.46 (11)  |
| O1—S1—C7     | 108.68 (11)  |
| O2—S1—N1     | 106.31 (11)  |
| O2—S1—C7     | 108.86 (11)  |
| N1—S1—C7     | 104.06 (11)  |
| S1—N1—H1     | 116 (2)      |
| C1—N1—S1     | 122.24 (17)  |
| C1—N1—H1     | 120 (2)      |
| C2—N2—H2A    | 108 (2)      |
| C2—N2—H2B    | 108.1 (18)   |
| H2A—N2—H2B   | 107 (3)      |
| N1—C1—H1A    | 108.4        |
| N1—C1—C2     | 106.87 (18)  |
| N1—C1—C6     | 113.39 (19)  |
| C2—C1—H1A    | 108.4        |
| C6—C1—H1A    | 108.4        |
| C6—C1—C2     | 111.36 (17)  |
| N2—C2—C1     | 113.59 (18)  |
| N2—C2—H2     | 107.1        |
| N2—C2—C3     | 109.98 (18)  |
| C1—C2—H2     | 107.1        |
| C3—C2—C1     | 111.70 (18)  |
| C3—C2—H2     | 107.1        |
| C2—C3—H3A    | 109.1        |
| C2—C3—H3B    | 109.1        |
| H3A—C3—H3B   | 107.9        |
| C4—C3—H3A    | 109.1        |
| C4—C3—H3B    | 109.1        |
| C3—C4—H4A    | 109.4        |
| C3—C4—H4B    | 109.4        |
| C3—C4—C5     | 111.02 (19)  |
| H4A—C4—H4B   | 108.0        |
| C5—C4—H4A    | 109.4        |
| C5—C4—H4B    | 109.4        |

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C4—C5—H5A 109.5 C12—C15—H15A 109.5
C4—C5—H5B 109.5 C12—C15—H15B 109.5
H5A—C5—H5B 108.1 C12—C15—H15C 109.5
C6—C5—C4 110.51 (19) H15A—C15—H15B 109.5
C6—C5—H5A 109.5 H15A—C15—H15C 109.5
C6—C5—H5B 109.5 H15B—C15—H15C 109.5

\[ S1—N1—C1—C2 \quad -156.04 (17) \quad C2—C1—C6—C5 \quad 55.2 (2) \]
\[ S1—N1—C1—C6 \quad 80.9 (2) \quad C2—C3—C4—C5 \quad -55.0 (3) \]
\[ S1—C7—C8—C9 \quad 177.22 (17) \quad C3—C4—C5—C6 \quad 56.3 (3) \]
\[ S1—C7—C8—C13 \quad -0.7 (3) \quad C4—C5—C6—C1 \quad -57.3 (3) \]
\[ S1—C7—C12—C11 \quad -175.90 (18) \quad C6—C1—C2—N2 \quad -177.74 (19) \]
\[ S1—C7—C12—C15 \quad 4.4 (3) \quad C6—C1—C2—C3 \quad -52.6 (2) \]
\[ O1—S1—N1—C1 \quad -46.1 (2) \quad C7—S1—N1—C1 \quad 70.4 (2) \]
\[ O1—S1—C7—C8 \quad -173.93 (17) \quad C7—C8—C9—C10 \quad -1.4 (3) \]
\[ O1—S1—C7—C12 \quad 4.7 (2) \quad C8—C7—C12—C11 \quad 2.7 (3) \]
\[ O2—S1—N1—C1 \quad -174.73 (18) \quad C8—C7—C12—C15 \quad -177.0 (2) \]
\[ O2—S1—C7—C8 \quad -44.7 (2) \quad C8—C9—C10—C11 \quad 2.8 (4) \]
\[ O2—S1—C7—C12 \quad 133.97 (19) \quad C8—C9—C10—C14 \quad -176.1 (2) \]
\[ N1—S1—C7—C8 \quad 68.36 (19) \quad C9—C10—C11—C12 \quad -1.4 (4) \]
\[ N1—S1—C7—C12 \quad -112.99 (19) \quad C10—C11—C12—C7 \quad -1.3 (4) \]
\[ N1—C1—C2—N2 \quad 57.9 (2) \quad C10—C11—C12—C15 \quad 178.4 (2) \]
\[ N1—C1—C2—C3 \quad -176.97 (18) \quad C12—C7—C8—C9 \quad -1.5 (3) \]
\[ N1—C1—C6—C5 \quad 175.8 (2) \quad C12—C7—C8—C13 \quad -179.4 (2) \]
\[ N2—C2—C3—C4 \quad 179.90 (18) \quad C13—C8—C9—C10 \quad 176.7 (2) \]
\[ C1—C2—C3—C4 \quad 52.8 (3) \quad C14—C10—C11—C12 \quad 177.4 (2) \]

**Hydrogen-bond geometry (Å, °)**

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|------|-------|-------|---------|
| N2—H2A···N1 | 0.89 (3) | 2.43 (3) | 2.877 (3) | 111.2 (2) |
| N1—H1···N2i | 0.79 (3) | 2.14 (3) | 2.921 (3) | 170.3 (2) |

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