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

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The title compound, $C_{15}H_{24}N_2O_2S$, was synthesized *via* a substitution reaction between the enantiopure (1S,2S)-(+)-1,2-diaminocyclohexane and 2,4,6-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 *et al.*, 2006; Palakurthy & Mandal, 2011). The use of sulfonamides as catalysts in asymmetric synthesis has also been reported (Lao *et al.*, 2009; Feng *et al.*, 2010; Jin *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 *et al.*, 2009; Sun *et al.*, 2012; Zhou *et al.*, 2014; Ruiz-Olalla *et al.*, 2015; Yang *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 *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 γ-amino acids (Horne & Gellman, 2008; Wiesner *et al.*, 2008; Chi *et al.*, 2008).
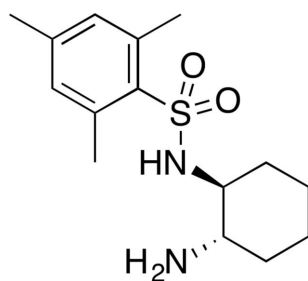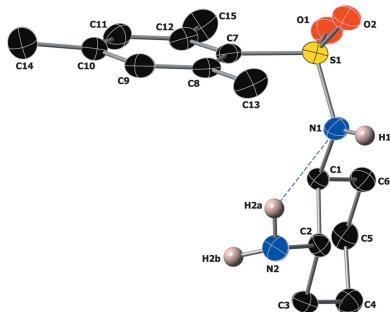
In line with our research interest in the synthesis of heterogeneous foldamers (Hayen *et al.*, 2004), we synthesized the title compound as a chiral organocatalyst for conjugate addition. This conjugate addition was then applied for the

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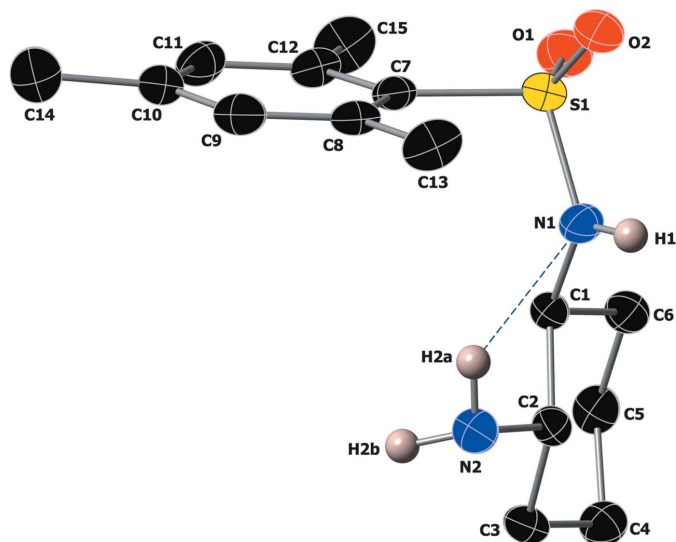
Figure 1
The asymmetric part of the unit cell along with the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. An intramolecular N—H···N interaction is shown with a blue dashed line. Only N—H hydrogens are shown for clarity.

synthesis of γ-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 sp^2-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 (FAVHEP; 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

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[i]	0.79 (3)	2.14 (3)	2.921 (3)	170 (3)

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

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 intermolecular hydrogen bond present between a donor sulfonamide N1—H1 and a nearby amine
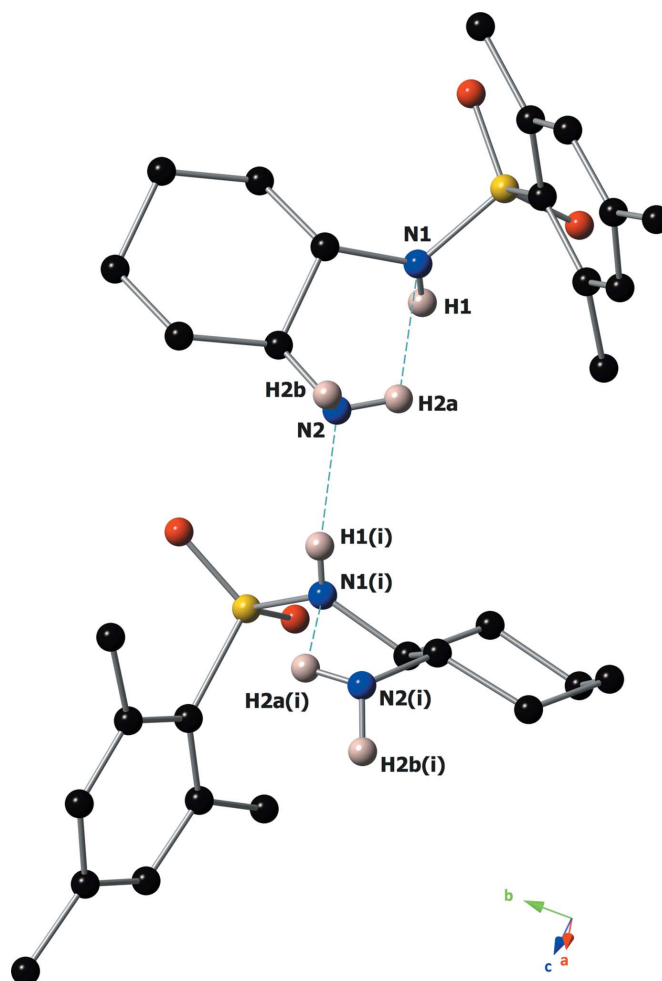
Figure 2
Intra- and intermolecular hydrogen-bonding interactions present in the crystal. Hydrogen bonds are drawn as blue dashed lines. Only N—H hydrogens are shown for clarity. [Symmetry code: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, -z + 1$.]

acceptor N atom [$D \cdots H = 0.860\,(7)$ Å; $H \cdots A = 2.160\,(8)$ Å; $D \cdots A = 3.011\,(8)$ Å; $D{-}H \cdots A = 169.9\,(5)°$].

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-di-aminocyclohexane rings as the amide substituent. In structure OTOPAP (Schwarz *et al.*, 2010), both amines of the *trans*-1,2-diaminocyclohexane ring are bonded to a mesitylsulfonamide group. Structure FAVHEP (Balsells *et al.*, 1998) is the same as the title compound, but is present as a racemic mixture that crystallized in the space group $P\overline{1}$.

5. Synthesis and crystallization

To a stirred solution of $(1S,2S)$-(+)-1,2-diaminocyclohexane (0.77 g, 6.74 mmol) in 5 ml of CH_2Cl_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_2Cl_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_2O (3 × 25 ml) and the aqueous layer was back-extracted with CH_2Cl_2 (20 ml). The combined organic extracts were dried over Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by column chromatography over silica gel (CH_2Cl_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_2Cl_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, H2*A* and H2*B*) were located in difference-Fourier maps and refined isotropically.

Acknowledgements

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{24}N_2O_2S$
M_r	296.42
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	173
a, b, c (Å)	6.5215 (4), 10.0202 (6), 23.3660 (15)
V (Å^3)	1526.89 (16)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.22
Crystal size (mm)	$0.37 \times 0.20 \times 0.15$
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.706, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25587, 2799, 2667
R_{int}	0.034
$(\sin \theta/\lambda)_{max}$ (Å^{-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
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.21
Absolute structure	Flack parameter x determined using 1098 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.00 (2)

Computer programs: *APEX2* ad *SAINT* (Bruker, 2013), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009; Bourhis *et al.*, 2015) and *CrystalMaker* (Palmer, 2007).

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supporting information

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

Felix N. Ngassa, Shannon M. Biros and Richard J. Staples

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

$C_{15}H_{24}N_2O_2S$	$D_x = 1.289$ Mg m^{-3}
$M_r = 296.42$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 9968 reflections
$a = 6.5215$ (4) Å	$\theta = 2.2–25.3°$
$b = 10.0202$ (6) Å	$\mu = 0.22$ mm^{-1}
$c = 23.3660$ (15) Å	$T = 173$ K
$V = 1526.89$ (16) Å^3	Block, colourless
$Z = 4$	$0.37 \times 0.20 \times 0.15$ mm
$F(000) = 640$	

Data collection

Bruker APEXII CCD diffractometer	25587 measured reflections
Radiation source: sealed tube	2799 independent reflections
Graphite monochromator	2667 reflections with $I > 2\sigma(I)$
Detector resolution: 8 pixels mm^{-1}	$R_{int} = 0.034$
φ and ω scans	$\theta_{max} = 25.4°$, $\theta_{min} = 1.7°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)	$h = -7 \rightarrow 7$
	$k = -12 \rightarrow 12$
	$l = -28 \rightarrow 28$
$T_{min} = 0.706$, $T_{max} = 0.745$	

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.029$	$w = 1/[\sigma^2(F_o^2) + (0.0313P)^2 + 0.5049P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.071$	
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
2799 reflections	$\Delta\rho_{max} = 0.19$ e Å^{-3}
196 parameters	$\Delta\rho_{min} = -0.21$ e Å^{-3}
0 restraints	
Hydrogen site location: mixed	

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 (Å^2)

	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*

H14B	1.0897	0.8789	0.8261	0.080*
H14C	1.0452	1.0327	0.8124	0.080*
C15	0.4607 (5)	0.6726 (3)	0.75300 (12)	0.0440 (7)
H15A	0.3236	0.7116	0.7569	0.066*
H15B	0.5071	0.6399	0.7903	0.066*
H15C	0.4559	0.5983	0.7258	0.066*
H2A	0.864 (5)	0.754 (3)	0.5537 (12)	0.047 (8)*
H1	0.484 (5)	0.768 (3)	0.5458 (13)	0.040 (8)*
H2B	1.003 (5)	0.645 (3)	0.5683 (13)	0.045 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
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)

C2—H2	1.0000	C12—C15	1.509 (3)
C2—C3	1.521 (3)	C13—H13A	0.9800
C3—H3A	0.9900	C13—H13B	0.9800
C3—H3B	0.9900	C13—H13C	0.9800
C3—C4	1.522 (3)	C14—H14A	0.9800
C4—H4A	0.9900	C14—H14B	0.9800
C4—H4B	0.9900	C14—H14C	0.9800
C4—C5	1.525 (3)	C15—H15A	0.9800
C5—H5A	0.9900	C15—H15B	0.9800
C5—H5B	0.9900	C15—H15C	0.9800
C5—C6	1.523 (3)		
O1—S1—O2	117.62 (12)	C1—C6—H6A	109.4
O1—S1—N1	110.46 (11)	C1—C6—H6B	109.4
O1—S1—C7	108.68 (11)	C5—C6—C1	111.33 (19)
O2—S1—N1	106.31 (11)	C5—C6—H6A	109.4
O2—S1—C7	108.86 (11)	C5—C6—H6B	109.4
N1—S1—C7	104.06 (11)	H6A—C6—H6B	108.0
S1—N1—H1	116 (2)	C8—C7—S1	117.96 (16)
C1—N1—S1	122.24 (17)	C12—C7—S1	121.78 (19)
C1—N1—H1	120 (2)	C12—C7—C8	120.2 (2)
C2—N2—H2A	108 (2)	C7—C8—C13	124.7 (2)
C2—N2—H2B	108.1 (18)	C9—C8—C7	118.8 (2)
H2A—N2—H2B	107 (3)	C9—C8—C13	116.5 (2)
N1—C1—H1A	108.4	C8—C9—H9	118.8
N1—C1—C2	106.87 (18)	C8—C9—C10	122.4 (2)
N1—C1—C6	113.39 (19)	C10—C9—H9	118.8
C2—C1—H1A	108.4	C9—C10—C14	120.6 (3)
C6—C1—H1A	108.4	C11—C10—C9	117.9 (2)
C6—C1—C2	111.36 (17)	C11—C10—C14	121.5 (2)
N2—C2—C1	113.59 (18)	C10—C11—H11	118.5
N2—C2—H2	107.1	C10—C11—C12	123.0 (2)
N2—C2—C3	109.98 (18)	C12—C11—H11	118.5
C1—C2—H2	107.1	C7—C12—C15	125.9 (2)
C3—C2—C1	111.70 (18)	C11—C12—C7	117.7 (2)
C3—C2—H2	107.1	C11—C12—C15	116.5 (2)
C2—C3—H3A	109.1	C8—C13—H13A	109.5
C2—C3—H3B	109.1	C8—C13—H13B	109.5
C2—C3—C4	112.32 (19)	C8—C13—H13C	109.5
H3A—C3—H3B	107.9	H13A—C13—H13B	109.5
C4—C3—H3A	109.1	H13A—C13—H13C	109.5
C4—C3—H3B	109.1	H13B—C13—H13C	109.5
C3—C4—H4A	109.4	C10—C14—H14A	109.5
C3—C4—H4B	109.4	C10—C14—H14B	109.5
C3—C4—C5	111.02 (19)	C10—C14—H14C	109.5
H4A—C4—H4B	108.0	H14A—C14—H14B	109.5
C5—C4—H4A	109.4	H14A—C14—H14C	109.5
C5—C4—H4B	109.4	H14B—C14—H14C	109.5

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	−156.04 (17)	C2—C1—C6—C5	55.2 (2)
S1—N1—C1—C6	80.9 (2)	C2—C3—C4—C5	−55.0 (3)
S1—C7—C8—C9	177.22 (17)	C3—C4—C5—C6	56.8 (3)
S1—C7—C8—C13	−0.7 (3)	C4—C5—C6—C1	−57.3 (3)
S1—C7—C12—C11	−175.90 (18)	C6—C1—C2—N2	−177.74 (19)
S1—C7—C12—C15	4.4 (3)	C6—C1—C2—C3	−52.6 (2)
O1—S1—N1—C1	−46.1 (2)	C7—S1—N1—C1	70.4 (2)
O1—S1—C7—C8	−173.93 (17)	C7—C8—C9—C10	−1.4 (3)
O1—S1—C7—C12	4.7 (2)	C8—C7—C12—C11	2.7 (3)
O2—S1—N1—C1	−174.73 (18)	C8—C7—C12—C15	−177.0 (2)
O2—S1—C7—C8	−44.7 (2)	C8—C9—C10—C11	2.8 (4)
O2—S1—C7—C12	133.97 (19)	C8—C9—C10—C14	−176.1 (2)
N1—S1—C7—C8	68.36 (19)	C9—C10—C11—C12	−1.4 (4)
N1—S1—C7—C12	−112.99 (19)	C10—C11—C12—C7	−1.3 (4)
N1—C1—C2—N2	57.9 (2)	C10—C11—C12—C15	178.4 (2)
N1—C1—C2—C3	−176.97 (18)	C12—C7—C8—C9	−1.5 (3)
N1—C1—C6—C5	175.8 (2)	C12—C7—C8—C13	−179.4 (2)
N2—C2—C3—C4	179.90 (18)	C13—C8—C9—C10	176.7 (2)
C1—C2—C3—C4	52.8 (3)	C14—C10—C11—C12	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)
N1—H1···N2[i]	0.79 (3)	2.14 (3)	2.921 (3)	170 (3)

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