

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

5,13-Disulfamoyl-1,9-diazatetracyclo- [7.7.1.0^{2,7}.0^{10,15}]heptadeca-2(7),3,5,10,- 12,14-hexaen-1-ium chloride

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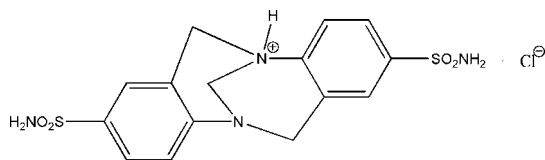
Received 31 August 2011; accepted 19 September 2011

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; disorder in solvent or counterion; R factor = 0.068; wR factor = 0.219; data-to-parameter ratio = 12.1.

In the title salt, $\text{C}_{15}\text{H}_{17}\text{N}_4\text{O}_4\text{S}_2^+\cdot\text{Cl}^-$, the chloride anion is disordered over two positions with occupancies of 0.776 (6) and 0.224 (6). The cation adopts an L shape and the dihedral angle between the benzene rings is 82.5 (3)°. In the crystal, inversion dimers of cations linked by pairs of $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds occur, with the bond arising from the protonated N atom. The cationic dimers are linked into chains *via* the disordered chloride ions by way of $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds and $\text{N}-\text{H}\cdots\text{O}$, $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{Cl}$ interactions also occur, which help to consolidate the three-dimensional network.

Related literature

For a related structure and background references to supramolecular networks, see: Jin *et al.* (2010).



Experimental

Crystal data

$\text{C}_{15}\text{H}_{17}\text{N}_4\text{O}_4\text{S}_2^+\cdot\text{Cl}^-$
 $M_r = 416.90$

Monoclinic, $P2_1/c$
 $a = 11.5247$ (11) Å

$b = 18.5693$ (16) Å
 $c = 8.1489$ (7) Å
 $\beta = 109.177$ (1)°
 $V = 1647.1$ (3) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 0.52$ mm⁻¹
 $T = 298$ K
 $0.40 \times 0.33 \times 0.27$ mm

Data collection

Bruker SMART CCD
diffractometer
Absorption correction: multi-scan
(*SADABS*; Bruker, 2002)
 $T_{\min} = 0.815$, $T_{\max} = 0.869$

8082 measured reflections
2895 independent reflections
1944 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.042$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.068$
 $wR(F^2) = 0.219$
 $S = 1.08$
2895 reflections

239 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.52$ e Å⁻³
 $\Delta\rho_{\min} = -0.96$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O2}^{\text{i}}$	0.89	2.26	3.081 (8)	153
$\text{N1}-\text{H1B}\cdots\text{Cl1}^{\text{ii}}$	0.89	2.26	3.141 (7)	170
$\text{N2}-\text{H2A}\cdots\text{Cl1}^{\text{iii}}$	0.89	2.19	3.042 (6)	160
$\text{N2}-\text{H2B}\cdots\text{O1}^{\text{iv}}$	0.89	2.46	3.109 (7)	130
$\text{N2}-\text{H2B}\cdots\text{O2}^{\text{iv}}$	0.89	2.36	3.240 (7)	168
$\text{N4}-\text{H4}\cdots\text{N2}^{\text{v}}$	0.91	2.02	2.922 (7)	173
$\text{C12}-\text{H12}\cdots\text{O3}^{\text{vi}}$	0.93	2.49	3.416 (7)	175
$\text{C13}-\text{H13A}\cdots\text{Cl1}^{\text{vii}}$	0.97	2.76	3.514 (7)	135
$\text{C14}-\text{H14A}\cdots\text{O4}^{\text{i}}$	0.97	2.50	3.212 (9)	130
$\text{C15}-\text{H15A}\cdots\text{O3}^{\text{viii}}$	0.97	2.52	3.443 (7)	158

Symmetry codes: (i) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (ii) $x + 1, y, z$; (iii) $x, -y + \frac{1}{2}, z + \frac{1}{2}$; (iv) $x - 1, -y + \frac{1}{2}, z - \frac{1}{2}$; (v) $-x + 1, -y + 1, -z + 1$; (vi) $-x + 1, -y + 1, -z + 2$; (vii) $x + 1, -y + \frac{1}{2}, z + \frac{1}{2}$; (viii) $x, y, z - 1$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINTE* (Bruker, 2002); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

We gratefully acknowledge financial support by the Education Office Foundation of Zhejiang Province (project No. Y201017321) and the innovation project of Zhejiang A & F University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6395).

References

- Bruker (2002). *SMART, SAINT and SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
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Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supporting information

Acta Cryst. (2011). E67, o2730 [https://doi.org/10.1107/S1600536811038189]

5,13-Disulfamoyl-1,9-diazatetracyclo- [7.7.1.0^{2,7}.0^{10,15}]heptadeca-2(7),3,5,10,12,14-hexaen-1-ium chloride

Yichao Xu, Shouwen Jin, Jianlong Zhu, Yingjia Liu and ChuanChuan Shi

S1. Comment

Organic salts based on hydrogen bonding are a research field receiving great attention in recent years. As an extension of our study concentrating on hydrogen bonded assembly of organic acid and organic base (Jin *et al.*, 2010), herein we report the crystal structure of 2,9-Dibenzenesulfonamide-1,5-diazaium-bicyclo[3.3.1]dimethanodibenzo chloride.

The crystal of the title compound of the formula C₁₅H₁₇ClN₄O₄S₂ was obtained by recrystallization of 2,9-Dibenzene-sulfonamide-1,5-diazaium- bicyclo[3.3.1]dimethanodibenzo from methanol and HCl solution.

The compound is a salt. The asymmetric unit of the compound consists of one monocation, and one chloride anion (Fig. 1), respectively.

The chloride anion is disordered over two positions with occupancies of 0.78, and 0.22 respectively. In the compound there is a mirror plane running through the C15 atom. Two cations formed dimers *via* the N—H···N hydrogen bond between the NH₂⁺ cation and the amino group with N—N separation of 2.922 (6) Å. The cation dimers were connected together *via* the chloride anion through CH—Cl, Cl—O, and N—H···Cl contacts to form one-dimensional chain (A) running along the *b* axis direction (Fig. 2). Such adjacent chains were combined together by the CH₂—O, and CH—O interactions to form two-dimensional sheet extending along the *bc* plane. Such kind of sheets were stacked along the *a* axis direction *via* the CH₂—Cl interactions to form three-dimensional network structure. It is worthy to note that there are one-dimensional chains (B) that are running through the three-dimensional network. And such kind of chains were connected with the three-dimensional network through the N—H···S, and N—H···O interactions.

S2. Experimental

A solution of 2,9-dibenzenesulfonamide-1,5-diazabicyclo[3.3.1]dimethanodibenzo (38 mg, 0.1 mmol) was dissolved in 5 ml of methanol and 1 ml of conc. HCl under continuous stirring. The solution was stirred for about 1 h at room temperature, then the solution was filtered into a test tube. The solution was left standing at room temperature for several days, colorless block crystals were isolated after slow evaporation of the solution in air at ambient temperature. The crystals were collected and dried in air to give the title compound.

S3. Refinement

Hydrogen atoms attached to the C atoms were placed in calculated positions with $d(\text{C—H}) = 0.93\text{--}0.97$ Å. Positions of the hydrogen atoms at the NH groups were located from the Fourier difference syntheses and refined independently. All U_{iso} values were restrained on U_{eq} values of the parent atoms.

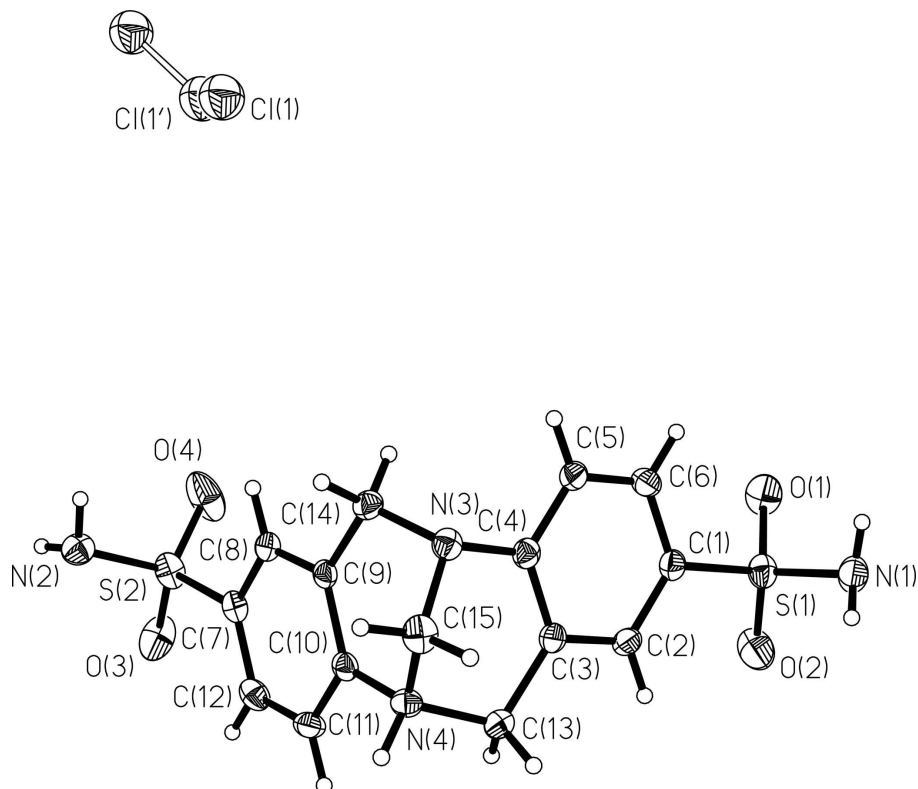


Figure 1

The structure of the title compound, showing displacement ellipsoids drawn at the 30% probability level.

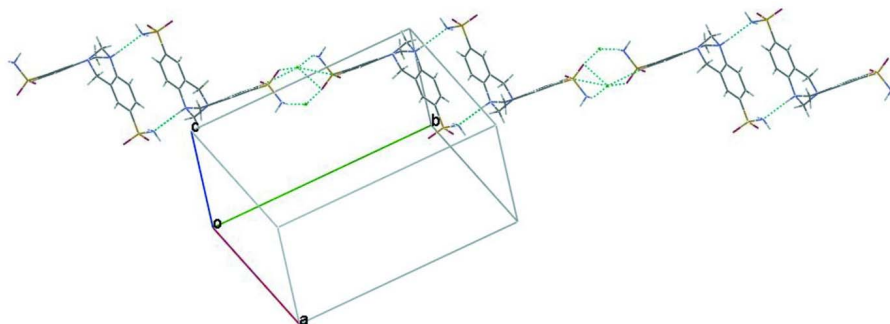


Figure 2

The one-dimensional doublechain formed through CH—O, and CH₂—O interactions running along the *a* axis direction.

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Crystal data

C₁₅H₁₇N₄O₄S₂⁺·Cl⁻

M_r = 416.90

Monoclinic, *P*2₁/*c*

Hall symbol: -*P* 2ybc

a = 11.5247 (11) Å

b = 18.5693 (16) Å

c = 8.1489 (7) Å

β = 109.177 (1)°

V = 1647.1 (3) Å³

Z = 4

F(000) = 864

D_x = 1.681 Mg m⁻³

Mo *Kα* radiation, λ = 0.71073 Å

μ = 0.52 mm⁻¹

$T = 298$ K $0.40 \times 0.33 \times 0.27$ mm
 Block, colorless

Data collection

Bruker SMART CCD diffractometer Radiation source: fine-focus sealed tube Graphite monochromator phi and ω scans Absorption correction: multi-scan (SADABS; Bruker, 2002) $T_{\min} = 0.815$, $T_{\max} = 0.869$	8082 measured reflections 2895 independent reflections 1944 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.042$ $\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.9^\circ$ $h = -11 \rightarrow 13$ $k = -21 \rightarrow 22$ $l = -9 \rightarrow 5$
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Refinement

Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.068$ $wR(F^2) = 0.219$ $S = 1.08$ 2895 reflections 239 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 $w = 1/[\sigma^2(F_o^2) + (0.0953P)^2 + 5.3108P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} < 0.001$ $\Delta\rho_{\text{max}} = 0.52 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.96 \text{ e } \text{\AA}^{-3}$
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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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C11	0.1069 (3)	0.02872 (18)	0.3829 (5)	0.0948 (11)	0.776 (6)
C11'	0.0764 (12)	0.0213 (7)	0.4728 (19)	0.0948 (11)	0.224 (6)
N1	1.2145 (4)	0.1555 (3)	0.6436 (7)	0.0489 (13)	
H1A	1.2289	0.1965	0.5969	0.073*	
H1B	1.1813	0.1236	0.5598	0.073*	
N2	0.2583 (4)	0.4134 (3)	0.6686 (6)	0.0436 (12)	
H2A	0.2080	0.4192	0.7302	0.065*	
H2B	0.2262	0.3815	0.5843	0.065*	
N3	0.6862 (4)	0.3219 (2)	0.2614 (5)	0.0342 (10)	
N4	0.7476 (4)	0.4335 (2)	0.4164 (6)	0.0350 (10)	
H4	0.7507	0.4818	0.3997	0.042*	
O1	1.0815 (4)	0.1016 (2)	0.7888 (6)	0.0581 (12)	
O2	1.1807 (4)	0.2171 (3)	0.8899 (6)	0.0684 (14)	
O3	0.4230 (4)	0.4292 (3)	0.9437 (5)	0.0658 (14)	

O4	0.3793 (6)	0.3081 (3)	0.8158 (8)	0.0860 (18)
S1	1.12094 (13)	0.17065 (8)	0.74765 (18)	0.0425 (4)
S2	0.38898 (14)	0.38395 (8)	0.79416 (19)	0.0440 (4)
C1	0.9909 (5)	0.2165 (3)	0.6090 (7)	0.0349 (12)
C2	0.9842 (5)	0.2910 (3)	0.6153 (7)	0.0356 (12)
H2	1.0470	0.3169	0.6947	0.043*
C3	0.8829 (4)	0.3271 (3)	0.5022 (7)	0.0325 (11)
C4	0.7906 (4)	0.2870 (3)	0.3842 (6)	0.0318 (11)
C5	0.7975 (5)	0.2124 (3)	0.3834 (7)	0.0361 (12)
H5	0.7337	0.1861	0.3071	0.043*
C6	0.8967 (5)	0.1769 (3)	0.4933 (7)	0.0381 (12)
H6	0.9011	0.1270	0.4907	0.046*
C7	0.4950 (5)	0.3985 (3)	0.6817 (7)	0.0336 (12)
C8	0.4905 (4)	0.3543 (3)	0.5427 (7)	0.0328 (11)
H8	0.4314	0.3183	0.5080	0.039*
C9	0.5745 (4)	0.3639 (3)	0.4549 (6)	0.0288 (11)
C10	0.6603 (4)	0.4199 (3)	0.5082 (6)	0.0301 (11)
C11	0.6638 (5)	0.4636 (3)	0.6472 (7)	0.0371 (12)
H11	0.7223	0.5000	0.6815	0.045*
C12	0.5815 (5)	0.4538 (3)	0.7349 (7)	0.0394 (13)
H12	0.5833	0.4834	0.8278	0.047*
C13	0.8742 (5)	0.4079 (3)	0.5131 (8)	0.0394 (13)
H13A	0.8962	0.4223	0.6339	0.047*
H13B	0.9320	0.4302	0.4648	0.047*
C14	0.5740 (5)	0.3144 (3)	0.3071 (7)	0.0352 (12)
H14A	0.5664	0.2649	0.3404	0.042*
H14B	0.5034	0.3254	0.2062	0.042*
C15	0.7088 (5)	0.3973 (3)	0.2424 (7)	0.0421 (13)
H15A	0.6348	0.4199	0.1664	0.051*
H15B	0.7728	0.4026	0.1901	0.051*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.093 (2)	0.091 (2)	0.107 (3)	-0.0023 (16)	0.0411 (18)	-0.0070 (19)
Cl1'	0.093 (2)	0.091 (2)	0.107 (3)	-0.0023 (16)	0.0411 (18)	-0.0070 (19)
N1	0.041 (3)	0.047 (3)	0.063 (3)	0.006 (2)	0.023 (2)	0.008 (2)
N2	0.046 (3)	0.049 (3)	0.037 (3)	-0.004 (2)	0.015 (2)	-0.007 (2)
N3	0.035 (2)	0.038 (2)	0.031 (2)	0.0010 (19)	0.0125 (18)	-0.0018 (19)
N4	0.037 (2)	0.027 (2)	0.043 (2)	-0.0031 (18)	0.016 (2)	0.0048 (19)
O1	0.061 (3)	0.058 (3)	0.058 (3)	0.007 (2)	0.023 (2)	0.023 (2)
O2	0.063 (3)	0.072 (3)	0.056 (3)	0.017 (2)	-0.001 (2)	-0.014 (2)
O3	0.051 (3)	0.113 (4)	0.034 (2)	0.005 (3)	0.015 (2)	-0.011 (2)
O4	0.115 (4)	0.051 (3)	0.127 (5)	0.026 (3)	0.087 (4)	0.040 (3)
S1	0.0381 (8)	0.0485 (9)	0.0396 (8)	0.0072 (6)	0.0111 (6)	0.0007 (6)
S2	0.0533 (9)	0.0450 (9)	0.0411 (8)	0.0103 (7)	0.0256 (7)	0.0109 (6)
C1	0.030 (3)	0.038 (3)	0.039 (3)	0.002 (2)	0.015 (2)	-0.001 (2)
C2	0.030 (3)	0.038 (3)	0.041 (3)	-0.006 (2)	0.013 (2)	-0.007 (2)

C3	0.030 (3)	0.035 (3)	0.037 (3)	-0.001 (2)	0.019 (2)	-0.003 (2)
C4	0.030 (3)	0.037 (3)	0.032 (3)	0.000 (2)	0.014 (2)	-0.003 (2)
C5	0.028 (3)	0.040 (3)	0.039 (3)	-0.001 (2)	0.010 (2)	-0.010 (2)
C6	0.041 (3)	0.031 (3)	0.047 (3)	-0.002 (2)	0.020 (3)	-0.005 (2)
C7	0.036 (3)	0.034 (3)	0.033 (3)	0.009 (2)	0.015 (2)	0.004 (2)
C8	0.027 (3)	0.033 (3)	0.035 (3)	0.003 (2)	0.007 (2)	0.001 (2)
C9	0.026 (2)	0.028 (3)	0.030 (3)	0.006 (2)	0.005 (2)	0.002 (2)
C10	0.030 (3)	0.026 (3)	0.031 (3)	0.006 (2)	0.005 (2)	0.004 (2)
C11	0.041 (3)	0.027 (3)	0.041 (3)	-0.004 (2)	0.011 (2)	-0.005 (2)
C12	0.049 (3)	0.035 (3)	0.033 (3)	0.007 (2)	0.012 (2)	-0.004 (2)
C13	0.031 (3)	0.035 (3)	0.052 (3)	-0.003 (2)	0.013 (2)	0.000 (2)
C14	0.030 (3)	0.039 (3)	0.034 (3)	-0.002 (2)	0.007 (2)	-0.007 (2)
C15	0.047 (3)	0.048 (3)	0.036 (3)	0.003 (3)	0.020 (3)	0.007 (3)

Geometric parameters (Å, °)

C11'—C11 ^h	2.11 (3)	C2—H2	0.9300
N1—S1	1.600 (5)	C3—C4	1.392 (7)
N1—H1A	0.8900	C3—C13	1.509 (7)
N1—H1B	0.8900	C4—C5	1.388 (7)
N2—S2	1.613 (5)	C5—C6	1.367 (7)
N2—H2A	0.8900	C5—H5	0.9300
N2—H2B	0.8900	C6—H6	0.9300
N3—C15	1.441 (7)	C7—C8	1.386 (7)
N3—C4	1.442 (6)	C7—C12	1.397 (8)
N3—C14	1.465 (6)	C8—C9	1.391 (7)
N4—C10	1.460 (6)	C8—H8	0.9300
N4—C13	1.490 (7)	C9—C10	1.401 (7)
N4—C15	1.499 (7)	C9—C14	1.513 (7)
N4—H4	0.9100	C10—C11	1.384 (7)
O1—S1	1.437 (5)	C11—C12	1.375 (7)
O2—S1	1.427 (5)	C11—H11	0.9300
O3—S2	1.425 (5)	C12—H12	0.9300
O4—S2	1.428 (5)	C13—H13A	0.9700
S1—C1	1.770 (5)	C13—H13B	0.9700
S2—C7	1.772 (5)	C14—H14A	0.9700
C1—C2	1.387 (7)	C14—H14B	0.9700
C1—C6	1.392 (7)	C15—H15A	0.9700
C2—C3	1.398 (7)	C15—H15B	0.9700
S1—N1—H1A	109.3	C4—C5—H5	119.5
S1—N1—H1B	109.2	C5—C6—C1	119.2 (5)
H1A—N1—H1B	109.5	C5—C6—H6	120.4
S2—N2—H2A	109.2	C1—C6—H6	120.4
S2—N2—H2B	109.2	C8—C7—C12	121.3 (5)
H2A—N2—H2B	109.5	C8—C7—S2	119.1 (4)
C15—N3—C4	111.8 (4)	C12—C7—S2	119.6 (4)
C15—N3—C14	109.0 (4)	C7—C8—C9	120.0 (5)

C4—N3—C14	112.7 (4)	C7—C8—H8	120.0
C10—N4—C13	113.2 (4)	C9—C8—H8	120.0
C10—N4—C15	111.4 (4)	C8—C9—C10	118.3 (4)
C13—N4—C15	107.1 (4)	C8—C9—C14	120.7 (4)
C10—N4—H4	108.3	C10—C9—C14	121.0 (4)
C13—N4—H4	108.3	C11—C10—C9	121.2 (5)
C15—N4—H4	108.3	C11—C10—N4	118.5 (4)
O2—S1—O1	117.1 (3)	C9—C10—N4	120.3 (4)
O2—S1—N1	107.9 (3)	C12—C11—C10	120.5 (5)
O1—S1—N1	106.7 (3)	C12—C11—H11	119.8
O2—S1—C1	108.0 (3)	C10—C11—H11	119.8
O1—S1—C1	108.2 (3)	C11—C12—C7	118.7 (5)
N1—S1—C1	108.8 (3)	C11—C12—H12	120.6
O3—S2—O4	119.1 (3)	C7—C12—H12	120.6
O3—S2—N2	106.3 (3)	N4—C13—C3	111.0 (4)
O4—S2—N2	108.5 (3)	N4—C13—H13A	109.4
O3—S2—C7	108.0 (3)	C3—C13—H13A	109.4
O4—S2—C7	108.0 (3)	N4—C13—H13B	109.4
N2—S2—C7	106.2 (2)	C3—C13—H13B	109.4
C2—C1—C6	120.7 (5)	H13A—C13—H13B	108.0
C2—C1—S1	120.1 (4)	N3—C14—C9	111.8 (4)
C6—C1—S1	119.1 (4)	N3—C14—H14A	109.3
C1—C2—C3	119.9 (5)	C9—C14—H14A	109.3
C1—C2—H2	120.1	N3—C14—H14B	109.3
C3—C2—H2	120.1	C9—C14—H14B	109.3
C4—C3—C2	118.9 (5)	H14A—C14—H14B	107.9
C4—C3—C13	121.5 (5)	N3—C15—N4	110.0 (4)
C2—C3—C13	119.6 (5)	N3—C15—H15A	109.7
C5—C4—C3	120.3 (5)	N4—C15—H15A	109.7
C5—C4—N3	118.8 (4)	N3—C15—H15B	109.7
C3—C4—N3	120.9 (5)	N4—C15—H15B	109.7
C6—C5—C4	121.0 (5)	H15A—C15—H15B	108.2
C6—C5—H5	119.5		
O2—S1—C1—C2	20.7 (5)	C12—C7—C8—C9	1.1 (7)
O1—S1—C1—C2	148.3 (4)	S2—C7—C8—C9	-178.7 (4)
N1—S1—C1—C2	-96.2 (5)	C7—C8—C9—C10	-1.5 (7)
O2—S1—C1—C6	-159.9 (4)	C7—C8—C9—C14	177.7 (5)
O1—S1—C1—C6	-32.2 (5)	C8—C9—C10—C11	1.5 (7)
N1—S1—C1—C6	83.3 (5)	C14—C9—C10—C11	-177.7 (5)
C6—C1—C2—C3	-1.2 (8)	C8—C9—C10—N4	-178.0 (4)
S1—C1—C2—C3	178.2 (4)	C14—C9—C10—N4	2.8 (7)
C1—C2—C3—C4	-0.3 (7)	C13—N4—C10—C11	76.1 (6)
C1—C2—C3—C13	178.2 (5)	C15—N4—C10—C11	-163.2 (5)
C2—C3—C4—C5	2.1 (7)	C13—N4—C10—C9	-104.4 (5)
C13—C3—C4—C5	-176.4 (5)	C15—N4—C10—C9	16.4 (6)
C2—C3—C4—N3	-178.1 (4)	C9—C10—C11—C12	-1.0 (8)
C13—C3—C4—N3	3.4 (7)	N4—C10—C11—C12	178.5 (5)

C15—N3—C4—C5	-162.8 (4)	C10—C11—C12—C7	0.5 (8)
C14—N3—C4—C5	74.0 (6)	C8—C7—C12—C11	-0.5 (8)
C15—N3—C4—C3	17.5 (6)	S2—C7—C12—C11	179.3 (4)
C14—N3—C4—C3	-105.8 (5)	C10—N4—C13—C3	75.6 (5)
C3—C4—C5—C6	-2.5 (8)	C15—N4—C13—C3	-47.6 (5)
N3—C4—C5—C6	177.7 (5)	C4—C3—C13—N4	13.2 (7)
C4—C5—C6—C1	1.0 (8)	C2—C3—C13—N4	-165.3 (4)
C2—C1—C6—C5	0.9 (8)	C15—N3—C14—C9	-48.8 (5)
S1—C1—C6—C5	-178.6 (4)	C4—N3—C14—C9	76.0 (5)
O3—S2—C7—C8	172.3 (4)	C8—C9—C14—N3	-166.0 (4)
O4—S2—C7—C8	42.2 (5)	C10—C9—C14—N3	13.3 (6)
N2—S2—C7—C8	-74.1 (5)	C4—N3—C15—N4	-54.7 (5)
O3—S2—C7—C12	-7.5 (5)	C14—N3—C15—N4	70.6 (5)
O4—S2—C7—C12	-137.6 (5)	C10—N4—C15—N3	-52.9 (6)
N2—S2—C7—C12	106.1 (4)	C13—N4—C15—N3	71.4 (5)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A \cdots O2 ⁱⁱ	0.89	2.26	3.081 (8)	153
N1—H1B \cdots C11 ⁱⁱⁱ	0.89	2.26	3.141 (7)	170
N2—H2A \cdots C11 ^{iv}	0.89	2.19	3.042 (6)	160
N2—H2B \cdots O1 ^v	0.89	2.46	3.109 (7)	130
N2—H2B \cdots O2 ^v	0.89	2.36	3.240 (7)	168
N4—H4 \cdots N2 ^{vi}	0.91	2.02	2.922 (7)	173
C12—H12 \cdots O3 ^{vii}	0.93	2.49	3.416 (7)	175
C13—H13A \cdots C11 ^{viii}	0.97	2.76	3.514 (7)	135
C14—H14A \cdots O4 ⁱⁱ	0.97	2.50	3.212 (9)	130
C15—H15A \cdots O3 ^{ix}	0.97	2.52	3.443 (7)	158

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