Benzene-1,2-diaminium bis(4-methylbenzene-1-sulfonate)

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The structure of the title salt, $C_6H_{10}N_2^{2+} \cdot 2C_7H_7O_3S^-$, consists of a unique benzene-1,2-diaminium dication charge balanced by a pair of crystallographically independent 4-methylbenzene-1-sulfonate anions. The cations and anions are interlinked by several N—H···O hydrogen bonds.

3D view
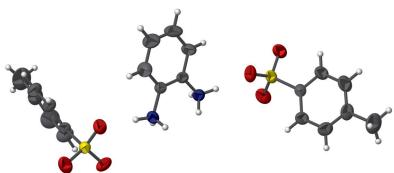
Chemical scheme
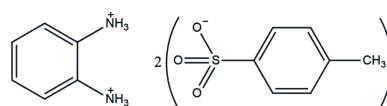
Structure description

The aromatic diamine, benzene-1,2-diamine also known as *o*-phenylenediamine, can function as a neutral ligand and bind to a metal *via* both amine N atoms (Koizumi & Fukuju, 2011; Guillén *et al.*, 2018) or by a single nitrogen in a monodentate fashion (Nelson *et al.*, 1982; Dickman, 2000). In addition, benzene-1,2-diamine can function as a charge-balancing dication in which both the amine N atoms are protonated (Raghavaiah *et al.*, 2006; Powers & Geiger, 2019) or as a monocation (Raghavaiah *et al.*, 2005; Mishra & Pallepogu, 2018). The structural diversity of the compounds of benzene-1,2-diamine in neutral or cationic form is highlighted by the results of a survey of the Cambridge Structural Database (CSD; Groom *et al.*, 2016), which had more than 220 hits for the above three types of compounds. Of these, a total of 79 deposits do not contain any metal ions and correspond to crystal structures containing only diprotonated benzene-1,2-diaminium cations (47 hits) and monoprotonated 2-aminoanilinium cations (55 hits). An example of a molecular salt of 4-methylbenzene-1-sulfonic acid containing both mono and diprotonated cations, namely 2-aminoanilinium benzene-1,2-diaminium tris(4-methylbenzene-1-sulfonate) (**2**) has been reported recently (Amirthakumar *et al.*, 2018).

In this report, we describe the crystal structure of the title compound, which was obtained by an aqueous reaction of the aromatic diamine with 4-methylbenzene-1-sulfonic acid in a 1:2 molar ratio, unlike **2**, which was isolated from a 1:1 reaction. The asymmetric unit of the title compound consists of an unique benzene-1,2-diaminium dication charge-balanced by a pair of crystallographically independent 4-methylbenzene-
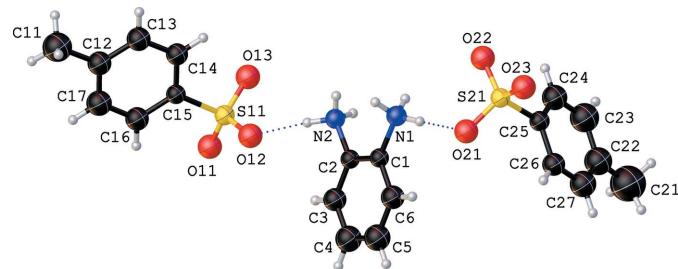
Figure 1
The crystal structure of **1** showing the atom-labelling scheme. Blue dotted lines indicate hydrogen bonds. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

Figure 3
A view along *b* axis of the unit-cell packing showing the interlinking of the dications with the monocations *via* N—H···O hydrogen bonds which are shown as dashed lines. For clarity, the H atoms attached to the C atoms are not shown.

1-sulfonate anions (Fig. 1) with all atoms located on general positions. The geometric parameters of the unique dication and the crystallographically independent anions are in normal ranges and are in agreement with reported data (Powers & Geiger, 2019).

All six oxygen atoms attached to the sulfur atom of the sulfonate moiety of the anion function as hydrogen-bond acceptors while the H atoms attached to the N atoms of the dication function as hydrogen-bond donors, resulting in a total of eight N—H···O hydrogen bonds of which six are intermolecular (Table 1). It is interesting to note that the dications and the unique anions are interlinked only *via* N—H···O hydrogen bonds, unlike in **2** for which both N—H···O and C—H···O hydrogen bonds were reported. Each anion is linked to three symmetry-related dications (Fig. 2) while each dication is hydrogen-bonded to six symmetry-related anions. The net result of the hydrogen-bonding interactions is the interlinking of the cations with the anions, resulting in alternating layers of cations and anions parallel to [010] (Fig. 3).

Synthesis and crystallization

Freshly recrystallized benzene-1,2-diamine (108 mg, 1 mmol) was dissolved in double-distilled water (10–15 ml) by heating the mixture. Into this, an aqueous solution of 4-methyl-

benzene-1-sulfonic acid (380 mg, 2 mmol) was added. The reaction mixture was heated to boiling and a pinch of activated charcoal was added. The hot solution was filtered and the clear filtrate was left aside for crystallization. After a few days, crystals of the title compound **1** slowly separated. The crystals were filtered and air dried. Yield 50%.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements
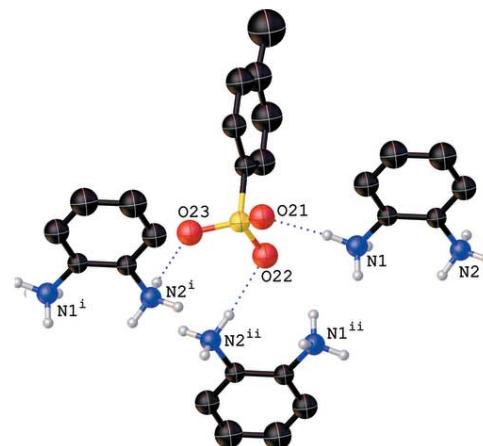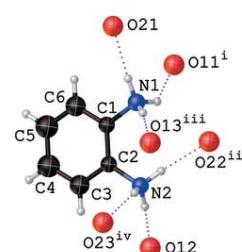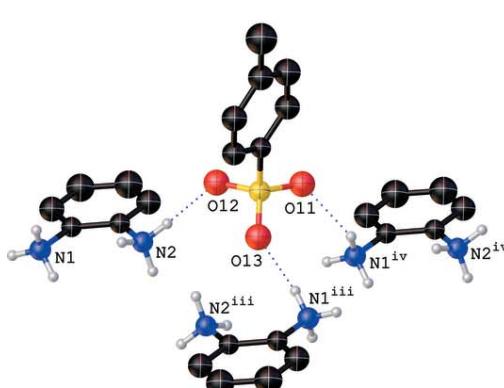
Figure 2
The hydrogen-bonding scheme around the two unique anions (left and right). For clarity, the H atoms of the aromatic ring are not shown. The hydrogen-bonding environment of the dication (middle) shows only the acceptor oxygen atoms of the unique anions. Symmetry codes: (i) *x*, *y* + 1, *z*; (ii) −*x* + 1, −*y* + 1, −*z* + 1; (iii) −*x* + 1, −*y*, −*z* + 1; (iv) *x*, *y* − 1, *z*.

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$A\cdots$O21	0.89	1.92	2.8062 (19)	175
N1—H1$B\cdots$O11^{i}	0.89	2.07	2.7509 (19)	133
N1—H1$B\cdots$O22^{ii}	0.89	2.31	2.9017 (18)	124
N1—H1$C\cdots$O13^{iii}	0.89	1.89	2.7733 (19)	170
N2—H2$A\cdots$O13^{iii}	0.89	2.46	2.9128 (19)	112
N2—H2$A\cdots$O23^{iv}	0.89	1.97	2.7820 (18)	151
N2—H2$B\cdots$O22^{ii}	0.89	1.98	2.8611 (19)	173
N2—H2$C\cdots$O12	0.89	1.84	2.7224 (19)	175

Symmetry codes: (i) $x, y + 1, z$; (ii) $-x + 1, -y + 1, -z + 1$; (iii) $-x + 1, -y, -z + 1$; (iv) $x, y - 1, z$.

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_{10}N_2^{2+}\cdot2C_7H_7O_3S^-$
M_r	452.53
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	293
a, b, c (Å)	29.1537 (9), 8.8739 (3), 19.9919 (6)
β (°)	123.621 (1)
V (Å³)	4306.9 (2)
Z	8
Radiation type	Mo $K\alpha$
μ (mm⁻¹)	0.29
Crystal size (mm)	$0.56 \times 0.15 \times 0.12$
Data collection	
Diffractometer	Bruker D8 Quest ECO
Absorption correction	Multi-scan (*SADABS*; Bruker, 2018)
T_{min}, T_{max}	0.696, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	59056, 6568, 4705
R_{int}	0.046
$(\sin \theta/\lambda)_{max}$ (Å⁻¹)	0.715
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.126, 1.07
No. of reflections	6568
No. of parameters	276
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å⁻³)	0.34, −0.39

Computer programs: *APEX3* and *SAINT* (Bruker, 2018), *SHELXT2014* (Sheldrick, 2015a), *SHELXL2018* (Sheldrick, 2015b), *OLEX2* (Dolomanov *et al.*, 2009) and *shelXle* (Hübschle *et al.*, 2011).

full crystallographic data

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Crystal data
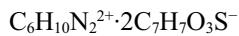
$C_6H_{10}N_2^{2+} \cdot 2C_7H_7O_3S^-$	$F(000) = 1904$
$M_r = 452.53$	$D_x = 1.396$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 29.1537$ (9) Å	Cell parameters from 9968 reflections
$b = 8.8739$ (3) Å	$\theta = 2.9$–29.9°
$c = 19.9919$ (6) Å	$\mu = 0.29$ mm^{-1}
$\beta = 123.621$ (1)°	$T = 293$ K
$V = 4306.9$ (2) Å^3	Block, colourless
$Z = 8$	$0.56 \times 0.14 \times 0.12$ mm

Data collection

Bruker D8 Quest ECO diffractometer	6568 independent reflections
Radiation source: Sealed Tube	4705 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.046$
Absorption correction: multi-scan (SADABS; Bruker, 2018)	$\theta_{max} = 30.5°$, $\theta_{min} = 2.9°$
$T_{min} = 0.696$, $T_{max} = 0.746$	$h = -41 \rightarrow 41$
59056 measured reflections	$k = -12 \rightarrow 12$
	$l = -28 \rightarrow 28$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2 + 2.9966P]$
$R[F^2 > 2\sigma(F^2)] = 0.040$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.126$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.07$	$\Delta\rho_{max} = 0.34$ e Å^{-3}
6568 reflections	$\Delta\rho_{min} = -0.39$ e Å^{-3}
276 parameters	Extinction correction: SHELXL2018 (Sheldrick, 2015b),
0 restraints	$F_c^* = kF_c[1+0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$
Hydrogen site location: inferred from neighbouring sites	Extinction coefficient: 0.0026 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. All hydrogen atoms were located in appropriate positions and were included in calculated positions and refined with a riding model for both C—H and N—H protons. C–H distances ranged from = 0.93 and 0.96 Å for aromatic and methyl H atoms, respectively, and 0.89 for NH_3^+ H atoms with $U_{iso}(H) = 1.2\ U_{eq}(C\text{-aromatic})$ and $U_{iso}(H) = 1.5\ U_{eq}(C\text{-methyl}, NH_3^+)$.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	y	z	$U_{iso}*/U_{eq}$
N1	0.52597 (6)	0.42385 (15)	0.43447 (8)	0.0399 (3)
H1A	0.516000	0.511465	0.408451	0.060*
H1B	0.552390	0.439398	0.485886	0.060*
H1C	0.497014	0.381592	0.430938	0.060*
N2	0.54019 (6)	0.10069 (15)	0.46813 (8)	0.0374 (3)
H2A	0.505767	0.066255	0.439229	0.056*
H2B	0.543473	0.168126	0.503495	0.056*
H2C	0.563230	0.024462	0.494094	0.056*
C1	0.54643 (6)	0.32416 (17)	0.39869 (9)	0.0349 (3)
C2	0.55343 (6)	0.17140 (17)	0.41510 (9)	0.0344 (3)
C3	0.57224 (8)	0.0796 (2)	0.37927 (12)	0.0505 (4)
H3	0.576521	−0.023317	0.389900	0.061*
C4	0.58462 (11)	0.1411 (3)	0.32770 (14)	0.0661 (6)
H4	0.597256	0.079592	0.303508	0.079*
C5	0.57830 (11)	0.2935 (3)	0.31201 (15)	0.0664 (6)
H5	0.586983	0.334936	0.277609	0.080*
C6	0.55909 (9)	0.3848 (2)	0.34726 (12)	0.0529 (4)
H6	0.554660	0.487571	0.336310	0.064*
S11	0.60971 (2)	−0.26457 (4)	0.57918 (2)	0.03904 (11)
O11	0.61408 (5)	−0.40103 (15)	0.54362 (8)	0.0562 (3)
O12	0.61358 (6)	−0.12891 (15)	0.54200 (8)	0.0563 (3)
O13	0.56134 (5)	−0.26132 (16)	0.58310 (9)	0.0573 (4)
C11	0.81185 (11)	−0.2503 (3)	0.92035 (15)	0.0827 (8)
H11A	0.833550	−0.338591	0.929269	0.124*
H11B	0.801302	−0.248348	0.958103	0.124*
H11C	0.833111	−0.161970	0.927333	0.124*
C12	0.76068 (8)	−0.2532 (2)	0.83564 (12)	0.0540 (5)
C13	0.71405 (8)	−0.1716 (2)	0.81418 (11)	0.0541 (5)
H13	0.713844	−0.113580	0.852757	0.065*
C14	0.66758 (7)	−0.1744 (2)	0.73639 (11)	0.0460 (4)
H14	0.636634	−0.118206	0.722766	0.055*
C15	0.66778 (6)	−0.26174 (17)	0.67934 (10)	0.0363 (3)
C16	0.71387 (7)	−0.3444 (2)	0.69966 (12)	0.0523 (4)
H16	0.713945	−0.403424	0.661270	0.063*
C17	0.76014 (8)	−0.3390 (3)	0.77780 (13)	0.0616 (5)
H17	0.791258	−0.394165	0.791294	0.074*
S21	0.45059 (2)	0.76496 (4)	0.35286 (2)	0.03714 (11)
O21	0.49995 (5)	0.70837 (16)	0.36096 (8)	0.0547 (3)
O22	0.44084 (6)	0.69248 (16)	0.40921 (7)	0.0559 (3)
O23	0.44971 (6)	0.92776 (14)	0.35764 (8)	0.0565 (4)

C21	0.26881 (15)	0.5602 (4)	0.01997 (17)	0.1233 (14)
H21A	0.233080	0.582893	0.009049	0.185*
H21B	0.272805	0.452969	0.018852	0.185*
H21C	0.272661	0.606499	−0.020056	0.185*
C22	0.31300 (11)	0.6205 (3)	0.10249 (13)	0.0742 (7)
C23	0.30782 (11)	0.6004 (3)	0.16652 (16)	0.0813 (7)
H23	0.275944	0.556751	0.157815	0.098*
C24	0.34940 (9)	0.6443 (3)	0.24375 (13)	0.0609 (5)
H24	0.345911	0.627550	0.286660	0.073*
C25	0.39576 (7)	0.71265 (18)	0.25587 (9)	0.0387 (3)
C26	0.40091 (9)	0.7360 (2)	0.19192 (11)	0.0496 (4)
H26	0.432285	0.782254	0.200184	0.060*
C27	0.35939 (11)	0.6905 (3)	0.11584 (12)	0.0665 (6)
H27	0.362871	0.707427	0.072940	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0434 (7)	0.0323 (6)	0.0424 (7)	0.0035 (5)	0.0229 (6)	−0.0005 (5)
N2	0.0435 (7)	0.0346 (6)	0.0376 (7)	0.0003 (5)	0.0246 (6)	0.0022 (5)
C1	0.0357 (7)	0.0340 (7)	0.0356 (7)	−0.0015 (6)	0.0202 (6)	−0.0014 (6)
C2	0.0390 (8)	0.0329 (7)	0.0352 (7)	−0.0019 (6)	0.0230 (6)	−0.0009 (6)
C3	0.0707 (12)	0.0390 (9)	0.0597 (11)	0.0038 (8)	0.0473 (10)	−0.0019 (8)
C4	0.0979 (17)	0.0598 (12)	0.0792 (15)	0.0033 (11)	0.0732 (14)	−0.0036 (11)
C5	0.0924 (16)	0.0672 (13)	0.0737 (14)	−0.0001 (12)	0.0673 (14)	0.0091 (11)
C6	0.0669 (12)	0.0435 (9)	0.0623 (11)	−0.0018 (8)	0.0444 (10)	0.0082 (8)
S11	0.03285 (19)	0.0358 (2)	0.0398 (2)	0.00174 (14)	0.01463 (16)	−0.00139 (15)
O11	0.0498 (7)	0.0493 (7)	0.0513 (7)	0.0054 (6)	0.0165 (6)	−0.0134 (6)
O12	0.0558 (8)	0.0497 (7)	0.0522 (7)	0.0056 (6)	0.0227 (6)	0.0147 (6)
O13	0.0324 (6)	0.0628 (9)	0.0694 (9)	−0.0034 (5)	0.0237 (6)	−0.0094 (7)
C11	0.0602 (14)	0.095 (2)	0.0504 (12)	0.0003 (12)	0.0039 (11)	−0.0007 (12)
C12	0.0433 (9)	0.0557 (11)	0.0440 (10)	−0.0025 (8)	0.0122 (8)	0.0027 (8)
C13	0.0534 (11)	0.0615 (12)	0.0427 (9)	−0.0035 (9)	0.0236 (8)	−0.0089 (8)
C14	0.0403 (8)	0.0516 (10)	0.0449 (9)	0.0032 (7)	0.0229 (7)	−0.0038 (7)
C15	0.0320 (7)	0.0356 (7)	0.0390 (8)	−0.0009 (6)	0.0182 (6)	0.0017 (6)
C16	0.0413 (9)	0.0563 (11)	0.0504 (10)	0.0096 (8)	0.0199 (8)	−0.0063 (8)
C17	0.0403 (10)	0.0659 (13)	0.0586 (12)	0.0134 (9)	0.0149 (9)	−0.0009 (10)
S21	0.0452 (2)	0.03159 (19)	0.03394 (19)	0.00202 (14)	0.02151 (17)	0.00074 (13)
O21	0.0502 (7)	0.0599 (8)	0.0523 (7)	0.0147 (6)	0.0274 (6)	0.0096 (6)
O22	0.0741 (9)	0.0606 (8)	0.0383 (6)	−0.0077 (7)	0.0345 (7)	−0.0003 (6)
O23	0.0581 (8)	0.0318 (6)	0.0582 (8)	0.0003 (5)	0.0188 (7)	−0.0062 (5)
C21	0.131 (3)	0.089 (2)	0.0642 (16)	−0.005 (2)	0.0007 (17)	−0.0314 (16)
C22	0.0841 (16)	0.0541 (12)	0.0475 (11)	0.0005 (11)	0.0132 (11)	−0.0131 (9)
C23	0.0700 (15)	0.0772 (17)	0.0764 (16)	−0.0281 (13)	0.0279 (13)	−0.0191 (13)
C24	0.0641 (12)	0.0657 (13)	0.0564 (11)	−0.0176 (10)	0.0355 (10)	−0.0091 (10)
C25	0.0486 (9)	0.0326 (7)	0.0356 (7)	0.0005 (6)	0.0237 (7)	−0.0019 (6)
C26	0.0659 (12)	0.0465 (10)	0.0406 (9)	0.0041 (8)	0.0320 (9)	0.0042 (7)
C27	0.0919 (17)	0.0610 (12)	0.0383 (9)	0.0128 (12)	0.0309 (11)	0.0004 (9)

data-3

Geometric parameters (Å, º)

N1—C1	1.4570 (19)	C13—C14	1.386 (3)
N2—C2	1.4561 (18)	C14—C15	1.382 (2)
C1—C6	1.380 (2)	C15—C16	1.380 (2)
C1—C2	1.383 (2)	C16—C17	1.389 (3)
C2—C3	1.383 (2)	S21—O21	1.4462 (14)
C3—C4	1.380 (3)	S21—O23	1.4490 (13)
C4—C5	1.378 (3)	S21—O22	1.4554 (13)
C5—C6	1.380 (3)	S21—C25	1.7602 (17)
S11—O11	1.4451 (13)	C21—C22	1.521 (3)
S11—O12	1.4517 (14)	C22—C27	1.373 (4)
S11—O13	1.4553 (14)	C22—C23	1.381 (4)
S11—C15	1.7671 (16)	C23—C24	1.390 (3)
C11—C12	1.515 (3)	C24—C25	1.375 (3)
C12—C17	1.377 (3)	C25—C26	1.383 (2)
C12—C13	1.382 (3)	C26—C27	1.379 (3)
C6—C1—C2	119.60 (15)	C16—C15—C14	120.25 (16)
C6—C1—N1	118.71 (15)	C16—C15—S11	119.46 (13)
C2—C1—N1	121.69 (13)	C14—C15—S11	120.27 (12)
C3—C2—C1	120.23 (14)	C15—C16—C17	119.57 (18)
C3—C2—N2	117.66 (14)	C12—C17—C16	121.09 (18)
C1—C2—N2	122.10 (13)	O21—S21—O23	113.06 (9)
C4—C3—C2	119.78 (17)	O21—S21—O22	111.63 (9)
C5—C4—C3	120.09 (18)	O23—S21—O22	111.81 (9)
C4—C5—C6	120.07 (18)	O21—S21—C25	105.80 (8)
C5—C6—C1	120.23 (18)	O23—S21—C25	107.28 (8)
O11—S11—O12	112.95 (9)	O22—S21—C25	106.77 (8)
O11—S11—O13	113.27 (8)	C27—C22—C23	118.7 (2)
O12—S11—O13	111.32 (8)	C27—C22—C21	121.4 (3)
O11—S11—C15	106.21 (7)	C23—C22—C21	119.9 (3)
O12—S11—C15	105.73 (8)	C22—C23—C24	121.2 (2)
O13—S11—C15	106.72 (8)	C25—C24—C23	119.1 (2)
C17—C12—C13	118.48 (17)	C24—C25—C26	120.16 (17)
C17—C12—C11	119.6 (2)	C24—C25—S21	121.00 (14)
C13—C12—C11	121.9 (2)	C26—C25—S21	118.79 (14)
C12—C13—C14	121.40 (18)	C27—C26—C25	119.8 (2)
C15—C14—C13	119.22 (17)	C22—C27—C26	121.0 (2)
C6—C1—C2—C3	−0.9 (2)	C14—C15—C16—C17	−0.2 (3)
N1—C1—C2—C3	179.13 (16)	S11—C15—C16—C17	178.16 (16)
C6—C1—C2—N2	−179.29 (16)	C13—C12—C17—C16	−0.2 (3)
N1—C1—C2—N2	0.8 (2)	C11—C12—C17—C16	179.8 (2)
C1—C2—C3—C4	0.7 (3)	C15—C16—C17—C12	0.5 (3)
N2—C2—C3—C4	179.15 (19)	C27—C22—C23—C24	−2.5 (4)
C2—C3—C4—C5	0.0 (4)	C21—C22—C23—C24	175.2 (3)
C3—C4—C5—C6	−0.6 (4)	C22—C23—C24—C25	1.8 (4)

C4—C5—C6—C1	0.4 (4)	C23—C24—C25—C26	−0.6 (3)
C2—C1—C6—C5	0.4 (3)	C23—C24—C25—S21	−177.95 (19)
N1—C1—C6—C5	−179.68 (19)	O21—S21—C25—C24	131.47 (17)
C17—C12—C13—C14	−0.3 (3)	O23—S21—C25—C24	−107.57 (17)
C11—C12—C13—C14	179.6 (2)	O22—S21—C25—C24	12.44 (18)
C12—C13—C14—C15	0.6 (3)	O21—S21—C25—C26	−45.95 (16)
C13—C14—C15—C16	−0.3 (3)	O23—S21—C25—C26	75.00 (16)
C13—C14—C15—S11	−178.67 (15)	O22—S21—C25—C26	−164.99 (14)
O11—S11—C15—C16	22.07 (17)	C24—C25—C26—C27	0.0 (3)
O12—S11—C15—C16	−98.17 (16)	S21—C25—C26—C27	177.46 (15)
O13—S11—C15—C16	143.20 (15)	C23—C22—C27—C26	1.9 (4)
O11—S11—C15—C14	−159.58 (14)	C21—C22—C27—C26	−175.7 (2)
O12—S11—C15—C14	80.18 (15)	C25—C26—C27—C22	−0.7 (3)
O13—S11—C15—C14	−38.45 (16)		

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1A⋯O21	0.89	1.92	2.8062 (19)	175
N1—H1B⋯O11[i]	0.89	2.07	2.7509 (19)	133
N1—H1B⋯O22[ii]	0.89	2.31	2.9017 (18)	124
N1—H1C⋯O13[iii]	0.89	1.89	2.7733 (19)	170
N2—H2A⋯O13[iii]	0.89	2.46	2.9128 (19)	112
N2—H2A⋯O23[iv]	0.89	1.97	2.7820 (18)	151
N2—H2B⋯O22[ii]	0.89	1.98	2.8611 (19)	173
N2—H2C⋯O12	0.89	1.84	2.7224 (19)	175

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, -y, -z+1$; (iv) $x, y-1, z$.