

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

1,3-Diammonio-1,2,3-trideoxy-*cis*-inositol sulfate

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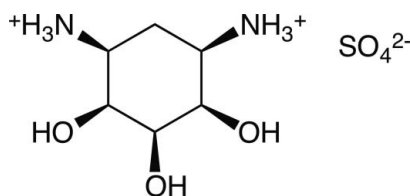
Received 13 March 2012; accepted 12 April 2012

 Key indicators: single-crystal X-ray study; $T = 200$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.026; wR factor = 0.066; data-to-parameter ratio = 10.3.

In the crystal structure of the title compound, $\text{C}_6\text{H}_{16}\text{N}_2\text{O}_3^{2+} \cdot \text{SO}_4^{2-}$, each cation forms three $\text{O}-\text{H} \cdots \text{O}$ and five $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds to six neighbouring sulfate anions. In addition, interlinking of the cations by $\text{N}-\text{H} \cdots \text{O}$ interactions is also observed. The cyclohexane ring adopts a chair conformation with two axial hydroxy groups. Although the separation of 2.928 Å is almost ideal for a hydrogen bond, intramolecular hydrogen bonding between these two hydroxy groups is not observed.

Related literature

The synthesis of the chloride salt, as well as formation of a Cu^{II} complex of 1,3-diamino-1,2,3-trideoxy-*cis*-inositol, was reported by Merten *et al.* (2012). A crystal structure determination of the chloride salt was performed by Neis *et al.* (2012). The importance of intramolecular hydrogen bonding in *syn*-1,3,5-trisubstituted cyclohexane derivatives has been discussed by Gencheva *et al.* (2000), Kramer *et al.* (1998), Kuppert *et al.* (2006), and Neis *et al.* (2010). Puckering parameters were calculated according to Cremer & Pople (1975). For the treatment of hydrogen atoms in *SHELXL*, see: Müller *et al.* (2006).



Experimental

Crystal data

 $\text{C}_6\text{H}_{16}\text{N}_2\text{O}_3^{2+} \cdot \text{SO}_4^{2-}$
 $M_r = 260.27$
 Monoclinic, $P2_1/n$
 $a = 9.2151$ (18) Å
 $b = 6.6673$ (13) Å
 $c = 17.267$ (4) Å

 $\beta = 101.46$ (3)°
 $V = 1039.7$ (4) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

 $\mu = 0.34$ mm⁻¹
 $T = 200$ K
 $0.30 \times 0.20 \times 0.15$ mm

Data collection

 Stoe IPDS image plate diffractometer
 6961 measured reflections

 1779 independent reflections
 1685 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.066$
 $S = 1.06$
 1779 reflections
 172 parameters
 9 restraints

 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.27$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.29$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{N1}-\text{H1A} \cdots \text{O4}^{\text{i}}$	0.87 (1)	2.09 (2)	2.9292 (17)	163 (2)
$\text{N1}-\text{H1B} \cdots \text{O3}^{\text{iii}}$	0.87 (2)	2.11 (2)	2.8125 (18)	138 (2)
$\text{N1}-\text{H1C} \cdots \text{O7}^{\text{iii}}$	0.85 (2)	2.04 (2)	2.882 (2)	170 (2)
$\text{N5}-\text{H5A} \cdots \text{O5}$	0.89 (2)	1.97 (2)	2.8538 (17)	173 (2)
$\text{N5}-\text{H5B} \cdots \text{O8}^{\text{iv}}$	0.86 (1)	2.02 (2)	2.8530 (18)	162 (2)
$\text{N5}-\text{H5C} \cdots \text{O7}^{\text{ii}}$	0.87 (2)	2.29 (2)	3.0852 (18)	153 (2)
$\text{N5}-\text{H5C} \cdots \text{O6}^{\text{ii}}$	0.87 (2)	2.34 (2)	3.0856 (19)	144 (2)
$\text{O4}-\text{H4O} \cdots \text{O6}$	0.85 (2)	1.86 (2)	2.7017 (16)	177 (2)
$\text{O2}-\text{H2O} \cdots \text{O8}^{\text{v}}$	0.86 (2)	1.97 (2)	2.8161 (15)	170 (2)
$\text{O3}-\text{H3O} \cdots \text{O7}^{\text{vi}}$	0.86 (2)	1.87 (2)	2.7149 (16)	167 (2)

 Symmetry codes: (i) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$; (ii) $x, y - 1, z$; (iii) $x - 1, y - 1, z$; (iv) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$; (v) $x - 1, y, z$; (vi) $-x + 1, -y + 1, -z$.

Data collection: *IPDS Software* (Stoe & Cie, 1997); cell refinement: *IPDS Software*; data reduction: *IPDS Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2011); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

We thank Dr Volker Huch (Universität des Saarlandes) for the collection of the data set.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2402).

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supporting information

Acta Cryst. (2012). E68, o1425–o1426 [doi:10.1107/S1600536812016029]

1,3-Diammonio-1,2,3-trideoxy-*cis*-inositol sulfate

Christian Neis, Günter J. Merten and Kaspar Hegetschweiler

S1. Comment

Due to the versatile metal- and hydrogen-binding properties, 1,3-diamino-1,2,3-trideoxy-*cis*-inositol has been found to be a promising building block for the construction of polynuclear metal complexes and extended hydrogen bonded networks (Merten *et al.*, 2012). The crystal structure of a corresponding hydrochloride $C_6H_{14}N_2O_3 \cdot 2HCl$ has recently been reported (Neis *et al.*, 2012). Similar to this chloride salt, the title compound contains 1,3-diammonio-1,2,3-trideoxy-*cis*-inositol dications with the cyclohexane ring adopting an almost ideal chair conformation (puckering parameters: $Q = 0.59 \text{ \AA}$, $\theta = 178.3^\circ$, $\varphi = 89.0^\circ$). In both salts, the cation has the same form with the two ammonium groups and one of the hydroxy groups in equatorial and the remaining two hydroxy groups in axial position. In the title compound, each cation is hydrogen-bonded to six sulfate counter ions by $O-H \cdots O$ and $N-H \cdots O$ interactions, one of the latter is bifurcated. These cation \cdots anion interactions constitute an extended three-dimensional network. Direct cation \cdots cation hydrogen bonding is also observed: One of the ammonium groups of each cation donates a hydrogen atom to the equatorial hydroxy group of a neighbouring cation and another hydrogen atom to the axial hydroxy group of an additional neighbour. Each cation is thus connected to a total of four neighbouring cations and these interactions generate double chains, which are oriented parallel to the crystallographic *b* axis. As already observed for the chloride salt, all $O-H$ and $N-H$ groups act as hydrogen donors, however, one of the axial hydroxy groups does not accept any hydrogen atom. We explain these observations by the well established stronger steric encumbrance of axial substituents. It is again worthy to note that the non-accepting axial hydroxy group does not form an intramolecular $O-H \cdots O$ hydrogen bond, even though the $O \cdots O$ separation of 2.928 \AA between the two axial oxygen atoms corresponds almost ideally to the value required for such an interaction. For corresponding structures with three axial hydroxy or amino groups in a *syn*-1,3,5-triaxial arrangement, it appears, however, that the formation of such intramolecular hydrogen bonds is often a prerequisite for a stable cyclohexane chair (Gencheva *et al.*, 2000; Kramer *et al.*, 1998; Kuppert *et al.*, 2006). The non-observance of such a hydrogen bond in the title compound further supports the conclusion that this type of interactions would be of minor importance in molecules having only two hydroxy groups in a 1,3-*syn*-axial arrangement.

S2. Experimental

The title compound has been obtained following the protocol given by Merten *et al.* (2012). 1H -NMR and ^{13}C -NMR properties are identical with the chloride salt (Neis *et al.*, 2012). Single crystals were grown from an aqueous solution (pH 2) by slow evaporation at 298 K.

S3. Refinement

All non-hydrogen atoms were refined using anisotropic displacement parameters. Hydrogen atoms were treated as recommended by Müller *et al.* (2006): A riding model was used for C-bonded hydrogen atoms. The positional parameters of the O- and N-bonded hydrogen atoms were refined using isotropic displacement parameters which were set to $1.5 \times U_{eq}$

of the pivot atom. In addition, restraints of 0.84 and 0.88 Å were used for the O—H and N—H distances, respectively.

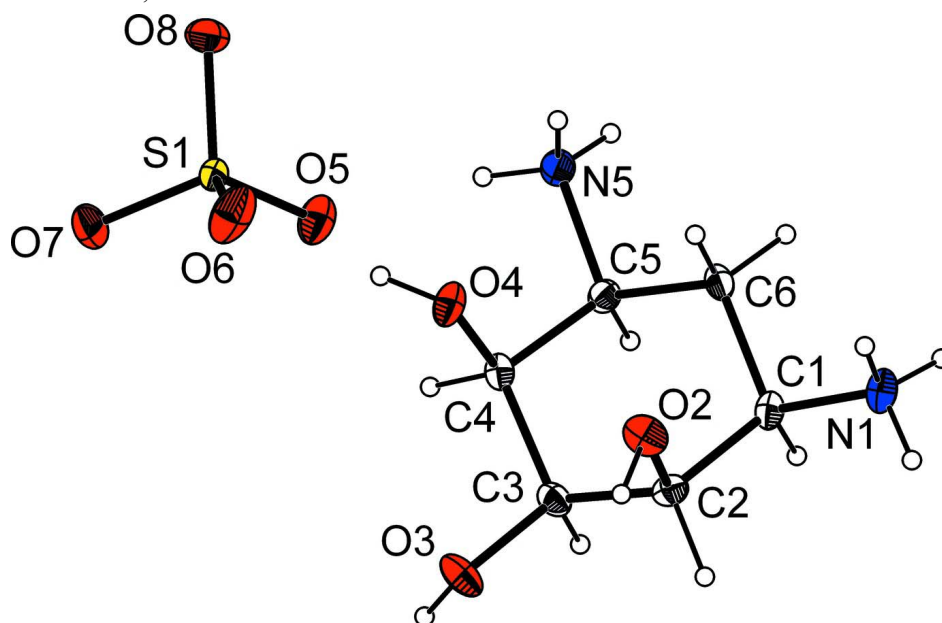


Figure 1

Molecular structure of the title compound with numbering scheme and displacement ellipsoids drawn at the 50% probability level.

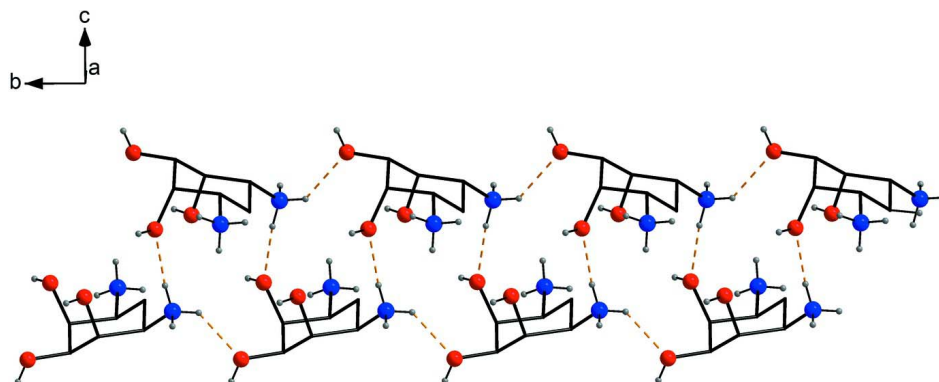


Figure 2

The double chain structure which is formed by hydrogen bonding between dication entities (ball and stick model).

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Crystal data

$C_6H_{16}N_2O_3^{2+} \cdot SO_4^{2-}$

$M_r = 260.27$

Monoclinic, $P2_1/n$

Hall symbol: $-P 2_1 n$

$a = 9.2151 (18) \text{ \AA}$

$b = 6.6673 (13) \text{ \AA}$

$c = 17.267 (4) \text{ \AA}$

$\beta = 101.46 (3)^\circ$

$V = 1039.7 (4) \text{ \AA}^3$

$Z = 4$

$F(000) = 552$

$D_x = 1.663 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3837 reflections

$\theta = 2.6\text{--}25.0^\circ$

$\mu = 0.34 \text{ mm}^{-1}$

$T = 200 \text{ K}$

Prism, colourless

$0.30 \times 0.20 \times 0.15 \text{ mm}$

Data collection

Stoe IPDS image plate
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

phi scans

6961 measured reflections

1779 independent reflections

1685 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.3^\circ$

$h = -10 \rightarrow 10$

$k = -7 \rightarrow 7$

$l = -20 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.026$

$wR(F^2) = 0.066$

$S = 1.06$

1779 reflections

172 parameters

9 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0259P)^2 + 0.7072P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.27 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.29 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C5	0.44604 (15)	-0.0876 (2)	0.10574 (8)	0.0129 (3)
H5	0.4373	-0.1399	0.0507	0.015*
C6	0.35712 (15)	-0.2238 (2)	0.15088 (8)	0.0149 (3)
H6A	0.3961	-0.3624	0.1521	0.018*
H6B	0.3684	-0.1762	0.2061	0.018*
C2	0.12716 (15)	-0.0111 (2)	0.10691 (8)	0.0139 (3)
H2	0.0241	-0.0171	0.0749	0.017*
C1	0.19415 (15)	-0.2228 (2)	0.11143 (8)	0.0136 (3)
H1	0.1839	-0.2768	0.0566	0.016*
C3	0.22081 (16)	0.1251 (2)	0.06417 (8)	0.0137 (3)
H3	0.2117	0.0722	0.0092	0.016*
C4	0.38668 (15)	0.1297 (2)	0.10194 (8)	0.0126 (3)
H4	0.4396	0.2105	0.0674	0.015*
N1	0.11358 (15)	-0.3591 (2)	0.15750 (8)	0.0171 (3)
H1A	0.124 (2)	-0.325 (3)	0.2070 (9)	0.026*
H1B	0.142 (2)	-0.481 (2)	0.1514 (10)	0.026*

H1C	0.0204 (17)	-0.360 (3)	0.1393 (10)	0.026*
N5	0.60555 (14)	-0.09248 (19)	0.14663 (8)	0.0151 (3)
H5A	0.6514 (19)	0.006 (3)	0.1269 (10)	0.023*
H5B	0.612 (2)	-0.084 (3)	0.1971 (9)	0.023*
H5C	0.642 (2)	-0.208 (2)	0.1385 (10)	0.023*
O4	0.41236 (12)	0.21890 (16)	0.17886 (6)	0.0177 (2)
H4O	0.4859 (19)	0.294 (3)	0.1786 (11)	0.027*
O2	0.12055 (12)	0.05338 (16)	0.18490 (6)	0.0188 (2)
H2O	0.0491 (19)	0.137 (3)	0.1815 (11)	0.028*
O3	0.15853 (12)	0.32218 (16)	0.05817 (6)	0.0206 (2)
H3O	0.171 (2)	0.369 (3)	0.0137 (9)	0.031*
S1	0.77047 (4)	0.40360 (5)	0.132375 (19)	0.01264 (13)
O7	0.80382 (13)	0.58885 (16)	0.09000 (6)	0.0268 (3)
O8	0.90424 (11)	0.34825 (16)	0.19086 (6)	0.0201 (2)
O5	0.72807 (12)	0.23732 (16)	0.07600 (6)	0.0221 (3)
O6	0.65015 (12)	0.45266 (18)	0.17466 (7)	0.0294 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C5	0.0114 (7)	0.0124 (7)	0.0148 (7)	-0.0003 (5)	0.0022 (5)	-0.0010 (5)
C6	0.0148 (7)	0.0096 (7)	0.0200 (7)	-0.0004 (5)	0.0027 (5)	0.0025 (5)
C2	0.0112 (7)	0.0156 (7)	0.0142 (6)	0.0004 (5)	0.0008 (5)	-0.0008 (5)
C1	0.0151 (7)	0.0118 (7)	0.0146 (6)	-0.0038 (5)	0.0043 (5)	-0.0007 (5)
C3	0.0165 (7)	0.0106 (7)	0.0137 (6)	0.0026 (5)	0.0024 (5)	0.0004 (5)
C4	0.0150 (7)	0.0104 (7)	0.0131 (6)	-0.0017 (5)	0.0044 (5)	-0.0001 (5)
N1	0.0178 (7)	0.0142 (6)	0.0205 (7)	-0.0052 (5)	0.0067 (5)	-0.0017 (5)
N5	0.0129 (6)	0.0132 (6)	0.0191 (6)	0.0008 (5)	0.0032 (5)	-0.0012 (5)
O4	0.0199 (5)	0.0158 (5)	0.0179 (5)	-0.0065 (4)	0.0045 (4)	-0.0047 (4)
O2	0.0209 (6)	0.0195 (5)	0.0172 (5)	0.0050 (4)	0.0069 (4)	-0.0003 (4)
O3	0.0269 (6)	0.0136 (5)	0.0223 (5)	0.0083 (4)	0.0073 (4)	0.0046 (4)
S1	0.0110 (2)	0.01085 (19)	0.0156 (2)	-0.00160 (12)	0.00125 (13)	0.00023 (12)
O7	0.0345 (7)	0.0183 (6)	0.0244 (6)	-0.0064 (5)	-0.0017 (5)	0.0082 (4)
O8	0.0183 (5)	0.0207 (5)	0.0193 (5)	0.0035 (4)	-0.0009 (4)	0.0023 (4)
O5	0.0255 (6)	0.0209 (6)	0.0205 (5)	-0.0077 (4)	0.0055 (4)	-0.0057 (4)
O6	0.0168 (6)	0.0289 (6)	0.0455 (7)	-0.0041 (5)	0.0134 (5)	-0.0149 (5)

Geometric parameters (Å, °)

C5—N5	1.4993 (18)	C4—O4	1.4312 (17)
C5—C6	1.5355 (19)	C4—H4	1.0000
C5—C4	1.5454 (19)	N1—H1A	0.870 (14)
C5—H5	1.0000	N1—H1B	0.867 (15)
C6—C1	1.521 (2)	N1—H1C	0.853 (15)
C6—H6A	0.9900	N5—H5A	0.885 (15)
C6—H6B	0.9900	N5—H5B	0.864 (14)
C2—O2	1.4265 (17)	N5—H5C	0.866 (15)
C2—C1	1.536 (2)	O4—H4O	0.845 (15)

C2—C3	1.5386 (19)	O2—H2O	0.855 (15)
C2—H2	1.0000	O3—H3O	0.856 (15)
C1—N1	1.4985 (18)	S1—O5	1.4758 (11)
C1—H1	1.0000	S1—O8	1.4768 (11)
C3—O3	1.4297 (17)	S1—O6	1.4802 (12)
C3—C4	1.538 (2)	S1—O7	1.4982 (11)
C3—H3	1.0000		
N5—C5—C6	108.67 (11)	C2—C3—H3	107.4
N5—C5—C4	110.25 (11)	O4—C4—C3	111.66 (11)
C6—C5—C4	110.85 (11)	O4—C4—C5	110.99 (11)
N5—C5—H5	109.0	C3—C4—C5	108.20 (11)
C6—C5—H5	109.0	O4—C4—H4	108.6
C4—C5—H5	109.0	C3—C4—H4	108.6
C1—C6—C5	110.43 (11)	C5—C4—H4	108.6
C1—C6—H6A	109.6	C1—N1—H1A	113.0 (13)
C5—C6—H6A	109.6	C1—N1—H1B	108.2 (12)
C1—C6—H6B	109.6	H1A—N1—H1B	112.8 (17)
C5—C6—H6B	109.6	C1—N1—H1C	112.2 (13)
H6A—C6—H6B	108.1	H1A—N1—H1C	105.8 (18)
O2—C2—C1	108.74 (11)	H1B—N1—H1C	104.5 (18)
O2—C2—C3	114.09 (11)	C5—N5—H5A	107.5 (12)
C1—C2—C3	107.97 (11)	C5—N5—H5B	109.5 (12)
O2—C2—H2	108.6	H5A—N5—H5B	113.7 (16)
C1—C2—H2	108.6	C5—N5—H5C	108.8 (12)
C3—C2—H2	108.6	H5A—N5—H5C	111.5 (17)
N1—C1—C6	107.99 (11)	H5B—N5—H5C	105.7 (17)
N1—C1—C2	110.35 (12)	C4—O4—H4O	103.2 (12)
C6—C1—C2	112.20 (11)	C2—O2—H2O	107.9 (12)
N1—C1—H1	108.7	C3—O3—H3O	106.1 (13)
C6—C1—H1	108.7	O5—S1—O8	109.81 (7)
C2—C1—H1	108.7	O5—S1—O6	111.42 (6)
O3—C3—C4	111.27 (11)	O8—S1—O6	108.86 (7)
O3—C3—C2	108.78 (11)	O5—S1—O7	110.50 (6)
C4—C3—C2	114.41 (11)	O8—S1—O7	108.39 (6)
O3—C3—H3	107.4	O6—S1—O7	107.77 (7)
C4—C3—H3	107.4		
N5—C5—C6—C1	179.85 (11)	O2—C2—C3—C4	65.11 (15)
C4—C5—C6—C1	58.54 (15)	C1—C2—C3—C4	-55.89 (14)
C5—C6—C1—N1	179.52 (11)	O3—C3—C4—O4	58.04 (15)
C5—C6—C1—C2	-58.64 (15)	C2—C3—C4—O4	-65.75 (15)
O2—C2—C1—N1	51.84 (14)	O3—C3—C4—C5	-179.54 (11)
C3—C2—C1—N1	176.11 (10)	C2—C3—C4—C5	56.67 (15)
O2—C2—C1—C6	-68.64 (14)	N5—C5—C4—O4	-53.77 (15)
C3—C2—C1—C6	55.63 (14)	C6—C5—C4—O4	66.61 (14)
O2—C2—C3—O3	-60.00 (15)	N5—C5—C4—C3	-176.61 (11)
C1—C2—C3—O3	179.00 (10)	C6—C5—C4—C3	-56.23 (15)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1A \cdots O4 ⁱ	0.87 (1)	2.09 (2)	2.9292 (17)	163 (2)
N1—H1B \cdots O3 ⁱⁱ	0.87 (2)	2.11 (2)	2.8125 (18)	138 (2)
N1—H1C \cdots O7 ⁱⁱⁱ	0.85 (2)	2.04 (2)	2.882 (2)	170 (2)
N5—H5A \cdots O5	0.89 (2)	1.97 (2)	2.8538 (17)	173 (2)
N5—H5B \cdots O8 ^{iv}	0.86 (1)	2.02 (2)	2.8530 (18)	162 (2)
N5—H5C \cdots O7 ⁱⁱ	0.87 (2)	2.29 (2)	3.0852 (18)	153 (2)
N5—H5C \cdots O6 ⁱⁱ	0.87 (2)	2.34 (2)	3.0856 (19)	144 (2)
O4—H4O \cdots O6	0.85 (2)	1.86 (2)	2.7017 (16)	177 (2)
O2—H2O \cdots O8 ^v	0.86 (2)	1.97 (2)	2.8161 (15)	170 (2)
O3—H3O \cdots O7 ^{vi}	0.86 (2)	1.87 (2)	2.7149 (16)	167 (2)

Symmetry codes: (i) $-x+1/2, y-1/2, -z+1/2$; (ii) $x, y-1, z$; (iii) $x-1, y-1, z$; (iv) $-x+3/2, y-1/2, -z+1/2$; (v) $x-1, y, z$; (vi) $-x+1, -y+1, -z$.