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Crystal structure of *catena*-poly[[[triaqua-strontium]-di-μ_2-glycinato] dibromide]

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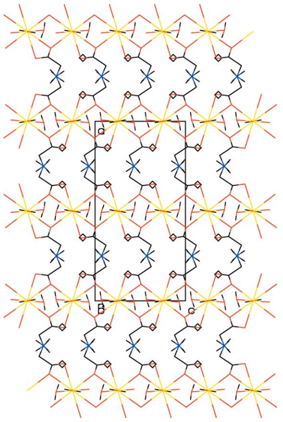
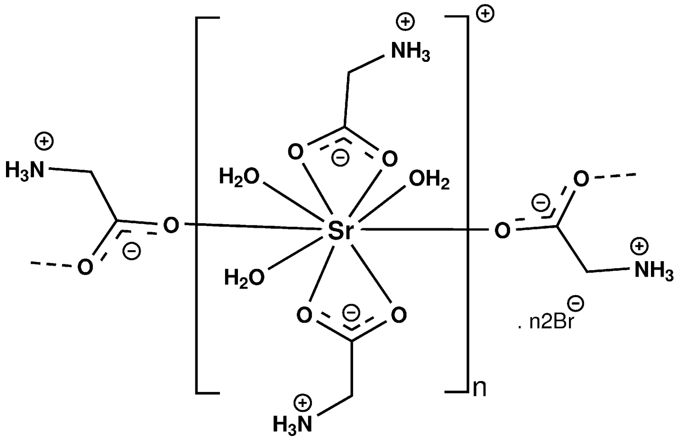
In the title coordination polymer, $\{[\mathrm{Sr}(\mathrm{C_2H_5NO_2})_2(\mathrm{H_2O})_3]\mathrm{Br_2}\}_n$, the Sr^{2+} ion and one of the water molecules are located on twofold rotation axes. The alkaline earth ion is nine-coordinated by three water O atoms and six O atoms of the carboxylate groups of four glycine ligands, two in a chelating mode and two in a monodentate mode. The glycine molecule exists in a zwitterionic form and bridges the cations into chains parallel to [001]. The Br^- counter-anions are located between the chains. Intermolecular hydrogen bonds are formed between the amino and carboxylate groups of neighbouring glycine ligands, generating a head-to-tail sequence. Adjacent head-to-tail sequences are further interconnected by intermolecular N—H···Br hydrogen-bonding interactions into sheets parallel to (100). O—H···Br and O—H···O hydrogen bonds involving the coordinating water molecules are also present, consolidating the three-dimensional hydrogen-bonding network.



1. Chemical context

Research in the field of coordination polymers has undergone rapid development in recent years due to their interesting structures and their wide range of applications as functional materials (Lyhs *et al.*, 2012). One of the simplest amino acids is glycine and some glycine–metal complexes have been reported previously (Fleck *et al.*, 2006 and references therein). The crystal structures of strontium combined with anions of amino acids are rare. As part of our ongoing investigations of the crystal and molecular structures of a series of metal complexes derived from amino acids (Sathiskumar *et al.*, 2015*a*,*b*; Balakrishnan *et al.*, 2013), we report here the crystal structure of a polymeric strontium–glycine complex, $\{[\mathrm{Sr}(\mathrm{C_2H_5NO_2})_2(\mathrm{H_2O})_3]\mathrm{Br_2}\}_n$, (I).



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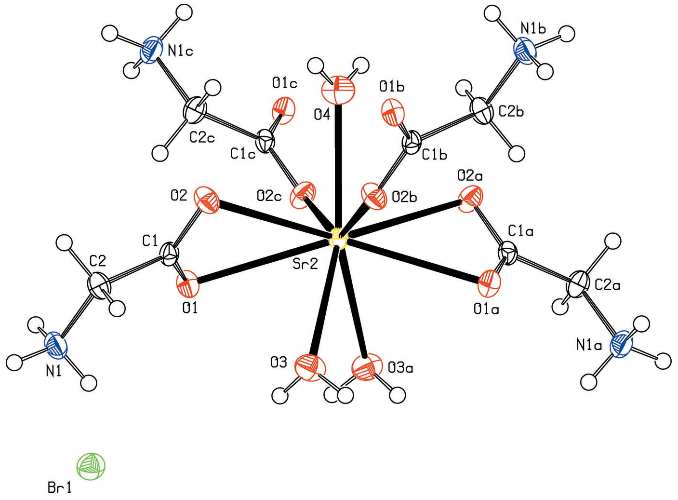

Figure 1
The coordination environment of Sr^{2+} in the crystal structure of (I). Displacement ellipsoids are drawn at the 40% probability level. [Symmetry codes: (*a*) $-x, y, \frac{1}{2} - z$; (*b*) $-x, 1 - y, 1 - z$; (*c*) $x, 1 - y, -\frac{1}{2} + z$].

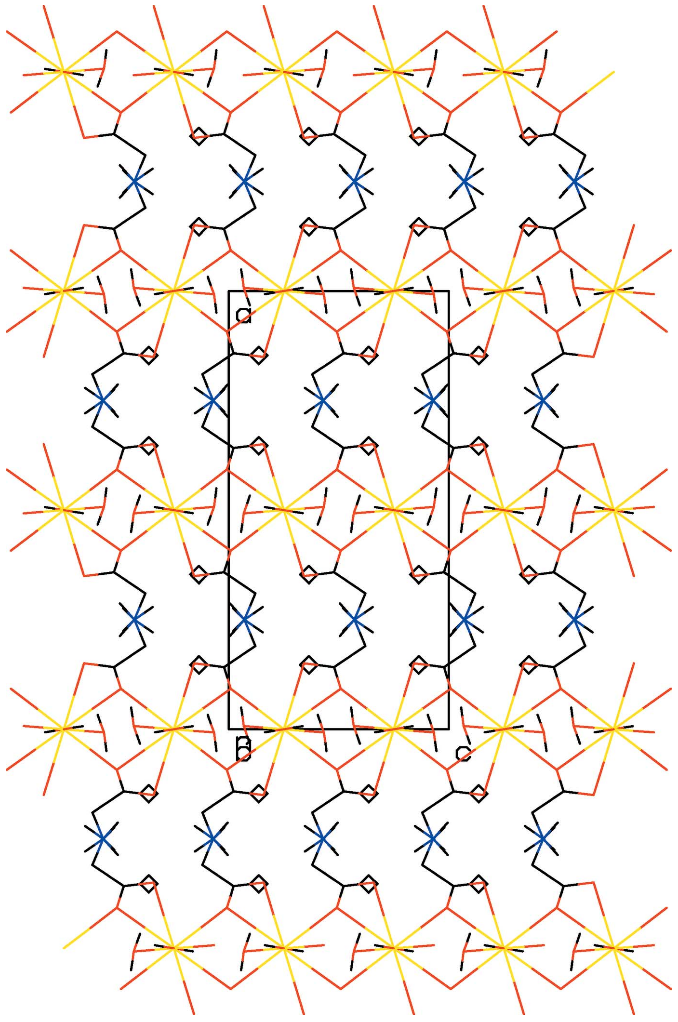

Figure 2
The crystal packing of (I) projected along [010]. H atoms have been omitted for clarity.

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1A⋯O1^{i}	0.88 (5)	2.00 (5)	2.879 (4)	175 (4)
N1—H1B⋯Br1^{ii}	0.88 (4)	2.58 (4)	3.450 (3)	179 (4)
N1—H1C⋯Br1^{iii}	0.89 (4)	2.51 (4)	3.321 (3)	152 (3)
O4—H4⋯O3^{iv}	0.83 (2)	2.01 (2)	2.828 (3)	166 (5)
O3—H3A⋯Br1^{ii}	0.84 (5)	2.50 (5)	3.335 (3)	170 (4)
O3—H3B⋯Br1^{v}	0.84 (2)	2.55 (3)	3.296 (3)	148 (4)

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

2. Structural commentary

The asymmetric unit of (I) contains one Sr^{2+} ion, one glycine ligand, one and a half water molecules and one bromide anion (Fig. 1). The Sr^{2+} cation and one of the water molecules (O4) are located on special positions with site symmetry 2. The bond lengths involving the carboxylate atoms and the protonation of the amino group reveal a zwitterionic form for the glycine ligand in (I). The Sr^{2+} ion is nine-coordinated by three oxygen atoms [Sr—O = 2.526 (4)–2.661 (2) Å] of water molecules and six carboxylate oxygen atoms of four glycine ligands [Sr—O = 2.605 (2)–2.703 (2) Å]. The glycine ligands coordinate each cation in a bis-bidentate and bis-monodentate way and simultaneously bridge two alkaline earth cations. As shown in Fig. 2, this coordination mode leads to the formation of polymeric chains running parallel to [001]. Adjacent Sr^{2+} ions are separated by 4.3497 (3) Å within a chain and the shortest Sr⋯Sr distance between neighbouring chains is 9.4960 (3) Å.

3. Supramolecular features

The crystal structure of (I) contains an intricate network of intermolecular N—H⋯O, N—H⋯Br, O—H⋯O and O—H⋯Br hydrogen bonds (Table 1). The protonated N atom of the glycine molecule is capable of forming three hydrogen-bonding interactions. One of them is the characteristic head-to-tail sequence in which amino acids are self-assembled through their amino and carboxylate groups (Sharma *et al.*, 2006; Selvaraj *et al.*, 2007; Balakrishnan *et al.*, 2013). In (I), the zwitterionic glycine molecules are arranged in linear arrays that run parallel to the [110] direction (Fig. 3), and adjacent glycine molecules are interconnected by an intermolecular N1—H1A⋯O1 hydrogen bond. This interaction can be described as a head-to-tail sequence having a $C(5)$ graph-set motif (Bernstein *et al.*, 1995). In each array, the Br^{-} counter anions bridge neighbouring glycines. Taken together, these three interactions form a hydrogen-bonded sheet extending parallel to (100). One of the water molecules (O3) acts as a donor for two different Br^{-} anions. These intermolecular O—H⋯Br interactions result in a cyclic dibromide motif as observed in the crystal structure of *N*,*N*′-dibenzyl-*N*,*N*,*N*′,*N*′-tetramethylethylenediammonium dibromide dihydrate (Srinivasan *et al.*, 2006). Within this motif, the distance between Br anions is 5.3398 (3) Å, and the distance between

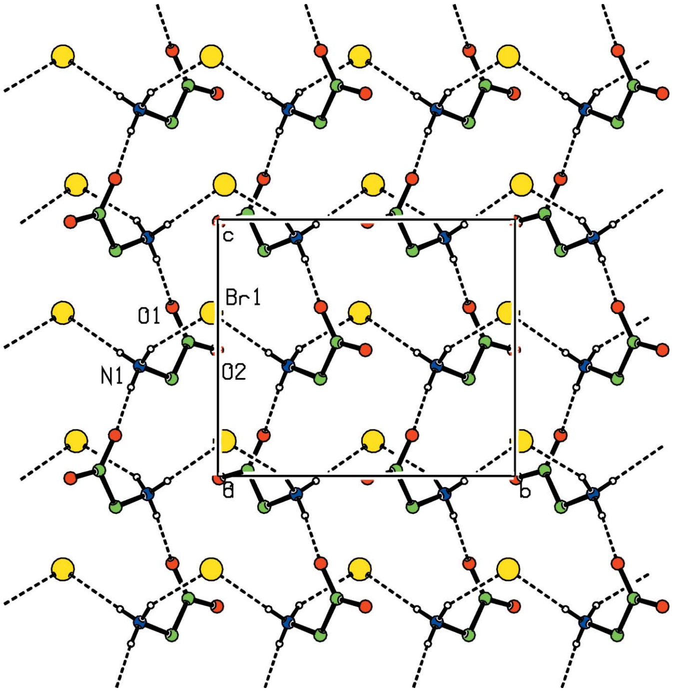

Figure 3
Zwitterionic glycine molecules are interconnected by intermolecular N—H···O and N—H···Br hydrogen bonds into (100) sheets.

water oxygen atoms (O3···O3′) is 3.932 (4) Å. Adjacent cylic dibromide motifs, which are parallel to [001], are interconnected by another water molecule (O4) (Table 1 and Fig. 4).

4. Synthesis and crystallization

Crystals of (I) were grown from an aqueous solution by slow solvent evaporation at room temperature. Analytical grade reagents glycine (Merck) and strontium bromide hexahydrate (Sigma–Aldrich) were taken in a 2:1 molar ratio, dissolved in double-distilled water and stirred well for 4 h using a temperature-controlled magnetic stirrer to yield a homogeneous mixture. The solution was finally filtered using Whatman filter paper. The beaker containing the solution was closed with a polythene sheet with two (or) three perforations and kept in a dust-free atmosphere for slow evaporation. Single crystals were harvested after a growth period of 20 days.

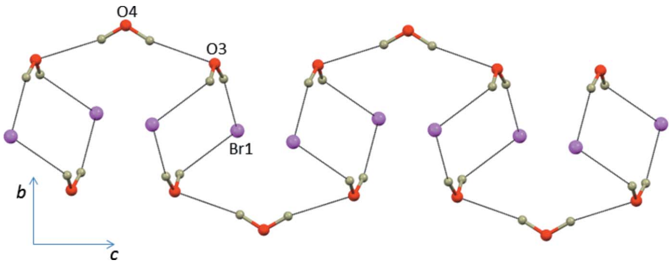

Figure 4
Cyclic dibromide motifs are interconnected by intermolecular O—H···O interactions.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Sr(C_2H_5NO_2)_2(H_2O)_3]Br_2$
M_r	451.63
Crystal system, space group	Orthorhombic, *Pbcn*
Temperature (K)	296
a, b, c (Å)	16.4198 (9), 9.5438 (5), 8.2402 (4)
V (Å^3)	1291.30 (12)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	10.38
Crystal size (mm)	0.15 × 0.10 × 0.10
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 1999)
T_{min}, T_{max}	0.251, 0.410
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22178, 1564, 1244
R_{int}	0.070
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.661
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.023, 0.057, 1.14
No. of reflections	1564
No. of parameters	99
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.86, −0.68

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SIR92* (Altomare *et al.*, 1995), *SHELXL2014* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The positions of the amino and water H atoms were located from difference Fourier maps. The O3—H3*B* and O4—H4 distances of the water molecules were restrained to 0.85 (2) Å. The remaining hydrogen atoms were placed in geometrically idealized positions (C—H = 0.97 Å) with $U_{iso}(H) = 1.2U_{eq}(C)$ and were constrained to ride on their parent atoms.

Acknowledgements

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supporting information

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Crystal structure of *catena*-poly[[[triaquastrontium]-di-μ_2-glycinato] dibromide]

Palanisamy Revathi, Thangavelu Balakrishnan, Kandasamy Ramamurthi and Subbiah Thamotharan

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1995); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015).

catena-Poly[[[triaquastrontium]-di-μ_2-glycinato] dibromide]

Crystal data

$[Sr(C_2H_5NO_2)_2(H_2O)_3]Br_2$
$M_r = 451.63$
Orthorhombic, *Pbcn*
$a = 16.4198\ (9)$ Å
$b = 9.5438\ (5)$ Å
$c = 8.2402\ (4)$ Å
$V = 1291.30\ (12)$ Å^3
$Z = 4$
$F(000) = 872$

$D_x = 2.323$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6100 reflections
$\theta = 2.5–27.8°$
$\mu = 10.38$ mm^{-1}
$T = 296$ K
Block, colourless
0.15 × 0.10 × 0.10 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: Sealed tube
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{min} = 0.251$, $T_{max} = 0.410$
22178 measured reflections

1564 independent reflections
1244 reflections with $I > 2\sigma(I)$
$R_{int} = 0.070$
$\theta_{max} = 28.0°$, $\theta_{min} = 2.5°$
$h = -21 \rightarrow 21$
$k = -12 \rightarrow 12$
$l = -9 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.057$
$S = 1.14$
1564 reflections
99 parameters
2 restraints
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0169P)^2 + 1.7773P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.86$ e Å^{-3}
$\Delta\rho_{min} = -0.67$ e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0086 (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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.14184 (17)	0.5997 (3)	0.4781 (4)	0.0178 (6)
C2	0.1901 (2)	0.6557 (3)	0.6205 (4)	0.0232 (7)
H2A	0.1529	0.6963	0.6989	0.028*
H2B	0.2183	0.5788	0.6729	0.028*
N1	0.2500 (2)	0.7627 (3)	0.5708 (4)	0.0263 (6)
O1	0.15044 (13)	0.6537 (2)	0.3416 (2)	0.0224 (5)
O2	0.09257 (13)	0.5034 (2)	0.5090 (3)	0.0251 (5)
O3	−0.00732 (17)	0.8029 (3)	0.4322 (3)	0.0308 (6)
O4	0.0000	0.3083 (4)	0.2500	0.0331 (8)
Br1	0.14700 (2)	0.97766 (4)	0.86395 (4)	0.02908 (12)
Sr2	0.0000	0.57306 (4)	0.2500	0.01637 (12)
H1A	0.279 (3)	0.793 (5)	0.654 (6)	0.062 (15)*
H1B	0.224 (2)	0.830 (4)	0.520 (5)	0.046 (13)*
H1C	0.287 (3)	0.726 (4)	0.505 (5)	0.044 (12)*
H4	−0.007 (3)	0.264 (4)	0.164 (4)	0.064 (15)*
H3A	0.033 (3)	0.853 (5)	0.404 (5)	0.059 (15)*
H3B	−0.0497 (19)	0.852 (4)	0.444 (6)	0.067 (16)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0131 (14)	0.0216 (15)	0.0186 (14)	0.0022 (11)	0.0002 (12)	−0.0025 (12)
C2	0.0231 (17)	0.0283 (18)	0.0183 (16)	−0.0036 (13)	−0.0017 (13)	−0.0028 (13)
N1	0.0224 (15)	0.0283 (17)	0.0283 (15)	−0.0035 (13)	−0.0052 (14)	−0.0055 (14)
O1	0.0204 (11)	0.0284 (12)	0.0184 (11)	−0.0046 (9)	−0.0007 (9)	0.0022 (9)
O2	0.0259 (12)	0.0277 (12)	0.0216 (11)	−0.0084 (9)	−0.0011 (9)	0.0018 (9)
O3	0.0295 (14)	0.0273 (14)	0.0356 (14)	−0.0015 (12)	0.0082 (12)	−0.0045 (11)
O4	0.044 (2)	0.031 (2)	0.0248 (19)	0.000	0.0019 (18)	0.000
Br1	0.02717 (19)	0.0276 (2)	0.0325 (2)	0.00143 (14)	0.00329 (15)	0.00078 (14)
Sr2	0.01582 (19)	0.0194 (2)	0.01391 (19)	0.000	−0.00064 (16)	0.000

Geometric parameters (Å, º)

C1—O1	1.246 (4)	O2—Sr2	2.703 (2)
C1—O2	1.251 (3)	O3—Sr2	2.661 (2)
C1—C2	1.513 (4)	O3—H3A	0.84 (5)
C1—Sr2	3.004 (3)	O3—H3B	0.842 (19)
C2—N1	1.477 (4)	O4—Sr2	2.526 (4)
C2—H2A	0.9700	O4—H4	0.833 (19)

C2—H2B	0.9700	Sr2—O2^{ii}	2.605 (2)
N1—H1A	0.88 (5)	Sr2—O2^{i}	2.605 (2)
N1—H1B	0.88 (4)	Sr2—O3^{iii}	2.661 (2)
N1—H1C	0.89 (4)	Sr2—O1^{iii}	2.695 (2)
O1—Sr2	2.695 (2)	Sr2—O2^{iii}	2.703 (2)
O2—Sr2^{i}	2.605 (2)	Sr2—C1^{iii}	3.004 (3)

O1—C1—O2	124.1 (3)	O1^{iii}—Sr2—O1	146.83 (10)
O1—C1—C2	119.7 (3)	O4—Sr2—O2^{iii}	75.77 (4)
O2—C1—C2	116.1 (3)	O2^{ii}—Sr2—O2^{iii}	69.96 (8)
O1—C1—Sr2	63.74 (15)	O2^{i}—Sr2—O2^{iii}	101.82 (7)
O2—C1—Sr2	64.13 (16)	O3^{iii}—Sr2—O2^{iii}	77.44 (7)
C2—C1—Sr2	157.1 (2)	O3—Sr2—O2^{iii}	128.53 (7)
N1—C2—C1	112.2 (3)	O1^{iii}—Sr2—O2^{iii}	48.23 (6)
N1—C2—H2A	109.2	O1—Sr2—O2^{iii}	143.76 (6)
C1—C2—H2A	109.2	O4—Sr2—O2	75.77 (4)
N1—C2—H2B	109.2	O2^{ii}—Sr2—O2	101.82 (7)
C1—C2—H2B	109.2	O2^{i}—Sr2—O2	69.96 (8)
H2A—C2—H2B	107.9	O3^{iii}—Sr2—O2	128.53 (7)
C2—N1—H1A	111 (3)	O3—Sr2—O2	77.44 (7)
C2—N1—H1B	108 (3)	O1^{iii}—Sr2—O2	143.76 (6)
H1A—N1—H1B	113 (4)	O1—Sr2—O2	48.23 (6)
C2—N1—H1C	111 (3)	O2^{iii}—Sr2—O2	151.53 (9)
H1A—N1—H1C	104 (4)	O4—Sr2—C1^{iii}	94.86 (6)
H1B—N1—H1C	109 (4)	O2^{ii}—Sr2—C1^{iii}	89.95 (7)
C1—O1—Sr2	91.77 (17)	O2^{i}—Sr2—C1^{iii}	92.77 (7)
C1—O2—Sr2^{i}	137.62 (19)	O3^{iii}—Sr2—C1^{iii}	67.17 (8)
C1—O2—Sr2	91.27 (18)	O3—Sr2—C1^{iii}	104.38 (8)
Sr2^{i}—O2—Sr2	110.04 (8)	O1^{iii}—Sr2—C1^{iii}	24.49 (7)
Sr2—O3—H3A	106 (3)	O1—Sr2—C1^{iii}	149.51 (7)
Sr2—O3—H3B	124 (3)	O2^{iii}—Sr2—C1^{iii}	24.60 (7)
H3A—O3—H3B	111 (4)	O2—Sr2—C1^{iii}	161.97 (7)
Sr2—O4—H4	120 (3)	O4—Sr2—C1	94.86 (6)
O4—Sr2—O2^{ii}	73.73 (5)	O2^{ii}—Sr2—C1	92.77 (7)
O4—Sr2—O2^{i}	73.73 (5)	O2^{i}—Sr2—C1	89.95 (7)
O2^{ii}—Sr2—O2^{i}	147.46 (10)	O3^{iii}—Sr2—C1	104.38 (8)
O4—Sr2—O3^{iii}	145.52 (6)	O3—Sr2—C1	67.17 (8)
O2^{ii}—Sr2—O3^{iii}	76.97 (7)	O1^{iii}—Sr2—C1	149.51 (7)
O2^{i}—Sr2—O3^{iii}	133.43 (8)	O1—Sr2—C1	24.49 (7)
O4—Sr2—O3	145.52 (6)	O2^{iii}—Sr2—C1	161.97 (7)
O2^{ii}—Sr2—O3	133.43 (8)	O2—Sr2—C1	24.60 (7)
O2^{i}—Sr2—O3	76.96 (7)	C1^{iii}—Sr2—C1	170.29 (11)
O3^{iii}—Sr2—O3	68.96 (11)	O4—Sr2—Sr2^{iv}	71.300 (10)
O4—Sr2—O1^{iii}	106.59 (5)	O2^{ii}—Sr2—Sr2^{iv}	35.72 (5)
O2^{ii}—Sr2—O1^{iii}	113.67 (6)	O2^{i}—Sr2—Sr2^{iv}	129.21 (5)
O2^{i}—Sr2—O1^{iii}	76.03 (7)	O3^{iii}—Sr2—Sr2^{iv}	74.32 (6)
O3^{iii}—Sr2—O1^{iii}	69.40 (8)	O3—Sr2—Sr2^{iv}	143.02 (6)
O3—Sr2—O1^{iii}	83.18 (8)	O1^{iii}—Sr2—Sr2^{iv}	80.00 (4)

O4—Sr2—O1	106.59 (5)	O1—Sr2—Sr2^{iv}	110.90 (4)
O2^{ii}—Sr2—O1	76.03 (7)	O2^{iii}—Sr2—Sr2^{iv}	34.24 (5)
O2^{i}—Sr2—O1	113.67 (6)	O2—Sr2—Sr2^{iv}	131.99 (5)
O3^{iii}—Sr2—O1	83.18 (8)	C1^{iii}—Sr2—Sr2^{iv}	55.55 (6)
O3—Sr2—O1	69.40 (8)	C1—Sr2—Sr2^{iv}	128.31 (6)
O1—C1—C2—N1	−6.2 (4)	O1—C1—O2—Sr2^{i}	−144.8 (2)
O2—C1—C2—N1	176.5 (3)	C2—C1—O2—Sr2^{i}	32.3 (4)
Sr2—C1—C2—N1	−98.5 (5)	Sr2—C1—O2—Sr2^{i}	−122.2 (3)
O2—C1—O1—Sr2	22.7 (3)	O1—C1—O2—Sr2	−22.6 (3)
C2—C1—O1—Sr2	−154.3 (2)	C2—C1—O2—Sr2	154.5 (2)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) *x*, −*y*+1, *z*−1/2; (iii) −*x*, *y*, −*z*+1/2; (iv) −*x*, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{v}	0.88 (5)	2.00 (5)	2.879 (4)	175 (4)
N1—H1*B*···Br1^{vi}	0.88 (4)	2.58 (4)	3.450 (3)	179 (4)
N1—H1*C*···Br1^{vii}	0.89 (4)	2.51 (4)	3.321 (3)	152 (3)
O4—H4···O3^{ii}	0.83 (2)	2.01 (2)	2.828 (3)	166 (5)
O3—H3*A*···Br1^{vi}	0.84 (5)	2.50 (5)	3.335 (3)	170 (4)
O3—H3*B*···Br1^{viii}	0.84 (2)	2.55 (3)	3.296 (3)	148 (4)

Symmetry codes: (ii) *x*, −*y*+1, *z*−1/2; (v) −*x*+1/2, −*y*+3/2, *z*+1/2; (vi) *x*, −*y*+2, *z*−1/2; (vii) −*x*+1/2, −*y*+3/2, *z*−1/2; (viii) −*x*, *y*, −*z*+3/2.