# Crystal structure of poly[[μ_2-diaqua-diaqua-μ_2-L-proline-κ^2O:O'-strontium] dibromide]

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In the title coordination polymer, $\{[Sr(C_5H_9NO_2)(H_2O)_4]Br_2\}_n$, the proline molecule exists in a zwitterionic form with one of the ring C atoms disordered over two sites [site-occupancy factors = 0.57 (6):0.43 (6)]. The Sr^{II} ion is nine-coordinated by six water O atoms, two monodentate and two μ_2-bridging, and three carboxylate O atoms of the proline ligands, with two bridging [Sr—O range = 2.524 (4)–2.800 (5) Å]. In the crystal, there is no direct interaction between the proline molecules. However, the proline and water molecules associate with the bromide counter-anions through a number of intermolecular O—H···Br and N—H···Br hydrogen-bonding interactions, giving a three-dimensional supramolecular structure.

1. Chemical context

The study of coordination polymers has been an area of rapid development in recent years due to their interesting structures and their wide range of applications as functional materials (Lyhs et al., 2012). Reports of the crystal structures of alkaline earth metal ions combined with anions of amino acids are very limited. As part of our ongoing investigations of the crystal and molecular structures of a series of metal complexes generated from amino acids (Revathi et al., 2015; Sathiskumar et al., 2015a,b; Balakrishnan et al., 2013), we report here the crystal structure of a polymeric strontium–proline complex, $\{[Sr(C_5H_9NO_2)(H_2O)_4]^{2+} 2(Br^-)\}_n$, (I).
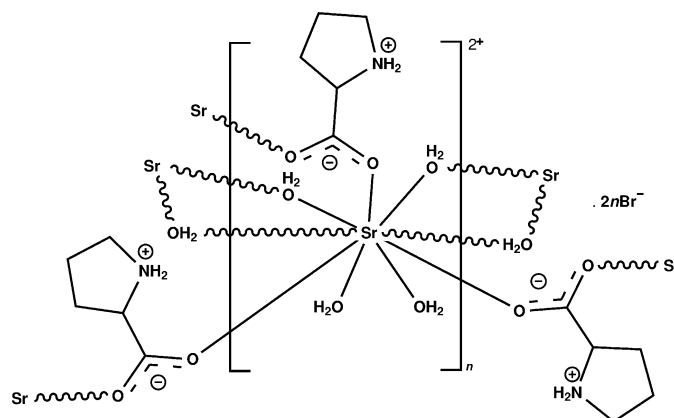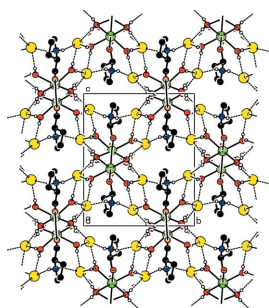
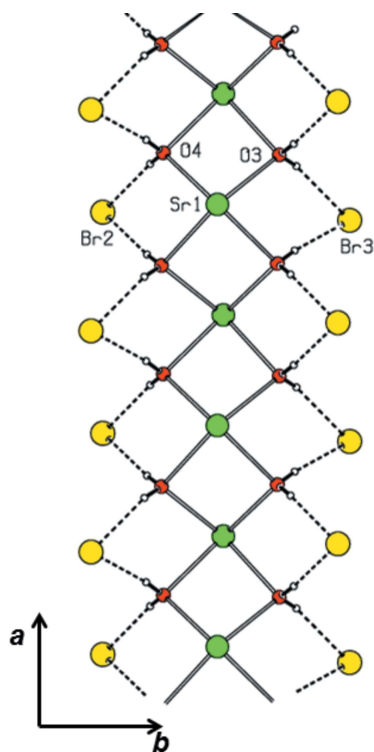## 2. Structural commentary

The asymmetric unit of the title complex (I) contains one Sr^{2+} ion, one bridging proline ligand and four water molecules, two of which are monodentate and two bridging, and two bromide
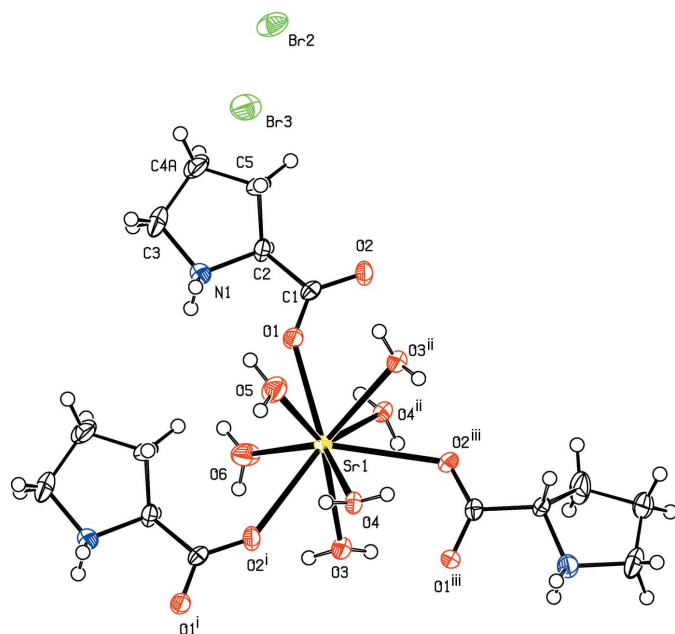
Figure 1
The coordination sphere of Sr^{2+} in the crystal structure of (I). Only the major components of the disordered proline ligands are shown. Displacement ellipsoids are drawn at the 50% probability level. For symmetry codes, see Table 1.

Table 1
Selected bond lengths (Å).

Sr1—O1	2.524 (4)	Sr1—O2^i	2.728 (4)
Sr1—O3	2.625 (6)	Sr1—O3^{ii}	2.707 (6)
Sr1—O4	2.630 (6)	Sr1—O4^{ii}	2.651 (5)
Sr1—O5	2.593 (5)	Sr1—O2^{iii}	2.800 (5)
Sr1—O6	2.582 (6)		

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

Table 2
Hydrogen-bond geometry (Å, °).

| $D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
N1—H1$A$$\cdots$Br2^i	0.90 (6)	2.52 (5)	3.374 (7)	159 (6)
N1—H1$B$$\cdots$Br3^i	0.90 (7)	2.40 (7)	3.240 (7)	156 (8)
O3—H3$C$$\cdots$Br3^{iv}	0.84 (7)	2.63 (7)	3.440 (6)	163 (7)
O3—H3$D$$\cdots$Br2^v	0.84 (7)	2.54 (7)	3.376 (6)	172 (5)
O4—H4$E$$\cdots$Br2^{vi}	0.85 (6)	2.47 (7)	3.281 (6)	162 (7)
O4—H4$F$$\cdots$Br3^{vii}	0.83 (6)	2.52 (6)	3.347 (6)	174 (6)
O5—H5$C$$\cdots$Br2^i	0.86 (5)	2.54 (5)	3.369 (6)	164 (6)
O5—H5$D$$\cdots$Br3^{vii}	0.84 (6)	2.48 (6)	3.304 (6)	166 (6)
O6—H6$C$$\cdots$Br2^v	0.83 (6)	2.58 (6)	3.393 (6)	167 (5)
O6—H6$D$$\cdots$Br3^i	0.85 (7)	2.56 (6)	3.378 (6)	162 (7)

Symmetry codes: (i) $x + 1, y, z$; (iv) $-x + \frac{3}{2}, -y + 1, z + \frac{1}{2}$; (v) $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$; (vi) $-x + \frac{3}{2}, -y, z + \frac{1}{2}$; (vii) $-x + 2, y - \frac{1}{2}, -z + \frac{1}{2}$.
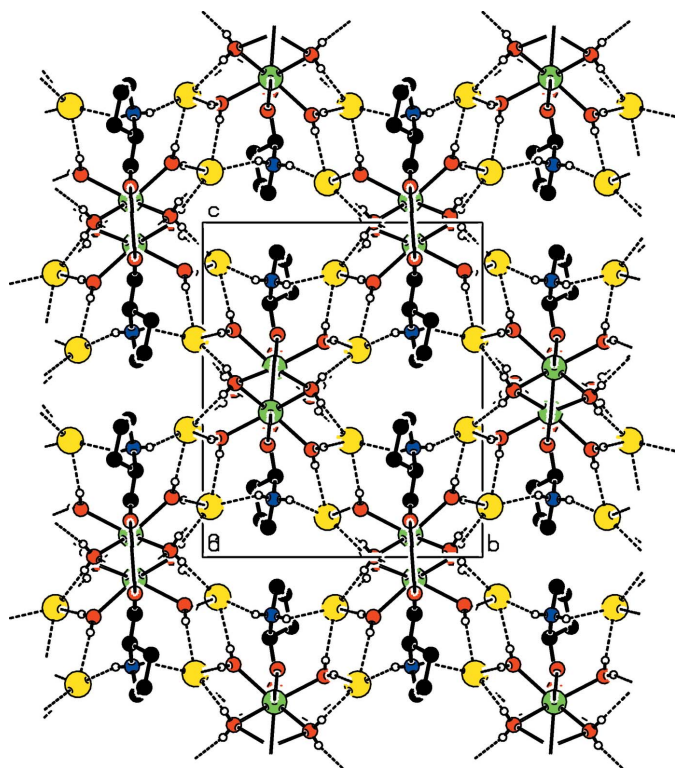
counter-anions (Fig. 1). In (I), the bond lengths involving the carboxylate atoms and the protonation of the amino group suggest that the proline molecule exists in a zwitterionic form. The Sr^{II} ion is nine-coordinated by six water oxygen atoms [Sr—O = 2.582 (6)–2.707 (5)Å] and three carboxylate oxygen atoms of zwitterionic proline ligands [Sr—O = 2.524 (4)–2.800 (4) Å; Table 1]. In the strontium–glycine complex, the Sr—O (water) and Sr—O(carboxylate) distances ranges are 2.526 (4)–2.661 (2) and 2.605 (2)–2.703 (2) Å, respectively (Revathi *et al.*, 2015). In (I), one of the carbon atoms (C4) of the pyrrolidine ring is disordered over two sites. In the major component of the pyrrolidine ring, there is a twist conformation on the C2—C5 bond with a pseudo-rotation angle $\Delta = 40.1 (14)°$ and a maximum torsion angle $\varphi_m = 43.8 (10)°$ for the atom sequence N1–C2–C5–C4A–C3 (Rao *et al.*, 1981). In the minor component, the pyrrolidine ring exhibits an envelope conformation on N1 with a pseudo-rotation angle $\Delta = 341.5 (19)°$ and a maximum torsion angle $\varphi_m = 36.0 (9)°$ for the atom sequence N1–C2–C5–C4B–C3 (Rao *et al.*, 1981). As shown in Fig. 2, the title complex forms a coordination polymeric chain that lies parallel to the *a* axis. Adjacent Sr^{II} ions are separated by 3.9387 (7) Å within a chain.

Figure 2
The Sr–water coordination polymeric chain substructure of (I), with peripheral water O—H$\cdots$Br hydrogen bonds shown as dashed lines.

3. Supramolecular features

The crystal structure of (I), is stabilized by intermolecular N—H$\cdots$Br and O—H$\cdots$Br hydrogen bonds (Table 2). One of the characteristic features observed in amino acid complexes is the head-to-tail sequence in which amino acids are self-associated through their amino and carboxylate groups (Sharma *et al.*, 2006; Selvaraj *et al.*, 2007; Balakrishnan *et al.*, 2013; Revathi *et al.*, 2015). In the crystal structure of the L-proline lithium bromide monohydrate complex, there is a head-to-tail sequence observed (Sathiskumar *et al.*, 2015a). In contrast, there is no direct hydrogen-bonding interaction between the proline molecules in (I).
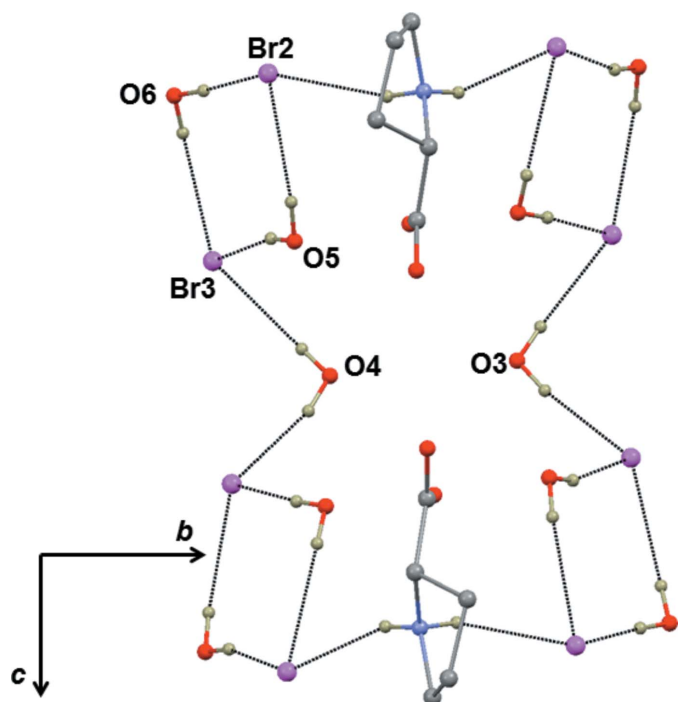
Figure 3
The butterfly-like supramolecular arrangements generated by inter-molecular N—H⋯Br and O—H⋯Br hydrogen bonds. Only atoms involved in hydrogen-bonding interactions are labelled.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Sr(C_5H_9NO_2)(H_2O)_4]Br_2$
M_r	434.63
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	296
a, b, c (Å)	6.7079 (4), 12.9125 (9), 15.4499 (11)
V (Å^3)	1338.20 (16)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	10.01
Crystal size (mm)	$0.15 \times 0.10 \times 0.10$
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SABABS*; Bruker, 2004)
T_{min}, T_{max}	0.26, 0.44
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	14183, 2345, 2081
R_{int}	0.068
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.032, 0.063, 1.07
No. of reflections	2345
No. of parameters	186
No. of restraints	26
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.60, −0.86
Absolute structure	Flack x determined using 788 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.008 (8)

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2004), *SIR92* (Altomare *et al.*, 1993), *SHELXL2014* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

As shown in Fig. 3, two water molecules and two bromide anions along with Sr^{2+} ions generate a hydrogen-bonded sheet which lies parallel to the *a* axis. Within this sheet, two Sr^{2+} ions and two water oxygens form a cyclic motif. Water molecules (O3 and O4) interconnect the bromide anions, forming a chain. In (I), two molecules (O5 and O6) act as donors for intermolecular O—H⋯Br hydrogen bonds. These hydrogen bonds generate a cyclic dibromide motif similar to that observed in a related structure (Revathi *et al.*, 2015). Adjacent dibromide motifs in (I), which run parallel to the *b* axis, are interconnected by proline ligands through intermolecular N—H⋯Br hydrogen bonds on both sides (Fig. 3). Adjacent supramolecular arrangements of cyclic dibromide ⋯proline⋯cyclic dibromide motifs are interlinked further by water molecules (O3 and O4) through O—H⋯Br hydrogen bonds. This entire arrangement forms a butterfly-like structure. The overall hydrogen-bonded supramolecular structure (Fig. 4) is three-dimensional.

4. Synthesis and crystallization

Single crystals of the title complex were obtained by slow evaporation from an aqueous solution of L-proline and

Figure 4
The crystal packing of (I) viewed along the *a* axis, with hydrogen bonds shown as dashed lines. C-bound H atoms have been omitted for clarity.

strontium bromide hexahydrate in a 1:1 stoichiometric molar ratio at 306 K. The prepared solution was stirred well and filtered. The resultant filtered solution was left undisturbed to allow evaporation. After 15 days, colourless prismatic crystals were harvested.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. One of the carbon (C4) atoms of the pyrrolidine ring appears to be disordered over two sites. These positions were defined for this atom and constrained refinement of the site-occupation factors led to a value of 0.57 (6) for the major component. The positions of amino and water H atoms were located from difference Fourier maps. Further, the O—H distances in the water molecules were restrained to 0.85 (2) Å. The N—H distances of amino group were also restrained, to 0.89 (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 atom. The Flack absolute structure parameter was determined to be 0.008 (8) (788 Friedel pairs; Parsons *et al.*, 2013), indicating an *S* configuration for C2, consistent with that for the parent L-proline (Kayushina & Vainshtein, 1965).

Acknowledgements

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Crystal structure of poly[[*μ₂*-diaqua-diaqua-*μ₂*-L-proline-*κ²O:O′*-strontium] dibromide]

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Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); 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).

Poly[[*μ₂*-diaqua-diaqua-*μ₂*-L-proline-*κ²O:O′*-\ strontium] dibromide]

Crystal data

$[Sr(C_5H_9NO_2)(H_2O)_4]Br_2$	$D_x = 2.157$ Mg m^{-3}
$M_r = 434.63$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 7063 reflections
$a = 6.7079$ (4) Å	$\theta = 2.6$–$28.5°$
$b = 12.9125$ (9) Å	$\mu = 10.01$ mm^{-1}
$c = 15.4499$ (11) Å	$T = 296$ K
$V = 1338.20$ (16) Å^3	Block, brown
$Z = 4$	$0.15 \times 0.10 \times 0.10$ mm
$F(000) = 840$	

Data collection

Bruker Kappa APEXII CCD diffractometer	2345 independent reflections
Radiation source: Sealed tube	2081 reflections with $I > 2\sigma(I)$
ω nd φ scan	$R_{int} = 0.068$
Absorption correction: multi-scan (SABABS; Bruker, 2004)	$\theta_{max} = 25.0°$, $\theta_{min} = 2.6°$
$T_{min} = 0.26$, $T_{max} = 0.44$	$h = -7 \rightarrow 7$
14183 measured reflections	$k = -15 \rightarrow 15$
	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0267P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.032$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.063$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.07$	$\Delta\rho_{max} = 0.60$ e Å^{-3}
2345 reflections	$\Delta\rho_{min} = -0.86$ e Å^{-3}
186 parameters	
26 restraints	
Hydrogen site location: mixed	

Absolute structure: Flack x determined using
788 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*,
2013)
Absolute structure parameter: 0.008 (8)

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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

	x	y	z	$U_{iso}*/U_{eq}$	Occ. (<1)
Sr1	1.34882 (8)	0.24302 (5)	0.43342 (4)	0.0174 (2)	
O1	1.0492 (6)	0.2322 (4)	0.3350 (3)	0.0257 (16)	
O2	0.7439 (6)	0.2420 (4)	0.3916 (3)	0.0243 (16)	
O3	1.5725 (8)	0.3885 (5)	0.5016 (4)	0.0243 (19)	
O4	1.5819 (8)	0.1162 (4)	0.5200 (4)	0.0213 (17)	
O5	1.3443 (9)	0.0648 (4)	0.3561 (4)	0.035 (2)	
O6	1.3860 (9)	0.3899 (5)	0.3212 (4)	0.038 (2)	
N1	0.9404 (8)	0.2529 (6)	0.1734 (4)	0.026 (2)	
C1	0.8660 (9)	0.2426 (5)	0.3307 (4)	0.018 (2)	
C2	0.7837 (9)	0.2600 (6)	0.2411 (4)	0.021 (2)	
C3	0.8370 (12)	0.2347 (7)	0.0890 (5)	0.042 (3)	
C4A	0.623 (2)	0.211 (3)	0.1117 (11)	0.034 (7)	0.57 (6)
C5	0.6277 (12)	0.1840 (7)	0.2082 (5)	0.042 (3)	
C4B	0.660 (5)	0.167 (3)	0.1117 (13)	0.035 (8)	0.43 (6)
Br2	0.18627 (12)	0.02641 (6)	0.15165 (6)	0.0389 (3)	
Br3	0.22307 (13)	0.44596 (7)	0.11973 (6)	0.0466 (3)	
H1A	1.024 (9)	0.199 (4)	0.180 (5)	0.02 (2)*	
H1B	1.033 (10)	0.303 (5)	0.175 (6)	0.05 (3)*	
H3C	1.522 (13)	0.429 (5)	0.538 (4)	0.06 (3)*	
H3D	1.622 (13)	0.422 (5)	0.460 (4)	0.07 (4)*	
H4E	1.532 (12)	0.085 (5)	0.563 (3)	0.05 (3)*	
H4F	1.640 (10)	0.075 (4)	0.487 (4)	0.04 (3)*	
H5C	1.281 (10)	0.060 (6)	0.308 (3)	0.06 (3)*	
H5D	1.450 (7)	0.030 (6)	0.353 (5)	0.06 (3)*	
H6C	1.478 (8)	0.432 (5)	0.327 (5)	0.03 (3)*	
H6D	1.319 (11)	0.402 (7)	0.276 (4)	0.09 (4)*	
H31	0.89720	0.17700	0.05850	0.0500*	0.57 (6)
H32	0.84480	0.29580	0.05270	0.0500*	0.57 (6)
H41	0.57440	0.15290	0.07800	0.0410*	0.57 (6)
H42	0.53890	0.27050	0.10120	0.0410*	0.57 (6)
H51	0.49920	0.19560	0.23530	0.0500*	0.57 (6)
H52	0.66830	0.11280	0.21770	0.0500*	0.57 (6)
H2	0.72630	0.32970	0.23900	0.0250*	
H33	0.92450	0.19970	0.04850	0.0500*	0.43 (6)
H34	0.79360	0.29960	0.06370	0.0500*	0.43 (6)
H43	0.68850	0.09490	0.09960	0.0420*	0.43 (6)

H44	0.54310	0.18790	0.07910	0.0420*	0.43 (6)
H53	0.49510	0.21140	0.21840	0.0500*	0.43 (6)
H54	0.63970	0.11870	0.23880	0.0500*	0.43 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.0142 (3)	0.0215 (4)	0.0165 (3)	0.0003 (3)	−0.0010 (3)	0.0006 (3)
O1	0.017 (2)	0.041 (3)	0.019 (3)	0.006 (2)	−0.001 (2)	−0.003 (3)
O2	0.024 (2)	0.033 (3)	0.016 (3)	0.004 (3)	0.004 (2)	0.002 (3)
O3	0.025 (3)	0.029 (3)	0.019 (4)	0.000 (2)	0.000 (3)	−0.003 (3)
O4	0.024 (3)	0.024 (3)	0.016 (3)	0.000 (2)	0.003 (3)	0.000 (3)
O5	0.033 (3)	0.044 (4)	0.029 (4)	0.006 (3)	−0.002 (3)	−0.010 (3)
O6	0.034 (4)	0.043 (4)	0.037 (4)	−0.012 (3)	−0.011 (3)	0.017 (3)
N1	0.022 (3)	0.035 (4)	0.022 (4)	−0.005 (4)	0.000 (3)	0.004 (4)
C1	0.025 (4)	0.011 (3)	0.017 (4)	−0.001 (3)	−0.003 (3)	−0.004 (3)
C2	0.024 (3)	0.026 (4)	0.013 (4)	0.005 (4)	0.002 (3)	0.000 (4)
C3	0.052 (5)	0.059 (6)	0.015 (4)	0.000 (5)	−0.001 (4)	−0.001 (4)
C4A	0.036 (10)	0.041 (15)	0.025 (9)	0.001 (8)	−0.007 (7)	−0.014 (9)
C5	0.035 (5)	0.066 (6)	0.025 (5)	−0.025 (4)	−0.006 (4)	−0.004 (5)
C4B	0.033 (13)	0.042 (17)	0.030 (11)	−0.010 (13)	0.005 (10)	−0.023 (11)
Br2	0.0357 (5)	0.0379 (5)	0.0432 (5)	0.0057 (4)	−0.0102 (4)	−0.0197 (4)
Br3	0.0505 (6)	0.0484 (6)	0.0409 (6)	−0.0239 (4)	−0.0107 (4)	0.0197 (5)

Geometric parameters (Å, º)

Sr1—O1	2.524 (4)	N1—H1A	0.90 (6)
Sr1—O3	2.625 (6)	N1—H1B	0.90 (7)
Sr1—O4	2.630 (6)	C1—C2	1.507 (9)
Sr1—O5	2.593 (5)	C2—C5	1.522 (11)
Sr1—O6	2.582 (6)	C3—C4A	1.509 (17)
Sr1—O2ⁱ	2.728 (4)	C3—C4B	1.52 (4)
Sr1—O3ⁱⁱ	2.707 (6)	C4A—C5	1.53 (2)
Sr1—O4ⁱⁱ	2.651 (5)	C4B—C5	1.52 (2)
Sr1—O2ⁱⁱⁱ	2.800 (5)	C2—H2	0.9800
O1—C1	1.238 (7)	C3—H31	0.9700
O2—C1	1.248 (8)	C3—H32	0.9700
O3—H3C	0.84 (7)	C3—H33	0.9700
O3—H3D	0.84 (7)	C3—H34	0.9700
O4—H4E	0.85 (6)	C4A—H41	0.9700
O4—H4F	0.83 (6)	C4A—H42	0.9700
O5—H5D	0.84 (6)	C4B—H43	0.9700
O5—H5C	0.86 (5)	C4B—H44	0.9700
O6—H6D	0.85 (7)	C5—H51	0.9700
O6—H6C	0.83 (6)	C5—H54	0.9700
N1—C3	1.496 (10)	C5—H52	0.9700
N1—C2	1.486 (8)	C5—H53	0.9700

O1—Sr1—O3	137.44 (18)	Sr1—O6—H6D	130 (6)
O1—Sr1—O4	138.19 (17)	Sr1—O6—H6C	119 (5)
O1—Sr1—O5	70.37 (18)	H6C—O6—H6D	111 (8)
O1—Sr1—O6	73.32 (18)	C2—N1—C3	107.2 (5)
O1—Sr1—O2^{i}	129.10 (14)	C3—N1—H1B	117 (6)
O1—Sr1—O3^{ii}	69.11 (17)	H1A—N1—H1B	97 (5)
O1—Sr1—O4^{ii}	70.35 (17)	C2—N1—H1A	114 (5)
O1—Sr1—O2^{iii}	112.66 (13)	C2—N1—H1B	115 (5)
O3—Sr1—O4	84.36 (18)	C3—N1—H1A	105 (5)
O3—Sr1—O5	145.76 (18)	O1—C1—C2	115.4 (5)
O3—Sr1—O6	71.85 (19)	O2—C1—C2	117.0 (5)
O2^{i}—Sr1—O3	62.82 (16)	O1—C1—O2	127.6 (6)
O3—Sr1—O3^{ii}	133.75 (19)	N1—C2—C5	102.2 (6)
O3—Sr1—O4^{ii}	77.67 (17)	N1—C2—C1	112.2 (5)
O2^{iii}—Sr1—O3	72.95 (16)	C1—C2—C5	117.6 (6)
O4—Sr1—O5	71.86 (18)	N1—C3—C4B	104.6 (10)
O4—Sr1—O6	137.87 (18)	N1—C3—C4A	105.7 (8)
O2^{i}—Sr1—O4	62.60 (16)	C3—C4A—C5	104.7 (10)
O3^{ii}—Sr1—O4	80.08 (17)	C3—C4B—C5	104.8 (19)
O4—Sr1—O4^{ii}	133.67 (19)	C2—C5—C4A	101.1 (12)
O2^{iii}—Sr1—O4	72.62 (16)	C2—C5—C4B	108.8 (15)
O5—Sr1—O6	110.10 (19)	N1—C2—H2	108.00
O2^{i}—Sr1—O5	84.14 (17)	C1—C2—H2	108.00
O3^{ii}—Sr1—O5	66.80 (19)	C5—C2—H2	108.00
O4^{ii}—Sr1—O5	136.53 (18)	N1—C3—H31	111.00
O2^{iii}—Sr1—O5	120.21 (17)	N1—C3—H32	111.00
O2^{i}—Sr1—O6	75.56 (17)	N1—C3—H33	111.00
O3^{ii}—Sr1—O6	140.90 (18)	N1—C3—H34	111.00
O4^{ii}—Sr1—O6	75.16 (19)	C4A—C3—H31	111.00
O2^{iii}—Sr1—O6	128.45 (18)	C4A—C3—H32	111.00
O2^{i}—Sr1—O3^{ii}	138.60 (17)	H31—C3—H32	109.00
O2^{i}—Sr1—O4^{ii}	136.37 (16)	C4B—C3—H33	111.00
O2^{i}—Sr1—O2^{iii}	118.24 (13)	C4B—C3—H34	111.00
O3^{ii}—Sr1—O4^{ii}	82.36 (17)	H33—C3—H34	109.00
O2^{iii}—Sr1—O3^{ii}	60.87 (16)	C3—C4A—H41	111.00
O2^{iii}—Sr1—O4^{ii}	61.37 (16)	C3—C4A—H42	111.00
Sr1—O1—C1	144.8 (4)	C5—C4A—H41	111.00
Sr1^{iv}—O2—C1	144.7 (4)	C5—C4A—H42	111.00
Sr1^{ii}—O2—C1	124.2 (4)	H41—C4A—H42	109.00
Sr1^{iv}—O2—Sr1^{ii}	90.87 (13)	H43—C4B—H44	109.00
Sr1—O3—Sr1^{iii}	95.2 (2)	C3—C4B—H44	111.00
Sr1—O4—Sr1^{iii}	96.47 (17)	C5—C4B—H43	111.00
H3C—O3—H3D	111 (6)	C3—C4B—H43	111.00
Sr1^{iii}—O3—H3C	115 (5)	C5—C4B—H44	111.00
Sr1^{iii}—O3—H3D	110 (5)	C2—C5—H52	112.00
Sr1—O3—H3C	119 (6)	C2—C5—H53	110.00
Sr1—O3—H3D	107 (5)	C2—C5—H51	112.00
H4E—O4—H4F	111 (6)	C4B—C5—H54	110.00

Sr1—O4—H4E	117 (5)	H53—C5—H54	108.00
Sr1—O4—H4F	111 (4)	C2—C5—H54	110.00
Sr1iii—O4—H4F	107 (4)	C4A—C5—H51	112.00
Sr1iii—O4—H4E	112 (5)	C4A—C5—H52	112.00
Sr1—O5—H5D	119 (5)	H51—C5—H52	109.00
Sr1—O5—H5C	118 (5)	C4B—C5—H53	110.00
H5C—O5—H5D	109 (7)		
O3—Sr1—O1—C1	−76.6 (8)	O5iii—Sr1iii—O3—Sr1	−158.1 (2)
O4—Sr1—O1—C1	101.4 (8)	O6iii—Sr1iii—O3—Sr1	−64.4 (3)
O5—Sr1—O1—C1	128.0 (8)	O1—Sr1—O4—Sr1iii	171.61 (16)
O6—Sr1—O1—C1	−112.8 (8)	O3—Sr1—O4—Sr1iii	−9.71 (18)
O2i—Sr1—O1—C1	−167.5 (7)	O5—Sr1—O4—Sr1iii	145.3 (2)
O3ii—Sr1—O1—C1	56.1 (8)	O6—Sr1—O4—Sr1iii	45.1 (3)
O4ii—Sr1—O1—C1	−33.0 (8)	O2i—Sr1—O4—Sr1iii	52.53 (16)
O2iii—Sr1—O1—C1	12.5 (8)	O3ii—Sr1—O4—Sr1iii	−146.0 (2)
O1iv—Sr1iv—O2—C1	5.3 (8)	O4ii—Sr1—O4—Sr1iii	−76.7 (3)
O3iv—Sr1iv—O2—C1	−125.2 (8)	O2iii—Sr1—O4—Sr1iii	−83.58 (18)
O4iv—Sr1iv—O2—C1	136.7 (8)	O3—Sr1iii—O4—Sr1	9.45 (18)
O5iv—Sr1iv—O2—C1	64.1 (8)	O2i—Sr1iii—O4—Sr1	−51.45 (16)
O6iv—Sr1iv—O2—C1	−48.4 (8)	O1iii—Sr1iii—O4—Sr1	79.93 (18)
O2ii—Sr1iv—O2—C1	−174.6 (7)	O3iii—Sr1iii—O4—Sr1	−128.6 (2)
O3iv—Sr1ii—O2—C1	127.5 (6)	O4iii—Sr1iii—O4—Sr1	−58.9 (3)
O4iv—Sr1ii—O2—C1	−135.0 (6)	O5iii—Sr1iii—O4—Sr1	53.5 (3)
O1ii—Sr1ii—O2—C1	175.1 (5)	O6iii—Sr1iii—O4—Sr1	157.2 (2)
O3ii—Sr1ii—O2—C1	−50.0 (5)	Sr1—O1—C1—O2	−19.8 (13)
O4ii—Sr1ii—O2—C1	39.4 (5)	Sr1—O1—C1—C2	158.9 (6)
O5ii—Sr1ii—O2—C1	95.3 (5)	Sr1iv—O2—C1—O1	−172.8 (5)
O6ii—Sr1ii—O2—C1	−98.7 (5)	Sr1ii—O2—C1—O1	13.2 (10)
O2iii—Sr1ii—O2—C1	−5.0 (6)	Sr1iv—O2—C1—C2	8.5 (11)
O1—Sr1—O3—Sr1iii	−171.81 (15)	Sr1ii—O2—C1—C2	−165.5 (4)
O4—Sr1—O3—Sr1iii	9.48 (18)	C2—N1—C3—C4A	−10.6 (17)
O5—Sr1—O3—Sr1iii	−36.0 (4)	C3—N1—C2—C5	34.0 (8)
O6—Sr1—O3—Sr1iii	−135.3 (2)	C3—N1—C2—C1	160.9 (6)
O2i—Sr1—O3—Sr1iii	−52.54 (16)	O1—C1—C2—N1	4.6 (9)
O3ii—Sr1—O3—Sr1iii	80.0 (3)	O2—C1—C2—C5	−58.5 (9)
O4ii—Sr1—O3—Sr1iii	146.5 (2)	O2—C1—C2—N1	−176.6 (6)
O2iii—Sr1—O3—Sr1iii	83.01 (17)	O1—C1—C2—C5	122.7 (7)
O4—Sr1iii—O3—Sr1	−9.45 (18)	N1—C2—C5—C4A	−43.4 (12)
O2i—Sr1iii—O3—Sr1	51.95 (16)	C1—C2—C5—C4A	−166.7 (12)
O1iii—Sr1iii—O3—Sr1	−81.27 (18)	N1—C3—C4A—C5	−17 (2)
O3iii—Sr1iii—O3—Sr1	55.3 (3)	C3—C4A—C5—C2	37 (2)
O4iii—Sr1iii—O3—Sr1	127.5 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Br2[i]	0.90 (6)	2.52 (5)	3.374 (7)	159 (6)
N1—H1*B*···Br3[i]	0.90 (7)	2.40 (7)	3.240 (7)	156 (8)
O3—H3*C*···Br3[v]	0.84 (7)	2.63 (7)	3.440 (6)	163 (7)
O3—H3*D*···Br2[vi]	0.84 (7)	2.54 (7)	3.376 (6)	172 (5)
O4—H4*E*···Br2[vii]	0.85 (6)	2.47 (7)	3.281 (6)	162 (7)
O4—H4*F*···Br3[viii]	0.83 (6)	2.52 (6)	3.347 (6)	174 (6)
O5—H5*C*···Br2[i]	0.86 (5)	2.54 (5)	3.369 (6)	164 (6)
O5—H5*D*···Br3[viii]	0.84 (6)	2.48 (6)	3.304 (6)	166 (6)
O6—H6*C*···Br2[vi]	0.83 (6)	2.58 (6)	3.393 (6)	167 (5)
O6—H6*D*···Br3[i]	0.85 (7)	2.56 (6)	3.378 (6)	162 (7)

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