

Synthesis, crystal structure and Hirshfeld surface analysis of $[\text{Sr}(\text{urea})(\text{NO}_3)_2]_n$

Aysanem Bektursinova,^a Zulfiya Djumanazarova,^a Zamira Uzakbergenova,^a Jamshid Ashurov,^b Akram A Khan,^c Shakhnoza Kadirova^d and Batirbay Torambetov^{d,c,*}

Received 16 December 2024

Accepted 23 December 2024

Edited by B. Therrien, University of Neuchâtel, Switzerland

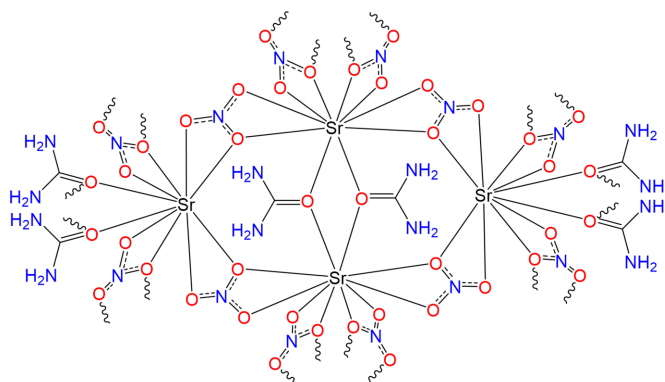
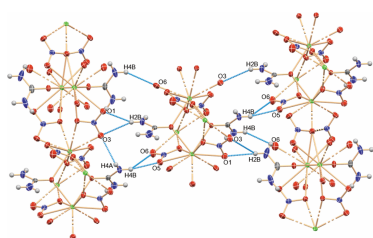
Keywords: crystal structure; strontium; caramid; urea; Hirshfeld surface analysis.**CCDC reference:** 2297418**Supporting information:** this article has supporting information at journals.iucr.org/e

^aKarakalpak State University, 1 Ch. Abdirov St Nukus, 230112, Uzbekistan, ^bInstitute of Bioorganic Chemistry, Academy of Sciences of Uzbekistan, M. Ulugbek St, 83, Tashkent, 100125, Uzbekistan, ^cPhysical and Materials Chemistry Division, CSIR-National Chemical Laboratory, Pune-411008, India, and ^dNational University of Uzbekistan named after Mirzo Ulugbek, 4 University St, Tashkent, 100174, Uzbekistan. *Correspondence e-mail: torambetov_b@mail.ru

The crystal structure of poly[di- μ_2 -nitrate- μ_2 -urea-strontium(II)], $[\text{Sr}(\text{NO}_3)_2(\text{CH}_4\text{N}_2\text{O})]_n$, was determined using single-crystal X-ray diffraction. Crystallizing in the orthorhombic space group $Aba2$, the asymmetric unit consists of an Sr^{II} cation, two nitrate anions, and two half urea molecules. The Sr^{II} cation adopts a distorted decahedral geometry coordinated by ten oxygen atoms, with Sr–O bond lengths ranging from 2.573 (3) to 2.847 (5) Å. The nitrate anions act as bidentate ligands, displaying both terminal and bridging coordination modes. The structure features a robust coordination network supported by hydrogen bonding. These results provide insight into the coordination behaviour of Sr^{II} with nitrate and urea ligands, contributing to the understanding of supramolecular architectures in metal–organic frameworks (MOFs).

1. Chemical context

The study of coordination polymers (CPs) and the crystal engineering of MOFs has garnered significant interest due to their diverse structural architectures and potential applications in catalysis, gas storage, and sensing (Allendorf & Stavila, 2015). Metal ions such as Sr^{II} have proven versatile in forming coordination complexes owing to their ability to adopt various coordination geometries (Kainat *et al.*, 2024). Ligands like urea and nitrate, capable of acting as terminal and bridging ligands, offer unique opportunities for the construction of supramolecular networks (Reek *et al.*, 2022). In this study, the polymeric complex $[\text{Sr}(\text{urea})(\text{NO}_3)_2]_n$ was synthesized and characterized.



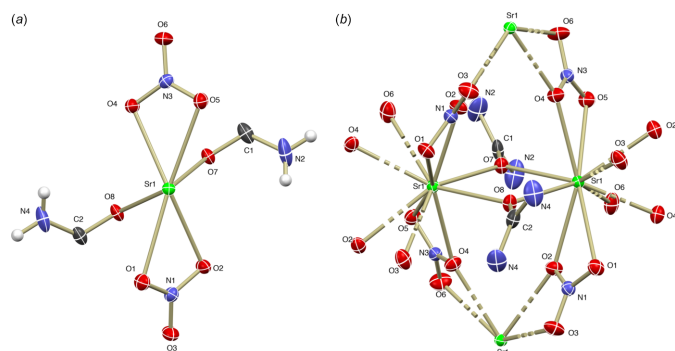


Figure 1
 (a) The asymmetric unit of $[\text{Sr}(\text{urea})(\text{NO}_3)_2]_n$ with the atom-labelling scheme and displacement ellipsoids drawn at the 30% probability level.
 (b) Extended coordination sphere of the polymeric complex.

2. Structural commentary

The crystal structure of the title compound $[\text{Sr}(\text{urea})(\text{NO}_3)_2]_n$ was determined in the orthorhombic space group $Aba2$. The asymmetric unit consists of an Sr^{II} cation, two nitrate anions, and one urea molecule. The Sr^{II} cation is coordinated by ten oxygen atoms, eight of which originate from nitrate anions and two from urea molecules, adopting a decahedral geometry (Fig. 1). The Sr^{II} cation forms a distorted decahedral coordination environment through interactions with oxygen atoms from the urea and nitrate ligands. The nitrate anions exhibit dual binding modes, participating in bidentate bridging interactions, which stabilize the structure through hydrogen bonds and intermolecular forces. Such versatility in coordination and binding contributes to the robust di-periodic layered network

Table 1
 Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N4}-\text{H4A}\cdots\text{O3}^{\text{i}}$	0.86	2.44	2.956 (6)	119
$\text{N4}-\text{H4B}\cdots\text{O5}^{\text{ii}}$	0.86	2.29	3.086 (6)	154
$\text{N4}-\text{H4B}\cdots\text{O6}^{\text{ii}}$	0.86	2.59	3.304 (7)	141
$\text{N2}-\text{H2A}\cdots\text{O6}^{\text{iii}}$	0.86	2.50	3.020 (6)	120
$\text{N2}-\text{H2B}\cdots\text{O1}^{\text{iv}}$	0.86	2.33	3.139 (7)	157
$\text{N2}-\text{H2B}\cdots\text{O3}^{\text{iv}}$	0.86	2.57	3.312 (6)	145

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

observed in the crystal structure. These findings provide insights into the design of Sr^{II} -based CPs and MOFs, highlighting the significance of urea and nitrate ligands in generating diverse structural motifs and functional materials (Preethi *et al.*, 2024).

3. Supramolecular features

In the crystal, closely associated molecules form a di-periodic sheet structure along the a - and b -axis directions. Along the c axis, molecules are connected by hydrogen bonds ($\text{N4}-\text{H4A}\cdots\text{O3}^{\text{ii}}$, $\text{N4}-\text{H4B}\cdots\text{O5}^{\text{vi}}$, $\text{N4}-\text{H4B}\cdots\text{O6}^{\text{vi}}$, $\text{N2}-\text{H2A}\cdots\text{O6}^{\text{i}}$, $\text{N2}-\text{H2B}\cdots\text{O1}^{\text{vii}}$, $\text{N2}-\text{H2B}\cdots\text{O3}^{\text{vii}}$; Table 1). The Sr–O (Sr-nitrate) bond lengths range from 2.622 (3) \AA to 2.847 (5) \AA , while the Sr–O (Sr-urea) bond lengths fall between 2.573 (3) \AA and 2.604 (3) \AA , reflecting variations due to ligand-field effects and steric factors (Fig. 1). The nitrate anions act as bidentate ligand, contributing to the coordination geometry in two distinct modes. First, two oxygen atoms from each nitrate molecule coordinate to the

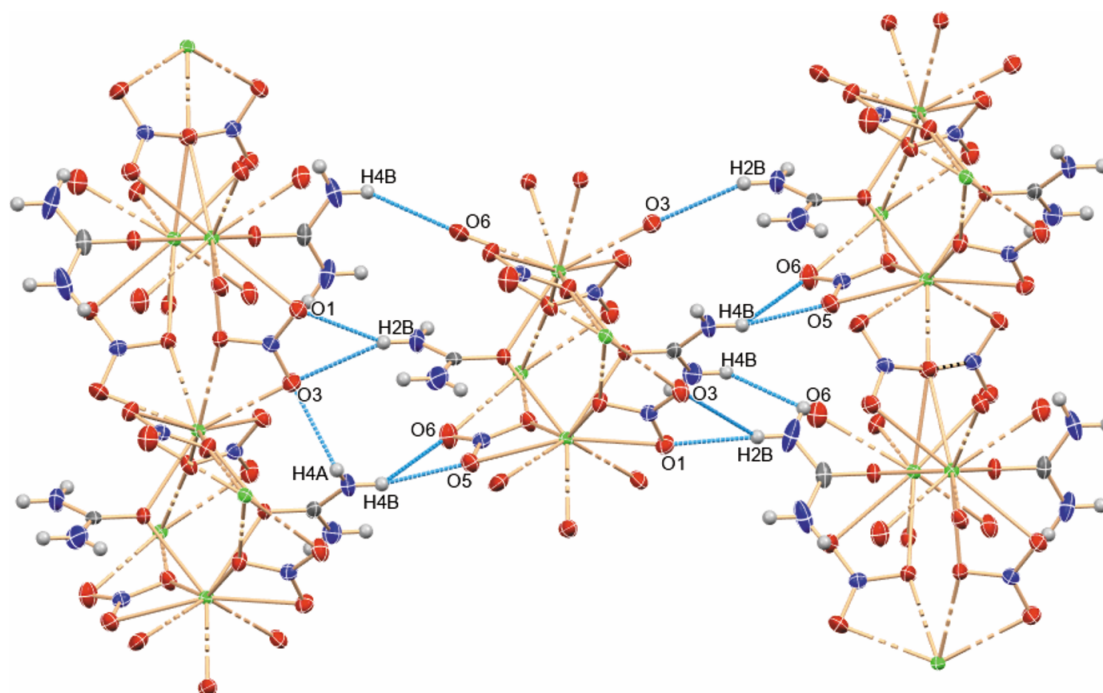


Figure 2
 Hydrogen-bonded chains (blue dashed lines) in the crystal of $[\text{Sr}(\text{urea})(\text{NO}_3)_2]_n$.

same Sr^{II} ion. Second, the oxygen atoms O7 and O8 are bidentate bridging ligands, connecting two Sr^{II} cations and forming a distorted parallelogram. The bond angles of the bridging oxygen atoms are 108.0 (2)° for (Sr–O7–Sr) and 106.13 (19)° for (Sr–O8–Sr). In the crystal structure, the urea molecules are located on a special position with a twofold rotation axis at (−*x*, −*y*, *z*), oriented along the [001] direction. This structural arrangement results in a stable coordination network supported by interactions between the Sr^{II} cations, nitrate anions, and urea (Fig. 2).

4. Database survey

A survey of the Cambridge Structural Database (CSD, Version 5.45, last updated March 2024; Groom *et al.*, 2016) revealed around 320 metal complexes where urea is directly bonded to a metal *via* oxygen, whereas only one structure where Sr is directly bonded to the oxygen atom of the urea molecule has been reported (MOXJUG; Schwarz & Streb, 2015). Moreover, no crystal structure similar to that of [Sr(urea)(NO₃)₂]_{*n*} has been reported.

5. Synthesis and crystallization

Strontium nitrate (Sr(NO₃)₂, 0.212 g, 1 mmol) and carbamide (urea, 0.12 g, 2 mmol) were each individually dissolved in 5 mL of a 1:1 volumetric mixture of water and ethanol, ensuring complete dissolution of both compounds. The solutions were mixed together and kept for 10 min in an ultrasonic bath. The obtained colourless solution was filtered and left for crystallization. Single crystals of the title complex suitable for X-ray analysis were obtained by slow evaporation of the solution over a period of 10 days.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All hydrogen atoms were located in difference-Fourier maps and refined using an isotropic approximation.

References

Allendorf, M. D. & Stavila, V. (2015). *CrystEngComm*, **17**, 229–246.
 Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Table 2

Experimental details.

Crystal data	
Chemical formula	[Sr(NO ₃) ₂ (CH ₄ N ₂ O)]
<i>M_r</i>	271.70
Crystal system, space group	Orthorhombic, <i>Ab</i> a2
Temperature (K)	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.3527 (1), 9.9701 (1), 17.0496 (2)
<i>V</i> (Å ³)	1589.83 (3)
<i>Z</i>	8
Radiation type	Cu <i>K</i> α
μ (mm ^{−1})	9.77
Crystal size (mm)	0.12 × 0.08 × 0.06
Data collection	
Diffractometer	XtaLAB Synergy, Single source at home/near, HyPix3000
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2022)
<i>T_{min}</i> , <i>T_{max}</i>	0.300, 1.000
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	6435, 1517, 1487
<i>R_{int}</i>	0.029
(sin θ/λ) _{max} (Å ^{−1})	0.614
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.021, 0.055, 1.07
No. of reflections	1517
No. of parameters	121
No. of restraints	1
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ^{−3})	0.74, −0.27
Absolute structure	Flack <i>x</i> ' determined using 678 quotients [(<i>I</i> ⁺) − (<i>I</i> [−])] / [(<i>I</i> ⁺) + (<i>I</i> [−])] (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	−0.020 (15)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT2018/2* (Sheldrick, 2015a), *SHELXL2016/6* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
 Kainat, S. F., Hawsawi, M. B., Mughal, E. U., Naeem, N., Almohyawi, A. M., Altass, H. M., Hussein, E. M., Sadiq, A., Moussa, Z., Abd-El-Aziz, A. S. & Ahmed, S. A. (2024). *RSC Adv.* **14**, 21464–21537.
 Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* **B69**, 249–259.
 Preethi, P. C., Harisankar, A., Maneesha, M., Sreeja, T. G., Al-Otaibi, J. S., Mary, Y. S. & Raghunandan, R. (2024). *Opt. Mater.* **154**, 115750.
 Reek, J. N., de Bruin, B., Pullen, S., Mooibroek, T. J., Kluwer, A. M. & Caumes, X. (2022). *Chem. Rev.* **122**, 12308–12369.
 Rigaku OD (2022). *CrysAlis PRO*. Rigaku Oxford Diffraction Ltd, Yarnton, Oxfordshire, England.
 Schwarz, B. & Streb, C. (2015). *Dalton Trans.* **44**, 4195–4199.
 Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
 Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.

supporting information

Acta Cryst. (2025). E81 [https://doi.org/10.1107/S2056989024012386]

Synthesis, crystal structure and Hirshfeld surface analysis of [Sr(urea)(NO₃)₂]_n

Aysanem Bektursinova, Zulfiya Djumanazarova, Zamira Uzakbergenova, Jamshid Ashurov, Akram A Khan, Shakhnoza Kadirova and Batirbay Torambetov

Computing details

Ooly[di- μ_2 -nitrate- μ_2 -urea-strontium(II)]

Crystal data

[Sr(NO₃)₂(CH₄N₂O)]

$M_r = 271.70$

Orthorhombic, *Aba2*

$a = 9.3527$ (1) Å

$b = 9.9701$ (1) Å

$c = 17.0496$ (2) Å

$V = 1589.83$ (3) Å³

$Z = 8$

$F(000) = 1056$

$D_x = 2.270$ Mg m⁻³

Cu *K* α radiation, $\lambda = 1.54184$ Å

Cell parameters from 5341 reflections

$\theta = 4.7$ – 71.3°

$\mu = 9.77$ mm⁻¹

$T = 293$ K

Block, colourless

$0.12 \times 0.08 \times 0.06$ mm

Data collection

XtaLAB Synergy, Single source at home/near,

HyPix3000

diffractometer

Radiation source: micro-focus sealed X-ray

tube, PhotonJet (Cu) X-ray Source

Mirror monochromator

Detector resolution: 10.0000 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(CrysAlisPro; Rigaku OD, 2022)

$T_{\min} = 0.300$, $T_{\max} = 1.000$

6435 measured reflections

1517 independent reflections

1487 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 71.2^\circ$, $\theta_{\min} = 5.2^\circ$

$h = -11 \rightarrow 10$

$k = -11 \rightarrow 12$

$l = -20 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.021$

$wR(F^2) = 0.055$

$S = 1.07$

1517 reflections

121 parameters

1 restraint

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0374P)^2 + 0.1494P]$

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

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

$\Delta\rho_{\max} = 0.74$ e Å⁻³

$\Delta\rho_{\min} = -0.27$ e Å⁻³

Extinction correction: *SHELXL2016/6*

(Sheldrick, 2015b),

$F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00038 (6)

Absolute structure: Flack x' determined using

678 quotients $[(I^-) - (I^+)] / [(I^-) + (I^+)]$ (Parsons *et al.*, 2013)

Absolute structure parameter: -0.020 (15)

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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sr1	0.66197 (3)	0.35686 (3)	0.50071 (5)	0.02435 (15)
O5	0.5691 (4)	0.2029 (4)	0.6237 (2)	0.0380 (8)
O7	0.500000	0.500000	0.5894 (3)	0.0317 (12)
O4	0.4300 (3)	0.2135 (4)	0.52232 (18)	0.0361 (8)
O8	0.500000	0.500000	0.4089 (3)	0.0328 (12)
O1	0.8252 (4)	0.4683 (4)	0.3800 (2)	0.0396 (9)
O2	0.7896 (4)	0.5891 (3)	0.48352 (18)	0.0367 (8)
O6	0.3592 (4)	0.1112 (5)	0.6265 (3)	0.0508 (10)
O3	0.8632 (4)	0.6835 (4)	0.3775 (2)	0.0463 (9)
C1	0.500000	0.500000	0.6641 (5)	0.042 (2)
N3	0.4530 (4)	0.1754 (4)	0.5924 (2)	0.0314 (8)
N4	0.4670 (6)	0.3903 (6)	0.2952 (3)	0.0610 (14)
H4A	0.445171	0.317865	0.319881	0.073*
H4B	0.467264	0.391253	0.244752	0.073*
N2	0.6152 (6)	0.5375 (8)	0.7034 (3)	0.0719 (18)
H2A	0.690719	0.562025	0.678455	0.086*
H2B	0.614571	0.537260	0.753809	0.086*
N1	0.8270 (4)	0.5799 (4)	0.4124 (3)	0.0312 (9)
C2	0.500000	0.500000	0.3348 (5)	0.038 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.0243 (2)	0.0232 (2)	0.0255 (2)	0.00128 (10)	0.0001 (2)	0.00073 (18)
O5	0.0368 (19)	0.0425 (19)	0.0346 (18)	−0.0014 (15)	−0.0072 (14)	0.0028 (15)
O7	0.037 (3)	0.036 (3)	0.022 (3)	0.006 (2)	0.000	0.000
O4	0.0326 (15)	0.0439 (18)	0.032 (2)	−0.0061 (14)	−0.0059 (11)	0.0078 (13)
O8	0.037 (3)	0.043 (3)	0.019 (3)	0.011 (2)	0.000	0.000
O1	0.049 (2)	0.031 (2)	0.038 (2)	−0.0005 (14)	0.0039 (14)	−0.0070 (15)
O2	0.0462 (16)	0.0334 (16)	0.030 (2)	−0.0066 (13)	0.0083 (14)	−0.0046 (12)
O6	0.051 (2)	0.059 (2)	0.043 (2)	−0.0199 (18)	0.0080 (18)	0.010 (2)
O3	0.065 (2)	0.037 (2)	0.036 (2)	−0.0119 (19)	0.0026 (19)	0.0080 (17)
C1	0.054 (5)	0.042 (5)	0.029 (5)	0.028 (4)	0.000	0.000
N3	0.029 (2)	0.0276 (18)	0.037 (2)	0.0002 (15)	0.0008 (16)	−0.0026 (16)
N4	0.084 (4)	0.072 (3)	0.028 (2)	0.021 (3)	−0.013 (3)	−0.016 (2)
N2	0.070 (4)	0.110 (5)	0.036 (3)	0.030 (4)	−0.021 (3)	−0.024 (3)
N1	0.0311 (19)	0.029 (2)	0.034 (2)	0.0006 (14)	−0.0019 (14)	−0.0016 (17)
C2	0.034 (4)	0.056 (6)	0.025 (5)	0.015 (4)	0.000	0.000

Geometric parameters (Å, °)

Sr1—O5	2.740 (4)	O4—N3	1.272 (5)
Sr1—O7	2.573 (3)	O8—C2	1.264 (10)
Sr1—O4	2.624 (3)	O1—N1	1.243 (6)
Sr1—O4 ⁱ	2.629 (3)	O2—N1	1.265 (5)
Sr1—O8	2.604 (3)	O6—N3	1.232 (5)
Sr1—O1	2.793 (4)	O3—N1	1.239 (6)
Sr1—O2 ⁱⁱ	2.723 (3)	C1—N2	1.322 (7)
Sr1—O2	2.622 (3)	C1—N2 ⁱⁱⁱ	1.322 (7)
Sr1—O6 ⁱ	2.847 (5)	N4—H4A	0.8600
Sr1—O3 ⁱⁱ	2.731 (4)	N4—H4B	0.8600
Sr1—N3	3.088 (4)	N4—C2	1.322 (7)
Sr1—N1	3.097 (4)	N2—H2A	0.8600
O5—N3	1.241 (5)	N2—H2B	0.8600
O7—C1	1.274 (11)		
O5—Sr1—O1	163.75 (10)	O2 ⁱⁱ —Sr1—N1	124.65 (11)
O5—Sr1—O6 ⁱ	72.03 (13)	O6 ⁱ —Sr1—N3	95.41 (13)
O5—Sr1—N3	23.62 (10)	O6 ⁱ —Sr1—N1	87.87 (13)
O5—Sr1—N1	158.76 (11)	O3 ⁱⁱ —Sr1—O5	101.94 (11)
O7—Sr1—O5	71.00 (11)	O3 ⁱⁱ —Sr1—O1	74.45 (12)
O7—Sr1—O4 ⁱ	128.84 (10)	O3 ⁱⁱ —Sr1—O6 ⁱ	134.94 (11)
O7—Sr1—O4	74.49 (8)	O3 ⁱⁱ —Sr1—N3	87.94 (12)
O7—Sr1—O8	72.94 (8)	O3 ⁱⁱ —Sr1—N1	97.10 (12)
O7—Sr1—O1	122.30 (10)	N3—Sr1—N1	169.13 (10)
O7—Sr1—O2	81.01 (8)	N3—O5—Sr1	94.1 (3)
O7—Sr1—O2 ⁱⁱ	134.83 (9)	Sr1—O7—Sr1 ⁱⁱⁱ	108.0 (2)
O7—Sr1—O6 ⁱ	82.92 (12)	C1—O7—Sr1	126.00 (10)
O7—Sr1—O3 ⁱⁱ	138.81 (11)	C1—O7—Sr1 ⁱⁱⁱ	126.00 (10)
O7—Sr1—N3	69.81 (9)	Sr1—O4—Sr1 ^{iv}	156.08 (14)
O7—Sr1—N1	100.42 (9)	N3—O4—Sr1	98.9 (2)
O4—Sr1—O5	47.58 (9)	N3—O4—Sr1 ^{iv}	102.3 (2)
O4 ⁱ —Sr1—O5	92.60 (10)	Sr1—O8—Sr1 ⁱⁱⁱ	106.13 (19)
O4—Sr1—O4 ⁱ	128.56 (4)	C2—O8—Sr1	126.94 (9)
O4—Sr1—O1	140.54 (10)	C2—O8—Sr1 ⁱⁱⁱ	126.94 (9)
O4 ⁱ —Sr1—O1	71.84 (10)	N1—O1—Sr1	92.1 (3)
O4—Sr1—O2 ⁱⁱ	67.60 (11)	Sr1—O2—Sr1 ^v	158.35 (14)
O4 ⁱ —Sr1—O2 ⁱⁱ	66.10 (11)	N1—O2—Sr1	99.7 (2)
O4 ⁱ —Sr1—O6 ⁱ	46.09 (10)	N1—O2—Sr1 ^v	97.4 (2)
O4—Sr1—O6 ⁱ	119.40 (13)	N3—O6—Sr1 ^{iv}	92.7 (3)
O4 ⁱ —Sr1—O3 ⁱⁱ	91.21 (11)	N1—O3—Sr1 ^v	97.7 (3)
O4—Sr1—O3 ⁱⁱ	72.06 (12)	O7—C1—N2	120.4 (4)
O4—Sr1—N3	24.02 (9)	O7—C1—N2 ⁱⁱⁱ	120.4 (4)
O4 ⁱ —Sr1—N3	112.09 (11)	N2 ⁱⁱⁱ —C1—N2	119.2 (8)
O4—Sr1—N1	150.61 (10)	Sr1—N3—Sr1 ^{iv}	110.78 (12)
O4 ⁱ —Sr1—N1	77.56 (10)	O5—N3—Sr1 ^{iv}	172.2 (3)
O8—Sr1—O5	125.63 (9)	O5—N3—Sr1	62.2 (2)

O8—Sr1—O4	84.36 (7)	O5—N3—O4	119.1 (4)
O8—Sr1—O4 ⁱ	141.75 (10)	O4—N3—Sr1 ^{iv}	54.49 (19)
O8—Sr1—O1	69.95 (10)	O4—N3—Sr1	57.1 (2)
O8—Sr1—O2	73.36 (8)	O6—N3—Sr1	173.7 (4)
O8—Sr1—O2 ⁱⁱ	124.70 (9)	O6—N3—Sr1 ^{iv}	64.3 (3)
O8—Sr1—O6 ⁱ	140.21 (11)	O6—N3—O5	122.4 (4)
O8—Sr1—O3 ⁱⁱ	80.46 (12)	O6—N3—O4	118.5 (4)
O8—Sr1—N3	104.90 (9)	H4A—N4—H4B	120.0
O8—Sr1—N1	66.70 (8)	C2—N4—H4A	120.0
O1—Sr1—O6 ⁱ	99.01 (12)	C2—N4—H4B	120.0
O1—Sr1—N3	162.17 (11)	C1—N2—H2A	120.0
O1—Sr1—N1	23.64 (11)	C1—N2—H2B	120.0
O2 ⁱⁱ —Sr1—O5	65.54 (10)	H2A—N2—H2B	120.0
O2—Sr1—O5	136.45 (11)	Sr1—N1—Sr1 ^v	114.45 (13)
O2—Sr1—O4 ⁱ	79.48 (11)	O1—N1—Sr1 ^v	177.6 (3)
O2—Sr1—O4	150.83 (11)	O1—N1—Sr1	64.3 (2)
O2—Sr1—O1	46.95 (10)	O1—N1—O2	119.2 (4)
O2 ⁱⁱ —Sr1—O1	102.69 (11)	O2—N1—Sr1 ^v	59.1 (2)
O2—Sr1—O2 ⁱⁱ	141.08 (5)	O2—N1—Sr1	56.5 (2)
O2 ⁱⁱ —Sr1—O6 ⁱ	94.76 (12)	O3—N1—Sr1	165.5 (3)
O2—Sr1—O6 ⁱ	71.96 (14)	O3—N1—Sr1 ^v	59.3 (3)
O2—Sr1—O3 ⁱⁱ	120.82 (11)	O3—N1—O1	122.4 (5)
O2 ⁱⁱ —Sr1—O3 ⁱⁱ	46.46 (10)	O3—N1—O2	118.4 (4)
O2 ⁱⁱ —Sr1—N3	65.51 (11)	O8—C2—N4 ⁱⁱⁱ	120.7 (4)
O2—Sr1—N3	149.57 (10)	O8—C2—N4	120.7 (4)
O2—Sr1—N1	23.74 (10)	N4—C2—N4 ⁱⁱⁱ	118.6 (8)
Sr1—O5—N3—O4	5.5 (4)	Sr1—O8—C2—N4 ⁱⁱⁱ	-117.5 (3)
Sr1—O5—N3—O6	-175.1 (4)	Sr1—O1—N1—O2	14.2 (4)
Sr1 ⁱⁱⁱ —O7—C1—N2	-117.6 (4)	Sr1—O1—N1—O3	-165.2 (4)
Sr1 ⁱⁱⁱ —O7—C1—N2 ⁱⁱⁱ	62.4 (4)	Sr1 ^v —O2—N1—Sr1	-166.7 (2)
Sr1—O7—C1—N2	62.4 (4)	Sr1—O2—N1—Sr1 ^v	166.7 (2)
Sr1—O7—C1—N2 ⁱⁱⁱ	-117.6 (4)	Sr1—O2—N1—O1	-15.3 (4)
Sr1 ^{iv} —O4—N3—Sr1	-168.9 (2)	Sr1 ^v —O2—N1—O1	178.0 (3)
Sr1—O4—N3—Sr1 ^{iv}	168.9 (2)	Sr1—O2—N1—O3	164.1 (3)
Sr1—O4—N3—O5	-5.8 (4)	Sr1 ^v —O2—N1—O3	-2.6 (4)
Sr1 ^{iv} —O4—N3—O5	-174.7 (3)	Sr1 ^{iv} —O6—N3—O5	175.3 (4)
Sr1 ^{iv} —O4—N3—O6	5.9 (5)	Sr1 ^{iv} —O6—N3—O4	-5.3 (4)
Sr1—O4—N3—O6	174.8 (4)	Sr1 ^v —O3—N1—Sr1	68.3 (14)
Sr1 ⁱⁱⁱ —O8—C2—N4 ⁱⁱⁱ	62.5 (3)	Sr1 ^v —O3—N1—O1	-178.0 (3)
Sr1—O8—C2—N4	62.5 (3)	Sr1 ^v —O3—N1—O2	2.6 (4)
Sr1 ⁱⁱⁱ —O8—C2—N4	-117.5 (3)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N4—H4A \cdots O3 ⁱⁱ	0.86	2.44	2.956 (6)	119

N4—H4B···O5 ^{vi}	0.86	2.29	3.086 (6)	154
N4—H4B···O6 ^{vi}	0.86	2.59	3.304 (7)	141
N2—H2A···O6 ⁱ	0.86	2.50	3.020 (6)	120
N2—H2B···O1 ^{vii}	0.86	2.33	3.139 (7)	157
N2—H2B···O3 ^{vii}	0.86	2.57	3.312 (6)	145

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