

catena-Poly[[[diaqua(2-fluorobenzoato- κ^2O,O')strontium]- μ_3 -2-fluorobenzoato- $\kappa^5O:O,O':O',F$] monohydrate]

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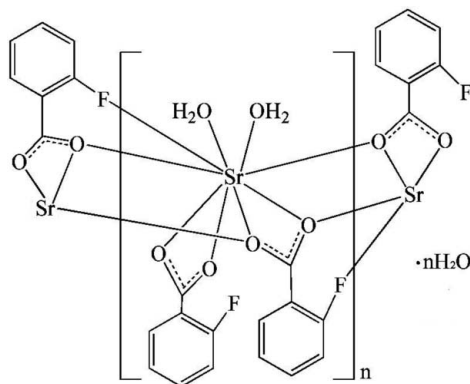
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Key indicators: single-crystal X-ray study; $T = 290$ K; mean $\sigma(C-C) = 0.008$ Å; R factor = 0.032; wR factor = 0.097; data-to-parameter ratio = 13.4.

In the title compound, $\{[\text{Sr}(\text{C}_7\text{H}_4\text{FO}_2)_2(\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}\}_n$, the Sr^{II} atom is coordinated by six O atoms and one F atom from four 2-fluorobenzoate ligands and two water molecules, resulting in an irregular SrFO_8 coordination environment. The μ_3 -2-fluorobenzoate ligand bridges three symmetry-related Sr^{II} atoms, giving rise to a chain structure extending along $[010]$. The polymeric chains are connected *via* $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds into a two-dimensional supramolecular structure parallel to (100) .

Related literature

For metal complexes with 2-fluorobenzoate ligands, see: Zhang *et al.* (2005a,b); Zhang (2006). For related structures, see: Zhang (2008, 2009).



Experimental

Crystal data

$[\text{Sr}(\text{C}_7\text{H}_4\text{FO}_2)_2(\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}$	$V = 1660.7$ (6) Å ³
$M_r = 419.87$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 12.515$ (3) Å	$\mu = 3.30$ mm ⁻¹
$b = 6.8232$ (14) Å	$T = 290$ K
$c = 19.489$ (4) Å	$0.22 \times 0.16 \times 0.12$ mm
$\beta = 93.71$ (3)°	

Data collection

Rigaku R-Axis RAPID diffractometer	12414 measured reflections
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	2912 independent reflections
$T_{\text{min}} = 0.535$, $T_{\text{max}} = 0.674$	2351 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.043$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$	218 parameters
$wR(F^2) = 0.097$	H-atom parameters constrained
$S = 1.28$	$\Delta\rho_{\text{max}} = 0.67$ e Å ⁻³
2912 reflections	$\Delta\rho_{\text{min}} = -0.68$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O5}-\text{H5A} \cdots \text{O7}^{\text{i}}$	0.82	2.11	2.854 (5)	152
$\text{O5}-\text{H5B} \cdots \text{O7}^{\text{ii}}$	0.82	2.14	2.914 (6)	158
$\text{O6}-\text{H6A} \cdots \text{O1}^{\text{iii}}$	0.82	2.10	2.791 (5)	142
$\text{O6}-\text{H6B} \cdots \text{O2}^{\text{ii}}$	0.82	2.22	2.901 (5)	140
$\text{O7}-\text{H7A} \cdots \text{O2}^{\text{ii}}$	0.82	2.01	2.800 (5)	161

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2410).

References

- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
 Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
 Rigaku/MS (2002). *CrystalStructure*. Rigaku/MS Inc., The Woodlands, Texas, USA.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Zhang, B.-S. (2006). *Z. Kristallogr. New Cryst. Struct.* **221**, 355–356.
 Zhang, B.-S. (2008). *Acta Cryst.* **E64**, m1055–m1056.
 Zhang, B.-S. (2009). *Acta Cryst.* **E65**, m1500.
 Zhang, B.-S., Zeng, X.-R., Fang, X.-N. & Huang, C.-F. (2005a). *Z. Kristallogr. New Cryst. Struct.* **220**, 141–142.
 Zhang, B.-S., Zeng, X.-R., Yu, Y.-Y., Fang, X.-N. & Huang, C.-F. (2005b). *Z. Kristallogr. New Cryst. Struct.* **220**, 75–76.

supporting information

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catena-Poly[[[diaqua(2-fluorobenzoato- κ^2 O,O')strontium]- μ_3 -2-fluorobenzoato- κ^5 O:O,O':O',F] monohydrate]

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S1. Comment

Metal ions with 2-fluorobenzoate ligands can form, among others, mononuclear and dinuclear complexes (Zhang, 2006; Zhang *et al.*, 2005a,b). However, very few complexes of 2-fluorobenzoate ligands with one-dimensional chain structure have been reported. In this paper, we report the synthesis and crystal structure of a one-dimensional chain strontium(II) complex with 2-fluorobenzoate.

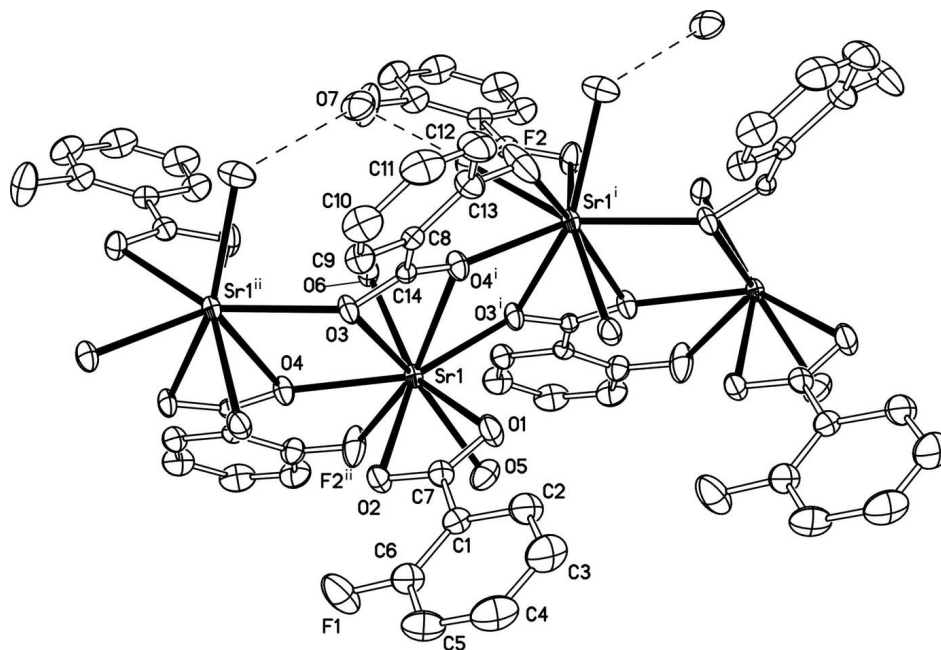
The crystal structure of the title compound is similar to those of the reported complexes (Zhang, 2008, 2009). The Sr^{II} atom is coordinated by six O atoms and one F atom from four 2-fluorobenzoate ligands and two water molecules in an irregular SrFO₈ coordination geometry. The μ_3 -2-fluorobenzoate ligand bridges three symmetry-related Sr^{II} atoms, giving rise to a chain structure extending along [0 1 0], with Sr—O bond lengths in the range of 2.463 (3) to 2.705 (3) Å and the Sr—F bond length being 2.908 (4) Å. Separation between Sr1 and Sr1ⁱ [symmetry code: (i) -x+1, y+1/2, -z+1/2] is 4.1869 (8) Å (Fig. 1). The polymeric chains are connected via O—H...O intermolecular hydrogen bonds (Table 2) between the coordinated and uncoordinated water molecules and the carboxylate groups of the 2-fluorobenzoate ligands into a two-dimensional supramolecular structure (Fig. 2).

S2. Experimental

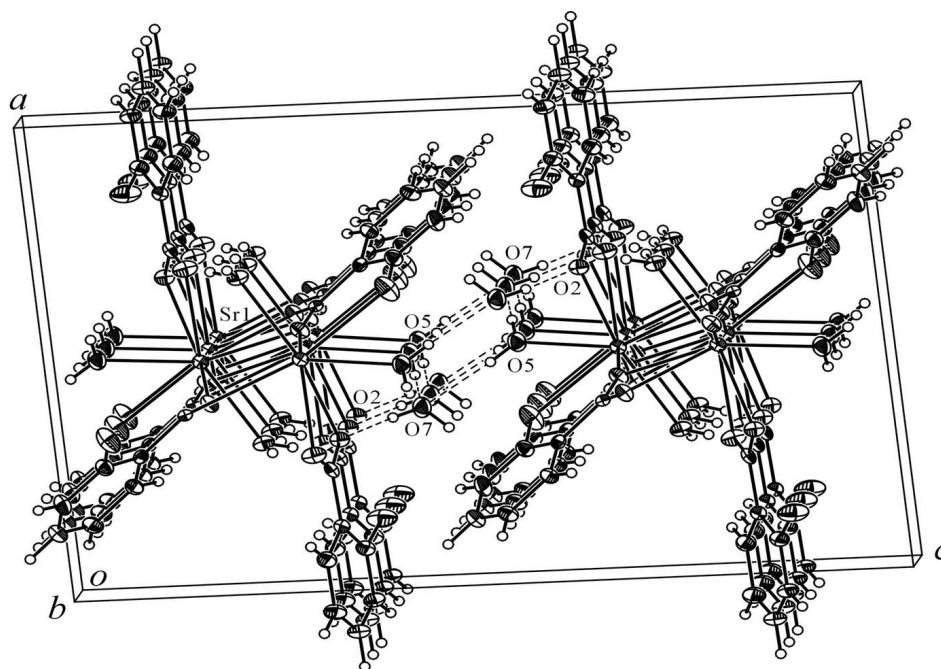
Sr(NO₃)₂ (0.109 g, 0.50 mmol) was dissolved in appropriate amount of water and then 1M Na₂CO₃ solution was added. SrCO₃ was obtained by filtration, which was washed with distilled water for 5 times. The freshly prepared SrCO₃, 2-fluorobenzoic acid (0.036 g, 0.25 mmol), 2,2'-bipyridine (0.039 g, 0.25 mmol) and CH₃OH/H₂O (v/v = 1:2, 15 ml) were mixed and stirred for 2 h. Subsequently, the resulting cream suspension was heated in a 23 ml Teflon-lined stainless steel autoclave at 433 K for 97 h. After the autoclave was cooled to room temperature in a procedure of 43 h, the solid was filtered off. The resulting filtrate was allowed to stand at room temperature, and slow evaporation for 6 weeks afforded colorless block single crystals.

S3. Refinement

C-bound H atoms were placed in calculated positions and refined as riding atoms, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms of water molecules were located in a difference Fourier map and refined with an O—H distance restraint of 0.82 (1) Å and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

**Figure 1**

The one-dimensional chain structure of the title compound. Displacement ellipsoids are drawn at the 40% probability level. H atoms have been omitted for clarity. Hydrogen bonds are shown as dashed lines. [Symmetry codes: (i) $-x+1, y+1/2, -z+1/2$; (ii) $-x+1, y-1/2, -z+1/2$.]

**Figure 2**

A packing diagram of the title compound, viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

catena-Poly[[[diaqua(2-fluorobenzoato- κ^2O,O')strontium]- μ_3 -2-fluorobenzoato- $\kappa^5O:O,O':O',F$] monohydrate]

Crystal data

[Sr(C₇H₄FO₂)₂(H₂O)₂] \cdot H₂O
M_r = 419.87
 Monoclinic, *P*2₁/*c*
 Hall symbol: -*P* 2ybc
a = 12.515 (3) Å
b = 6.8232 (14) Å
c = 19.489 (4) Å
 β = 93.71 (3)°
V = 1660.7 (6) Å³
Z = 4

F(000) = 840
D_x = 1.679 Mg m⁻³
 Mo *K* α radiation, λ = 0.71073 Å
 Cell parameters from 2912 reflections
 θ = 3.2–25.0°
 μ = 3.30 mm⁻¹
T = 290 K
 Block, colorless
 0.22 × 0.16 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID
 diffractometer
 Radiation source: rotation anode
 Graphite monochromator
 ω scans
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
T_{min} = 0.535, *T_{max}* = 0.674

12414 measured reflections
 2912 independent reflections
 2351 reflections with *I* > 2 σ (*I*)
R_{int} = 0.043
 θ_{\max} = 25.0°, θ_{\min} = 3.2°
h = -14→14
k = -7→8
l = -23→23

Refinement

Refinement on *F*²
 Least-squares matrix: full
R[*F*² > 2 σ (*F*²)] = 0.032
wR(*F*²) = 0.097
S = 1.28
 2912 reflections
 218 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods
 Secondary atom site location: difference Fourier
 map

Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.P)^2 + 5.2938P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.67 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.68 \text{ e } \text{Å}^{-3}$
 Extinction correction: SHELXL97 (Sheldrick,
 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.0066 (5)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U_{iso}</i> */ <i>U_{eq}</i>
Sr1	0.49560 (4)	0.13650 (6)	0.18761 (2)	0.02804 (17)
F1	0.8456 (3)	-0.2517 (6)	0.1198 (2)	0.0793 (13)
F2	0.6409 (3)	0.4689 (5)	0.4237 (2)	0.0751 (12)
O1	0.6953 (3)	0.2536 (5)	0.1848 (2)	0.0513 (11)
O2	0.6718 (3)	-0.0557 (5)	0.15556 (19)	0.0398 (9)
O3	0.5848 (3)	-0.0267 (4)	0.30415 (18)	0.0366 (8)
O4	0.4430 (3)	-0.2113 (5)	0.18799 (19)	0.0386 (9)
O5	0.5122 (3)	0.2790 (6)	0.0668 (2)	0.0581 (11)
H5A	0.4729	0.2551	0.0325	0.087*
H5B	0.5570	0.3656	0.0634	0.087*
O6	0.3191 (3)	0.1157 (5)	0.24982 (19)	0.0414 (9)
H6A	0.3064	0.0463	0.2827	0.062*

H6B	0.3006	0.2265	0.2602	0.062*
O7	0.3815 (3)	0.1569 (6)	0.4433 (2)	0.0602 (12)
H7A	0.3644	0.2184	0.4082	0.090*
H7B	0.3370	0.1511	0.4723	0.090*
C1	0.8510 (4)	0.0722 (8)	0.1647 (3)	0.0356 (12)
C2	0.9161 (5)	0.2282 (10)	0.1858 (3)	0.0525 (16)
H2	0.8851	0.3423	0.2014	0.063*
C3	1.0267 (5)	0.2175 (12)	0.1841 (4)	0.069 (2)
H3	1.0689	0.3235	0.1989	0.082*
C4	1.0738 (5)	0.0520 (13)	0.1607 (4)	0.069 (2)
H4	1.1478	0.0459	0.1593	0.083*
C5	1.0123 (4)	-0.1044 (11)	0.1394 (3)	0.0595 (18)
H5	1.0439	-0.2176	0.1235	0.071*
C6	0.9030 (4)	-0.0920 (9)	0.1419 (3)	0.0472 (14)
C7	0.7313 (4)	0.0909 (7)	0.1680 (2)	0.0340 (12)
C8	0.6861 (4)	0.1429 (7)	0.3916 (2)	0.0301 (11)
C9	0.7526 (4)	-0.0162 (8)	0.4058 (3)	0.0406 (13)
H9	0.7459	-0.1266	0.3779	0.049*
C10	0.8289 (5)	-0.0148 (10)	0.4606 (3)	0.0572 (17)
H10	0.8724	-0.1236	0.4694	0.069*
C11	0.8399 (5)	0.1477 (12)	0.5016 (3)	0.0640 (19)
H11	0.8915	0.1485	0.5382	0.077*
C12	0.7760 (5)	0.3100 (10)	0.4897 (3)	0.0594 (18)
H12	0.7830	0.4197	0.5180	0.071*
C13	0.7012 (4)	0.3044 (8)	0.4344 (3)	0.0429 (13)
C14	0.6027 (3)	0.1360 (7)	0.3328 (2)	0.0241 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.0313 (3)	0.0191 (2)	0.0333 (3)	-0.00040 (19)	-0.00080 (18)	0.0008 (2)
F1	0.050 (2)	0.060 (2)	0.128 (4)	0.0046 (19)	0.008 (2)	-0.038 (2)
F2	0.105 (3)	0.046 (2)	0.069 (3)	0.020 (2)	-0.030 (2)	-0.0262 (19)
O1	0.043 (2)	0.030 (2)	0.082 (3)	-0.0060 (18)	0.011 (2)	-0.015 (2)
O2	0.037 (2)	0.0299 (19)	0.052 (2)	-0.0019 (16)	0.0028 (17)	-0.0079 (17)
O3	0.049 (2)	0.0202 (17)	0.039 (2)	-0.0012 (16)	-0.0090 (17)	-0.0037 (15)
O4	0.044 (2)	0.0245 (18)	0.045 (2)	-0.0049 (16)	-0.0090 (17)	-0.0026 (16)
O5	0.063 (3)	0.068 (3)	0.043 (2)	-0.017 (2)	-0.001 (2)	0.013 (2)
O6	0.0369 (19)	0.0283 (19)	0.060 (2)	-0.0018 (16)	0.0105 (17)	0.0053 (18)
O7	0.072 (3)	0.064 (3)	0.045 (2)	0.014 (2)	0.004 (2)	0.013 (2)
C1	0.030 (3)	0.043 (3)	0.033 (3)	-0.002 (2)	0.000 (2)	0.001 (2)
C2	0.044 (3)	0.062 (4)	0.051 (4)	-0.012 (3)	0.001 (3)	-0.012 (3)
C3	0.040 (4)	0.097 (6)	0.069 (5)	-0.027 (4)	0.000 (3)	-0.012 (4)
C4	0.028 (3)	0.112 (6)	0.068 (5)	-0.001 (4)	0.005 (3)	-0.003 (4)
C5	0.032 (3)	0.085 (5)	0.061 (4)	0.016 (3)	0.007 (3)	-0.007 (4)
C6	0.036 (3)	0.057 (4)	0.048 (3)	-0.007 (3)	-0.001 (3)	-0.006 (3)
C7	0.039 (3)	0.035 (3)	0.026 (3)	-0.003 (2)	-0.009 (2)	-0.001 (2)
C8	0.032 (3)	0.029 (2)	0.030 (3)	-0.003 (2)	0.007 (2)	0.002 (2)

C9	0.038 (3)	0.041 (3)	0.042 (3)	0.006 (2)	-0.004 (2)	0.005 (3)
C10	0.042 (3)	0.073 (5)	0.055 (4)	0.016 (3)	-0.006 (3)	0.013 (4)
C11	0.049 (4)	0.098 (6)	0.043 (4)	-0.005 (4)	-0.011 (3)	0.000 (4)
C12	0.069 (4)	0.071 (5)	0.037 (4)	-0.005 (4)	-0.009 (3)	-0.012 (3)
C13	0.044 (3)	0.042 (3)	0.041 (3)	0.002 (3)	-0.003 (3)	-0.006 (3)
C14	0.021 (2)	0.023 (2)	0.029 (2)	0.000 (2)	0.0043 (18)	0.000 (2)

Geometric parameters (Å, °)

Sr1—O4	2.463 (3)	C1—C6	1.384 (8)
Sr1—O3 ⁱ	2.518 (3)	C1—C2	1.387 (7)
Sr1—O5	2.568 (4)	C1—C7	1.509 (7)
Sr1—O6	2.591 (3)	C2—C3	1.388 (8)
Sr1—O1	2.627 (4)	C2—H2	0.9300
Sr1—O2	2.674 (3)	C3—C4	1.365 (10)
Sr1—O4 ⁱ	2.703 (4)	C3—H3	0.9300
Sr1—O3	2.705 (3)	C4—C5	1.364 (9)
Sr1—F2 ⁱⁱ	2.908 (4)	C4—H4	0.9300
F1—C6	1.359 (6)	C5—C6	1.375 (7)
F2—C13	1.361 (6)	C5—H5	0.9300
F2—Sr1 ⁱ	2.908 (4)	C8—C9	1.385 (7)
O1—C7	1.250 (6)	C8—C13	1.387 (7)
O2—C7	1.261 (6)	C8—C14	1.500 (6)
O3—C14	1.256 (5)	C9—C10	1.386 (8)
O3—Sr1 ⁱⁱ	2.518 (3)	C9—H9	0.9300
O4—C14 ⁱⁱ	1.244 (5)	C10—C11	1.369 (9)
O4—Sr1 ⁱⁱ	2.703 (4)	C10—H10	0.9300
O5—H5A	0.8200	C11—C12	1.377 (9)
O5—H5B	0.8200	C11—H11	0.9300
O6—H6A	0.8200	C12—C13	1.382 (8)
O6—H6B	0.8200	C12—H12	0.9300
O7—H7A	0.8200	C14—O4 ⁱ	1.244 (5)
O7—H7B	0.8200		
O4—Sr1—O3 ⁱ	140.48 (11)	H6A—O6—H6B	105.5
O4—Sr1—O5	113.89 (13)	H7A—O7—H7B	116.6
O3 ⁱ —Sr1—O5	76.65 (13)	C6—C1—C2	115.9 (5)
O4—Sr1—O6	73.14 (11)	C6—C1—C7	124.8 (5)
O3 ⁱ —Sr1—O6	70.37 (11)	C2—C1—C7	119.3 (5)
O5—Sr1—O6	124.86 (13)	C1—C2—C3	121.4 (6)
O4—Sr1—O1	123.21 (12)	C1—C2—H2	119.3
O3 ⁱ —Sr1—O1	96.20 (11)	C3—C2—H2	119.3
O5—Sr1—O1	74.49 (14)	C4—C3—C2	120.2 (6)
O6—Sr1—O1	150.09 (12)	C4—C3—H3	119.9
O4—Sr1—O2	75.68 (11)	C2—C3—H3	119.9
O3 ⁱ —Sr1—O2	143.25 (11)	C5—C4—C3	120.1 (6)
O5—Sr1—O2	81.65 (13)	C5—C4—H4	119.9
O6—Sr1—O2	145.41 (11)	C3—C4—H4	119.9

O1—Sr1—O2	49.04 (11)	C4—C5—C6	119.0 (6)
O4—Sr1—O4 ⁱ	115.34 (9)	C4—C5—H5	120.5
O3 ⁱ —Sr1—O4 ⁱ	71.56 (10)	C6—C5—H5	120.5
O5—Sr1—O4 ⁱ	129.93 (12)	F1—C6—C5	116.5 (6)
O6—Sr1—O4 ⁱ	78.62 (11)	F1—C6—C1	120.0 (5)
O1—Sr1—O4 ⁱ	71.71 (12)	C5—C6—C1	123.4 (6)
O2—Sr1—O4 ⁱ	101.95 (11)	O1—C7—O2	122.4 (5)
O4—Sr1—O3	72.34 (10)	O1—C7—C1	117.5 (4)
O3 ⁱ —Sr1—O3	117.84 (8)	O2—C7—C1	120.0 (5)
O5—Sr1—O3	150.73 (12)	O1—C7—Sr1	60.2 (3)
O6—Sr1—O3	84.40 (11)	O2—C7—Sr1	62.3 (3)
O1—Sr1—O3	78.54 (12)	C1—C7—Sr1	175.0 (3)
O2—Sr1—O3	72.10 (11)	C9—C8—C13	116.5 (5)
O4 ⁱ —Sr1—O3	47.70 (10)	C9—C8—C14	120.5 (4)
O4—Sr1—F2 ⁱⁱ	58.61 (10)	C13—C8—C14	123.1 (4)
O3 ⁱ —Sr1—F2 ⁱⁱ	100.89 (11)	C8—C9—C10	121.6 (6)
O5—Sr1—F2 ⁱⁱ	62.81 (12)	C8—C9—H9	119.2
O6—Sr1—F2 ⁱⁱ	81.40 (12)	C10—C9—H9	119.2
O1—Sr1—F2 ⁱⁱ	128.15 (13)	C11—C10—C9	119.6 (6)
O2—Sr1—F2 ⁱⁱ	94.95 (12)	C11—C10—H10	120.2
O4 ⁱ —Sr1—F2 ⁱⁱ	160.00 (12)	C9—C10—H10	120.2
O3—Sr1—F2 ⁱⁱ	130.94 (9)	C10—C11—C12	121.1 (6)
C13—F2—Sr1 ⁱ	137.0 (3)	C10—C11—H11	119.4
C7—O1—Sr1	95.5 (3)	C12—C11—H11	119.4
C7—O2—Sr1	93.0 (3)	C11—C12—C13	117.8 (6)
C14—O3—Sr1 ⁱ	147.1 (3)	C11—C12—H12	121.1
C14—O3—Sr1	93.5 (3)	C13—C12—H12	121.1
Sr1 ⁱⁱ —O3—Sr1	106.53 (12)	F2—C13—C12	116.0 (5)
C14 ⁱⁱ —O4—Sr1	157.5 (3)	F2—C13—C8	120.7 (5)
C14 ⁱⁱ —O4—Sr1 ⁱⁱ	93.9 (3)	C12—C13—C8	123.3 (5)
Sr1—O4—Sr1 ⁱⁱ	108.21 (12)	O4 ⁱ —C14—O3	122.0 (4)
Sr1—O5—H5A	126.3	O4 ⁱ —C14—C8	120.3 (4)
Sr1—O5—H5B	116.3	O3—C14—C8	117.6 (4)
H5A—O5—H5B	117.0	O4 ⁱ —C14—Sr1	62.1 (2)
Sr1—O6—H6A	127.7	O3—C14—Sr1	62.2 (2)
Sr1—O6—H6B	109.2	C8—C14—Sr1	162.0 (3)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H5A \cdots O7 ⁱⁱⁱ	0.82	2.11	2.854 (5)	152
O5—H5B \cdots O7 ⁱ	0.82	2.14	2.914 (6)	158
O6—H6A \cdots O1 ⁱⁱ	0.82	2.10	2.791 (5)	142
O6—H6B \cdots O2 ⁱ	0.82	2.22	2.901 (5)	140
O7—H7A \cdots O2 ⁱ	0.82	2.01	2.800 (5)	161

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