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catena-Poly[[[aqua[2-(6-chloropyridin-3-yl)acetato-κ*O*]sodium]-di-μ-aqua] monohydrate]

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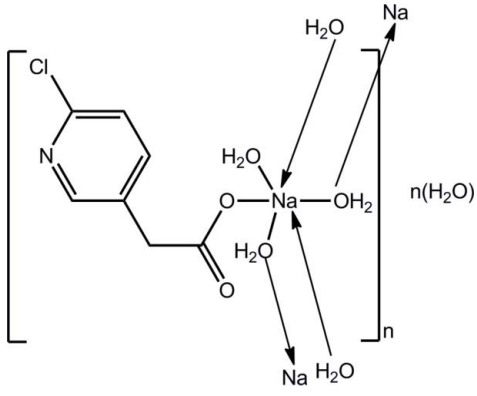
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.084; data-to-parameter ratio = 14.4.

The crystal structure of the title compound, $\{[Na(C_7H_5ClNO_2)(H_2O)_3]\cdot H_2O\}_n$, features polymeric chains along [010]. The Na^+ cation is octahedrally coordinated by four bridging water molecules, a terminal water molecule and an O atom derived from a monodentate carboxylate ligand. Adjacent polyhedra share two O···O edges. The polymeric chains are linked into a three-dimensional network *via* O—H···O and O—H···N hydrogen bonds.

Related literature

For a related structure, see: Guo *et al.* (2004).



Experimental

Crystal data

$[Na(C_7H_5ClNO_2)(H_2O)_3]\cdot H_2O$
M_r = 265.62
Monoclinic, $P2_1/c$
a = 12.4695 (12) Å
b = 5.5377 (5) Å
c = 17.0557 (17) Å
β = 91.190 (1)°
V = 1177.48 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 298 K
0.47 × 0.21 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.844, T_{max} = 0.964
5621 measured reflections
2082 independent reflections
1558 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.084
S = 1.05
2082 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected bond lengths (Å).

Na1—O1	2.3632 (15)	Na1—O4	2.4239 (17)
Na1—O5^{i}	2.3872 (16)	Na1—O3	2.5142 (17)
Na1—O3^{ii}	2.4032 (16)	Na1—O5	2.5187 (16)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O4^{iii}	0.85	2.06	2.893 (2)	168
O4—H4A···O2^{iv}	0.85	1.91	2.762 (2)	175
O3—H3B···O6^{v}	0.85	1.97	2.775 (2)	159
O4—H4B···O2^{v}	0.85	1.98	2.824 (2)	169
O5—H5A···O6^{v}	0.85	2.08	2.886 (2)	157
O5—H5B···O1^{ii}	0.85	2.07	2.9214 (19)	175
O6—H6A···N1^{vi}	0.85	2.05	2.900 (2)	173
O6—H6B···O2	0.85	1.95	2.796 (2)	176

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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: TK5075).

References

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supporting information

Acta Cryst. (2012). E**68**, m584 [doi:10.1107/S1600536812014092]

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S1. Comment

In the title compound (Fig. 1), (I), the Na atom has a distorted O_6 octahedral environment formed by a terminal water molecule O4, four O atoms derived from μ_2-bridging water molecules and one carboxylate (O1) atom of the 6-chloro-3-pyridineacetate ligand (Table 1). Each coordination octahedron shares two O···O edges with two adjacent octahedra, thus producing infinite chains. Similar chains were found in the structure of sodium carboxynitrobenzoate tetrahydrate (Guo, 2004). In (I), the chains are linked into a three-dimensional network *via* O—H···O and O—H···N hydrogen bonds (Table 2 and Fig. 2).

S2. Experimental

To a solution of 6-chloro-3-pyridineacetic acid (1 mmol) in doubly-distilled water (60 ml), a solution of an equimolar amount of sodium hydroxide in doubly-distilled water (40 ml) was added drop wise at room temperature. After vigorous stirring for 4 h, the resulting mixture was evaporated *in vacuo* to a volume of about 20 ml and filtered hot. The filtrate was then set aside for crystallization at room temperature. Two weeks later, colourless crystals of the title compound were isolated.

S3. Refinement

The H atoms were placed in geometrically idealized positions (O—H = 0.85, C—H = 0.93–0.97 Å) and treated as riding on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(O) or U_{iso}(H) = 1.2U_{eq}(C).

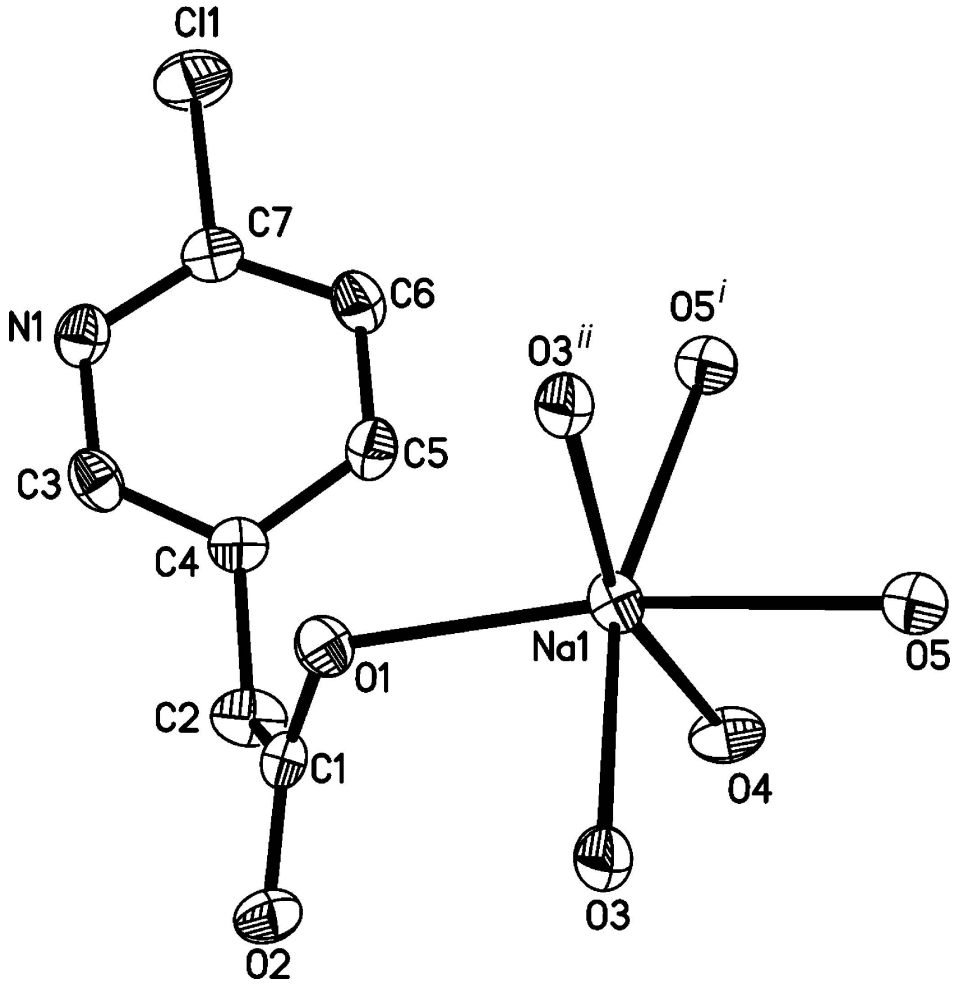

Figure 1

The coordination environment around the Na atom showing numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry codes: *i* - *x* + 1, -*y* + 1, -*z* + 1; *ii* - *x* + 1, -*y* + 2, -*z* + 1. The lattice water molecule and hydrogen atoms have been omitted.

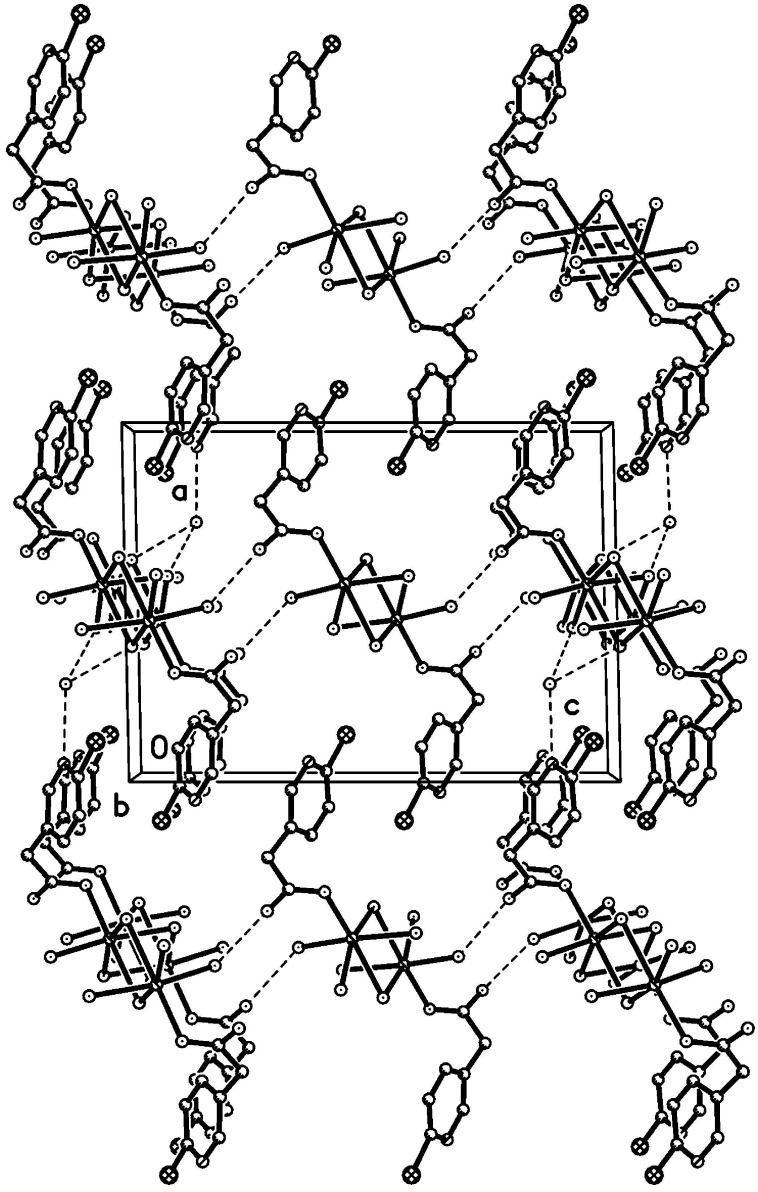

Figure 2

Packing diagram of (I), showing hydrogen bonds as dashed lines.

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$c = 17.0557\ (17)$ Å
$\beta = 91.190\ (1)°$
$V = 1177.48\ (19)$ Å^3
$Z = 4$
$F(000) = 552$
$D_x = 1.498$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5621 reflections
$\theta = 2.4–27.1°$
$\mu = 0.37$ mm^{-1}
$T = 298$ K
Block, colourless
0.47 × 0.21 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.844, T_{max} = 0.964
5621 measured reflections
2082 independent reflections
1558 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 25.0°, θ_{min} = 1.6°
$h = -9 \rightarrow 14$
$k = -6 \rightarrow 6$
$l = -19 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.084
S = 1.05
2082 reflections
145 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
$w = 1/[\sigma^2(F_o^2) + (0.0308P)^2 + 0.4882P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O6	0.73121 (12)	1.2862 (3)	0.13436 (9)	0.0499 (4)
Na1	0.55064 (6)	0.74749 (14)	0.44657 (5)	0.0350 (2)
Cl1	1.11649 (5)	0.25311 (12)	0.44137 (4)	0.0589 (2)
N1	1.04684 (13)	0.6295 (3)	0.36393 (11)	0.0399 (5)
O1	0.69179 (11)	0.9744 (3)	0.39281 (8)	0.0363 (4)
O2	0.64644 (11)	1.1400 (3)	0.27723 (8)	0.0395 (4)
O3	0.42626 (11)	1.0983 (3)	0.42246 (8)	0.0412 (4)
H3A	0.4419	1.2194	0.3943	0.049*
H3B	0.3694	1.0368	0.4027	0.049*
O4	0.51265 (12)	0.4951 (3)	0.33326 (9)	0.0453 (4)
H4A	0.5559	0.3922	0.3147	0.054*
H4B	0.4714	0.5431	0.2961	0.054*
O5	0.37654 (11)	0.6269 (2)	0.50779 (8)	0.0381 (4)
H5A	0.3354	0.6360	0.4675	0.046*
H5B	0.3590	0.7388	0.5391	0.046*
H6A	0.7978	1.2532	0.1339	0.046*

H6B	0.7082	1.2413	0.1786	0.046*
C1	0.70075 (15)	0.9966 (4)	0.32056 (12)	0.0311 (5)
C2	0.78312 (18)	0.8466 (4)	0.27717 (13)	0.0461 (6)
H2A	0.7443	0.7362	0.2428	0.055*
H2B	0.8230	0.9552	0.2440	0.055*
C3	0.97016 (17)	0.7608 (4)	0.32733 (13)	0.0398 (5)
H3	0.9909	0.9016	0.3021	0.048*
C4	0.86306 (16)	0.7010 (4)	0.32460 (12)	0.0337 (5)
C5	0.83412 (18)	0.4939 (4)	0.36460 (13)	0.0395 (5)
H5	0.7623	0.4490	0.3662	0.047*
C6	0.91043 (18)	0.3544 (4)	0.40187 (13)	0.0428 (6)
H6	0.8919	0.2143	0.4284	0.051*
C7	1.01530 (17)	0.4294 (4)	0.39851 (12)	0.0368 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O6	0.0327 (9)	0.0665 (11)	0.0504 (10)	0.0073 (8)	0.0012 (7)	0.0212 (8)
Na1	0.0387 (5)	0.0315 (4)	0.0349 (5)	−0.0025 (4)	0.0060 (4)	0.0001 (4)
Cl1	0.0542 (4)	0.0584 (4)	0.0637 (4)	0.0218 (3)	−0.0098 (3)	−0.0013 (3)
N1	0.0308 (10)	0.0401 (11)	0.0491 (11)	0.0015 (9)	0.0052 (9)	−0.0046 (9)
O1	0.0378 (8)	0.0405 (8)	0.0310 (8)	−0.0005 (7)	0.0078 (6)	0.0007 (7)
O2	0.0328 (8)	0.0476 (9)	0.0378 (9)	0.0095 (7)	−0.0022 (7)	−0.0004 (8)
O3	0.0423 (9)	0.0397 (9)	0.0413 (9)	−0.0108 (7)	−0.0040 (7)	0.0033 (7)
O4	0.0487 (9)	0.0488 (9)	0.0382 (9)	0.0147 (8)	−0.0060 (7)	−0.0062 (7)
O5	0.0420 (9)	0.0361 (8)	0.0361 (8)	0.0018 (7)	−0.0001 (7)	−0.0013 (7)
C1	0.0249 (10)	0.0327 (11)	0.0357 (12)	−0.0057 (9)	0.0008 (9)	−0.0015 (10)
C2	0.0482 (14)	0.0550 (14)	0.0352 (12)	0.0189 (12)	0.0073 (10)	−0.0003 (11)
C3	0.0409 (13)	0.0340 (11)	0.0449 (13)	0.0021 (10)	0.0143 (10)	0.0043 (11)
C4	0.0349 (12)	0.0371 (12)	0.0294 (11)	0.0074 (9)	0.0065 (9)	−0.0050 (9)
C5	0.0321 (12)	0.0382 (12)	0.0482 (14)	−0.0036 (10)	0.0032 (10)	−0.0029 (11)
C6	0.0455 (14)	0.0326 (12)	0.0504 (14)	−0.0013 (11)	0.0070 (11)	0.0043 (11)
C7	0.0390 (13)	0.0366 (12)	0.0347 (12)	0.0090 (10)	0.0016 (10)	−0.0067 (10)

Geometric parameters (Å, º)

O6—H6A	0.8500	O3—H3B	0.8500
O6—H6B	0.8502	O4—H4A	0.8500
Na1—O1	2.3632 (15)	O4—H4B	0.8500
Na1—O5^{i}	2.3872 (16)	O5—Na1^{i}	2.3872 (16)
Na1—O3^{ii}	2.4032 (16)	O5—H5A	0.8499
Na1—O4	2.4239 (17)	O5—H5B	0.8500
Na1—O3	2.5142 (17)	C1—C2	1.524 (3)
Na1—O5	2.5187 (16)	C2—C4	1.505 (3)
Na1—Na1^{i}	3.5391 (15)	C2—H2A	0.9700
Na1—Na1^{ii}	3.5823 (15)	C2—H2B	0.9700
Cl1—C7	1.744 (2)	C3—C4	1.376 (3)
N1—C7	1.319 (3)	C3—H3	0.9300

N1—C3	1.344 (3)	C4—C5	1.386 (3)
O1—C1	1.246 (2)	C5—C6	1.371 (3)
O2—C1	1.271 (2)	C5—H5	0.9300
O3—Na1^{ii}	2.4032 (16)	C6—C7	1.374 (3)
O3—H3A	0.8500	C6—H6	0.9300
H6A—O6—H6B	107.0	Na1—O3—H3B	105.2
O1—Na1—O5^{i}	107.88 (6)	H3A—O3—H3B	106.9
O1—Na1—O3^{ii}	95.50 (6)	Na1—O4—H4A	124.6
O5^{i}—Na1—O3^{ii}	88.18 (5)	Na1—O4—H4B	121.3
O1—Na1—O4	97.59 (6)	H4A—O4—H4B	108.1
O5^{i}—Na1—O4	79.97 (5)	Na1^{i}—O5—Na1	92.30 (5)
O3^{ii}—Na1—O4	164.52 (6)	Na1^{i}—O5—H5A	122.3
O1—Na1—O3	89.29 (5)	Na1—O5—H5A	99.2
O5^{i}—Na1—O3	162.45 (6)	Na1^{i}—O5—H5B	122.0
O3^{ii}—Na1—O3	86.51 (6)	Na1—O5—H5B	107.6
O4—Na1—O3	101.86 (6)	H5A—O5—H5B	107.8
O1—Na1—O5	163.18 (6)	O1—C1—O2	125.41 (19)
O5^{i}—Na1—O5	87.70 (5)	O1—C1—C2	120.11 (19)
O3^{ii}—Na1—O5	78.27 (5)	O2—C1—C2	114.48 (18)
O4—Na1—O5	91.24 (6)	C4—C2—C1	118.45 (18)
O3—Na1—O5	74.85 (5)	C4—C2—H2A	107.7
O1—Na1—Na1^{i}	152.66 (6)	C1—C2—H2A	107.7
O5^{i}—Na1—Na1^{i}	45.32 (4)	C4—C2—H2B	107.7
O3^{ii}—Na1—Na1^{i}	80.43 (4)	C1—C2—H2B	107.7
O4—Na1—Na1^{i}	84.15 (5)	H2A—C2—H2B	107.1
O3—Na1—Na1^{i}	117.20 (5)	N1—C3—C4	124.5 (2)
O5—Na1—Na1^{i}	42.37 (4)	N1—C3—H3	117.8
O1—Na1—Na1^{ii}	93.18 (5)	C4—C3—H3	117.8
O5^{i}—Na1—Na1^{ii}	130.38 (5)	C3—C4—C5	116.4 (2)
O3^{ii}—Na1—Na1^{ii}	44.47 (4)	C3—C4—C2	121.4 (2)
O4—Na1—Na1^{ii}	142.25 (6)	C5—C4—C2	122.1 (2)
O3—Na1—Na1^{ii}	42.04 (4)	C6—C5—C4	120.6 (2)
O5—Na1—Na1^{ii}	71.35 (4)	C6—C5—H5	119.7
Na1^{i}—Na1—Na1^{ii}	102.08 (4)	C4—C5—H5	119.7
C7—N1—C3	116.48 (18)	C5—C6—C7	117.5 (2)
C1—O1—Na1	121.26 (13)	C5—C6—H6	121.2
Na1^{ii}—O3—Na1	93.49 (6)	C7—C6—H6	121.2
Na1^{ii}—O3—H3A	102.7	N1—C7—C6	124.4 (2)
Na1—O3—H3A	123.6	N1—C7—Cl1	115.97 (16)
Na1^{ii}—O3—H3B	126.5	C6—C7—Cl1	119.60 (17)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O4^{iii}	0.85	2.06	2.893 (2)	168

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