catena-Poly[[diaquarubidium(I)]-(μ₂-3-carboxypyrazine-2-carboxylato)-(μ₂-pyrazine-2,3-dicarboxylic acid)]

Mustafa Tombul[a]* and Kutalmis Guven[b]

[a]Department of Chemistry, Faculty of Art and Science, University of Kırıkkale, Campus, Yahsihan, 71450 Kırıkkale, Turkey, and [b]Department of Physics, Faculty of Art and Science, University of Kirikkale, Campus, Yahsihan, 71450 Kırıkkale, Turkey
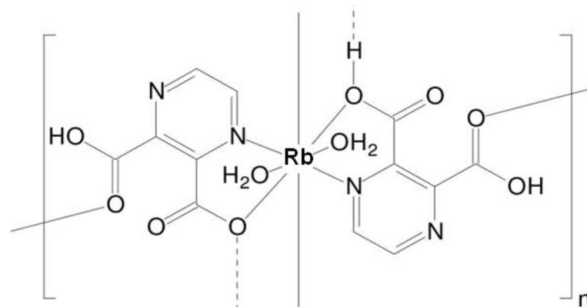Correspondence e-mail: mustafatombul38@gmail.com

The structural unit of the title compound, $[Rb(C_6H_3N_2O_4)-(C_6H_4N_2O_4)(H_2O)_2]_n$, consists of one rubidium cation, one hydrogen pyrazine-2,3-dicarboxylate anion, one pyrazine-2,3-dicarboxylic acid molecule and two water molecules. This formulation is repeated twice in the asymmetric unit as the rubidium cation lies on an inversion centre. Each anion or acid molecule is linked to two rubidium cations, while the rubidium cation has close contacts to four symmetry-equivalent organic ligands, with two different coordination modes towards this cation. In addition, each rubidium cation is coordinated by two water O atoms, raising the coordination number to eight. One of the carboxyl groups of the acid holds its H atom, which forms a hydrogen bond to a coordinated water molecule. The other carboxyl group is deprotonated in half of the ligands and protonated in the other half, taking part in a strong O—H···O hydrogen bond disordered over an inversion centre. The stabilization of the crystal structure is further assisted by O—H···O and O—H···N hydrogen-bonding interactions involving the water molecules and carboxylate O atoms.

Related literature

Pyrazine-2,3-dicarboxylic acid (Takusagawa & Shimada, 1973) and its dianion (Richard *et al.*, 1973; Nepveu *et al.*, 1993) have been used in the construction of multi-dimensional frameworks. A variety of metal–pyrazine-2,3-dicarboxylic acid complexes have been characterized, including the calcium (Ptasiewicz-Bak & Leciejewicz, 1997a; Starosta & Leciejewicz, 2005), magnesium (Ptasiewicz-Bak & Leciejewicz, 1997b), sodium (Tombul *et al.*, 2006), caesium (Tombul *et al.*, 2007), potassium (Tombul *et al.*, 2008a) and lithium (Tombul *et al.*, 2008b) complexes. For Rb—N bond lengths, see: Yang *et al.* (2008); Cametti *et al.* (2005); Wiesbrock & Schmidbaur (2003); Shannon (1976); Devi & Vidyasagar (2000).

Experimental

Crystal data

$[Rb(C_6H_3N_2O_4)(C_6H_4N_2O_4)-(H_2O)_2]$	$\beta = 81.424\ (19)°$
$M_r = 456.72$	$\gamma = 65.322\ (18)°$
Triclinic, $P\bar{1}$	$V = 414.32\ (16)$ Å³
$a = 7.452\ (2)$ Å	$Z = 1$
$b = 7.8640\ (15)$ Å	Mo $K\alpha$ radiation
$c = 8.3280\ (12)$ Å	$\mu = 3.05$ mm⁻¹
$\alpha = 69.111\ (12)°$	$T = 298\ (2)$ K
	$0.20 \times 0.15 \times 0.06$ mm

Data collection

Rigaku AFC-7S diffractometer	1604 reflections with $I > 2\sigma(I)$
Absorption correction: numerical (Clark & Reid, 1995)	$R_{int} = 0.048$
$T_{min} = 0.581$, $T_{max} = 0.838$	3 standard reflections every 150 reflections intensity decay: none
5329 measured reflections	
5057 independent reflections	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.219$	
$S = 0.98$	$\Delta\rho_{max} = 1.35$ e Å⁻³
5057 reflections	$\Delta\rho_{min} = -1.91$ e Å⁻³
133 parameters	
1 restraint	

Table 1
Selected geometric parameters (Å, °).

Rb1—O3ⁱ	2.987 (3)	Rb1—O5	3.096 (4)
Rb1—N2ⁱⁱ	3.007 (3)	Rb1—O1	3.137 (3)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H1···O3ⁱᵛ	0.93	1.55 (1)	2.468 (3)	170 (1)
O5—H5A···N1	0.84 (9)	2.07 (9)	2.888 (3)	168 (7)
O5—H5B···O4ᵛ	0.82 (6)	1.94 (6)	2.753 (3)	170.39 (5)
O2—H2···O5ᵛⁱ	0.82	1.79	2.596 (6)	166 (1)

Symmetry codes: (iv) $-x + 1, -y + 2, -z$; (v) $x, y - 1, z$; (vi) $-x + 2, -y, -z + 1$.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1997); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN for Windows* (Molecular Structure Corporation, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to

metal-organic compounds

refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2450).

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supporting information

catena-Poly[[diaquarubidium(I)](*µ*₂-3-carboxypyrazine-2-carboxylato)(*µ*₂-pyrazine-2,3-dicarboxylic acid)]

Mustafa Tombul and Kutalmis Guven

S1. Comment

Pyrazine-2,3-dicarboxylic acid (Takusagawa & Shimada, 1973) and its dianion (Richard *et al.*, 1973; Nepveu *et al.*, 1993) have been reported to be well suited for the construction of multidimensional frameworks (nD, n = 1–3), owing to the presence of two adjacent carboxylate groups (O donor atoms) as substituents on the N-heterocyclic pyrazine ring (N donor atoms). In recent years, a variety of metal-organic compound of pyrazine-2,3-dicarboxylic acid have been characterized crystallographically owing to growing interest in supramolecular chemistry. Examples are including the calcium (Ptasiewicz-Bak & Leciejewicz, 1997*a*; Starosta & Leciejewicz, 2005), magnesium (Ptasiewicz-Bak & Leciejewicz, 1997*b*), sodium (Tombul *et al.*, 2006), caesium (Tombul *et al.*, 2007) and potassium (Tombul *et al.*, 2008*a*) and lithium (Tombul *et al.*, 2008*b*) complexes. Continuation our research on Group I dicarboxylates, we present here the synthesis and crystal structure of the hydrated polymeric rubidium complex, (I), formed with pyrazine-2,3-dicarboxylic acid.

The structural unit of the title compound, (I), contains one rubidium cation, one hydrogen pyrazine-2,3-dicarboxylate anion, one pyrazine-2,3-dicarboxylic acid molecule and two water molecules; this is twice in the asymmetric unit, since the rubidium ion lies on an inversion centre. This compound is isostructural with the corresponding potassium and caesium complexes, which are fully described previously (Tombul *et al.*, 2008*a*; Tombul *et al.*, 2007). Pyrazine-2,3-di-carboxylic acid is, on average, only half deprotonated at one of the carboxylate groups (O3^{ii} and O3^{iii}) complete the charge balance of the cation. Taking a larger domain of the crystal structure, the anion or acid molecule is linked to two rubidium cations, while the Rb⁺ cation is surrounded by four organic ligands, two of which are coordinated by employing both N and O atoms and the other two are coordinated solely by O atoms. In addition, each rubidium cation is coordinated by two water molecules, raising a coordination number of eight. The inner coordination sphere accommodates comprises six oxygen atoms (O1, O1^{i}, O3^{ii}, O3^{iii}, O5 and O5^{i}), together with two nitrogen atoms (N2^{ii} and N2^{iii}). The planes of the carboxylic/carboxylate groups (O1/C1/C2/O2) and (O3/C6/C5/O4) form dihedral angles with the ring (C2/C3/C4/C5/N1/N2) plane of 75.87 (16) and 6.65 (21), respectively. The Rb—O distances are in the range from 2.987 (3) Å to 3.137 (3) Å, which are well within the range reported in the literature for other rubidium complexes (Yang *et al.* 2008; Cametti *et al.*, 2005; Wiesbrock & Schmidbaur, 2003; Shannon, 1976; Devi & Vidyasagar, 2000). Rb—N bond lengths also lie within the normal ranges found for similar bonds in the literature (Yang *et al.* 2008).

In the crystal structure, an asymmetric strong hydrogen bond occurs, linking carboxylate O atoms O—H···O [O···O = 2.468 (3) 2.596 (2) Å respectively]. Atom H1 is involved in this bond and maintains the charge balance within the structure. The water molecules are involved in normal, slightly bent, hydrogen bonds with hydrogen pyrazine-2,3-di-carboxylate (Table 2); the acceptors are carboxylate O atoms and N atoms of the aromatic ring. The polymeric complex is linked in a three-dimensional manner by further numerous intermolecular O—H···O and O—H···N hydrogen bonds (Fig.

2 and Table 2)

S2. Experimental

Rb~2~CO~3~ (462 mg, 2 mmol) was carefully added to an aqueous solution (20 ml) of pyrazine 2,3-dicarboxylic acid (672 mg, 4 mmol), until no further bubbles formed. The reaction mixture produced a colourless and clear solution which was stirred at 323 K for 200 min., until it solidified. The solid product was then redissolved in water (5 ml) and allowed to stand for three days at ambient temperature, after which transparent fine crystals were harvested.

S3. Refinement

The H5A atom of water molecule was located in a difference map. The position of H5B atom was obtained from difference map and then its position was refined with riding constraint.The other hydyrogen atoms (H1, H2, H3, H4) were repositioned geometrically. (C—H = 0.93 Å, O—H = 0.93 Å and O—H = 0.82 Å) and U\ĩso\~(H) (in the range 1.2–1.5 times U\~eq\~ of the parent atom).
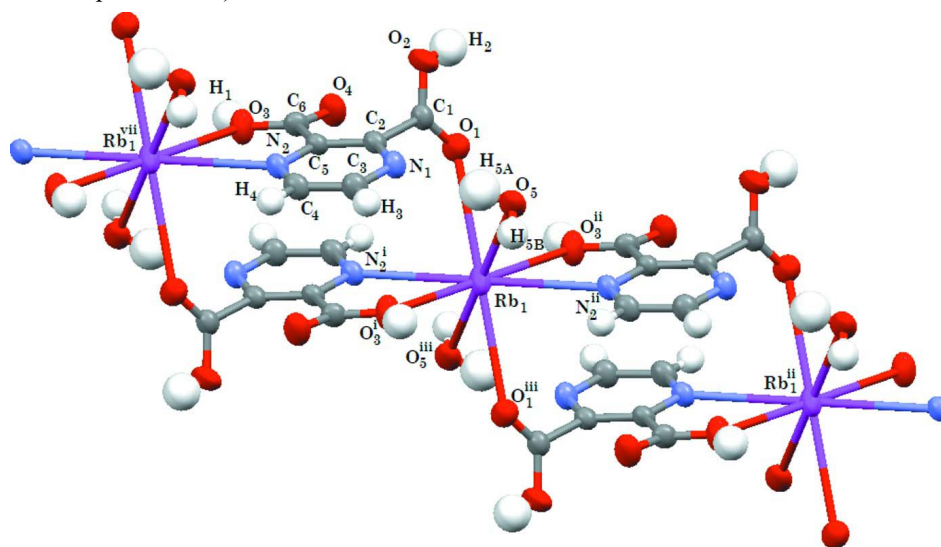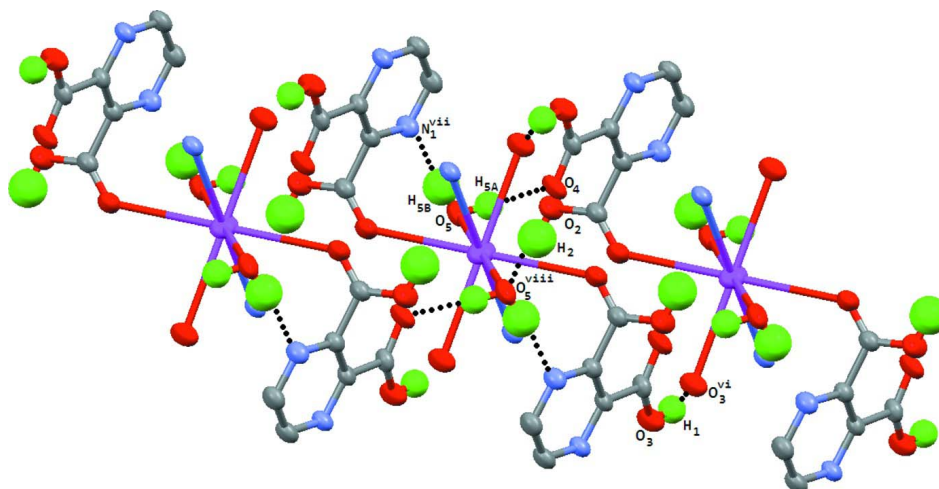

Figure 1

A perspective view diagram of the structure of (I) together with asymmetric units. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $1 - x$, $1 - y$, $-z$, (ii) $1 + x$, $y - 1$, z, (iii) $-x + 2$, $-y$, $-z$, (vii) $x - 1$, $y + 1$, z].

Figure 2

Hydrogen bongd diagram of (I). Dashed lines indicate hydrogen bonds. (H atoms of carbons were ommited for clarity).

catena-**Poly[[diaquarubidium(I)](*μ*₂-3-carboxypyrazine-2- carboxylato)(*μ*₂-pyrazine-2,3-dicarboxylic acid)]**

Crystal data

[Rb(C₆H₃N₂O₄)(C₆H₄N₂O₄)(H₂O)₂]
$M_r = 456.72$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.452 (2)$ Å
$b = 7.8640 (15)$ Å
$c = 8.3280 (12)$ Å
$\alpha = 69.111 (12)°$
$\beta = 81.424 (19)°$
$\gamma = 65.322 (18)°$
$V = 414.32 (16)$ Å³

$Z = 1$
$F(000) = 228$
$D_x = 1.830$ Mg m⁻³
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 2.6$–$9.2°$
$\mu = 3.05$ mm⁻¹
$T = 298$ K
Prism, colourless
$0.20 \times 0.15 \times 0.06$ mm

Data collection

Rigaku AFC-7S
   diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω–2θ scans
Absorption correction: numerical
   (Clark & Reid, 1995)
$T_{min} = 0.581$, $T_{max} = 0.838$
5329 measured reflections

5057 independent reflections
1604 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 40.0°$, $\theta_{min} = 2.6°$
$h = -13 \rightarrow 13$
$k = -12 \rightarrow 13$
$l = 0 \rightarrow 15$
3 standard reflections every 150 reflections
   intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.219$
$S = 0.98$
5057 reflections
133 parameters
1 restraint

Primary atom site location: structure-invariant
   direct methods
Secondary atom site location: difference Fourier
   map
Hydrogen site location: inferred from
   neighbouring sites
H atoms treated by a mixture of independent
   and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0711P)^2 + 0.5448P]$
 where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.35$ e Å^{-3}

$\Delta\rho_{min} = -1.91$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Extinction coefficient: 0.093 (11)

Special details

Experimental. [analytical numeric absorption correction using a multifaceted crystal model based on expressions derived (Clark & Reid, 1995)]

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Rb1	1.0000	0.0000	0.0000	0.0474 (3)	
O1	0.9512 (4)	0.1940 (5)	0.2826 (4)	0.0451 (7)	
O2	0.8035 (5)	0.3205 (6)	0.4927 (4)	0.0555 (9)	
H2	0.9157	0.2906	0.5229	0.083*	
O3	0.4264 (4)	0.8765 (4)	0.0673 (4)	0.0472 (7)	
H1	0.4742	0.9762	0.0256	0.071*	0.50
O4	0.7256 (4)	0.6622 (5)	0.1716 (5)	0.0497 (8)	
O5	0.8582 (5)	−0.1900 (5)	0.3618 (5)	0.0520 (8)	
N1	0.5456 (5)	0.1950 (5)	0.3236 (4)	0.0367 (7)	
N2	0.2959 (4)	0.5834 (5)	0.1521 (4)	0.0333 (6)	
C1	0.8065 (5)	0.2816 (5)	0.3520 (5)	0.0335 (7)	
C2	0.6004 (5)	0.3460 (5)	0.2892 (4)	0.0307 (7)	
C3	0.3632 (6)	0.2399 (6)	0.2753 (5)	0.0390 (8)	
H3	0.3190	0.1392	0.2980	0.047*	
C4	0.2388 (6)	0.4346 (6)	0.1918 (5)	0.0372 (8)	
H4	0.1117	0.4612	0.1629	0.045*	
C5	0.4790 (5)	0.5392 (5)	0.1997 (4)	0.0297 (7)	
C6	0.5508 (6)	0.7044 (5)	0.1459 (5)	0.0344 (8)	
H5A	0.761 (12)	−0.087 (12)	0.364 (10)	0.10 (3)*	
H5B	0.816 (8)	−0.243 (8)	0.316 (6)	0.057 (16)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rb1	0.0433 (4)	0.0367 (3)	0.0434 (4)	−0.0028 (2)	−0.0063 (2)	−0.0051 (2)
O1	0.0316 (14)	0.0510 (17)	0.0607 (19)	−0.0160 (13)	−0.0025 (13)	−0.0265 (15)
O2	0.0423 (16)	0.079 (2)	0.0460 (17)	−0.0112 (16)	−0.0128 (13)	−0.0312 (17)
O3	0.0395 (15)	0.0302 (13)	0.069 (2)	−0.0180 (12)	−0.0093 (14)	−0.0036 (13)
O4	0.0393 (15)	0.0428 (16)	0.075 (2)	−0.0207 (13)	−0.0172 (14)	−0.0157 (15)
O5	0.0471 (18)	0.0489 (18)	0.066 (2)	−0.0120 (15)	−0.0233 (15)	−0.0253 (16)

N1	0.0360 (16)	0.0293 (14)	0.0426 (17)	−0.0139 (12)	−0.0078 (13)	−0.0053 (12)
N2	0.0290 (14)	0.0350 (15)	0.0375 (16)	−0.0144 (12)	−0.0070 (12)	−0.0088 (12)
C1	0.0304 (17)	0.0321 (17)	0.0395 (19)	−0.0143 (14)	−0.0057 (14)	−0.0089 (14)
C2	0.0299 (16)	0.0340 (17)	0.0304 (17)	−0.0148 (14)	−0.0030 (13)	−0.0093 (13)
C3	0.040 (2)	0.0370 (19)	0.046 (2)	−0.0223 (16)	−0.0045 (16)	−0.0094 (16)
C4	0.0324 (17)	0.043 (2)	0.041 (2)	−0.0219 (16)	−0.0042 (15)	−0.0096 (16)
C5	0.0307 (16)	0.0325 (16)	0.0300 (16)	−0.0147 (13)	−0.0050 (13)	−0.0100 (13)
C6	0.0397 (19)	0.0314 (17)	0.0400 (19)	−0.0200 (15)	−0.0049 (15)	−0.0113 (14)

Geometric parameters (Å, º)

Rb1—O3^i	2.987 (3)	O4—C6	1.234 (5)
Rb1—O3^{ii}	2.987 (3)	O5—H5A	0.84 (9)
Rb1—N2^{ii}	3.007 (3)	O5—H5B	0.82 (6)
Rb1—N2^i	3.007 (3)	N1—C2	1.336 (5)
Rb1—O5	3.096 (4)	N1—C3	1.340 (5)
Rb1—O5^{iii}	3.096 (4)	N2—C4	1.326 (5)
Rb1—O1^{iii}	3.137 (3)	N2—C5	1.344 (4)
Rb1—O1	3.137 (3)	N2—Rb1^{iv}	3.007 (3)
Rb1—H5B	3.16 (5)	C1—C2	1.513 (5)
O1—C1	1.204 (5)	C2—C5	1.389 (5)
O2—C1	1.307 (5)	C3—C4	1.391 (6)
O2—H2	0.8210	C3—H3	0.9300
O3—C6	1.274 (5)	C4—H4	0.9300
O3—Rb1^{iv}	2.987 (3)	C5—C6	1.506 (5)
O3—H1	0.9299		
O3^i—Rb1—O3^{ii}	180.00 (14)	O5^{iii}—Rb1—H5B	165.0 (3)
O3^i—Rb1—N2^{ii}	126.56 (8)	O1^{iii}—Rb1—H5B	104.1 (4)
O3^{ii}—Rb1—N2^{ii}	53.44 (8)	O1—Rb1—H5B	76.0 (10)
O3^i—Rb1—N2^i	53.44 (8)	C1—O1—Rb1	131.4 (2)
O3^{ii}—Rb1—N2^i	126.56 (8)	C1—O2—H2	111.2
N2^{ii}—Rb1—N2^i	180.0	C6—O3—Rb1^{iv}	128.1 (2)
O3^i—Rb1—O5	78.94 (9)	C6—O3—H1	116.0
O3^{ii}—Rb1—O5	101.06 (9)	Rb1^{iv}—O3—H1	115.9
N2^{ii}—Rb1—O5	70.89 (9)	Rb1—O5—H5A	95 (5)
N2^i—Rb1—O5	109.11 (9)	Rb1—O5—H5B	87 (4)
O3^i—Rb1—O5^{iii}	101.06 (9)	H5A—O5—H5B	104 (6)
O3^{ii}—Rb1—O5^{iii}	78.94 (9)	C2—N1—C3	116.8 (3)
N2^{ii}—Rb1—O5^{iii}	109.11 (9)	C4—N2—C5	117.1 (3)
N2^i—Rb1—O5^{iii}	70.89 (9)	C4—N2—Rb1^{iv}	119.0 (2)
O5—Rb1—O5^{iii}	180.00 (13)	C5—N2—Rb1^{iv}	123.5 (2)
O3^i—Rb1—O1^{iii}	81.24 (8)	O1—C1—O2	126.2 (3)
O3^{ii}—Rb1—O1^{iii}	98.76 (8)	O1—C1—C2	121.8 (3)
N2^{ii}—Rb1—O1^{iii}	76.07 (8)	O2—C1—C2	111.8 (3)
N2^i—Rb1—O1^{iii}	103.93 (8)	N1—C2—C5	121.9 (3)
O5—Rb1—O1^{iii}	118.29 (9)	N1—C2—C1	113.0 (3)
O5^{iii}—Rb1—O1^{iii}	61.71 (9)	C5—C2—C1	125.1 (3)

O3^i—Rb1—O1	98.76 (8)	N1—C3—C4	121.2 (3)
O3^{ii}—Rb1—O1	81.24 (8)	N1—C3—H3	119.4
N2^{ii}—Rb1—O1	103.93 (8)	C4—C3—H3	119.4
N2^i—Rb1—O1	76.07 (8)	N2—C4—C3	122.0 (3)
O5—Rb1—O1	61.71 (9)	N2—C4—H4	119.0
O5^{iii}—Rb1—O1	118.29 (9)	C3—C4—H4	119.0
O1^{iii}—Rb1—O1	180.00 (14)	N2—C5—C2	120.9 (3)
O3^i—Rb1—H5B	70.4 (9)	N2—C5—C6	117.8 (3)
O3^{ii}—Rb1—H5B	109.6 (9)	C2—C5—C6	121.2 (3)
N2^{ii}—Rb1—H5B	69.3 (10)	O4—C6—O3	125.3 (3)
N2^i—Rb1—H5B	110.7 (10)	O4—C6—C5	118.4 (3)
O5—Rb1—H5B	15.1 (10)	O3—C6—C5	116.1 (3)
O3^i—Rb1—O1—C1	4.0 (4)	Rb1^{iv}—N2—C4—C3	−174.7 (3)
O3^{ii}—Rb1—O1—C1	−176.0 (4)	N1—C3—C4—N2	1.8 (7)
N2^{ii}—Rb1—O1—C1	−127.2 (4)	C4—N2—C5—C2	−1.2 (5)
N2^i—Rb1—O1—C1	52.8 (4)	Rb1^{iv}—N2—C5—C2	171.6 (3)
O5—Rb1—O1—C1	−68.3 (4)	C4—N2—C5—C6	176.2 (3)
O5^{iii}—Rb1—O1—C1	111.7 (4)	Rb1^{iv}—N2—C5—C6	−11.0 (4)
Rb1—O1—C1—O2	164.6 (3)	N1—C2—C5—N2	3.7 (6)
Rb1—O1—C1—C2	−10.4 (6)	C1—C2—C5—N2	−178.5 (3)
C3—N1—C2—C5	−3.4 (6)	N1—C2—C5—C6	−173.6 (3)
C3—N1—C2—C1	178.7 (3)	C1—C2—C5—C6	4.2 (6)
O1—C1—C2—N1	72.3 (5)	Rb1^{iv}—O3—C6—O4	−179.2 (3)
O2—C1—C2—N1	−103.3 (4)	Rb1^{iv}—O3—C6—C5	5.3 (5)
O1—C1—C2—C5	−105.6 (5)	N2—C5—C6—O4	−171.9 (4)
O2—C1—C2—C5	78.8 (5)	C2—C5—C6—O4	5.5 (6)
C2—N1—C3—C4	0.7 (6)	N2—C5—C6—O3	3.9 (5)
C5—N2—C4—C3	−1.5 (6)	C2—C5—C6—O3	−178.7 (4)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H1···O3^v	0.93	1.55 (1)	2.468 (3)	170 (1)
O5—H5*A*···N1	0.84 (9)	2.07 (9)	2.888 (3)	168 (7)
O5—H5*B*···O4^{vi}	0.82 (6)	1.94 (6)	2.753 (3)	170 (1)
O2—H2···O5^{vii}	0.82	1.79	2.596 (6)	166 (1)

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