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2-Amino-5-chloropyridinium *cis*-diaquadioxalatochromate(III) sesquihydrate

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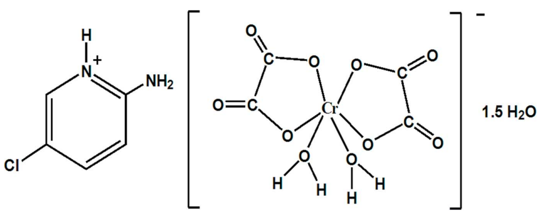
Key indicators: single-crystal X-ray study; *T* = 298 K; mean σ(C–C) = 0.004 Å; *R* factor = 0.029; *wR* factor = 0.074; data-to-parameter ratio = 14.0.

In the crystal structure of the title compound, $(C_5H_6ClN_2)[Cr(C_2O_4)_2(H_2O)_2]\cdot 1.5H_2O$, the Cr^{III} atom adopts a distorted octahedral geometry being coordinated by two O atoms of two *cis* water molecules and four O atoms from two chelating oxalate dianions. The *cis*-diaquadioxalatochromate(III) anions, 2-amino-5-chloropyridinium cations and uncoordinated water molecules are linked into a three-dimensional supramolecular array by O—H···O and N—H···O hydrogen-bonding interactions. One of the two independent lattice water molecules is situated on a twofold rotation axis.

Related literature

For structural characterization of salts containing the $[Cr(C_2O_4)_2(H_2O)_2]^-$ anion with various cations see: Bélombé *et al.* (2009); Nenwa *et al.* (2010); Chérif *et al.* (2011). For the building of hybrid supramolecular networks, see: Zhang *et al.* (2000); Paraschiv *et al.* (2007). For discussion of hydrogen bonding, see: Blessing (1986); Brown (1976).



Experimental

Crystal data

$(C_5H_6ClN_2)[Cr(C_2O_4)_2(H_2O)_2]\cdot$-
$1.5H_2O$
M_r = 420.66
Orthorhombic, *Fdd*2
a = 11.376 (2) Å
b = 53.041 (3) Å
c = 10.413 (2) Å
V = 6283.1 (17) $Å^3$
Z = 16
Mo *Kα* radiation
μ = 0.96 mm^{-1}
T = 298 K
0.42 × 0.32 × 0.13 mm

Data collection

Enraf–Nonius CAD-4
diffractometer
Absorption correction: ψ scan
(North *et al.*, 1968)
T_{min} = 0.792, T_{max} = 0.882
3854 measured reflections
3414 independent reflections
3180 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
2 standard reflections every 120 min
intensity decay: 5%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.074
S = 1.07
3414 reflections
243 parameters
8 restraints
H atoms treated by a mixture of
independent and constrained
refinement
$\Delta\rho_{max}$ = 0.30 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.31 e $Å^{-3}$
Absolute structure: Flack (1983),
1608 Friedel pairs
Flack parameter: 0.000 (18)

Table 1
Selected bond lengths (Å).

Cr—O1	1.9618 (19)	Cr—O6	1.9642 (18)
Cr—O2	1.9907 (19)	Cr—O1*W*	1.9978 (18)
Cr—O5	1.9547 (19)	Cr—O2*W*	1.9891 (19)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H11*W*···$O4^{i}$	0.85 (2)	1.84 (3)	2.686 (3)	172 (3)
O1*W*—H12*W*···$O3^{ii}$	0.85 (2)	1.94 (3)	2.769 (3)	163 (3)
O2*W*—H21*W*···$O3^{iii}$	0.90 (2)	1.91 (2)	2.775 (3)	161 (3)
O2*W*—H21*W*···$O4^{iii}$	0.90 (2)	2.37 (3)	2.909 (3)	118 (2)
O2*W*—H22*W*···$O4W^{iv}$	0.89 (2)	1.89 (3)	2.770 (3)	176 (3)
O3*W*—H31*W*···$O2^{v}$	0.88 (2)	2.12 (4)	2.979 (3)	167 (4)
O3*W*—H32*W*···O1	0.88 (2)	2.03 (4)	2.861 (3)	157 (4)
O4*W*—H4*W*···O6	0.90 (2)	2.12 (3)	3.011 (3)	173 (3)
N1—H1*A*···$O8^{vi}$	0.86	2.15	2.911 (4)	147
N1—H1*B*···$O3W^{iv}$	0.86	2.07	2.900 (4)	161
N2—H2···$O8^{vi}$	0.86	2.13	2.900 (4)	150
N2—H2···$O7^{vi}$	0.86	2.25	2.897 (4)	132

Symmetry codes: (i) $-x+\frac{1}{2}, -y, z-\frac{1}{2}$; (ii) $-x+1, -y, z$; (iii) $x-\frac{1}{2}, y, z-\frac{1}{2}$; (iv) $x-\frac{1}{2}, y, z+\frac{1}{2}$; (v) $x+\frac{1}{2}, y, z-\frac{1}{2}$; (vi) $x-\frac{1}{4}, -y+\frac{1}{4}, z+\frac{3}{4}$.

Data collection: *CAD-4 EXPRESS* (Duisenberg, 1992; Macíček & Yordanov, 1992); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2416).

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supplementary materials

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2-Amino-5-chloropyridinium *cis*-diaquadioxalatochromate(III) sesquihydrate

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Comment

It is well known that the use of hydrogen-bonding and *π-π* stacking interactions is a successful way to obtain a large variety of hybrid (organic/inorganic) compounds with extended supramolecular networks through self-assembly (Zhang *et al.*, 2000; Paraschiv *et al.*, 2007). Following this strategy, we recently published the structure of an organic-inorganic hybrid salt: 4-aminopyridinium *trans*-diaquadioxalatochromate(III) monohydrate (Chérif *et al.*, 2011). In this contribution, we report the crystal structure of an homologous salt with 2-amino-5-chloropyridinium as the organic cation.

The title compound appears to be the first member of salts of general formula (organic cation)$[Cr(C_2O_4)_2(H_2O)_2].xH_2O$ where $x = 0$ or $x = 1$ in which the complex anion $[Cr(C_2O_4)_2(H_2O)_2]^-$ adopts the *cis* geometry. The asymmetric unit is formed by a $[Cr(C_2O_4)_2(H_2O)_2]^-$ anion, a $(C_5H_6ClN_2)^+$ cation and 1.5 water molecules [The O4W atom is located on a special position (1/2, 0, *z*)] (Fig. 1). In the complex anion, each chromium atom is six-coordinated in a distorted octahedral geometry with two O water molecules in *cis* position and four oxalato-O atoms from two chelating oxalate groups (Table 1). The four Cr—O(ox) distances range from 1.955 (2) to 1.991 (2) Å; three of them in the range 1.955 (2)–1.965 (2) Å are comparable to those reported in similar compounds (Bélombé *et al.*, 2009; Nenwa *et al.*, 2010; Chérif *et al.*, 2011) but the last one, Cr—O2, is slightly longer. The Cr—O(water) distances are shorter than those observed for the quinolinium and 4-dimethylaminopyridinium compounds (Bélombé *et al.*, 2009; Nenwa *et al.*, 2010).

The structure can be described as segregated positive $(C_5H_6ClN_2)^+$ and negative $[[Cr(C_2O_4)_2(H_2O)_2]^- + H_2O]$ layers parallel to (010) (Fig. 2) and interconnected *via* N—H···O and O—H···O hydrogen bonds (Blessing, 1986; Brown, 1976). In fact, an extensive network of hydrogen bonds contributes to the stabilization of the structure. O—H···O hydrogen bonds involving all water molecules and some of the oxalato-O atoms provide the cohesion of the positive layers. The two N atoms of $(C_5H_6ClN_2)^+$ are hydrogen bonded to the peripheral O atoms of the oxalate groups (O8 and O7) and to the solvent water molecules (O3W) connecting the positive and negative layers (Fig. 3, Table 2).

Experimental

Ethanol solutions of $C_5H_5ClN_2$ (1 mmol) (10 mL) and $H_2C_2O_4.2H_2O$ (2 mmol) (10 mL) were added to $CrCl_3.6H_2O$ (1 mmol) dissolved in 10 mL of ethanol and stirred for 5 h. The resulting violet solution was left at room temperature and crystals suitable for X-ray diffraction were obtained after two weeks of slow evaporation.

Refinement

All non hydrogen atoms were treated anisotropically. Water H atoms were initially located in a difference Fourier map and refined with restraints: d(O—H)=0.90 (2) Å and $U_{iso}(H)=1.5U_{eq}(O)$. All other H atoms were constrained to an ideal geometry with d(C—H)=0.93 Å, d(N—H)=0.86 Å and $U_{iso}(H)=1.2U_{eq}$(C or N).

Computing details

Data collection: *CAD-4 EXPRESS* (Duisenberg, 1992; Macíček & Yordanov, 1992); cell refinement: *CAD-4 EXPRESS* (Duisenberg, 1992; Macíček & Yordanov, 1992); data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

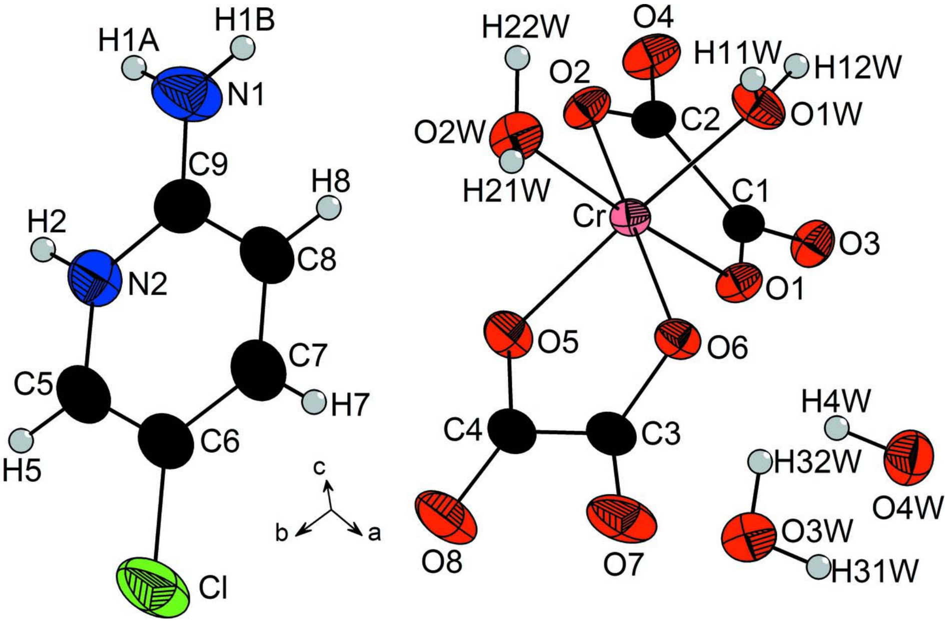

Figure 1

The asymmetric unit of $(C_5H_6ClN_2)[Cr(C_2O_4)_2(H_2O)_2].1.5H_2O$ with the atom-numbering scheme. Thermal ellipsoids are drawn at the 50% probability level for non-H atoms.

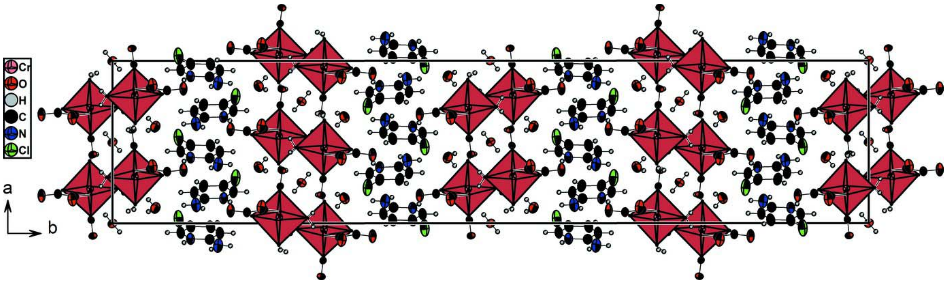

Figure 2

Projection of $(C_5H_6ClN_2)[Cr(C_2O_4)_2(H_2O)_2].1.5H_2O$ structure along the *c* axis.

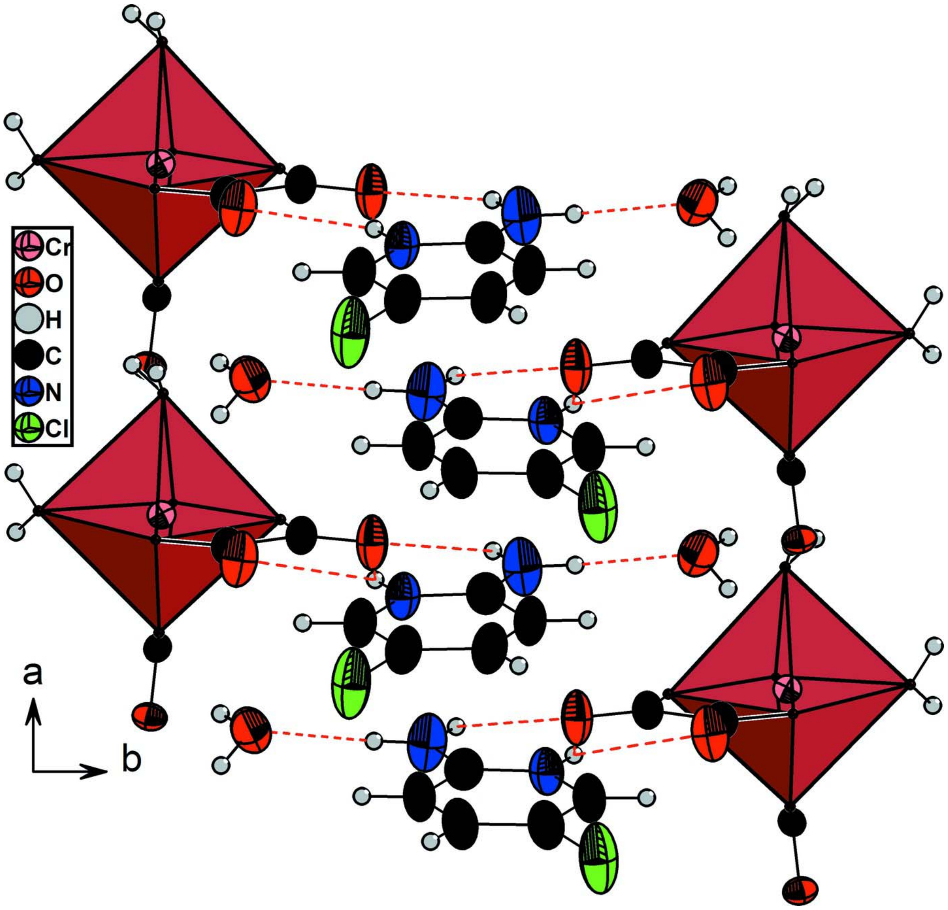

Figure 3

N—H···O hydrogen bonds (dashed lines) in $(C_5H_6ClN_2)[Cr(C_2O_4)_2(H_2O)_2].1.5H_2O$ showing the connection between positive and negative layers.

2-Amino-5-chloropyridinium *cis*-diaquadioxalatochromate(III) sesquihydrate

Crystal data

$(C_5H_6ClN_2)[Cr(C_2O_4)_2(H_2O)_2]\cdot 1.5H_2O$	$F(000) = 3424$
$M_r = 420.66$	$D_x = 1.779$ Mg m^{-3}
Orthorhombic, *Fdd*2	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: F 2 -2d	Cell parameters from 25 reflections
$a = 11.376$ (2) Å	$\theta = 10$–$15°$
$b = 53.041$ (3) Å	$\mu = 0.96$ mm^{-1}
$c = 10.413$ (2) Å	$T = 298$ K
$V = 6283.1$ (17) Å^3	Prism, violet
$Z = 16$	0.42 × 0.32 × 0.13 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	Absorption correction: ψ scan (North *et al.*, 1968)
Radiation source: fine-focus sealed tube	$T_{min} = 0.792$, $T_{max} = 0.882$
Graphite monochromator	3854 measured reflections
$\omega/2\theta$ scans	3414 independent reflections
	3180 reflections with $I > 2\sigma(I)$

R_{int} = 0.022
θ_{max} = 27.0°, θ_{min} = 2.7°
$h = -14 \rightarrow 1$
$k = -1 \rightarrow 67$
$l = -13 \rightarrow 13$
2 standard reflections every 120 min
intensity decay: 5%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.074$
$S = 1.07$
3414 reflections
243 parameters
8 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0316P)^2 + 13.7688P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Absolute structure: Flack (1983), 1608 Friedel pairs
Flack parameter: 0.000 (18)

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cr	0.28854 (3)	0.029597 (7)	0.12687 (3)	0.01808 (9)
O1	0.45606 (16)	0.02882 (3)	0.17139 (17)	0.0219 (4)
O2	0.27072 (17)	0.03331 (4)	0.31611 (17)	0.0238 (4)
O3	0.57607 (15)	0.02584 (3)	0.34029 (18)	0.0245 (4)
O4	0.37907 (17)	0.03041 (4)	0.49507 (17)	0.0295 (4)
O5	0.29574 (17)	0.06593 (3)	0.09653 (16)	0.0286 (4)
O6	0.32410 (18)	0.02782 (3)	−0.05749 (16)	0.0228 (4)
O7	0.3518 (3)	0.05318 (4)	−0.2259 (2)	0.0467 (6)
O8	0.3288 (3)	0.09378 (4)	−0.0606 (2)	0.0471 (6)
O1W	0.28282 (17)	−0.00790 (3)	0.1438 (2)	0.0289 (4)
H11W	0.228 (2)	−0.0153 (6)	0.103 (3)	0.043*
H12W	0.313 (3)	−0.0148 (6)	0.210 (3)	0.043*
O2W	0.11515 (17)	0.03017 (4)	0.10241 (18)	0.0297 (5)
H21W	0.086 (3)	0.0282 (7)	0.023 (2)	0.045*
H22W	0.075 (3)	0.0209 (6)	0.158 (3)	0.045*
O3W	0.5956 (2)	0.05669 (5)	−0.0077 (3)	0.0541 (7)
H31W	0.646 (3)	0.0476 (8)	−0.052 (4)	0.081*
H32W	0.572 (4)	0.0474 (8)	0.058 (3)	0.081*
O4W	0.5000	0.0000	−0.2206 (3)	0.0366 (7)
H4W	0.448 (3)	0.0093 (7)	−0.177 (3)	0.055*

C1	0.4779 (2)	0.02831 (4)	0.2921 (2)	0.0186 (5)
C2	0.3677 (2)	0.03087 (4)	0.3782 (2)	0.0204 (5)
C3	0.3332 (2)	0.04963 (5)	−0.1130 (3)	0.0264 (5)
C4	0.3183 (3)	0.07223 (5)	−0.0199 (3)	0.0290 (6)
C5	0.1933 (3)	0.15991 (6)	0.3233 (3)	0.0418 (8)
H5	0.1933	0.1774	0.3230	0.050*
C6	0.2315 (3)	0.14673 (6)	0.2190 (3)	0.0423 (7)
C7	0.2297 (3)	0.12042 (6)	0.2198 (3)	0.0438 (8)
H7	0.2549	0.1114	0.1482	0.053*
C8	0.1909 (3)	0.10801 (6)	0.3254 (3)	0.0422 (8)
H8	0.1899	0.0905	0.3262	0.051*
C9	0.1518 (3)	0.12160 (6)	0.4344 (3)	0.0379 (7)
N1	0.1138 (3)	0.11041 (6)	0.5402 (3)	0.0565 (9)
H1A	0.0913	0.1193	0.6047	0.068*
H1B	0.1115	0.0942	0.5445	0.068*
N2	0.1552 (3)	0.14686 (5)	0.4280 (2)	0.0394 (6)
H2	0.1319	0.1553	0.4938	0.047*
Cl	0.27889 (13)	0.162724 (19)	0.08436 (9)	0.0737 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr	0.02037 (17)	0.02121 (17)	0.01267 (16)	−0.00028 (16)	−0.00167 (15)	0.00091 (14)
O1	0.0205 (9)	0.0299 (10)	0.0153 (8)	−0.0020 (7)	−0.0002 (7)	−0.0005 (7)
O2	0.0199 (9)	0.0364 (10)	0.0152 (8)	0.0007 (7)	0.0009 (7)	−0.0006 (7)
O3	0.0202 (9)	0.0318 (10)	0.0217 (9)	0.0023 (7)	−0.0022 (7)	−0.0021 (7)
O4	0.0292 (10)	0.0449 (12)	0.0144 (9)	−0.0055 (8)	−0.0002 (8)	−0.0022 (7)
O5	0.0426 (11)	0.0237 (9)	0.0195 (10)	0.0004 (8)	0.0002 (8)	−0.0017 (7)
O6	0.0323 (10)	0.0215 (9)	0.0147 (9)	−0.0017 (7)	0.0003 (8)	−0.0004 (6)
O7	0.0840 (19)	0.0369 (12)	0.0193 (10)	−0.0082 (12)	0.0086 (11)	0.0046 (9)
O8	0.0819 (18)	0.0244 (11)	0.0352 (12)	−0.0008 (11)	0.0065 (12)	0.0055 (9)
O1W	0.0335 (10)	0.0240 (9)	0.0290 (11)	−0.0057 (8)	−0.0117 (8)	0.0064 (8)
O2W	0.0230 (10)	0.0415 (12)	0.0247 (12)	−0.0020 (8)	−0.0070 (8)	0.0010 (8)
O3W	0.0566 (16)	0.0432 (14)	0.0626 (17)	0.0086 (12)	0.0283 (14)	0.0134 (12)
O4W	0.0340 (16)	0.0394 (18)	0.0365 (16)	0.0055 (13)	0.000	0.000
C1	0.0209 (12)	0.0191 (11)	0.0160 (11)	−0.0019 (9)	0.0000 (10)	−0.0007 (9)
C2	0.0211 (11)	0.0225 (11)	0.0177 (11)	−0.0028 (9)	0.0009 (10)	0.0008 (10)
C3	0.0349 (13)	0.0254 (12)	0.0189 (12)	−0.0019 (10)	−0.0013 (11)	0.0022 (10)
C4	0.0372 (14)	0.0234 (13)	0.0263 (13)	−0.0009 (11)	0.0028 (11)	0.0011 (11)
C5	0.063 (2)	0.0263 (15)	0.0361 (16)	0.0034 (14)	0.0054 (16)	−0.0047 (12)
C6	0.062 (2)	0.0331 (16)	0.0318 (15)	0.0050 (15)	0.0083 (16)	−0.0007 (13)
C7	0.069 (2)	0.0321 (15)	0.0305 (15)	0.0067 (15)	0.0075 (16)	−0.0089 (13)
C8	0.064 (2)	0.0254 (14)	0.0373 (16)	0.0024 (15)	0.0092 (16)	−0.0069 (12)
C9	0.0452 (19)	0.0375 (16)	0.0311 (15)	−0.0007 (14)	0.0043 (13)	−0.0044 (13)
N1	0.092 (3)	0.0399 (16)	0.0380 (16)	−0.0064 (16)	0.0192 (17)	−0.0017 (13)
N2	0.0595 (18)	0.0302 (13)	0.0284 (12)	0.0027 (12)	0.0068 (12)	−0.0092 (11)
Cl	0.1375 (11)	0.0385 (5)	0.0451 (5)	0.0074 (6)	0.0346 (7)	0.0065 (4)

Geometric parameters (Å, º)

Cr—O1	1.9618 (19)	O3W—H32W	0.883 (19)
Cr—O2	1.9907 (19)	O4W—H4W	0.897 (18)
Cr—O5	1.9547 (19)	C1—C2	1.547 (3)
Cr—O6	1.9642 (18)	C3—C4	1.551 (4)
Cr—O1W	1.9978 (18)	C5—N2	1.363 (4)
Cr—O2W	1.9891 (19)	C5—C6	1.363 (4)
O1—C1	1.282 (3)	C5—H5	0.9300
O2—C2	1.286 (3)	C6—C7	1.396 (4)
O3—C1	1.231 (3)	C6—Cl	1.725 (3)
O4—C2	1.224 (3)	C7—C8	1.355 (5)
O5—C4	1.284 (3)	C7—H7	0.9300
O6—C3	1.297 (3)	C8—C9	1.417 (4)
O7—C3	1.209 (3)	C8—H8	0.9300
O8—C4	1.225 (3)	C9—N1	1.324 (4)
O1W—H11W	0.850 (18)	C9—N2	1.342 (4)
O1W—H12W	0.850 (18)	N1—H1A	0.8600
O2W—H21W	0.896 (18)	N1—H1B	0.8600
O2W—H22W	0.885 (18)	N2—H2	0.8600
O3W—H31W	0.880 (19)		
O5—Cr—O1	91.04 (8)	O4—C2—C1	119.3 (2)
O5—Cr—O6	83.15 (7)	O2—C2—C1	114.4 (2)
O1—Cr—O6	91.71 (8)	O7—C3—O6	125.9 (3)
O5—Cr—O2W	90.33 (9)	O7—C3—C4	120.4 (2)
O1—Cr—O2W	173.68 (8)	O6—C3—C4	113.7 (2)
O6—Cr—O2W	94.58 (8)	O8—C4—O5	126.1 (3)
O5—Cr—O2	93.82 (8)	O8—C4—C3	119.7 (2)
O1—Cr—O2	82.36 (7)	O5—C4—C3	114.3 (2)
O6—Cr—O2	173.31 (9)	N2—C5—C6	118.6 (3)
O2W—Cr—O2	91.39 (8)	N2—C5—H5	120.7
O5—Cr—O1W	175.72 (9)	C6—C5—H5	120.7
O1—Cr—O1W	89.42 (8)	C5—C6—C7	120.2 (3)
O6—Cr—O1W	92.58 (8)	C5—C6—Cl	119.7 (3)
O2W—Cr—O1W	89.67 (9)	C7—C6—Cl	120.1 (3)
O2—Cr—O1W	90.46 (8)	C8—C7—C6	119.7 (3)
C1—O1—Cr	114.86 (16)	C8—C7—H7	120.2
C2—O2—Cr	113.60 (17)	C6—C7—H7	120.2
C4—O5—Cr	114.69 (16)	C7—C8—C9	120.3 (3)
C3—O6—Cr	114.13 (16)	C7—C8—H8	119.8
Cr—O1W—H11W	116 (2)	C9—C8—H8	119.8
Cr—O1W—H12W	119 (3)	N1—C9—N2	119.9 (3)
H11W—O1W—H12W	120 (3)	N1—C9—C8	122.8 (3)
Cr—O2W—H21W	119 (2)	N2—C9—C8	117.3 (3)
Cr—O2W—H22W	115 (2)	C9—N1—H1A	120.0
H21W—O2W—H22W	110 (3)	C9—N1—H1B	120.0
H31W—O3W—H32W	107 (5)	H1A—N1—H1B	120.0
O3—C1—O1	125.3 (2)	C9—N2—C5	123.8 (3)
O3—C1—C2	120.5 (2)	C9—N2—H2	118.1

O1—C1—C2	114.2 (2)	C5—N2—H2	118.1
O4—C2—O2	126.3 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H11*W*···O4$^{\rm i}$	0.85 (2)	1.84 (3)	2.686 (3)	172 (3)
O1*W*—H12*W*···O3$^{\rm ii}$	0.85 (2)	1.94 (3)	2.769 (3)	163 (3)
O2*W*—H21*W*···O3$^{\rm iii}$	0.90 (2)	1.91 (2)	2.775 (3)	161 (3)
O2*W*—H21*W*···O4$^{\rm iii}$	0.90 (2)	2.37 (3)	2.909 (3)	118 (2)
O2*W*—H22*W*···O4*W*$^{\rm iv}$	0.89 (2)	1.89 (3)	2.770 (3)	176 (3)
O3*W*—H31*W*···O2$^{\rm v}$	0.88 (2)	2.12 (4)	2.979 (3)	167 (4)
O3*W*—H32*W*···O1	0.88 (2)	2.03 (4)	2.861 (3)	157 (4)
O4*W*—H4*W*···O6	0.90 (2)	2.12 (3)	3.011 (3)	173 (3)
N1—H1*A*···O8$^{\rm vi}$	0.86	2.15	2.911 (4)	147
N1—H1*B*···O3*W*$^{\rm iv}$	0.86	2.07	2.900 (4)	161
N2—H2···O8$^{\rm vi}$	0.86	2.13	2.900 (4)	150
N2—H2···O7$^{\rm vi}$	0.86	2.25	2.897 (4)	132

Symmetry codes: (i) $-x+1/2, -y, z-1/2$; (ii) $-x+1, -y, z$; (iii) $x-1/2, y, z-1/2$; (iv) $x-1/2, y, z+1/2$; (v) $x+1/2, y, z-1/2$; (vi) $x-1/4, -y+1/4, z+3/4$.