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trans-Aqua(4,7-diazadecane-1,10-diamine-κ^4N)fluoridochromium(III) bis(perchlorate) monohydrate

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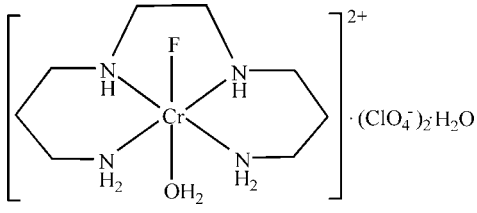
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.011 Å; H-atom completeness 93%; R factor = 0.077; wR factor = 0.228; data-to-parameter ratio = 17.9.

In the title compound, $[CrF(C_8H_{20}N_4)(H_2O)](ClO_4)_2\cdot H_2O$, the Cr atom is in a slightly distorted octahedral environment, coordinated by four N atoms of the 4,7-diazadecane-1,10-diamine ligand, one water molecule and an F atom *trans* to water. The five-membered chelate ring is in a *gauche* form, while the two six-membered chelate rings are in chair conformations. The crystal structure is stabilized by several hydrogen bonds.

Related literature

For the synthesis, see: Glerup *et al.* (1970). For related structures, see: Brencic *et al.* (1985); Choi *et al.* (1995, 2004, 2006, 2008). For other related literature, see: Choi & Hoggard (1992); Poon & Pun (1980); Stearns & Armstrong (1992).



Experimental

Crystal data

$[CrF(C_8H_{20}N_4)(H_2O)](ClO_4)_2\cdot H_2O$
M_r = 480.23
Monoclinic, $P2_1/c$
a = 9.950 (1) Å
b = 16.893 (2) Å
c = 12.008 (1) Å
β = 108.65 (1)°
V = 1912.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.94 mm^{-1}
T = 298 (2) K
0.43 × 0.30 × 0.25 mm

Data collection

Stoe Stadi-4 diffractometer
Absorption correction: numerical (*X-SHAPE*; Stoe, 1996)
T_{min} = 0.686, T_{max} = 0.889
4347 measured reflections
4347 independent reflections
3245 reflections with $I > 2\sigma(I)$
3 standard reflections
frequency: 60 min
intensity decay: 3.1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.228
S = 1.09
4347 reflections
243 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.07 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1OA···F^{i}	0.86 (6)	1.72 (6)	2.564 (5)	168 (8)
O1W—H1OB···O2W	0.74 (6)	1.92 (6)	2.617 (6)	158 (7)
N1—H1AN···O2^{ii}	0.91	2.42	3.332 (11)	177
N2—H1$N2$···O7^{iii}	0.91	2.45	3.154 (10)	134
N3—H3BN···O5	0.90	2.36	3.242 (10)	167
N4—H4BN···O5	0.90	2.43	3.062 (10)	127
C1—H1B···O4^{iv}	0.97	2.53	3.141 (13)	121

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

Data collection: *STADI4* (Stoe & Cie, 1996); cell refinement: *STADI4*; data reduction: *X-RED* (Stoe & Cie, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2211).

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supporting information

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trans-Aqua(4,7-diazadecane-1,10-diamine-κ^4N)fluoridochromium(III) bis(perchlorate) monohydrate

Jong-Ha Choi and Uk Lee

S1. Comment

Acyclic flexible 4,7-diazadecane-1,10-diamine (3,2,3-tet) and its related tetradentate ligands provide a rich field of geometric and conformational isomers in octahedral transition metal complexes (Choi *et al.*, 2008). The electronic absorption and infrared spectra often can be used diagnostically to identify the geometric isomers of chromium(III) complexes complexes (Poon & Pun, 1980; Choi & Hoggard, 1992). However, it should be noted that the assignments based on spectroscopic investigations are not always conclusive (Stearns & Armstrong, 1992). [Cr(3,2,3-tet)F(H_2O)]X_2 can adopt a diverse stereochemistry and configuration, but no structures have been reported. Thus we here report the crystal structure of the title complex (Fig. 1) in order to confirm the geometric configuration.

There are one fluorine atom and one water molecule coordinated to the chromium atom in a trans arrangement with an F—Cr—O1w bond angle of 179.5 (2)°. The rest of the coordination sites are occupied by four nitrogen atoms from 3,2,3-tet ligand in the equatorial plane. The mean Cr—N bond length of 2.079 (4) Å is normal, agreeing with literature values (Choi *et al.*, 1995; Choi *et al.*, 2004). The Cr—N1 and Cr—N2 bond lengths of 2.068 (5) and 2.070 (4) Å of secondary amines are slightly shorter than Cr—N3 and Cr—N4 distances of 2.082 (5) and 2.095 (4) Å of primary amines. The Cr—F distance of 1.881 (3) Å and Cr—O1W of 1.996 (4) Å are also compararble to the values of 1.870 (1) Å and 2.023 (2) Å found in trans-[Cr([15]aneN4)F_2]ClO_4 (Choi *et al.*, 2006) and trans-[Cr(NH_3)$_4$Cl(H_2O)]Cl_2 (Brencic *et al.*, 1985), respectively. The short Cr—F bond length suggests a strong bond.

The uncoordinated ClO_4^- anions and one water molecule remain outside the coordination sphere. There is an extensive hydrogen bonding network (Table 2) between the oxygens of the ClO_4^- anions, fluorine atom, water molecule, C—H and the N—H groups of the 3,2,3-tet ligand as shown in Figure 2. These hydrogen-bonded networks help to stabilize the crystal structure.

S2. Experimental

As starting material, trans-[Cr(3,2,3-tet)F_2]ClO_4 was prepared according to the literature (Glerup *et al.*, 1970). The complex trans-[Cr(3,2,3-tet)F_2]ClO_4 was dissolved in 0.2 M $HClO_4$. The solution was heated at 333 K for 50 min and then a saturated solution of sodium perchlorate was added. Dark red crystals suitable for an X-ray structural determination were deposited over several days as the solution evaporated.

S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å for aromatic H atoms and 0.98 Å for methyl H atoms, respectively, and with U_{iso}(H) = 1.2U_{eq}(C) for aromatic and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms. H atoms of O1w were located in a difference Fourier map and refined with constraints. Reasonable positions of H atoms for O2w could not obtained from a difference Fourier map.

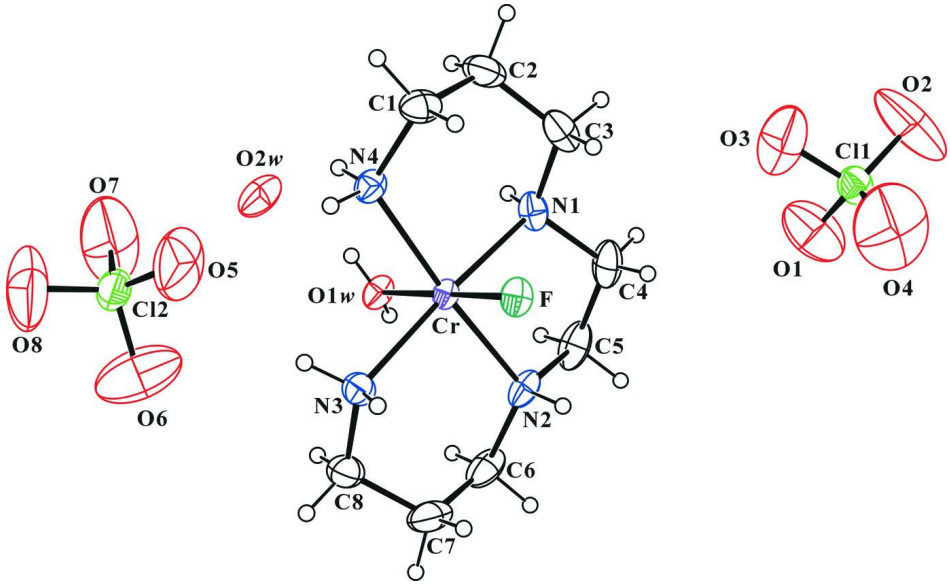

Figure 1

Molecular structure (30% probability ellipsoids) of the title compound.

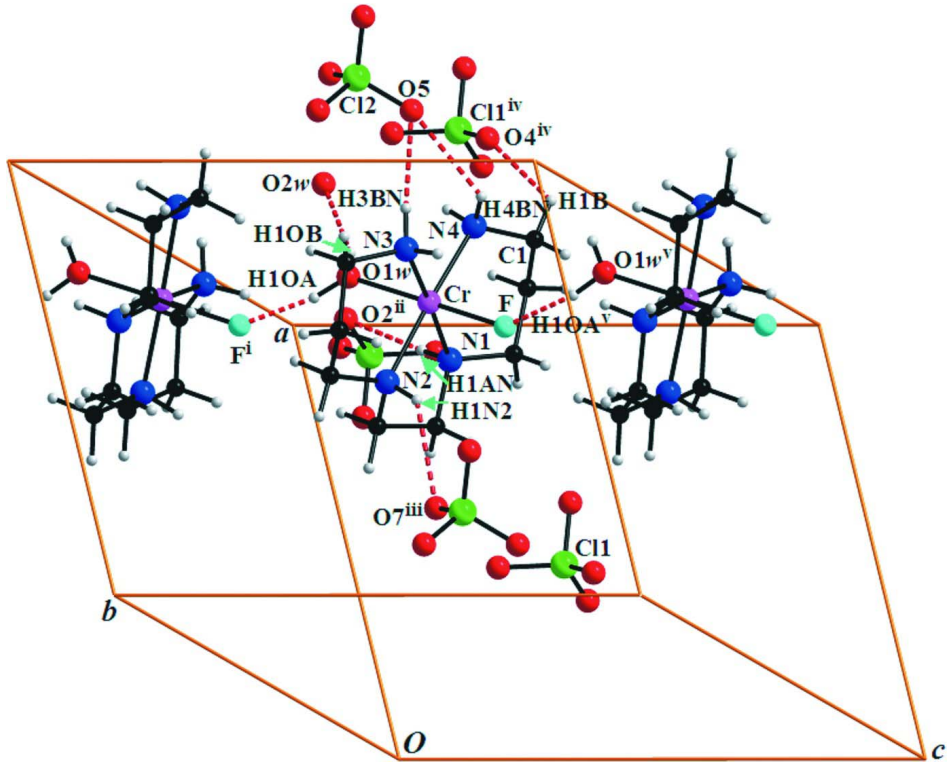

Figure 2

Hydrogen-bond interactions (dashed lines) in the title compound. [Symmetry codes: (i) x, -y+3/2, z-1/2; (ii) -x+1, -y+1, -z+1; (iii) x-1, y, z; (iv) x+1, y, z; (v) x, -y+3/2, z+1/2.]

trans-Aqua(4,7-diazadecane-1,10-diamine-κ^4N)fluoridochromium(III) bis(perchlorate) monohydrate

Crystal data

$[CrF(C_8H_{20}N_4)(H_2O)](ClO_4)_2\cdot H_2O$
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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.950$ (1) Å
$b = 16.893$ (2) Å
$c = 12.008$ (1) Å
$\beta = 108.65$ (1)°
$V = 1912.4$ (4) Å^3
$Z = 4$
$F(000) = 996$
$D_x = 1.668$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 32 reflections
$\theta = 19.0$–20.8°
$\mu = 0.94$ mm^{-1}
$T = 298$ K
Block, dark red
0.43 × 0.30 × 0.25 mm

Data collection

Stoe Stadi-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: numerical (*X-SHAPE*; Stoe, 1996)
$T_{min} = 0.686$, $T_{max} = 0.889$
4347 measured reflections
4347 independent reflections
3245 reflections with $I > 2\sigma(I)$
$R_{int} = 0.000$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.2°$
$h = -12\rightarrow12$
$k = 0\rightarrow21$
$l = 0\rightarrow15$
3 standard reflections every 60 min
intensity decay: 3.1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.076$
$wR(F^2) = 0.228$
$S = 1.09$
4347 reflections
243 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.1014P)^2 + 6.2787P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.07$ e Å^{-3}
$\Delta\rho_{min} = -0.60$ e Å^{-3}

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.

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 $F^2 > 2$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	0.77207 (8)	0.74161 (4)	0.61410 (6)	0.0294 (2)
Cl1	0.25308 (17)	0.51481 (9)	0.64339 (13)	0.0538 (4)
Cl2	1.24851 (16)	0.84876 (12)	0.62990 (16)	0.0643 (5)

F	0.7140 (3)	0.74557 (18)	0.7485 (2)	0.0404 (7)
N1	0.6809 (5)	0.6308 (3)	0.5748 (4)	0.0458 (11)
H1AN	0.7106	0.6106	0.5164	0.055*
N2	0.5732 (4)	0.7824 (3)	0.5160 (4)	0.0454 (11)
H1N2	0.5272	0.7928	0.5688	0.055*
N3	0.8507 (5)	0.8564 (3)	0.6485 (4)	0.0435 (10)
H3AN	0.8338	0.8731	0.7139	0.052*
H3BN	0.9455	0.8539	0.6654	0.052*
N4	0.9663 (4)	0.6910 (3)	0.7114 (4)	0.0414 (10)
H4AN	1.0105	0.6748	0.6607	0.050*
H4BN	1.0203	0.7291	0.7565	0.050*
C1	0.9611 (7)	0.6231 (4)	0.7887 (5)	0.0523 (14)
H1A	0.9198	0.6405	0.8476	0.063*
H1B	1.0569	0.6051	0.8291	0.063*
C2	0.8750 (8)	0.5550 (4)	0.7202 (7)	0.0643 (18)
H2A	0.8905	0.5089	0.7711	0.077*
H2B	0.9095	0.5423	0.6554	0.077*
C3	0.7171 (8)	0.5710 (4)	0.6718 (6)	0.0639 (18)
H3A	0.6679	0.5219	0.6425	0.077*
H3B	0.6840	0.5898	0.7348	0.077*
C4	0.5235 (7)	0.6431 (5)	0.5235 (6)	0.0643 (19)
H4A	0.4797	0.5967	0.4788	0.077*
H4B	0.4827	0.6510	0.5860	0.077*
C5	0.4968 (6)	0.7142 (5)	0.4451 (5)	0.065 (2)
H5A	0.5311	0.7049	0.3791	0.078*
H5B	0.3959	0.7252	0.4147	0.078*
C6	0.5603 (7)	0.8554 (5)	0.4447 (5)	0.0629 (19)
H6A	0.4607	0.8690	0.4110	0.076*
H6B	0.5972	0.8452	0.3805	0.076*
C7	0.6384 (8)	0.9245 (4)	0.5152 (7)	0.068 (2)
H7A	0.6117	0.9719	0.4677	0.082*
H7B	0.6070	0.9311	0.5833	0.082*
C8	0.7971 (7)	0.9183 (4)	0.5569 (6)	0.0586 (16)
H8A	0.8289	0.9063	0.4904	0.070*
H8B	0.8372	0.9690	0.5885	0.070*
O1	0.2360 (12)	0.5429 (5)	0.5295 (7)	0.143 (3)
O2	0.1991 (14)	0.4382 (5)	0.6357 (8)	0.183 (5)
O3	0.3986 (11)	0.5079 (10)	0.6805 (16)	0.257 (8)
O4	0.2177 (16)	0.5591 (8)	0.7161 (12)	0.231 (7)
O5	1.1848 (9)	0.8171 (7)	0.7049 (9)	0.173 (5)
O6	1.1523 (12)	0.9046 (7)	0.5676 (8)	0.186 (5)
O7	1.2769 (14)	0.7974 (8)	0.5576 (17)	0.277 (10)
O8	1.3760 (9)	0.8831 (8)	0.6872 (10)	0.188 (5)
O1W	0.8322 (4)	0.7379 (3)	0.4706 (3)	0.0412 (9)
H1OA	0.782 (7)	0.743 (4)	0.398 (6)	0.07 (2)*
H1OB	0.896 (6)	0.714 (4)	0.474 (5)	0.046 (19)*
O2W	1.0660 (6)	0.6849 (4)	0.4419 (5)	0.0841 (17)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr	0.0281 (4)	0.0384 (4)	0.0229 (4)	−0.0002 (3)	0.0098 (3)	−0.0013 (3)
Cl1	0.0632 (9)	0.0531 (8)	0.0533 (8)	−0.0025 (7)	0.0302 (7)	−0.0047 (6)
Cl2	0.0436 (8)	0.0758 (11)	0.0728 (11)	−0.0005 (7)	0.0175 (7)	0.0124 (9)
F	0.0427 (16)	0.0559 (18)	0.0266 (13)	−0.0032 (13)	0.0166 (12)	−0.0043 (12)
N1	0.049 (3)	0.050 (3)	0.044 (2)	−0.015 (2)	0.022 (2)	−0.013 (2)
N2	0.032 (2)	0.073 (3)	0.032 (2)	0.010 (2)	0.0118 (17)	0.001 (2)
N3	0.048 (3)	0.040 (2)	0.048 (3)	−0.0004 (19)	0.022 (2)	−0.0008 (19)
N4	0.035 (2)	0.051 (3)	0.037 (2)	0.0042 (19)	0.0107 (18)	0.0039 (19)
C1	0.064 (4)	0.053 (3)	0.042 (3)	0.014 (3)	0.019 (3)	0.010 (3)
C2	0.083 (5)	0.036 (3)	0.078 (5)	0.007 (3)	0.032 (4)	0.011 (3)
C3	0.082 (5)	0.048 (3)	0.071 (4)	−0.019 (3)	0.038 (4)	−0.002 (3)
C4	0.043 (3)	0.082 (5)	0.068 (4)	−0.026 (3)	0.018 (3)	−0.027 (4)
C5	0.033 (3)	0.113 (6)	0.041 (3)	−0.008 (3)	0.001 (2)	−0.018 (4)
C6	0.048 (3)	0.097 (5)	0.045 (3)	0.030 (3)	0.017 (3)	0.029 (3)
C7	0.077 (5)	0.060 (4)	0.077 (5)	0.033 (4)	0.036 (4)	0.022 (4)
C8	0.067 (4)	0.044 (3)	0.077 (4)	0.008 (3)	0.041 (4)	0.012 (3)
O1	0.220 (10)	0.118 (6)	0.095 (5)	−0.040 (6)	0.058 (6)	−0.005 (5)
O2	0.337 (15)	0.099 (6)	0.131 (7)	−0.105 (8)	0.099 (9)	−0.011 (5)
O3	0.109 (8)	0.285 (16)	0.40 (2)	0.041 (10)	0.120 (11)	0.135 (16)
O4	0.320 (17)	0.204 (12)	0.246 (13)	−0.030 (11)	0.198 (13)	−0.117 (10)
O5	0.113 (6)	0.241 (12)	0.196 (10)	−0.005 (7)	0.091 (7)	0.089 (9)
O6	0.198 (10)	0.226 (12)	0.105 (6)	0.110 (9)	0.007 (6)	0.029 (7)
O7	0.226 (13)	0.185 (11)	0.53 (3)	−0.062 (9)	0.278 (17)	−0.190 (15)
O8	0.091 (6)	0.270 (13)	0.173 (9)	−0.082 (7)	0.002 (5)	0.040 (9)
O1W	0.0369 (19)	0.063 (2)	0.0266 (17)	0.0085 (18)	0.0144 (15)	0.0048 (16)
O2W	0.061 (3)	0.110 (5)	0.088 (4)	0.030 (3)	0.033 (3)	0.003 (3)

Geometric parameters (Å, º)

Cr—F	1.881 (3)	N4—H4BN	0.900
Cr—O1W	1.997 (3)	C1—C2	1.511 (10)
Cr—N1	2.068 (5)	C1—H1A	0.970
Cr—N2	2.070 (4)	C1—H1B	0.970
Cr—N3	2.082 (5)	C2—C3	1.516 (10)
Cr—N4	2.095 (4)	C2—H2A	0.970
Cl1—O4	1.282 (8)	C2—H2B	0.970
Cl1—O3	1.377 (11)	C3—H3A	0.970
Cl1—O2	1.392 (8)	C3—H3B	0.970
Cl1—O1	1.405 (8)	C4—C5	1.498 (11)
Cl2—O7	1.321 (10)	C4—H4A	0.970
Cl2—O8	1.364 (8)	C4—H4B	0.970
Cl2—O5	1.365 (7)	C5—H5A	0.970
Cl2—O6	1.381 (9)	C5—H5B	0.970
N1—C3	1.496 (8)	C6—C7	1.504 (11)
N1—C4	1.502 (8)	C6—H6A	0.970

N1—H1AN	0.910	C6—H6B	0.970
N2—C6	1.484 (8)	C7—C8	1.499 (10)
N2—C5	1.488 (8)	C7—H7A	0.970
N2—H1N2	0.910	C7—H7B	0.970
N3—C8	1.488 (8)	C8—H8A	0.970
N3—H3AN	0.900	C8—H8B	0.970
N3—H3BN	0.900	O1W—H1OA	0.86 (6)
N4—C1	1.487 (7)	O1W—H1OB	0.74 (6)
N4—H4AN	0.900		

F—Cr—O1W	179.49 (16)	N4—C1—C2	112.0 (5)
F—Cr—N1	89.72 (16)	N4—C1—H1A	109.2
O1W—Cr—N1	90.30 (18)	C2—C1—H1A	109.2
F—Cr—N2	88.63 (15)	N4—C1—H1B	109.2
O1W—Cr—N2	90.87 (17)	C2—C1—H1B	109.2
N1—Cr—N2	84.3 (2)	H1A—C1—H1B	107.9
F—Cr—N3	89.77 (16)	C1—C2—C3	114.3 (5)
O1W—Cr—N3	90.17 (18)	C1—C2—H2A	108.7
N1—Cr—N3	176.23 (19)	C3—C2—H2A	108.7
N2—Cr—N3	91.9 (2)	C1—C2—H2B	108.7
F—Cr—N4	91.04 (15)	C3—C2—H2B	108.7
O1W—Cr—N4	89.47 (17)	H2A—C2—H2B	107.6
N1—Cr—N4	90.98 (19)	N1—C3—C2	112.4 (5)
N2—Cr—N4	175.3 (2)	N1—C3—H3A	109.1
N3—Cr—N4	92.77 (19)	C2—C3—H3A	109.1
O4—Cl1—O3	108.6 (11)	N1—C3—H3B	109.1
O4—Cl1—O2	113.8 (8)	C2—C3—H3B	109.1
O3—Cl1—O2	106.6 (9)	H3A—C3—H3B	107.9
O4—Cl1—O1	119.5 (9)	C5—C4—N1	108.7 (5)
O3—Cl1—O1	97.5 (8)	C5—C4—H4A	109.9
O2—Cl1—O1	108.9 (5)	N1—C4—H4A	109.9
O7—Cl2—O8	104.5 (8)	C5—C4—H4B	109.9
O7—Cl2—O5	114.7 (9)	N1—C4—H4B	109.9
O8—Cl2—O5	112.8 (7)	H4A—C4—H4B	108.3
O7—Cl2—O6	110.5 (10)	N2—C5—C4	107.8 (5)
O8—Cl2—O6	110.7 (8)	N2—C5—H5A	110.1
O5—Cl2—O6	103.7 (7)	C4—C5—H5A	110.1
C3—N1—C4	111.9 (5)	N2—C5—H5B	110.1
C3—N1—Cr	117.1 (4)	C4—C5—H5B	110.1
C4—N1—Cr	107.0 (4)	H5A—C5—H5B	108.5
C3—N1—H1AN	106.8	N2—C6—C7	112.8 (5)
C4—N1—H1AN	106.8	N2—C6—H6A	109.0
Cr—N1—H1AN	106.8	C7—C6—H6A	109.0
C6—N2—C5	112.3 (5)	N2—C6—H6B	109.0
C6—N2—Cr	119.7 (4)	C7—C6—H6B	109.0
C5—N2—Cr	106.8 (4)	H6A—C6—H6B	107.8
C6—N2—H1N2	105.7	C8—C7—C6	115.7 (6)
C5—N2—H1N2	105.7	C8—C7—H7A	108.4

Cr—N2—H1N2	105.7	C6—C7—H7A	108.4
C8—N3—Cr	119.0 (4)	C8—C7—H7B	108.4
C8—N3—H3AN	107.6	C6—C7—H7B	108.4
Cr—N3—H3AN	107.6	H7A—C7—H7B	107.4
C8—N3—H3BN	107.6	N3—C8—C7	112.7 (5)
Cr—N3—H3BN	107.6	N3—C8—H8A	109.0
H3AN—N3—H3BN	107.0	C7—C8—H8A	109.0
C1—N4—Cr	116.9 (4)	N3—C8—H8B	109.0
C1—N4—H4AN	108.1	C7—C8—H8B	109.0
Cr—N4—H4AN	108.1	H8A—C8—H8B	107.8
C1—N4—H4BN	108.1	Cr—O1W—H1OA	129 (5)
Cr—N4—H4BN	108.1	Cr—O1W—H1OB	117 (5)
H4AN—N4—H4BN	107.3	H1OA—O1W—H1OB	109 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*OA*···F^{i}	0.86 (6)	1.72 (6)	2.564 (5)	168 (8)
O1*W*—H1*OB*···O2*W*	0.74 (6)	1.92 (6)	2.617 (6)	158 (7)
N1—H1*AN*···O2^{ii}	0.91	2.42	3.332 (11)	177
N2—H1*N*2···O7^{iii}	0.91	2.45	3.154 (10)	134
N3—H3*BN*···O5	0.90	2.36	3.242 (10)	167
N4—H4*BN*···O5	0.90	2.43	3.062 (10)	127
C1—H1*B*···O4^{iv}	0.97	2.53	3.141 (13)	121

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