

Crystal structure of *fac*-aquatricarbonyl[(*S*)-valinato- κ^2N,O]rhenium(I)Kseniia O. Piletska,^{a*} Kostiantyn V. Domasevitch^b and Alexander V. Shtemenko^a^aDepartment of Inorganic Chemistry, Ukrainian State University of Chemical Technology, Gagarin Ave. 8, Dnipropetrovsk 49005, Ukraine, and ^bInorganic Chemistry Department, National Taras Shevchenko University of Kyiv, Volodymyrska Street 64/13, Kyiv 01601, Ukraine. *Correspondence e-mail: ksenijapiletska@gmail.com

Received 19 March 2016

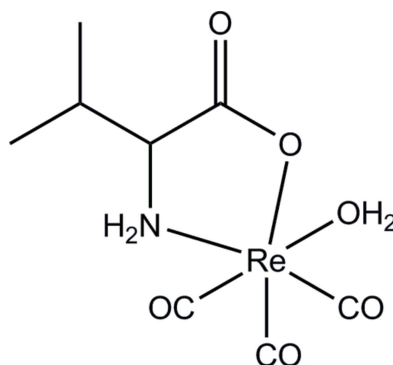
Accepted 28 March 2016

Edited by M. Weil, Vienna University of
Technology, Austria**Keywords:** crystal structure; rhenium carbonyl
complex; valine.**CCDC reference:** 1469075**Supporting information:** this article has
supporting information at journals.iucr.org/e

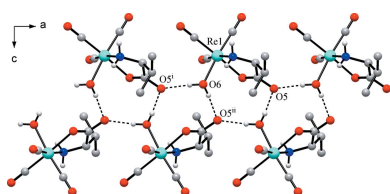
In the molecule of the title compound, [Re(C₅H₁₀NO₂)(CO)₃(H₂O)], the Re^I atom adopts a distorted octahedral coordination sphere defined by one aqua and three carbonyl ligands as well as one amino N and one carboxylate O atom of the chelating valinate anion. The carbonyl ligands are arranged in a *fac*-configuration around the Re^I ion. In the crystal, an intricate hydrogen-bonding system under participation of two O—H, two N—H and one C—H donor groups and the carboxylate and carbonyl O atoms as acceptor groups contribute to the formation of a three-dimensional supramolecular network.

1. Chemical context

The syntheses of metal–organic compounds, which are capable of visualization of biomolecules, is receiving growing interest in biocoordination chemistry (Coogan & Fernández-Moreira, 2014). For the labeling of biomolecules, octahedral *fac*-tricarbonyl complexes of Tc and Re are the most promising compounds (Alberto, 2007; Coogan *et al.*, 2014). The compact *M*(CO)₃-core (*M* = Tc, Re) allows labeling of low molecular weight substrates under retention of activity and specificity. In this context, Re(CO)₃⁺ compounds are of interest as the closest non-radioactive analogs of ^{99m}Tc-based systems, which could be particularly important for visualization and immunotherapy. Studies of the cytotoxicity of rhenium carbonyl complexes also suggest their specific anticancer activity (Leonidova & Gasser, 2014).



Most of the known Re(CO)₃⁺ complexes with biologically essential substrates comprise tridentate co-ligands, *e.g.* histidinato-*O,N,N'* (Alberto *et al.*, 1999), methioninato-*N,O,S* (He *et al.*, 2005), 2,3-diaminopropionato-*N,N',O* (Liu *et al.*, 2006), completing the coordination octahedra of the central ions. At



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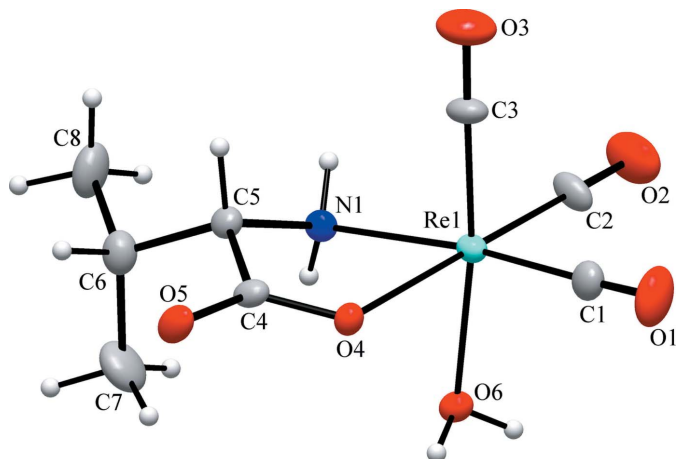


Figure 1
The molecular structure of the title complex, with displacement ellipsoids drawn at the 40% probability level.

the same time, coordinatively unsaturated complexes of bidentate aminocarboxylates could be suited for interactions with additional ligands, such as guanine bases (Zobi *et al.* 2005*a*), thus allowing an attractive scenario for the assembly of mixed-ligand systems.

In this communication, we report the synthesis and crystal structure of a novel $\text{Re}(\text{CO})_3^+$ complex with valine and water as co-ligands. Following the findings of Zobi *et al.* (2005*b*), sufficient reactivity of this compound towards DNA may be anticipated.

2. Structural commentary

In the molecule of the title compound (Fig. 1), the Re^{I} ion resides in a slightly distorted octahedral coordination environment, with a facial arrangement of three nearly equidistant carbonyl ligands [Re1–C bond lengths are in the range 1.881 (7)–1.909 (7) Å]. The compound crystallizes in the chiral space group $P2_12_12_1$, with the *S*-enantiomer of the valinate anion present in the selected crystal. The anion coordinates in a bidentate-chelating fashion through the amino N and one carboxylate O atoms, with Re1–N1 and Re1–O4 bond lengths of 2.195 (5) and 2.122 (4) Å, respectively. The five-

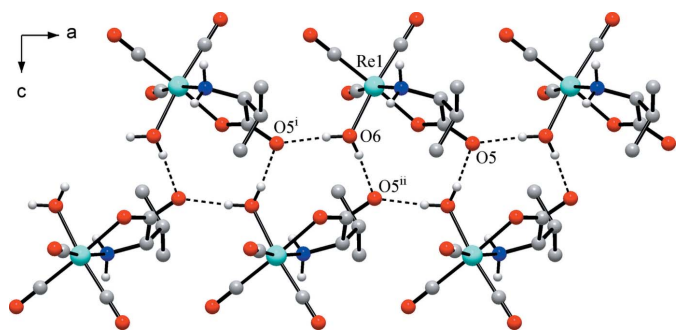


Figure 2
Primary supramolecular interactions involving rather strong O–H...O bonds that produce chains parallel to the *a* axis. [Symmetry codes: (i) $x - 1, y, z$; (ii) $x - 0.5, -y + 0.5, -z + 1$.]

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

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
O6–H1W...O5 ⁱ	0.85	1.85	2.693 (5)	175
O6–H2W...O5 ⁱⁱ	0.85	1.88	2.723 (5)	175
N1–H1N...O3 ⁱⁱⁱ	0.90	2.15	2.979 (7)	153
N1–H2N...O1 ^{iv}	0.90	2.41	3.103 (6)	133
C5–H5...O2 ^v	0.99	2.59	3.527 (7)	158

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

membered chelate ring [bite angle N1–Re1–O4 = 74.62 (18)°] has the expected envelope conformation, with the atoms of the Re1–O4–C4–C5 fragment being coplanar within 0.035 (3) Å and the N1 flap atom deviating from the given mean plane by 0.547 (6) Å. The Re1–O6 bond involving the aqua ligand [2.175 (5) Å] is slightly longer than the one with the carboxyl O atom. The CO ligands coordinate in an almost linear fashion, with O–C–Re bond angles spanning a range from 175.5 (7) to 179.9 (8)°, while the corresponding C–Re1–C angles are within 87.1 (3)–89.8 (2)°. All other bond length and angles are comparable to those found for related Re^{I} complexes (Rajendran *et al.*, 2000).

3. Supramolecular features

In the crystal, the packing of the molecules is governed by an intricate system of hydrogen bonds, including classical

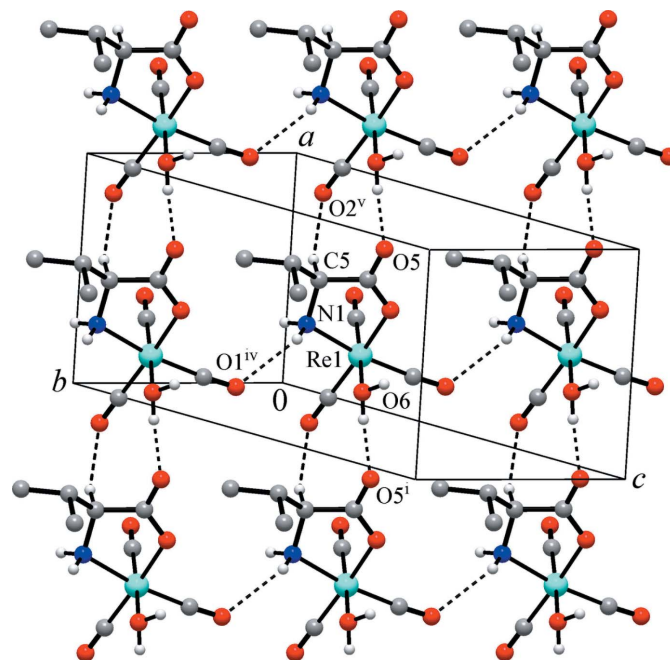


Figure 3
The crystal structure of the title complex showing all hydrogen-bonding interactions (O–H...O, N–H...O and C–H...O) as dashed lines. The isopropyl CH-hydrogen atoms were omitted for clarity. [Symmetry codes: (i) $x - 1, y, z$; (iv) $x, y + 1, z$; (v) $x + 1, y, z$.]

Table 2
Experimental details.

Crystal data	
Chemical formula	[Re(C ₅ H ₁₀ NO ₂)(CO) ₃ (H ₂ O)]
<i>M</i> _r	404.39
Crystal system, space group	Orthorhombic, <i>P</i> 2 ₁ 2 ₁ 2 ₁
Temperature (K)	213
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.1229 (5), 7.2913 (7), 22.6098 (18)
<i>V</i> (Å ³)	1174.24 (17)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	10.36
Crystal size (mm)	0.16 × 0.12 × 0.12
Data collection	
Diffractometer	Stoe Imaging plate diffraction system
Absorption correction	Numerical (<i>X-SHAPE</i> and <i>X-RED</i> ; Stoe, 2001)
<i>T</i> _{min} , <i>T</i> _{max}	0.288, 0.370
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	10442, 2809, 2546
<i>R</i> _{int}	0.040
(sin θ/λ) _{max} (Å ⁻¹)	0.660
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.022, 0.047, 0.99
No. of reflections	2809
No. of parameters	147
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	1.68, -0.91
Absolute structure	Flack <i>x</i> determined using 990 quotients [(<i>I</i> ⁺) - (<i>I</i> ⁻)] / [(<i>I</i> ⁺) + (<i>I</i> ⁻)] (Parsons <i>et al.</i> , 2013).
Absolute structure parameter	-0.018 (10)

Computer programs: *IPDS Software* (Stoe, 2000), *SHELXS97* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 1999) and *WinGX* (Farrugia, 2012).

O—H...O and N—H...O bonds and weaker C—H...O interactions (Table 1). Two rather strong and nearly linear O—H...O bonds are observed between the aqua ligand and the non-coordinating carboxylate O atoms of two symmetry-related neighbouring molecules. The amino group forms two weaker N—H...O bonds to carbonyl O atom acceptor groups of two neighbouring molecules. Each non-coordinating carboxylate O atom accepts two such bonds, yielding hydrogen-bonded chains parallel to the *a*-axis direction (Fig. 2), whereas the N—H...O bonds expand the hydrogen-bonding system into a three-dimensional network. Additional C—H...O interactions consolidate this arrangement (Fig. 3). The combination of O—H...O and C—H...O (involving the chiral C5 atom) bonds may be important for the observed enantioselective packing of the chiral moieties (Petkova *et al.*, 2001).

4. Synthesis and crystallization

To a solution of DL-valine (0.116 g, 0.984 mmol) in 5 ml of water, a solution of triaquatricarbonylrhenium(I) bromide (0.100 g, 0.246 mmol) in 10 ml of methanol was added. The reaction mixture was heated and stirred at 343 K under a steady stream of argon for 4 h. After cooling to room

temperature, the solution was left to evaporate in air for a period of a few days. After removal of the methanol co-solvent, a colourless crystalline product formed. The precipitate was collected by suction filtration, washed with water and then with a 50 ml portion of petroleum ether and dried (yield: 0.068 g, 68%). Suitable single crystals were obtained by slow diffusion of hexane vapor into a methanol solution of the complex. IR (KBr, cm⁻¹): ν_{as}(CO) 2028 (*s*), ν_s(CO) 1905 (*s*).

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound hydrogen atoms were placed geometrically and refined using a riding model, with C—H = 0.97 Å and *U*_{iso}(H) = 1.5*U*_{eq}(C) for methyl and with C—H = 0.99 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C) for methine groups. N- and O-bound hydrogen atoms were found from difference maps and refined with N—H = 0.90 Å, O—H = 0.85 Å and *U*_{iso}(H) = 1.2*U*_{eq}(N,O).

Acknowledgements

This work was supported by the fund Grant for Science Research (No. 0111U000111) from the Ministry of Education and Science of Ukraine. We also thank EU COST Action CM 1105 for supporting this study.

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supporting information

Acta Cryst. (2016). E72, 590-592 [https://doi.org/10.1107/S2056989016005235]

Crystal structure of *fac*-aquatricarbonyl[(*S*)-valinato- κ^2 N,O]rhenium(I)

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Computing details

Data collection: *IPDS Software* (Stoe, 2000); cell refinement: *IPDS Software* (Stoe, 2000); data reduction: *IPDS Software* (Stoe, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

fac-Aquatricarbonyl[(*S*)-valinato- κ^2 N,O]rhenium(I)

Crystal data

[Re(C₅H₁₀NO₂)(CO)₃(H₂O)]

$M_r = 404.39$

Orthorhombic, $P2_12_12_1$

$a = 7.1229$ (5) Å

$b = 7.2913$ (7) Å

$c = 22.6098$ (18) Å

$V = 1174.24$ (17) Å³

$Z = 4$

$F(000) = 760$

$D_x = 2.287$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 8000 reflections

$\theta = 2.9$ – 28.0°

$\mu = 10.36$ mm⁻¹

$T = 213$ K

Prism, colorless

$0.16 \times 0.12 \times 0.12$ mm

Data collection

Stoe Imaging plate diffraction system
diffractometer

Radiation source: fine-focus sealed tube

φ oscillation scans

Absorption correction: numerical
(*X-SHAPE* and *X-RED*; Stoe, 2001)

$T_{\min} = 0.288$, $T_{\max} = 0.370$

10442 measured reflections

2809 independent reflections

2546 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.040$

$\theta_{\max} = 28.0^\circ$, $\theta_{\min} = 2.9^\circ$

$h = -9 \rightarrow 9$

$k = -9 \rightarrow 9$

$l = -29 \rightarrow 29$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.022$

$wR(F^2) = 0.047$

$S = 0.99$

2809 reflections

147 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: mixed

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0254P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 1.68$ e Å⁻³

$\Delta\rho_{\min} = -0.91$ e Å⁻³

Absolute structure: Flack x determined using
990 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons *et al.*,
2013).

Absolute structure parameter: -0.018 (10)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Re1	0.27215 (3)	0.24317 (4)	0.36414 (2)	0.01911 (8)
O1	0.1402 (9)	−0.1539 (7)	0.3751 (3)	0.0475 (16)
O2	−0.0548 (9)	0.3311 (10)	0.2820 (3)	0.059 (2)
O3	0.4865 (10)	0.1103 (10)	0.2566 (3)	0.0510 (17)
O4	0.4953 (6)	0.2146 (6)	0.42564 (19)	0.0201 (10)
O5	0.7729 (7)	0.3107 (6)	0.4559 (2)	0.0296 (11)
O6	0.1463 (7)	0.3556 (6)	0.4439 (2)	0.0216 (10)
H1W	0.0276	0.3449	0.4455	0.032*
H2W	0.1929	0.3046	0.4744	0.032*
N1	0.4095 (7)	0.5125 (7)	0.3670 (3)	0.0202 (10)
H1N	0.4012	0.5560	0.3298	0.030*
H2N	0.3545	0.5944	0.3913	0.030*
C1	0.1826 (10)	−0.0024 (10)	0.3716 (4)	0.0300 (15)
C2	0.0674 (10)	0.2983 (10)	0.3127 (3)	0.0309 (18)
C3	0.4063 (11)	0.1628 (11)	0.2973 (3)	0.0283 (16)
C4	0.6284 (10)	0.3294 (9)	0.4248 (3)	0.0215 (14)
C5	0.6095 (10)	0.4941 (9)	0.3839 (3)	0.0216 (14)
H5	0.6814	0.4668	0.3475	0.026*
C6	0.6917 (11)	0.6706 (9)	0.4109 (4)	0.0319 (16)
H6	0.8235	0.6446	0.4220	0.038*
C7	0.5880 (13)	0.7280 (13)	0.4668 (4)	0.048 (2)
H7A	0.4638	0.7721	0.4565	0.072*
H7B	0.6574	0.8250	0.4864	0.072*
H7C	0.5768	0.6236	0.4931	0.072*
C8	0.6942 (12)	0.8254 (9)	0.3654 (5)	0.0424 (19)
H8A	0.5664	0.8610	0.3561	0.064*
H8B	0.7566	0.7837	0.3298	0.064*
H8C	0.7613	0.9298	0.3816	0.064*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Re1	0.01711 (11)	0.02296 (11)	0.01726 (10)	0.00198 (16)	−0.00083 (9)	−0.00125 (15)
O1	0.035 (3)	0.027 (3)	0.081 (5)	−0.005 (2)	−0.001 (3)	0.002 (3)
O2	0.038 (4)	0.091 (5)	0.048 (4)	0.017 (3)	−0.016 (3)	−0.006 (3)
O3	0.060 (5)	0.061 (4)	0.032 (3)	0.016 (3)	0.012 (3)	−0.006 (3)
O4	0.018 (2)	0.020 (3)	0.023 (2)	−0.0010 (17)	−0.0010 (17)	0.0027 (17)
O5	0.015 (2)	0.043 (2)	0.030 (2)	0.0011 (19)	−0.005 (2)	0.0118 (19)
O6	0.019 (2)	0.024 (2)	0.022 (2)	0.0027 (18)	0.0015 (19)	0.0026 (18)

N1	0.020 (3)	0.020 (2)	0.020 (3)	0.0023 (19)	-0.002 (3)	0.003 (2)
C1	0.020 (4)	0.037 (4)	0.032 (4)	-0.002 (3)	-0.004 (3)	0.000 (3)
C2	0.023 (4)	0.043 (5)	0.026 (4)	0.011 (3)	-0.010 (3)	-0.010 (3)
C3	0.027 (4)	0.041 (4)	0.016 (3)	0.006 (3)	0.005 (3)	-0.001 (3)
C4	0.017 (4)	0.028 (3)	0.019 (3)	0.005 (3)	0.003 (3)	0.002 (2)
C5	0.017 (3)	0.025 (3)	0.023 (3)	0.002 (2)	0.000 (2)	0.000 (2)
C6	0.024 (4)	0.031 (3)	0.041 (4)	0.000 (3)	-0.005 (3)	-0.001 (3)
C7	0.055 (5)	0.039 (5)	0.050 (5)	0.005 (5)	-0.006 (4)	-0.022 (4)
C8	0.033 (5)	0.027 (3)	0.066 (6)	-0.007 (3)	-0.002 (5)	0.004 (4)

Geometric parameters (Å, °)

Re1—C3	1.881 (7)	N1—H1N	0.9004
Re1—C2	1.908 (7)	N1—H2N	0.9004
Re1—C1	1.909 (7)	C4—C5	1.520 (9)
Re1—O4	2.122 (4)	C5—C6	1.539 (9)
Re1—O6	2.175 (5)	C5—H5	0.9900
Re1—N1	2.195 (5)	C6—C7	1.523 (11)
O1—C1	1.148 (9)	C6—C8	1.526 (11)
O2—C2	1.139 (9)	C6—H6	0.9900
O3—C3	1.148 (9)	C7—H7A	0.9700
O4—C4	1.265 (8)	C7—H7B	0.9700
O5—C4	1.255 (8)	C7—H7C	0.9700
O6—H1W	0.8498	C8—H8A	0.9700
O6—H2W	0.8503	C8—H8B	0.9700
N1—C5	1.482 (8)	C8—H8C	0.9700
C3—Re1—C2	88.0 (3)	O5—C4—O4	122.3 (6)
C3—Re1—C1	87.1 (3)	O5—C4—C5	119.9 (6)
C2—Re1—C1	89.8 (3)	O4—C4—C5	117.8 (6)
C3—Re1—O4	96.6 (3)	N1—C5—C4	108.3 (5)
C2—Re1—O4	173.0 (2)	N1—C5—C6	113.1 (5)
C1—Re1—O4	95.8 (3)	C4—C5—C6	112.8 (6)
C3—Re1—O6	173.2 (3)	N1—C5—H5	107.5
C2—Re1—O6	96.4 (3)	C4—C5—H5	107.5
C1—Re1—O6	98.2 (3)	C6—C5—H5	107.5
O4—Re1—O6	78.61 (18)	C7—C6—C8	111.2 (7)
C3—Re1—N1	94.4 (3)	C7—C6—C5	111.9 (6)
C2—Re1—N1	99.8 (3)	C8—C6—C5	110.9 (7)
C1—Re1—N1	170.4 (3)	C7—C6—H6	107.5
O4—Re1—N1	74.62 (18)	C8—C6—H6	107.5
O6—Re1—N1	79.7 (2)	C5—C6—H6	107.5
C4—O4—Re1	119.1 (4)	C6—C7—H7A	109.5
Re1—O6—H1W	114.3	C6—C7—H7B	109.5
Re1—O6—H2W	110.2	H7A—C7—H7B	109.5
H1W—O6—H2W	108.2	C6—C7—H7C	109.5
C5—N1—Re1	110.8 (4)	H7A—C7—H7C	109.5
C5—N1—H1N	109.6	H7B—C7—H7C	109.5

Re1—N1—H1N	105.0	C6—C8—H8A	109.5
C5—N1—H2N	108.7	C6—C8—H8B	109.5
Re1—N1—H2N	114.7	H8A—C8—H8B	109.5
H1N—N1—H2N	107.9	C6—C8—H8C	109.5
O1—C1—Re1	175.5 (7)	H8A—C8—H8C	109.5
O2—C2—Re1	179.9 (8)	H8B—C8—H8C	109.5
O3—C3—Re1	178.6 (7)		
Re1—O4—C4—O5	-173.0 (5)	O5—C4—C5—C6	-37.3 (9)
Re1—O4—C4—C5	6.6 (7)	O4—C4—C5—C6	143.1 (6)
Re1—N1—C5—C4	-31.1 (6)	N1—C5—C6—C7	60.3 (8)
Re1—N1—C5—C6	-156.7 (5)	C4—C5—C6—C7	-63.0 (8)
O5—C4—C5—N1	-163.1 (6)	N1—C5—C6—C8	-64.5 (8)
O4—C4—C5—N1	17.2 (8)	C4—C5—C6—C8	172.2 (6)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O6—H1 <i>W</i> ...O5 ⁱ	0.85	1.85	2.693 (5)	175
O6—H2 <i>W</i> ...O5 ⁱⁱ	0.85	1.88	2.723 (5)	175
N1—H1 <i>N</i> ...O3 ⁱⁱⁱ	0.90	2.15	2.979 (7)	153
N1—H2 <i>N</i> ...O1 ^{iv}	0.90	2.41	3.103 (6)	133
C5—H5...O2 ^v	0.99	2.59	3.527 (7)	158

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