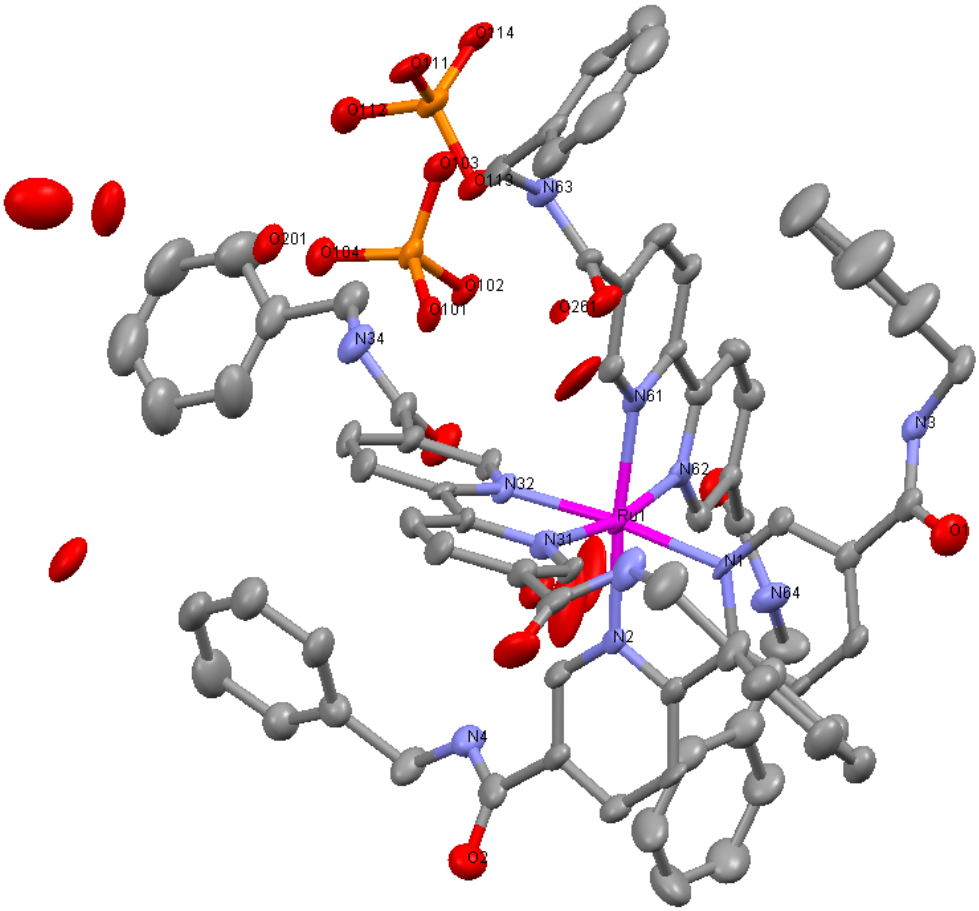
Electronic Supplementary Information for Dalton Transactions

The comparison of *fac* and *mer* ruthenium(II) trischelate complexes in anion binding.

Naomi A. C. Baker, Neil McGaughey, Nicholas C. Fletcher,* Aleksey V. Chernikov, Peter N. Horton and Michael B. Hursthouse

Sup. Fig. 1, Plot of $[Ru(L1)_3](H_2PO_4)_2$ with ellipsoids at 50% probability. Significant atoms have been numbers, and hydrogen atoms have been deleted for clarity.



Supplementary Table 1. Selected Angles and bond lengths for $[Ru(L1)_3](H_2PO_4)_2$ [Å and °].

Ru1-N2	2.033(6)	N2-Ru1-N61	174.0(2)
Ru1-N61	2.046(6)	N61-Ru1-N32	88.4(2)
Ru1-N32	2.049(6)	N2-Ru1-N1	78.8(3)
Ru1-N1	2.061(6)	N61-Ru1-N1	96.4(2)
Ru1-N62	2.061(6)	N32-Ru1-N1	172.9(2)
Ru1-N31	2.063(6)	N2-Ru1-N62	97.9(2)
		N61-Ru1-N62	78.6(2)
		N32-Ru1-N62	94.2(2)
		N1-Ru1-N62	92.0(2)
		N2-Ru1-N31	92.2(2)
		N61-Ru1-N31	91.8(2)
		N32-Ru1-N31	78.6(3)
		N1-Ru1-N31	95.9(2)
		N62-Ru1-N31	168.2(2)

Symmetry transformations used to generate equivalent atoms:
(i) –x+1,–y+1,–z (ii) x,y,z–1 (iii) –x+1,–y,–z
(iv) –x+2,–y+1,–z (v) x,y+1,z (vi) x,y,z+1 (vii) –x+1,–y,–z+1

Supplementary Table 2. Hydrogen bonds observed in structure of $[Ru(L1)_3](H_2PO_4)_2$ [Å and °] [Å and °].

D–H···*A*	*d*(*D*–H)	*d*(H···*A*)	*d*(*D*···*A*)	∠(*DHA*)
N3–H3A···O114^{i}	0.88	1.87	2.725(9)	165.0
N4–H4A···O241	0.88	2.00	2.835(9)	157.8
N33–H33A···O231^{ii}	0.88	2.09	2.911(10)	155.7
N34–H34A···O201	0.88	2.02	2.853(9)	158.3
N63–H63A···O103	0.88	2.23	2.842(9)	125.9
N64–H64A···O1^{iii}	0.88	1.94	2.801(9)	164.2
O101–H101···O104^{iv}	0.84	1.70	2.531(7)	168.0
O102–H102···O113	0.84	1.73	2.568(7)	175.3
O111–H111···O103	0.84	1.84	2.665(7)	169.1
O201–H201···O104	0.86	1.82	2.670(8)	170.1
O201–H202···O211	0.85	1.85	2.690(8)	167.2
O211–H211···O221	0.86	1.97	2.807(10)	163.1
O211–H212···O61^{iv}	0.86	2.02	2.785(8)	149.0
O221–H222···O2^{v}	0.86	1.97	2.830(9)	178.2
O231–H231···O61^{vi}	0.85	1.95	2.795(7)	172.9
O241–H241···O32	0.85	2.03	2.819(8)	153.1
O241–H242···O281	0.85	2.23	3.025(7)	156.1
O241–H242···O271	0.85	1.79	2.638(17)	171.0
O251–H251···O62	0.85	2.05	2.888(11)	170.9
O251–H252···O32	0.85	2.00	2.811(12)	160.6
O261–H261···O113	0.85	1.99	2.799(10)	159.9
O261–H262···O251	0.85	2.19	2.696(17)	118.4
O271–H272···O62	0.85	2.56	3.231(12)	136.5
O281–H282···O271^{vii}	0.85	2.09	2.818(18)	143.4

Symmetry transformations used to generate equivalent atoms:
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(iv) –x+2,–y+1,–z (v) x,y+1,z (vi) x,y,z+1 (vii) –x+1,–y,–z+1