Supplementary material

Table S1: Cu Coordination Geometry in PPLO

Angle		Triangular pyramidal[a] (His 528 at the apex)		Tetrahedral		Square pyramidal[a,b] (one equatorial ligand is missing; O_{axial} at the apex)	
	Measured	Ideal	Distortion	Ideal	Distortion	Ideal	Distortion
H528-Cu-H530	99.2°	90°	9.2°	109.5°	10.3°	90°	9.2°
H528-Cu-H694	100.0°	90°	10.0°	109.5°	9.4°	90°	10.0°
H530-Cu-H694	135.2°	120°	15.2°	109.5°	25.7°	180°	44.8°
H530-Cu-O_{axial}	106.1°	120°	13.9°	109.5°	3.4°	90°	16.1°
H528-Cu-O_{axial}	96.1°	90°	6.1°	109.5°	13.4°	90°	6.1°
H694-Cu-O_{axial}	111.6°	120°	8.5°	109.5°	2.1°	90°	21.6°
Average Distortion			10.5°		10.7°		18.0°
Deviation of Cu from base[a,b]			0.3 Å				0.6 Å
Cu distance from centre[c,d]					0.35 Å		

[a]The triangular pyramid has $N^{\varepsilon 2}$(His 528) at the apex and $N^{\varepsilon 2}$(His 530), $N^{\delta 1}$(His 964) and O_{axial} at the base.

[b]The square pyramid has O_{axial} at the apex, the N(His) atoms and a missing atom at the base.

[c]The centre of the tetrahedron is the unweighted mean position of $N^{\varepsilon 2}$(His 528), $N^{\varepsilon 2}$(His 530), $N^{\delta 1}$(His 964) and O_{axial}.