Table 1. Crystal data and structure refinement for [Tl(L-GluH)].

Identification code	[Tl(L-GluH)]	
Empirical formula	C5 H8 N O4 Tl	
Formula weight	350.49	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 9.4286(5) Å	α= 90°
	b = 5.3264(3) Å	β= 107.162(2)°
	c = 15.7265(9) Å	γ = 90°
Volume	754.63(7) $Å^3$	
Z	4	
Density (calculated)	3.085 Mg/m^3	
Absorption coefficient	21.368 mm^{-1}	
F(000)	632	
Crystal size	0.23 x 0.19 x 0.06 mm^3	
Theta range for data collection	2.26 to 36.00°	
Index ranges	-15<=h<=15, -8<=k<=8, -26<=l<=26	
Reflections collected	39491	
Independent reflections	7161 [R(int) = 0.0476]	
Completeness to theta = 36.00°	100.0 %	
Max. and min. transmission	0.3462 and 0.0834	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7161 / 1 / 200	
Goodness-of-fit on F^2	1.100	
Final R indices [I>2sigma(I)]	R1 = 0.0277, wR2 = 0.0707	
R indices (all data)	R1 = 0.0297, wR2 = 0.0719	
Absolute structure parameter	0.007(7)	
Extinction coefficient	0.0057(2)	
Largest diff. peak and hole	3.455 and -1.395 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [Tl(L-GluH)]. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Tl(1)	3274(1)	429(1)	-821(1)	10(1)
Tl(2)	1828(1)	5540(1)	807(1)	8(1)
O(1)	4363(3)	-1659(6)	769(2)	12(1)
O(2)	4230(3)	2515(6)	816(2)	12(1)
O(3)	8211(3)	3222(6)	4188(2)	10(1)
O(4)	7404(3)	-746(5)	4081(2)	12(1)
O(5)	1601(3)	5197(6)	-909(2)	16(1)
O(6)	-591(3)	5837(6)	-676(2)	14(1)
O(7)	-2148(3)	220(5)	-3532(2)	12(1)
O(8)	-3282(3)	3727(6)	-4159(2)	10(1)
N(1)	5519(3)	5052(6)	4083(2)	9(1)
N(2)	-827(3)	6083(6)	-4189(2)	8(1)
C(1)	7206(4)	1566(7)	4022(2)	7(1)
C(2)	5613(3)	2550(7)	3680(2)	7(1)
C(3)	5105(4)	2793(7)	2667(2)	10(1)
C(4)	5037(4)	277(9)	2202(2)	10(1)
C(5)	4507(3)	377(12)	1196(2)	9(1)
C(6)	-2131(4)	2430(7)	-3809(2)	8(1)
C(7)	-628(3)	3636(7)	-3704(2)	7(1)
C(8)	254(4)	3978(7)	-2720(2)	10(1)
C(9)	-572(3)	5424(10)	-2176(2)	11(1)
C(10)	216(4)	5463(12)	-1181(2)	11(1)

Table 3. Bond lengths [Å] and angles [°] for [Tl(L-GluH)].

Tl(1)-O(1)	2.651(3)
Tl(1)-O(1)#1	2.697(3)
Tl(1)-O(2)	2.703(3)
Tl(2)-O(5)	2.649(3)
Tl(2)-O(6)	2.744(3)
Tl(2)-O(6)#2	2.746(3)
Tl(2)-O(2)	2.776(3)
O(1)-C(5)	1.261(6)
O(1)-Tl(1)#3	2.697(3)
O(2)-C(5)	1.276(7)
O(3)-C(1)	1.264(4)
O(4)-C(1)	1.245(4)
O(5)-C(10)	1.257(4)
O(6)-C(10)	1.266(4)
O(6)-Tl(2)#4	2.746(3)
O(7)-C(6)	1.257(4)
O(8)-C(6)	1.267(4)
N(1)-C(2)	1.490(5)
N(1)-H(1A)	0.9101
N(1)-H(1B)	0.9097
N(1)-H(1C)	0.9096
N(2)-C(7)	1.493(4)
N(2)-H(2A)	0.9101
N(2)-H(2B)	0.9097
N(2)-H(2C)	0.9096
C(1)-C(2)	1.531(5)
C(2)-C(3)	1.528(5)
C(2)-H(2)	0.9800
C(3)-C(4)	1.519(6)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.513(5)
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700

C(6)-C(7)	1.521(4)
C(7)-C(8)	1.537(5)
C(7)-H(7)	0.9800
C(8)-C(9)	1.524(6)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-C(10)	1.522(5)
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700

O(1)-Tl(1)-O(1)#1	97.25(7)
O(1)-Tl(1)-O(2)	49.19(8)
O(1)#1-Tl(1)-O(2)	72.20(9)
O(5)-Tl(2)-O(6)	48.76(8)
O(5)-Tl(2)-O(6)#2	87.48(9)
O(6)-Tl(2)-O(6)#2	76.15(7)
O(5)-Tl(2)-O(2)	77.62(8)
O(6)-Tl(2)-O(2)	120.65(8)
O(6)#2-Tl(2)-O(2)	78.39(9)
C(5)-O(1)-Tl(1)	95.3(3)
C(5)-O(1)-Tl(1)#3	121.3(2)
Tl(1)-O(1)-Tl(1)#3	110.87(11)
C(5)-O(2)-Tl(1)	92.5(2)
C(5)-O(2)-Tl(2)	125.1(2)
Tl(1)-O(2)-Tl(2)	101.05(8)
C(10)-O(5)-Tl(2)	95.9(2)
C(10)-O(6)-Tl(2)	91.2(2)
C(10)-O(6)-Tl(2)#4	114.7(3)
Tl(2)-O(6)-Tl(2)#4	110.14(10)
C(2)-N(1)-H(1A)	109.2
C(2)-N(1)-H(1B)	109.9
H(1A)-N(1)-H(1B)	109.5
C(2)-N(1)-H(1C)	109.3
H(1A)-N(1)-H(1C)	109.5
H(1B)-N(1)-H(1C)	109.4
C(7)-N(2)-H(2A)	109.2

C(7)-N(2)-H(2B)	109.5
H(2A)-N(2)-H(2B)	109.5
C(7)-N(2)-H(2C)	109.7
H(2A)-N(2)-H(2C)	109.5
H(2B)-N(2)-H(2C)	109.4
O(4)-C(1)-O(3)	126.0(4)
O(4)-C(1)-C(2)	118.4(3)
O(3)-C(1)-C(2)	115.6(3)
N(1)-C(2)-C(3)	109.2(3)
N(1)-C(2)-C(1)	109.4(3)
C(3)-C(2)-C(1)	111.6(3)
N(1)-C(2)-H(2)	108.9
C(3)-C(2)-H(2)	108.9
C(1)-C(2)-H(2)	108.9
C(4)-C(3)-C(2)	112.5(3)
C(4)-C(3)-H(3A)	109.1
C(2)-C(3)-H(3A)	109.1
C(4)-C(3)-H(3B)	109.1
C(2)-C(3)-H(3B)	109.1
H(3A)-C(3)-H(3B)	107.8
C(5)-C(4)-C(3)	115.2(4)
C(5)-C(4)-H(4A)	108.5
C(3)-C(4)-H(4A)	108.5
C(5)-C(4)-H(4B)	108.5
C(3)-C(4)-H(4B)	108.5
H(4A)-C(4)-H(4B)	107.5
O(1)-C(5)-O(2)	122.9(3)
O(1)-C(5)-C(4)	118.4(5)
O(2)-C(5)-C(4)	118.7(5)
O(7)-C(6)-O(8)	124.4(3)
O(7)-C(6)-C(7)	117.7(3)
O(8)-C(6)-C(7)	117.9(3)
N(2)-C(7)-C(6)	109.9(3)
N(2)-C(7)-C(8)	111.1(3)
C(6)-C(7)-C(8)	111.7(3)
N(2)-C(7)-H(7)	108.0

C(6)-C(7)-H(7)	108.0
C(8)-C(7)-H(7)	108.0
C(9)-C(8)-C(7)	114.3(3)
C(9)-C(8)-H(8A)	108.7
C(7)-C(8)-H(8A)	108.7
C(9)-C(8)-H(8B)	108.7
C(7)-C(8)-H(8B)	108.7
H(8A)-C(8)-H(8B)	107.6
C(10)-C(9)-C(8)	114.1(3)
C(10)-C(9)-H(9A)	108.7
C(8)-C(9)-H(9A)	108.7
C(10)-C(9)-H(9B)	108.7
C(8)-C(9)-H(9B)	108.7
H(9A)-C(9)-H(9B)	107.6
O(5)-C(10)-O(6)	124.1(3)
O(5)-C(10)-C(9)	119.4(3)
O(6)-C(10)-C(9)	116.4(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y+1/2,-z #2 -x,y-1/2,-z #3 -x+1,y-1/2,-z

#4 -x,y+1/2,-z

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for [Tl(L-GluH)]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Tl(1)	11(1)	9(1)	7(1)	0(1)	0(1)	0(1)
Tl(2)	11(1)	8(1)	5(1)	-1(1)	1(1)	1(1)
O(1)	16(2)	8(1)	12(1)	-2(1)	4(1)	1(1)
O(2)	17(2)	10(1)	7(1)	2(1)	2(1)	1(1)
O(3)	7(1)	9(1)	14(1)	-3(1)	2(1)	0(1)
O(4)	13(1)	8(1)	15(1)	2(1)	3(1)	2(1)
O(5)	14(1)	20(1)	10(1)	-2(1)	-2(1)	3(1)
O(6)	19(1)	17(1)	6(1)	0(1)	4(1)	2(1)
O(7)	15(1)	8(1)	14(1)	2(1)	6(1)	-1(1)
O(8)	7(1)	11(1)	11(1)	-1(1)	3(1)	-1(1)
N(1)	9(1)	10(1)	7(1)	0(1)	4(1)	3(1)
N(2)	8(1)	8(1)	7(1)	1(1)	3(1)	-2(1)
C(1)	5(1)	10(1)	5(1)	0(1)	1(1)	2(1)
C(2)	7(1)	8(1)	8(1)	1(1)	4(1)	0(1)
C(3)	14(2)	10(2)	5(1)	1(1)	1(1)	1(1)
C(4)	18(1)	6(1)	4(1)	-2(1)	-1(1)	-7(1)
C(5)	8(1)	10(2)	8(1)	1(2)	2(1)	1(2)
C(6)	10(1)	9(1)	5(1)	-3(1)	3(1)	-3(1)
C(7)	7(1)	9(1)	5(1)	0(1)	2(1)	0(1)
C(8)	9(1)	14(2)	5(1)	1(1)	1(1)	1(1)
C(9)	14(1)	16(2)	3(1)	3(1)	0(1)	-2(2)
C(10)	16(1)	5(1)	9(1)	-1(2)	0(1)	-4(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for [Tl(L-GluH)].

	x	y	z	U(eq)
H(1A)	5870	4927	4686	10
H(1B)	4560	5583	3925	10
H(1C)	6079	6175	3887	10
H(2A)	-1354	5826	-4768	9
H(2B)	78	6736	-4161	9
H(2C)	-1326	7173	-3936	9
H(2)	4951	1381	3859	9
H(3A)	4130	3564	2481	12
H(3B)	5785	3889	2485	12
H(4A)	6019	-469	2385	12
H(4B)	4380	-823	2403	12
H(7)	-59	2519	-3976	8
H(8A)	514	2335	-2454	12
H(8B)	1170	4855	-2686	12
H(9A)	-714	7140	-2391	14
H(9B)	-1546	4680	-2274	14

Table 6. Torsion angles [°] for [Tl(L-GluH)].

O(1)#1-Tl(1)-O(1)-C(5)	60.84(18)
O(2)-Tl(1)-O(1)-C(5)	1.98(18)
O(1)#1-Tl(1)-O(1)-Tl(1)#3	-65.59(16)
O(2)-Tl(1)-O(1)-Tl(1)#3	-124.46(16)
O(1)-Tl(1)-O(2)-C(5)	-1.95(17)
O(1)#1-Tl(1)-O(2)-C(5)	-118.8(2)
O(1)-Tl(1)-O(2)-Tl(2)	-128.42(15)
O(1)#1-Tl(1)-O(2)-Tl(2)	114.69(10)
O(5)-Tl(2)-O(2)-C(5)	-127.1(3)
O(6)-Tl(2)-O(2)-C(5)	-103.2(3)
O(6)#2-Tl(2)-O(2)-C(5)	-37.1(3)
O(5)-Tl(2)-O(2)-Tl(1)	-26.03(10)
O(6)-Tl(2)-O(2)-Tl(1)	-2.15(14)
O(6)#2-Tl(2)-O(2)-Tl(1)	63.92(9)
O(6)-Tl(2)-O(5)-C(10)	-1.0(3)
O(6)#2-Tl(2)-O(5)-C(10)	72.8(3)
O(2)-Tl(2)-O(5)-C(10)	151.4(3)
O(5)-Tl(2)-O(6)-C(10)	0.9(3)
O(6)#2-Tl(2)-O(6)-C(10)	-98.0(3)
O(2)-Tl(2)-O(6)-C(10)	-30.8(3)
O(5)-Tl(2)-O(6)-Tl(2)#4	-115.96(14)
O(6)#2-Tl(2)-O(6)-Tl(2)#4	145.08(14)
O(2)-Tl(2)-O(6)-Tl(2)#4	-147.68(9)
O(4)-C(1)-C(2)-N(1)	150.4(3)
O(3)-C(1)-C(2)-N(1)	-32.1(4)
O(4)-C(1)-C(2)-C(3)	-88.7(4)
O(3)-C(1)-C(2)-C(3)	88.8(4)
N(1)-C(2)-C(3)-C(4)	-174.9(3)
C(1)-C(2)-C(3)-C(4)	64.0(4)
C(2)-C(3)-C(4)-C(5)	178.7(3)
Tl(1)-O(1)-C(5)-O(2)	-3.8(3)
Tl(1)#3-O(1)-C(5)-O(2)	114.6(3)
Tl(1)-O(1)-C(5)-C(4)	176.3(2)
Tl(1)#3-O(1)-C(5)-C(4)	-65.3(4)

Tl(1)-O(2)-C(5)-O(1)	3.7(3)
Tl(2)-O(2)-C(5)-O(1)	109.1(3)
Tl(1)-O(2)-C(5)-C(4)	-176.4(2)
Tl(2)-O(2)-C(5)-C(4)	-71.1(4)
C(3)-C(4)-C(5)-O(1)	-176.9(3)
C(3)-C(4)-C(5)-O(2)	3.2(4)
O(7)-C(6)-C(7)-N(2)	171.5(3)
O(8)-C(6)-C(7)-N(2)	-9.3(4)
O(7)-C(6)-C(7)-C(8)	-64.7(4)
O(8)-C(6)-C(7)-C(8)	114.5(3)
N(2)-C(7)-C(8)-C(9)	68.6(4)
C(6)-C(7)-C(8)-C(9)	-54.5(4)
C(7)-C(8)-C(9)-C(10)	172.3(4)
Tl(2)-O(5)-C(10)-O(6)	1.9(6)
Tl(2)-O(5)-C(10)-C(9)	179.9(5)
Tl(2)-O(6)-C(10)-O(5)	-1.8(6)
Tl(2)#4-O(6)-C(10)-O(5)	111.1(5)
Tl(2)-O(6)-C(10)-C(9)	-179.9(4)
Tl(2)#4-O(6)-C(10)-C(9)	-67.0(5)
C(8)-C(9)-C(10)-O(5)	25.3(7)
C(8)-C(9)-C(10)-O(6)	-156.5(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y+1/2,-z #2 -x,y-1/2,-z #3 -x+1,y-1/2,-z

#4 -x,y+1/2,-z