

Table 1. Crystal data and structure refinement for structure17.

Identification code	structure17
Empirical formula	C12 H9 Cl N2 O4
Formula weight	280.66
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 7.3104(5) Å α = 107.7590(10)°. b = 7.5438(5) Å β = 94.8030(10)°. c = 10.9411(7) Å γ = 91.6970(10)°.
Volume	571.64(7) Å ³
Z	2
Calculated density	1.631 Mg/m ³
Absorption coefficient	0.347 mm ⁻¹
F(000)	288
Crystal size	0.33 x 0.13 x 0.05 mm ³
Theta range for data collection	1.96 to 27.47°.
Limiting indices	-9<=h<=9, -9<=k<=9, -14<=l<=14
Reflections collected	5534
Independent reflections	2614 [R(int) = 0.0153]
Completeness to theta = 27.47°	99.2 %
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.806
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2614 / 0 / 172
Goodness-of-fit on F ²	1.062
Final R indices [I>2sigma(I)]	R1 = 0.0378, wR2 = 0.0960
R indices (all data)	R1 = 0.0425, wR2 = 0.0990
Largest diff. peak and hole	0.343 and -0.290 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct17. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	2257(1)	2533(1)	-856(1)	23(1)
O(1)	5010(2)	9174(2)	6959(1)	23(1)
O(2)	2238(2)	10126(2)	6532(1)	24(1)
O(3)	11234(2)	3553(2)	3963(1)	31(1)
O(4)	11661(2)	1449(2)	2085(1)	27(1)
N(1)	3274(2)	5981(2)	2212(1)	21(1)
N(2)	5598(2)	3577(2)	1151(1)	18(1)
C(1)	1945(2)	7082(2)	2694(2)	24(1)
C(2)	2004(2)	8124(2)	3984(2)	22(1)
C(3)	3522(2)	8033(2)	4812(2)	18(1)
C(4)	4920(2)	6886(2)	4327(2)	18(1)
C(5)	4728(2)	5883(2)	3020(2)	18(1)
C(6)	6104(2)	4598(2)	2386(1)	17(1)
C(7)	7812(2)	4345(2)	2940(1)	18(1)
C(8)	8944(2)	3079(2)	2202(1)	18(1)
C(9)	8396(2)	2121(2)	914(2)	21(1)
C(10)	6672(2)	2391(2)	413(2)	22(1)
C(11)	3681(2)	9166(2)	6212(2)	19(1)
C(12)	10737(2)	2737(2)	2853(2)	20(1)

Table 3. Bond lengths [Å] and angles [°] for struct17.

O(1)-C(11)	1.215(2)
O(2)-C(11)	1.3086(18)
O(3)-C(12)	1.2011(19)
O(4)-C(12)	1.3203(19)
N(1)-C(1)	1.333(2)
N(1)-C(5)	1.343(2)
N(2)-C(10)	1.332(2)
N(2)-C(6)	1.3493(19)
C(1)-C(2)	1.387(2)
C(2)-C(3)	1.389(2)
C(3)-C(4)	1.392(2)
C(3)-C(11)	1.502(2)
C(4)-C(5)	1.392(2)
C(5)-C(6)	1.483(2)
C(6)-C(7)	1.385(2)
C(7)-C(8)	1.391(2)
C(8)-C(9)	1.391(2)
C(8)-C(12)	1.506(2)
C(9)-C(10)	1.378(2)
C(1)-N(1)-C(5)	118.12(14)
C(10)-N(2)-C(6)	123.91(13)
N(1)-C(1)-C(2)	122.93(15)
C(1)-C(2)-C(3)	118.69(15)
C(2)-C(3)-C(4)	119.20(14)
C(2)-C(3)-C(11)	121.00(14)
C(4)-C(3)-C(11)	119.80(14)
C(5)-C(4)-C(3)	117.81(14)
N(1)-C(5)-C(4)	123.25(14)
N(1)-C(5)-C(6)	113.53(13)
C(4)-C(5)-C(6)	123.22(14)
N(2)-C(6)-C(7)	118.20(14)
N(2)-C(6)-C(5)	115.25(13)
C(7)-C(6)-C(5)	126.55(14)
C(6)-C(7)-C(8)	119.13(14)
C(9)-C(8)-C(7)	120.58(14)
C(9)-C(8)-C(12)	121.42(14)
C(7)-C(8)-C(12)	117.97(13)
C(10)-C(9)-C(8)	118.15(14)
N(2)-C(10)-C(9)	119.93(14)
O(1)-C(11)-O(2)	124.16(14)
O(1)-C(11)-C(3)	123.13(14)
O(2)-C(11)-C(3)	112.71(13)
O(3)-C(12)-O(4)	124.60(14)
O(3)-C(12)-C(8)	122.39(14)
O(4)-C(12)-C(8)	113.00(13)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct17.
The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	19(1)	28(1)	18(1)	3(1)	-3(1)	2(1)
O(1)	18(1)	29(1)	22(1)	6(1)	-1(1)	6(1)
O(2)	19(1)	30(1)	18(1)	1(1)	1(1)	10(1)
O(3)	23(1)	41(1)	22(1)	-1(1)	-5(1)	13(1)
O(4)	20(1)	34(1)	22(1)	2(1)	-2(1)	13(1)
N(1)	18(1)	24(1)	20(1)	5(1)	-2(1)	4(1)
N(2)	15(1)	21(1)	18(1)	6(1)	-3(1)	3(1)
C(1)	17(1)	29(1)	24(1)	7(1)	-3(1)	6(1)
C(2)	16(1)	24(1)	25(1)	6(1)	1(1)	7(1)
C(3)	16(1)	18(1)	20(1)	6(1)	1(1)	2(1)
C(4)	15(1)	19(1)	20(1)	7(1)	-1(1)	1(1)
C(5)	15(1)	18(1)	20(1)	7(1)	0(1)	1(1)
C(6)	17(1)	18(1)	17(1)	6(1)	1(1)	1(1)
C(7)	17(1)	19(1)	16(1)	5(1)	0(1)	1(1)
C(8)	15(1)	20(1)	19(1)	7(1)	0(1)	2(1)
C(9)	21(1)	22(1)	19(1)	4(1)	2(1)	7(1)
C(10)	23(1)	23(1)	17(1)	3(1)	0(1)	4(1)
C(11)	16(1)	19(1)	21(1)	7(1)	3(1)	2(1)
C(12)	16(1)	23(1)	19(1)	6(1)	1(1)	4(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct17.

	x	y	z	U(eq)
H(2A)	2385	10735	7320	36
H(4A)	12646	1308	2490	40
H(2B)	4493	3701	813	22
H(1)	911	7155	2128	29
H(2)	1026	8885	4296	27
H(4)	5971	6790	4871	21
H(7)	8205	5026	3811	21
H(9)	9190	1303	394	25
H(10)	6249	1733	-458	26

