

Table 1. Crystal data and structure refinement for struct21.

Identification code	struct21	
Empirical formula	C16 H16 N2 O4	
Formula weight	300.31	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 3.9463(2) Å b = 13.7018(8) Å c = 13.5187(8) Å	$\alpha = 90^\circ$. $\beta = 93.1920(10)^\circ$. $\gamma = 90^\circ$.
Volume	729.84(7) Å ³	
Z	2	
Calculated density	1.367 Mg/m ³	
Absorption coefficient	0.100 mm ⁻¹	
F(000)	316	
Crystal size	0.28 x 0.15 x 0.13 mm ³	
Theta range for data collection	2.12 to 24.99 °.	
Limiting indices	-4 ≤ h ≤ 4, -16 ≤ k ≤ 16, -16 ≤ l ≤ 16	
Reflections collected	7560	
Independent reflections	1290 [R(int) = 0.0213]	
Completeness to theta = 24.99°	99.9 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	1290 / 0 / 101	
Goodness-of-fit on F ²	1.090	
Final R indices [I > 2σ(I)]	R1 = 0.0337, wR2 = 0.0926	
R indices (all data)	R1 = 0.0365, wR2 = 0.0952	
Largest diff. peak and hole	0.173 and -0.159 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct21. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(2)	2626(2)	6328(1)	1261(1)	31(1)
O(1)	1300(3)	7616(1)	2187(1)	41(1)
N(1)	6518(3)	9061(1)	-801(1)	29(1)
C(5)	5095(3)	9459(1)	-13(1)	26(1)
C(3)	3995(3)	7887(1)	672(1)	27(1)
C(6)	2506(3)	7280(1)	1461(1)	28(1)
C(4)	3834(3)	8894(1)	741(1)	27(1)
C(7)	1185(3)	5677(1)	1979(1)	32(1)
C(2)	5464(3)	7474(1)	-140(1)	30(1)
C(1)	6694(3)	8092(1)	-848(1)	31(1)
C(8)	1564(4)	4658(1)	1592(1)	40(1)

Table 3. Bond lengths [Å] and angles [°] for struct21.

O(2)-C(6)	1.3328(15)
O(2)-C(7)	1.4573(14)
O(1)-C(6)	1.2058(14)
N(1)-N(1)#1	1.198(2)
N(1)-C(1)	1.3319(16)
N(1)-C(5)	1.3472(15)
C(5)-N(1)#1	1.3274(15)
C(5)-C(4)	1.3931(16)
C(5)-C(5)#2	1.486(2)
C(3)-C(4)	1.3844(18)
C(3)-C(2)	1.3908(16)
C(3)-C(6)	1.4978(16)
C(7)-C(8)	1.5014(18)
C(2)-C(1)	1.3856(17)
C(1)-N(1)#1	1.8397(17)
C(6)-O(2)-C(7)	116.35(9)
N(1)#1-N(1)-C(1)	93.14(7)
N(1)#1-N(1)-C(5)	62.54(6)
C(1)-N(1)-C(5)	117.76(10)
N(1)#1-C(5)-N(1)	53.23(10)
N(1)#1-C(5)-C(4)	100.62(10)
N(1)-C(5)-C(4)	122.37(11)
N(1)#1-C(5)-C(5)#2	113.98(12)
N(1)-C(5)-C(5)#2	116.50(12)
C(4)-C(5)-C(5)#2	121.12(13)
C(4)-C(3)-C(2)	118.75(11)
C(4)-C(3)-C(6)	119.00(10)
C(2)-C(3)-C(6)	122.23(11)
O(1)-C(6)-O(2)	124.00(11)
O(1)-C(6)-C(3)	123.74(11)
O(2)-C(6)-C(3)	112.26(10)
C(3)-C(4)-C(5)	119.04(10)
O(2)-C(7)-C(8)	106.68(10)
C(1)-C(2)-C(3)	118.30(12)
N(1)-C(1)-C(2)	123.76(11)
N(1)-C(1)-N(1)#1	40.57(8)
C(2)-C(1)-N(1)#1	98.57(9)

Symmetry transformations used to generate equivalent atoms: