

Table 1. Crystal data and structure refinement for struct23.

Identification code	struct23	
Empirical formula	C20 H24 N2 O4	
Formula weight	356.41	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	$a = 7.4910(15) \text{ Å}$ $b = 8.0010(16) \text{ Å}$ $c = 15.233(3) \text{ Å}$	$\alpha = 90^\circ$ $\beta = 92.19(3)^\circ$ $\gamma = 90^\circ$
Volume	912.3(3) Å ³	
Z	2	
Calculated density	1.297 Mg/m ³	
Absorption coefficient	0.091 mm ⁻¹	
F(000)	380	
Crystal size	0.40 x 0.25 x 0.13 mm ³	
Theta range for data collection	2.68 to 27.86 °.	
Limiting indices	-9<=h<=9, -10<=k<=10, -19<=l<=19	
Reflections collected	12461	
Independent reflections	2157 [R(int) = 0.0553]	
Completeness to theta = 27.86°	99.2 %	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2157 / 0 / 118	
Goodness-of-fit on F ²	1.052	
Final R indices [I>2sigma(I)]	R1 = 0.0471, wR2 = 0.1378	
R indices (all data)	R1 = 0.0877, wR2 = 0.1885	
Largest diff. peak and hole	0.365 and -0.429 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct23. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(2)	8857(1)	1996(2)	5888(1)	31(1)
C(4)	13053(2)	4128(2)	5606(1)	26(1)
N(1)	13623(2)	4329(2)	4069(1)	27(1)
O(1)	10666(2)	3189(2)	6923(1)	37(1)
C(2)	10928(2)	3039(2)	4546(1)	28(1)
C(3)	11444(2)	3338(2)	5418(1)	25(1)
C(8)	6069(2)	638(2)	6131(1)	29(1)
C(6)	10303(2)	2844(2)	6164(1)	27(1)
C(7)	7629(2)	1518(2)	6573(1)	34(1)
C(5)	14120(2)	4594(2)	4915(1)	24(1)
C(9)	4661(2)	192(3)	6786(1)	37(1)
C(10)	3090(2)	-755(2)	6373(1)	36(1)
C(1)	12058(2)	3572(2)	3899(1)	30(1)

Table 3. Bond lengths [Å] and angles [°] for struct23.

O(2)-C(6)	1.332(2)
O(2)-C(7)	1.467(2)
C(4)-C(3)	1.381(2)
C(4)-C(5)	1.396(2)
N(1)-C(1)	1.336(2)
N(1)-C(5)	1.345(2)
O(1)-C(6)	1.210(2)
C(2)-C(1)	1.390(2)
C(2)-C(3)	1.390(2)
C(3)-C(6)	1.500(2)
C(8)-C(7)	1.502(2)
C(8)-C(9)	1.522(2)
C(5)-C(5)#1	1.484(3)
C(9)-C(10)	1.516(2)
C(6)-O(2)-C(7)	115.67(13)
C(3)-C(4)-C(5)	119.10(14)
C(1)-N(1)-C(5)	117.76(14)
C(1)-C(2)-C(3)	118.02(15)
C(4)-C(3)-C(2)	119.03(15)
C(4)-C(3)-C(6)	118.80(14)
C(2)-C(3)-C(6)	122.18(15)
C(7)-C(8)-C(9)	111.28(14)
O(1)-C(6)-O(2)	124.57(15)
O(1)-C(6)-C(3)	123.37(15)
O(2)-C(6)-C(3)	112.06(14)
O(2)-C(7)-C(8)	107.57(13)
N(1)-C(5)-C(4)	122.33(14)
N(1)-C(5)-C(5)#1	116.63(17)
C(4)-C(5)-C(5)#1	121.04(17)
C(10)-C(9)-C(8)	113.06(14)
N(1)-C(1)-C(2)	123.74(15)

Symmetry transformations used to generate equivalent atoms:
#1 -x+3,-y+1,-z+1

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct23.
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}
O(2)	27(1)	41(1)	26(1)	1(1)	4(1)	-7(1)
C(4)	27(1)	27(1)	23(1)	2(1)	-2(1)	2(1)
N(1)	28(1)	31(1)	23(1)	0(1)	0(1)	-2(1)
O(1)	35(1)	52(1)	26(1)	2(1)	1(1)	-9(1)
C(2)	25(1)	29(1)	29(1)	-1(1)	-1(1)	-1(1)
C(3)	25(1)	24(1)	26(1)	2(1)	2(1)	4(1)
C(8)	29(1)	30(1)	27(1)	2(1)	3(1)	0(1)
C(6)	25(1)	31(1)	25(1)	3(1)	0(1)	1(1)
C(7)	32(1)	47(1)	24(1)	4(1)	6(1)	-7(1)
C(5)	27(1)	23(1)	23(1)	2(1)	0(1)	4(1)
C(9)	35(1)	50(1)	27(1)	3(1)	5(1)	-8(1)
C(10)	33(1)	43(1)	34(1)	5(1)	6(1)	-4(1)
C(1)	29(1)	35(1)	24(1)	-3(1)	-2(1)	-2(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct23.

	x	y	z	U(eq)
H(4)	13420	4348	6184	31
H(2)	9859	2498	4399	33
H(8A)	6483	-374	5852	34
H(8B)	5542	1353	5676	34
H(7A)	7225	2503	6879	41
H(7B)	8226	783	6996	41
H(9A)	5209	-483	7251	44
H(9B)	4228	1212	7048	44
H(10A)	2240	-990	6812	55
H(10B)	3502	-1786	6129	55
H(10C)	2532	-90	5915	55
H(1)	11704	3391	3315	35

