

Table 1. Crystal data and structure refinement for structure3.

Identification code	structure3
Empirical formula	C13.50 H9.50 Mn N2.50 O4.50
Formula weight	333.68
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 15.6763(10) Å α = 90°. b = 10.2423(6) Å β = 102.249(1)° c = 16.7755(10) Å γ = 90°.
Volume	2632.2(3) Å ³
Z	8
Calculated density	1.684 Mg/m ³
Absorption coefficient	1.026 mm ⁻¹
F(000)	1352
Crystal size	0.15 x 0.11 x 0.02 mm ³
Theta range for data collection	2.48 to 25.00°.
Limiting indices	-18<=h<=18, -12<=k<=12, -19<=l<=19
Reflections collected	10077
Independent reflections	2312 [R(int) = 0.0414]
Completeness to theta = 25.00°	99.6%
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.897
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2312 / 1 / 213
Goodness-of-fit on F ²	1.267
Final R indices [I>2sigma(I)]	R1 = 0.0478, wR2 = 0.0935
R indices (all data)	R1 = 0.0522, wR2 = 0.0952
Largest diff. peak and hole	0.425 and -0.352 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mn(1)	1433(1)	5990(1)	222(1)	10(1)
N(1)	1497(2)	4685(3)	1346(2)	14(1)
C(1)	1027(2)	4908(3)	1911(2)	17(1)
C(2)	1201(2)	4325(3)	2671(2)	18(1)
C(3)	1892(2)	3462(3)	2862(2)	14(1)
C(4)	2378(2)	3207(3)	2274(2)	15(1)
C(5)	2172(2)	3845(3)	1530(2)	13(1)
C(6)	2736(2)	3733(3)	919(2)	11(1)
C(7)	3308(2)	2701(3)	925(2)	13(1)
C(8)	3894(2)	2748(3)	414(2)	13(1)
C(9)	3888(2)	3826(3)	-80(2)	19(1)
C(10)	3271(2)	4786(4)	-84(2)	21(1)
N(2)	2685(2)	4744(3)	397(2)	15(1)
C(11)	2155(2)	2864(3)	3707(2)	13(1)
O(1)	2886(2)	2317(2)	3862(1)	16(1)
O(2)	1637(2)	3007(2)	4175(1)	17(1)
C(12)	4542(2)	1657(3)	416(2)	13(1)
O(3)	4299(1)	524(2)	544(1)	15(1)
O(4)	5273(1)	2000(2)	303(1)	18(1)
O(5)	0	7357(4)	2500	47(1)
C(13)	-247(5)	8363(9)	2776(5)	34(2)
N(3)	-100(40)	9552(7)	2520(30)	39(6)
C(14)	-487(14)	10704(15)	2824(10)	126(8)
C(15)	423(8)	9716(14)	1906(7)	65(3)

Table 3. Bond lengths [Å] and angles [°] for struct3.

Mn (1) -O (2) #1	2.117 (2)
Mn (1) -O (4) #2	2.120 (2)
Mn (1) -O (1) #3	2.158 (2)
Mn (1) -O (3) #4	2.178 (2)
Mn (1) -N (1)	2.296 (3)
Mn (1) -N (2)	2.307 (3)
N (1) -C (1)	1.337 (4)
N (1) -C (5)	1.347 (4)
C (1) -C (2)	1.382 (5)
C (2) -C (3)	1.382 (5)
C (3) -C (4)	1.393 (5)
C (3) -C (11)	1.519 (4)
C (4) -C (5)	1.385 (4)
C (5) -C (6)	1.494 (4)
C (6) -N (2)	1.347 (4)
C (6) -C (7)	1.385 (4)
C (7) -C (8)	1.383 (5)
C (8) -C (9)	1.380 (5)
C (8) -C (12)	1.510 (4)
C (9) -C (10)	1.378 (5)
C (10) -N (2)	1.346 (4)
C (11) -O (2)	1.252 (4)
C (11) -O (1)	1.252 (4)
O (1) -Mn (1) #5	2.158 (2)
O (2) -Mn (1) #6	2.117 (2)
C (12) -O (4)	1.251 (4)
C (12) -O (3)	1.254 (4)
O (3) -Mn (1) #4	2.178 (2)
O (4) -Mn (1) #7	2.120 (2)
O (5) -C (13)	1.225 (9)
O (5) -C (13) #8	1.225 (9)
C (13) -N (3)	1.326 (13)

N (3) -C (14)	1.462 (12)
N (3) -C (15)	1.463 (16)
O (2) #1-Mn (1) -O (4) #2	95.69 (9)
O (2) #1-Mn (1) -O (1) #3	98.39 (9)
O (4) #2-Mn (1) -O (1) #3	87.02 (9)
O (2) #1-Mn (1) -O (3) #4	90.57 (9)
O (4) #2-Mn (1) -O (3) #4	91.95 (9)
O (1) #3-Mn (1) -O (3) #4	171.04 (9)
O (2) #1-Mn (1) -N (1)	167.37 (9)
O (4) #2-Mn (1) -N (1)	96.91 (9)
O (1) #3-Mn (1) -N (1)	81.53 (9)
O (3) #4-Mn (1) -N (1)	89.77 (9)
O (2) #1-Mn (1) -N (2)	95.69 (9)
O (4) #2-Mn (1) -N (2)	168.34 (9)
O (1) #3-Mn (1) -N (2)	88.80 (9)
O (3) #4-Mn (1) -N (2)	90.48 (9)
N (1) -Mn (1) -N (2)	71.69 (9)
C (1) -N (1) -C (5)	118.0 (3)
C (1) -N (1) -Mn (1)	123.2 (2)
C (5) -N (1) -Mn (1)	117.1 (2)
N (1) -C (1) -C (2)	123.3 (3)
C (3) -C (2) -C (1)	118.8 (3)
C (2) -C (3) -C (4)	118.4 (3)
C (2) -C (3) -C (11)	121.3 (3)
C (4) -C (3) -C (11)	120.2 (3)
C (5) -C (4) -C (3)	119.4 (3)
N (1) -C (5) -C (4)	122.0 (3)
N (1) -C (5) -C (6)	116.2 (3)
C (4) -C (5) -C (6)	121.6 (3)
N (2) -C (6) -C (7)	122.7 (3)
N (2) -C (6) -C (5)	115.2 (3)
C (7) -C (6) -C (5)	122.0 (3)
C (8) -C (7) -C (6)	118.9 (3)
C (9) -C (8) -C (7)	118.7 (3)

C(9)-C(8)-C(12)	120.8(3)
C(7)-C(8)-C(12)	120.5(3)
C(10)-C(9)-C(8)	119.2(3)
N(2)-C(10)-C(9)	122.9(3)
C(10)-N(2)-C(6)	117.4(3)
C(10)-N(2)-Mn(1)	125.3(2)
C(6)-N(2)-Mn(1)	116.1(2)
O(2)-C(11)-O(1)	127.5(3)
O(2)-C(11)-C(3)	117.0(3)
O(1)-C(11)-C(3)	115.4(3)
C(11)-O(1)-Mn(1) #5	136.2(2)
C(11)-O(2)-Mn(1) #6	144.0(2)
O(4)-C(12)-O(3)	127.4(3)
O(4)-C(12)-C(8)	115.4(3)
O(3)-C(12)-C(8)	117.1(3)
C(12)-O(3)-Mn(1) #4	134.4(2)
C(12)-O(4)-Mn(1) #7	134.2(2)
C(13)-O(5)-C(13) #8	65.5(8)
O(5)-C(13)-N(3)	124.3(10)
C(13)-N(3)-C(14)	121.3(15)
C(13)-N(3)-C(15)	119.4(10)
C(14)-N(3)-C(15)	119.2(13)

Symmetry transformations used to generate equivalent atoms:

#1 $x, -y+1, z-1/2$ #2 $x-1/2, y+1/2, z$
#3 $-x+1/2, y+1/2, -z+1/2$ #4 $-x+1/2, -y+1/2, -z$
#5 $-x+1/2, y-1/2, -z+1/2$ #6 $x, -y+1, z+1/2$
#7 $x+1/2, y-1/2, z$ #8 $-x, y, -z+1/2$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct3.

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}
Mn (1)	10 (1)	13 (1)	9 (1)	0 (1)	3 (1)	2 (1)
N (1)	12 (1)	17 (2)	14 (1)	1 (1)	4 (1)	1 (1)
C (1)	14 (2)	22 (2)	17 (2)	2 (1)	5 (1)	6 (1)
C (2)	18 (2)	27 (2)	13 (2)	1 (1)	10 (1)	4 (1)
C (3)	15 (2)	15 (2)	13 (2)	0 (1)	3 (1)	-1 (1)
C (4)	15 (2)	15 (2)	17 (2)	1 (1)	5 (1)	4 (1)
C (5)	12 (2)	14 (2)	13 (2)	-2 (1)	5 (1)	0 (1)
C (6)	9 (2)	14 (2)	9 (2)	-2 (1)	0 (1)	-2 (1)
C (7)	14 (2)	16 (2)	10 (2)	4 (1)	0 (1)	2 (1)
C (8)	11 (2)	15 (2)	12 (2)	-6 (1)	1 (1)	-3 (1)
C (9)	18 (2)	21 (2)	20 (2)	4 (2)	11 (1)	5 (1)
C (10)	20 (2)	25 (2)	21 (2)	9 (2)	10 (2)	5 (2)
N (2)	14 (1)	18 (2)	13 (1)	1 (1)	4 (1)	2 (1)
C (11)	16 (2)	10 (2)	13 (2)	-2 (1)	3 (1)	-2 (1)
O (1)	15 (1)	21 (1)	13 (1)	4 (1)	3 (1)	5 (1)
O (2)	20 (1)	22 (1)	11 (1)	-1 (1)	8 (1)	3 (1)
C (12)	11 (2)	20 (2)	8 (2)	-2 (1)	1 (1)	2 (1)
O (3)	15 (1)	15 (1)	13 (1)	-1 (1)	2 (1)	0 (1)
O (4)	13 (1)	18 (1)	24 (1)	-1 (1)	10 (1)	4 (1)
O (5)	52 (3)	35 (3)	56 (3)	0	16 (2)	0
C (13)	30 (5)	47 (6)	22 (4)	12 (4)	1 (3)	3 (4)
N (3)	50 (20)	35 (3)	31 (5)	5 (9)	14 (9)	14 (8)
C (14)	220 (20)	76 (11)	96 (12)	12 (9)	71 (13)	85 (13)
C (15)	61 (7)	85 (9)	47 (7)	29 (6)	11 (6)	-29 (7)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct3.

	x	y	z	U(eq)
H(1)	550	5498	1783	21
H(2)	851	4514	3055	21
H(4)	2847	2601	2383	18
H(7)	3298	1974	1274	16
H(9)	4305	3907	-414	22
H(10)	3260	5508	-441	25
H(13)	-559	8286	3201	40
H(14A)	-824	10435	3226	189
H(14B)	-873	11148	2369	189
H(14C)	-20	11300	3081	189
H(15A)	651	8865	1782	97
H(15B)	911	10307	2115	97
H(15C)	62	10085	1408	97

