

Table 1. Crystal data and structure refinement for 1.

Identification code	4g
Empirical formula	C ₃₀ H ₂₈ N ₄ O ₈
Formula weight	572.56
Temperature	293 (2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁ /c
Unit cell dimensions	a = 9.5660(10) Å alpha = 90° b = 18.271(2) Å beta = 93.750(10)° c = 15.602(2) Å gamma = 90°
Volume, Z	2721.1(5) Å ³ , 4
Density (calculated)	1.398 Mg/m ³
Absorption coefficient	0.103 mm ⁻¹
F(000)	1200
Crystal size	0.3 x 0.3 x 0.2 mm
θ range for data collection	2.13 to 20.00°
Limiting indices	-10 ≤ h ≤ 8, 0 ≤ k ≤ 17, -15 ≤ l ≤ 14
Reflections collected	2629
Independent reflections	2433 (R _{int} = 0.0267)
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2211 / 0 / 379

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Goodness-of-fit on F^2 1.056
Final R indices [$I > 2\sigma(I)$] R1 = 0.0494, wR2 = 0.1147
R indices (all data) R1 = 0.0824, wR2 = 0.1356
Largest diff. peak and hole 0.203 and -0.204 eÅ⁻³

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	9108(3)	460(2)	2243(2)	47(1)
O(2)	11081(4)	-178(2)	2181(3)	88(1)
O(3)	10209(5)	2079(2)	2036(2)	71(1)
O(4)	5953(5)	3191(2)	2020(3)	91(1)
O(5)	6494(4)	1816(2)	3352(2)	51(1)
O(6)	5447(4)	2764(2)	3968(2)	82(1)
O(7)	8547(4)	-159(2)	3999(2)	62(1)
O(8)	4242(4)	803(2)	4329(3)	78(1)
N(1)	8526(5)	1752(2)	1003(3)	53(1)
N(2)	8056(5)	2592(2)	2068(3)	55(1)
N(3)	6432(5)	384(2)	4107(2)	46(1)
N(4)	6783(5)	-453(2)	3006(3)	48(1)
C(1)	6466(7)	-886(3)	-716(4)	96(2)
C(2)	7230(6)	-543(3)	66(4)	62(2)
C(3)	7158(5)	-855(3)	869(4)	61(2)
C(4)	7811(5)	-551(3)	1606(3)	49(1)
C(5)	8537(5)	98(3)	1507(3)	45(1)
C(6)	8633(5)	439(3)	727(3)	52(1)
C(7)	7979(6)	105(3)	13(3)	61(2)
C(8)	10440(6)	285(3)	2532(4)	58(2)
C(9)	10919(5)	730(3)	3286(3)	63(2)
C(10)	9378(6)	1167(3)	666(3)	61(2)
C(11)	6720(7)	2757(3)	1689(4)	66(2)
C(12)	6357(7)	2384(3)	904(4)	68(2)
C(13)	7232(7)	1899(3)	611(3)	64(2)
C(14)	9032(8)	2139(3)	1721(4)	56(2)
C(15)	8466(6)	2946(3)	2892(3)	65(2)
C(16)	8725(6)	2422(2)	3631(3)	48(1)
C(17)	9985(5)	2462(3)	4116(3)	52(1)
C(18)	10306(5)	2013(3)	4809(3)	50(1)
C(19)	9323(5)	1496(3)	5003(3)	49(1)

C (20)	8044 (5)	1425 (2)	4536 (3)	43 (1)
C (21)	7765 (5)	1907 (3)	3859 (3)	45 (1)
C (22)	5380 (6)	2268 (3)	3475 (3)	57 (1)
C (23)	4140 (6)	2054 (3)	2907 (4)	79 (2)
C (24)	11717 (5)	2053 (3)	5307 (3)	71 (2)
C (25)	7026 (5)	850 (3)	4805 (3)	54 (1)
C (26)	4987 (7)	418 (3)	3908 (4)	58 (2)
C (27)	4509 (6)	-16 (3)	3178 (4)	66 (2)
C (28)	5393 (7)	-409 (3)	2764 (3)	58 (2)
C (29)	7340 (7)	-79 (3)	3724 (3)	46 (1)
C (30)	7704 (6)	-886 (3)	2485 (3)	60 (2)

Table 4. Bond lengths [Å] and angles [°] for 1.

O(1)-C(8)	1.362(6)	O(1)-C(5)	1.404(5)
O(2)-C(8)	1.198(6)	O(3)-C(14)	1.204(6)
O(4)-C(11)	1.219(6)	O(5)-C(22)	1.373(6)
O(5)-C(21)	1.416(5)	O(6)-C(22)	1.187(6)
O(7)-C(29)	1.214(6)	O(8)-C(26)	1.222(6)
N(1)-C(13)	1.371(6)	N(1)-C(14)	1.385(6)
N(1)-C(10)	1.463(6)	N(2)-C(14)	1.384(7)
N(2)-C(11)	1.405(7)	N(2)-C(15)	1.471(6)
N(3)-C(29)	1.377(6)	N(3)-C(26)	1.398(6)
N(3)-C(25)	1.467(6)	N(4)-C(28)	1.361(6)
N(4)-C(29)	1.387(6)	N(4)-C(30)	1.469(6)
C(1)-C(2)	1.516(7)	C(2)-C(3)	1.382(7)
C(2)-C(7)	1.388(7)	C(3)-C(4)	1.389(7)
C(4)-C(5)	1.388(6)	C(4)-C(30)	1.513(6)
C(5)-C(6)	1.377(6)	C(6)-C(7)	1.383(7)
C(6)-C(10)	1.515(6)	C(8)-C(9)	1.478(7)
C(11)-C(12)	1.425(7)	C(12)-C(13)	1.320(7)
C(15)-C(16)	1.507(6)	C(16)-C(21)	1.377(6)
C(16)-C(17)	1.383(6)	C(17)-C(18)	1.376(6)
C(18)-C(19)	1.380(6)	C(18)-C(24)	1.514(6)
C(19)-C(20)	1.388(6)	C(20)-C(21)	1.388(6)
C(20)-C(25)	1.511(6)	C(22)-C(23)	1.486(7)
C(26)-C(27)	1.437(7)	C(27)-C(28)	1.312(7)
C(8)-O(1)-C(5)	117.7(4)	C(22)-O(5)-C(21)	119.8(4)
C(13)-N(1)-C(14)	121.2(5)	C(13)-N(1)-C(10)	119.4(5)
C(14)-N(1)-C(11)	119.4(5)	C(14)-N(2)-C(11)	125.6(5)
C(14)-N(2)-C(15)	117.2(5)	C(11)-N(2)-C(15)	117.2(5)
C(29)-N(3)-C(26)	125.0(5)	C(29)-N(3)-C(25)	117.0(5)
C(26)-N(3)-C(25)	117.9(4)	C(28)-N(4)-C(29)	120.8(5)
C(28)-N(4)-C(30)	119.2(5)	C(29)-N(4)-C(30)	119.9(5)
C(3)-C(2)-C(7)	117.6(5)	C(3)-C(2)-C(1)	120.5(5)
C(7)-C(2)-C(1)	121.8(6)	C(2)-C(3)-C(4)	122.5(5)
C(5)-C(4)-C(3)	116.9(5)	C(5)-C(4)-C(30)	120.7(5)
C(3)-C(4)-C(30)	122.4(5)	C(6)-C(5)-C(4)	123.2(5)
C(6)-C(5)-O(1)	117.7(4)	C(4)-C(5)-O(1)	118.9(5)
C(5)-C(6)-C(7)	117.4(5)	C(5)-C(6)-C(10)	120.8(5)
C(7)-C(6)-C(10)	121.8(5)	C(6)-C(7)-C(2)	122.4(5)

O(2) -C(8) -O(1)	120.7(5)	O(2) -C(8) -C(9)	127.6(5)
O(1) -C(8) -C(9)	111.6(5)	N(1) -C(10) -C(6)	110.1(4)
O(4) -C(11) -N(2)	121.2(6)	O(4) -C(11) -C(12)	123.8(6)
N(2) -C(11) -C(12)	115.0(6)	C(13) -C(12) -C(11)	119.6(6)
C(12) -C(13) -N(1)	123.4(5)	O(3) -C(14) -N(2)	122.2(5)
O(3) -C(14) -N(1)	123.5(6)	N(2) -C(14) -N(1)	114.3(6)
N(2) -C(15) -C(16)	114.2(4)	C(21) -C(16) -C(17)	117.8(4)
C(21) -C(16) -C(15)	123.6(5)	C(17) -C(16) -C(15)	118.6(5)
C(18) -C(17) -C(16)	122.8(5)	C(17) -C(18) -C(19)	117.3(5)
C(17) -C(18) -C(24)	121.4(5)	C(19) -C(18) -C(24)	121.2(5)
C(18) -C(19) -C(20)	122.6(5)	C(21) -C(20) -C(19)	117.4(5)
C(21) -C(20) -C(25)	123.9(5)	C(19) -C(20) -C(25)	118.8(4)
C(16) -C(21) -C(20)	122.1(5)	C(16) -C(21) -O(5)	119.9(4)
C(20) -C(21) -O(5)	117.7(4)	O(6) -C(22) -O(5)	122.7(5)
O(6) -C(22) -C(23)	126.5(6)	O(5) -C(22) -C(23)	110.8(5)
N(3) -C(25) -C(20)	115.0(4)	O(8) -C(26) -N(3)	120.6(5)
O(8) -C(26) -C(27)	125.2(6)	N(3) -C(26) -C(27)	114.2(5)
C(28) -C(27) -C(26)	120.7(6)	C(27) -C(28) -N(4)	123.0(5)
O(7) -C(29) -N(3)	122.2(5)	O(7) -C(29) -N(4)	122.2(5)
N(3) -C(29) -N(4)	115.7(5)	N(4) -C(30) -C(4)	111.3(4)

Table 5. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha)^2 U_{11} + \dots + 2hka^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
O(1)	39(2)	50(2)	51(2)	-6(2)	2(2)	-1(2)
O(2)	61(3)	96(3)	105(3)	-38(3)	-4(2)	26(2)
O(3)	69(3)	73(3)	71(3)	0(2)	4(2)	-18(2)
O(4)	123(4)	67(3)	83(3)	0(2)	0(3)	38(3)
O(5)	55(3)	46(2)	50(2)	1(2)	-6(2)	6(2)
O(6)	84(3)	84(3)	76(3)	-33(2)	-14(2)	21(2)
O(7)	53(3)	59(2)	73(3)	4(2)	-9(2)	11(2)
O(8)	56(3)	95(3)	82(3)	-17(2)	13(2)	6(2)
N(1)	69(4)	49(3)	42(3)	2(2)	6(3)	-3(3)
N(2)	79(4)	35(3)	49(3)	7(2)	0(3)	-3(3)
N(3)	41(3)	48(3)	49(3)	4(2)	5(2)	-4(2)
N(4)	45(3)	41(3)	57(3)	0(2)	5(2)	-7(2)
C(1)	103(5)	101(5)	82(4)	-30(4)	-14(4)	-18(4)
C(2)	53(4)	71(4)	63(4)	-16(3)	1(3)	-2(3)
C(3)	55(4)	51(3)	77(4)	-16(3)	8(3)	-7(3)
C(4)	48(3)	37(3)	62(4)	-7(3)	11(3)	3(3)
C(5)	40(3)	47(3)	48(4)	-9(3)	2(3)	2(3)
C(6)	52(4)	56(4)	47(4)	-9(3)	8(3)	-3(3)
C(7)	67(4)	67(4)	51(4)	-4(3)	14(3)	-1(3)
C(8)	53(5)	52(4)	67(4)	-7(3)	7(3)	4(3)
C(9)	48(4)	68(4)	73(4)	-17(3)	-5(3)	3(3)
C(10)	67(4)	65(4)	52(3)	0(3)	18(3)	-7(3)
C(11)	104(6)	39(4)	56(4)	20(3)	11(4)	10(4)
C(12)	91(5)	55(4)	57(4)	7(3)	0(3)	6(4)
C(13)	88(5)	54(4)	48(3)	8(3)	-10(4)	-13(4)
C(14)	76(5)	44(4)	49(4)	9(3)	9(4)	-9(4)
C(15)	92(5)	47(3)	55(4)	1(3)	2(3)	-14(3)
C(16)	61(4)	34(3)	47(3)	-2(3)	0(3)	-7(3)
C(17)	60(4)	45(3)	51(3)	-11(3)	10(3)	-15(3)
C(18)	44(4)	54(4)	52(4)	-17(3)	2(3)	-1(3)
C(19)	53(4)	51(3)	42(3)	-2(2)	1(3)	7(3)

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C(20)	47(4)	40(3)	41(3)	-2(3)	1(3)	2(3)
C(21)	48(4)	44(3)	41(3)	-6(3)	-7(3)	4(3)
C(22)	52(4)	60(4)	57(4)	6(3)	-10(3)	2(3)
C(23)	66(4)	71(4)	96(4)	1(3)	-24(4)	9(3)
C(24)	57(4)	80(4)	73(4)	-14(3)	-10(3)	-5(3)
C(25)	64(4)	57(3)	41(3)	4(3)	7(3)	-3(3)
C(26)	49(5)	60(4)	65(4)	8(3)	9(3)	-6(3)
C(27)	43(4)	82(4)	72(4)	-3(4)	6(3)	-8(3)
C(28)	46(4)	61(4)	67(4)	-7(3)	4(3)	-18(3)
C(29)	49(4)	34(3)	55(4)	12(3)	3(3)	-1(3)
C(30)	66(4)	39(3)	74(4)	-5(3)	10(3)	-1(3)

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H (1A)	6629 (7)	-600 (3)	-1215 (4)	144
H (1B)	5480 (7)	-900 (3)	-636 (4)	144
H (1C)	6806 (7)	-1374 (3)	-790 (4)	144
H (3A)	6652 (5)	-1286 (3)	917 (4)	73
H (7A)	8042 (6)	322 (3)	-522 (3)	73
H (9A)	10185 (5)	1058 (3)	3428 (3)	95
H (9B)	11731 (5)	1007 (3)	3155 (3)	95
H (9C)	11152 (5)	413 (3)	3765 (3)	95
H (10A)	10276 (6)	1146 (3)	991 (3)	73
H (10B)	9548 (6)	1269 (3)	71 (3)	73
H (12A)	5509 (7)	2481 (3)	600 (4)	82
H (13A)	6956 (7)	1644 (3)	112 (3)	77
H (15A)	7734 (6)	3286 (3)	3031 (3)	78
H (15B)	9312 (6)	3229 (3)	2828 (3)	78
H (17A)	10642 (5)	2806 (3)	3968 (3)	62
H (19A)	9526 (5)	1183 (3)	5464 (3)	58
H (23A)	4368 (6)	1635 (3)	2573 (4)	118
H (23B)	3876 (6)	2453 (3)	2530 (4)	118
H (23C)	3375 (6)	1937 (3)	3252 (4)	118
H (24A)	11748 (5)	1701 (3)	5765 (3)	106
H (24B)	11852 (5)	2535 (3)	5542 (3)	106
H (24C)	12444 (5)	1947 (3)	4930 (3)	106
H (25A)	7501 (5)	540 (3)	5236 (3)	65
H (25B)	6263 (5)	1093 (3)	5071 (3)	65
H (27A)	3563 (6)	-17 (3)	2997 (4)	79
H (28A)	5055 (7)	-671 (3)	2283 (3)	70
H (30C)	7340 (6)	-1380 (3)	2424 (3)	71
H (30A)	8630 (6)	-914 (3)	2776 (3)	71

Table 1. Crystal data and structure refinement for 1.

Identification code	4J.Ethanol
Empirical formula	$C_{54}H_{54}N_8O_{13}$
Formula weight	1023.05
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	$a = 11.346(3)$ Å $\alpha = 90^\circ$ $b = 17.125(3)$ Å $\beta = 102.63(2)^\circ$ $c = 25.281(5)$ Å $\gamma = 90^\circ$
Volume, Z	4793(2) Å ³ , 4
Density (calculated)	1.418 Mg/m ³
Absorption coefficient	0.103 mm ⁻¹
F(000)	2152
Crystal size	0.4 x 0.3 x 0.3 mm
θ range for data collection	1.45 to 20.00°
Limiting indices	$0 \leq h \leq 8$, $0 \leq k \leq 16$, $-24 \leq l \leq 23$
Reflections collected	4404
Independent reflections	4105 ($R_{int} = 0.0976$)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3140 / 2 / 416

Goodness-of-fit on F^2 1.015

Final R indices [I>2 σ (I)] R1 = 0.0979, WR2 = 0.2262

R indices (all data) R1 = 0.2557, WR2 = 0.3546

Largest diff. peak and hole 0.362 and -0.255 eÅ⁻³

Table 2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N(1)	5121(10)	5944(6)	2164(5)	38(3)
N(2)	6042(11)	5365(7)	1525(5)	46(4)
N(3)	1097(10)	3967(8)	333(5)	52(4)
N(4)	161(11)	4683(7)	920(5)	46(4)
N(5)	11292(11)	7987(7)	1584(5)	44(4)
N(6)	10331(11)	7387(7)	2207(5)	50(4)
N(7)	5470(11)	8704(7)	964(5)	47(4)
N(8)	6521(10)	9449(7)	435(5)	43(4)
O(1)	2126(9)	6396(5)	1320(4)	56(3)
O(2)	5895(10)	5785(7)	3066(4)	78(4)
O(3)	4381(9)	6113(6)	1262(4)	60(3)
O(4)	3714(9)	5222(6)	241(4)	52(3)
O(5)	1405(9)	5262(6)	439(4)	58(3)
O(6)	-1191(9)	4101(6)	1348(4)	66(4)
O(7)	8943(9)	8141(6)	316(4)	60(3)
O(8)	13071(10)	8590(6)	1848(4)	65(3)
O(9)	9563(9)	7266(6)	1319(4)	57(3)
O(10)	7338(9)	6920(6)	1380(4)	61(3)
O(11)	6767(10)	8147(6)	490(4)	64(3)
O(12)	6234(10)	10758(6)	385(5)	68(4)
C(1)	2041(13)	5956(9)	1750(6)	41(4)
C(2)	1033(13)	5497(9)	1730(6)	43(4)
C(3)	865(13)	5076(8)	2172(6)	41(4)
C(4)	1721(14)	5116(9)	2660(6)	48(5)
C(5)	2751(14)	5540(8)	2672(6)	51(5)
C(6)	2934(13)	5959(9)	2232(6)	41(4)
C(7)	4085(13)	6420(9)	2278(6)	53(5)
C(8)	6010(15)	5662(9)	2602(7)	50(5)
C(9)	6971(13)	5231(8)	2453(6)	42(4)
C(10)	6925(14)	5101(9)	1936(6)	45(5)
C(11)	5129(16)	5816(10)	1631(7)	46(5)

C (12)	5990 (13)	5127 (8)	957 (6)	45 (4)
C (13)	5163 (13)	4419 (9)	794 (6)	42 (4)
C (14)	4028 (13)	4500 (9)	460 (6)	36 (4)
C (15)	3311 (12)	3864 (9)	345 (5)	36 (4)
C (16)	3702 (14)	3131 (9)	563 (6)	53 (5)
C (17)	4834 (15)	3072 (10)	887 (7)	60 (5)
C (18)	5593 (14)	3696 (9)	1008 (6)	54 (5)
C (19)	2031 (13)	3916 (10)	-6 (6)	57 (5)
C (20)	441 (14)	3315 (10)	448 (6)	55 (5)
C (21)	-293 (15)	3335 (10)	779 (6)	65 (5)
C (22)	-531 (15)	4033 (10)	1046 (7)	46 (5)
C (23)	927 (15)	4683 (11)	561 (7)	45 (5)
C (24)	68 (14)	5447 (9)	1193 (6)	63 (5)
C (25)	5308 (15)	2274 (10)	1135 (7)	83 (6)
C (26)	1501 (15)	4638 (10)	3141 (6)	73 (6)
C (27)	9424 (14)	8853 (9)	515 (6)	41 (4)
C (28)	8701 (13)	9536 (9)	402 (6)	44 (4)
C (29)	9218 (13)	10237 (9)	570 (6)	42 (4)
C (30)	10389 (13)	10286 (9)	862 (6)	39 (4)
C (31)	11053 (14)	9606 (8)	999 (6)	45 (4)
C (32)	10552 (13)	8886 (9)	833 (6)	38 (4)

C(33)	11287(13)	8169(8)	1003(6)	39(4)
C(34)	12234(17)	8229(10)	1991(7)	56(5)
C(35)	12154(16)	8064(10)	2524(7)	70(6)
C(36)	11236(16)	7675(10)	2614(7)	63(5)
C(37)	10360(15)	7525(9)	1681(7)	36(4)
C(38)	9347(13)	6916(10)	2341(7)	59(5)
C(39)	8159(14)	7383(10)	2274(6)	53(5)
C(40)	8003(14)	7836(9)	2710(7)	55(5)
C(41)	6982(14)	8303(9)	2681(6)	50(5)
C(42)	6099(14)	8282(9)	2216(6)	55(5)
C(43)	6225(14)	7857(9)	1758(6)	48(5)
C(44)	7268(14)	7393(9)	1816(6)	46(5)
C(45)	5326(14)	7918(9)	1236(6)	61(5)
C(46)	4939(15)	9353(10)	1107(6)	56(5)
C(47)	5151(14)	10043(9)	927(6)	52(5)
C(48)	5960(15)	10132(11)	568(7)	55(5)
C(49)	6237(15)	8734(10)	629(6)	44(4)
C(50)	7396(13)	9495(9)	81(6)	49(5)
C(51)	10938(14)	11070(9)	1051(6)	60(5)
C(52)	6782(15)	8783(10)	3163(6)	75(6)
C(53)	6799(27)	12855(18)	-79(12)	130
C(54)	7407(30)	12080(20)	44(14)	161
O(13)	7704(36)	12108(24)	582(16)	392

Table 4. Bond lengths [Å] and angles [°] for 1.

N(1)-C(11)	1.37(2)	N(1)-C(8)	1.41(2)
N(1)-C(7)	1.51(2)	N(2)-C(10)	1.35(2)
N(2)-C(11)	1.37(2)	N(2)-C(12)	1.48(2)
N(3)-C(23)	1.39(2)	N(3)-C(20)	1.41(2)
N(3)-C(19)	1.50(2)	N(4)-C(23)	1.39(2)
N(4)-C(22)	1.44(2)	N(4)-C(24)	1.49(2)
N(5)-C(34)	1.38(2)	N(5)-C(37)	1.39(2)
N(5)-C(33)	1.50(2)	N(6)-C(37)	1.36(2)
N(6)-C(36)	1.38(2)	N(6)-C(38)	1.48(2)
N(7)-C(49)	1.34(2)	N(7)-C(46)	1.35(2)
N(7)-C(45)	1.53(2)	N(8)-C(49)	1.38(2)
N(8)-C(48)	1.41(2)	N(8)-C(50)	1.48(2)
O(1)-C(1)	1.34(2)	O(2)-C(8)	1.23(2)
O(3)-C(11)	1.23(2)	O(4)-C(14)	1.37(2)
O(5)-C(23)	1.20(2)	O(6)-C(22)	1.19(2)
O(7)-C(27)	1.38(2)	O(8)-C(34)	1.25(2)
O(9)-C(37)	1.22(2)	O(10)-C(44)	1.38(2)
O(11)-C(49)	1.26(2)	O(12)-C(48)	1.23(2)
C(1)-C(2)	1.38(2)	C(1)-C(6)	1.41(2)
C(2)-C(3)	1.38(2)	C(2)-C(24)	1.55(2)
C(3)-C(4)	1.40(2)	C(4)-C(5)	1.37(2)
C(4)-C(26)	1.53(2)	C(5)-C(6)	1.38(2)
C(6)-C(7)	1.51(2)	C(8)-C(9)	1.43(2)
C(9)-C(10)	1.32(2)	C(12)-C(13)	1.53(2)
C(13)-C(14)	1.38(2)	C(13)-C(18)	1.40(2)
C(14)-C(15)	1.35(2)	C(15)-C(16)	1.40(2)
C(15)-C(19)	1.53(2)	C(16)-C(17)	1.37(2)
C(17)-C(18)	1.36(2)	C(17)-C(25)	1.55(2)
C(20)-C(21)	1.30(2)	C(21)-C(22)	1.43(2)
C(27)-C(32)	1.36(2)	C(27)-C(28)	1.42(2)
C(28)-C(29)	1.36(2)	C(28)-C(50)	1.53(2)
C(29)-C(30)	1.37(2)	C(30)-C(31)	1.39(2)
C(30)-C(51)	1.51(2)	C(31)-C(32)	1.38(2)
C(32)-C(33)	1.49(2)	C(34)-C(35)	1.40(2)
C(35)-C(36)	1.30(2)	C(38)-C(39)	1.54(2)
C(39)-C(44)	1.36(2)	C(39)-C(40)	1.39(2)
C(40)-C(41)	1.40(2)	C(41)-C(42)	1.37(2)
C(41)-C(52)	1.53(2)	C(42)-C(43)	1.40(2)

C(43)-C(44)	1.41(2)	C(43)-C(45)	1.49(2)
C(46)-C(47)	1.31(2)	C(47)-C(48)	1.43(2)
C(53)-C(54)	1.50(2)	C(54)-O(13)	1.33(3)
C(11)-N(1)-C(8)	124.1(14)	C(11)-N(1)-C(7)	116.6(13)
C(8)-N(1)-C(7)	119.2(12)	C(10)-N(2)-C(11)	120.3(14)
C(10)-N(2)-C(12)	121.1(13)	C(11)-N(2)-C(12)	118.4(13)
C(23)-N(3)-C(20)	119.1(13)	C(23)-N(3)-C(19)	118.0(14)
C(20)-N(3)-C(19)	122.9(14)	C(23)-N(4)-C(22)	126.6(14)
C(23)-N(4)-C(24)	114.8(14)	C(22)-N(4)-C(24)	118.6(13)
C(34)-N(5)-C(37)	123(2)	C(34)-N(5)-C(33)	120.5(14)
C(37)-N(5)-C(33)	116.9(13)	C(37)-N(6)-C(36)	120(2)
C(37)-N(6)-C(38)	120.2(14)	C(36)-N(6)-C(38)	120.1(14)
C(49)-N(7)-C(46)	122(2)	C(49)-N(7)-C(45)	117.6(13)
C(46)-N(7)-C(45)	120.3(13)	C(49)-N(8)-C(48)	120.0(14)
C(49)-N(8)-C(50)	120.1(13)	C(48)-N(8)-C(50)	120.0(13)
O(1)-C(1)-C(2)	119.8(14)	O(1)-C(1)-C(6)	122.3(14)
C(2)-C(1)-C(6)	118(2)	C(3)-C(2)-C(1)	122.1(14)
C(3)-C(2)-C(24)	119.0(14)	C(1)-C(2)-C(24)	119.0(14)
C(2)-C(3)-C(4)	120(2)	C(5)-C(4)-C(3)	118(2)
C(5)-C(4)-C(26)	123.5(14)	C(3)-C(4)-C(26)	118.2(14)

C(4) - C(5) - C(6)	123(2)	C(5) - C(6) - C(1)	119(2)
C(5) - C(6) - C(7)	119.4(14)	C(1) - C(6) - C(7)	121.1(14)
N(1) - C(7) - C(6)	113.6(12)	O(2) - C(8) - N(1)	119(2)
O(2) - C(8) - C(9)	126(2)	N(1) - C(8) - C(9)	115(2)
C(10) - C(9) - C(8)	119(2)	C(9) - C(10) - N(2)	125(2)
O(3) - C(11) - N(1)	122(2)	O(3) - C(11) - N(2)	121(2)
N(1) - C(11) - N(2)	117(2)	N(2) - C(12) - C(13)	111.7(12)
C(14) - C(13) - C(18)	122(2)	C(14) - C(13) - C(12)	121.2(14)
C(18) - C(13) - C(12)	117.1(14)	C(15) - C(14) - O(4)	123.2(14)
C(15) - C(14) - C(13)	119(2)	O(4) - C(14) - C(13)	117.5(14)
C(14) - C(15) - C(16)	120.7(14)	C(14) - C(15) - C(19)	121.9(14)
C(16) - C(15) - C(19)	117.3(14)	C(17) - C(16) - C(15)	118(2)
C(18) - C(17) - C(16)	123(2)	C(18) - C(17) - C(25)	117(2)
C(16) - C(17) - C(25)	120(2)	C(17) - C(18) - C(13)	117(2)
N(3) - C(19) - C(15)	111.9(12)	C(21) - C(20) - N(3)	124(2)
C(20) - C(21) - C(22)	123(2)	O(6) - C(22) - C(21)	127(2)
O(6) - C(22) - N(4)	121(2)	C(21) - C(22) - N(4)	112(2)
O(5) - C(23) - N(4)	124(2)	O(5) - C(23) - N(3)	121(2)
N(4) - C(23) - N(3)	116(2)	N(4) - C(24) - C(2)	110.3(13)
C(32) - C(27) - O(7)	119.8(14)	C(32) - C(27) - C(28)	121(2)
O(7) - C(27) - C(28)	119.2(14)	C(29) - C(28) - C(27)	118(2)
C(29) - C(28) - C(50)	120.5(14)	C(27) - C(28) - C(50)	121(2)
C(28) - C(29) - C(30)	122(2)	C(29) - C(30) - C(31)	119(2)
C(29) - C(30) - C(51)	120.5(14)	C(31) - C(30) - C(51)	120.2(14)
C(32) - C(31) - C(30)	121(2)	C(27) - C(32) - C(31)	119(2)
C(27) - C(32) - C(33)	122.2(14)	C(31) - C(32) - C(33)	118.6(14)
C(32) - C(33) - N(5)	109.6(11)	O(8) - C(34) - N(5)	117(2)
O(8) - C(34) - C(35)	126(2)	N(5) - C(34) - C(35)	117(2)
C(36) - C(35) - C(34)	120(2)	C(35) - C(36) - N(6)	123(2)
O(9) - C(37) - N(6)	120(2)	O(9) - C(37) - N(5)	123(2)
N(6) - C(37) - N(5)	117(2)	N(6) - C(38) - C(39)	112.2(13)
C(44) - C(39) - C(40)	118(2)	C(44) - C(39) - C(38)	125(2)
C(40) - C(39) - C(38)	117.5(14)	C(41) - C(40) - C(39)	122(2)
C(42) - C(41) - C(40)	118(2)	C(42) - C(41) - C(52)	119(2)
C(40) - C(41) - C(52)	122(2)	C(41) - C(42) - C(43)	122(2)
C(42) - C(43) - C(44)	116(2)	C(42) - C(43) - C(45)	122(2)
C(44) - C(43) - C(45)	122.1(14)	C(39) - C(44) - O(10)	121(2)
C(39) - C(44) - C(43)	123(2)	O(10) - C(44) - C(43)	116.2(14)
C(43) - C(45) - N(7)	109.9(13)	C(47) - C(46) - N(7)	122(2)
C(46) - C(47) - C(48)	121(2)	O(12) - C(48) - N(8)	118(2)
O(12) - C(48) - C(47)	125(2)	N(8) - C(48) - C(47)	117(2)
O(11) - C(49) - N(7)	124(2)	O(11) - C(49) - N(8)	117(2)
N(7) - C(49) - N(8)	119(2)	N(8) - C(50) - C(28)	112.5(12)

O(13) - C(54) - C(53) 101(3)

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha)^2 U_{11} + \dots + 2hka b U_{12}]$$

	U11	U22	U33	U23	U13	U12
N(1)	39(9)	28(8)	52(9)	-16(7)	20(7)	1(7)
N(2)	50(9)	48(9)	44(8)	-22(7)	17(7)	-8(8)
N(3)	33(9)	92(12)	34(8)	-12(8)	14(7)	-4(8)
N(4)	52(9)	45(9)	36(8)	0(7)	-1(7)	9(8)
N(5)	47(9)	36(8)	51(9)	-10(7)	17(7)	7(7)
N(6)	44(10)	42(9)	67(11)	16(8)	18(8)	12(7)
N(7)	43(9)	52(9)	47(9)	-4(8)	11(7)	6(7)
N(8)	35(9)	40(9)	53(9)	-3(7)	10(7)	4(7)
O(1)	54(8)	28(6)	81(8)	5(6)	4(6)	-7(6)
O(2)	76(10)	109(10)	55(8)	-14(8)	29(7)	-6(8)
O(3)	57(8)	70(9)	56(8)	25(7)	14(6)	4(7)
O(4)	57(7)	45(7)	50(7)	19(6)	4(6)	2(6)
O(5)	73(9)	45(7)	62(8)	6(6)	31(6)	-3(7)
O(6)	44(8)	89(9)	76(8)	-38(7)	40(7)	-9(7)
O(7)	63(8)	67(8)	46(7)	-20(6)	2(6)	24(7)
O(8)	55(8)	72(8)	70(8)	-5(7)	17(7)	-12(7)
O(9)	46(8)	65(9)	60(8)	-1(7)	9(6)	-10(6)
O(10)	62(8)	46(7)	69(8)	-8(7)	-2(6)	6(6)
O(11)	65(8)	58(8)	75(8)	-19(7)	26(7)	2(7)
O(12)	66(9)	47(8)	89(9)	-2(7)	16(7)	11(7)

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H(1A)	2766(9)	6637(5)	1386(4)	84
H(4A)	3045(9)	5199(6)	38(4)	78
H(7A)	8260(9)	8207(6)	132(4)	90
H(10A)	7963(9)	6664(6)	1452(4)	92
H(3A)	182(13)	4765(8)	2145(6)	49
H(5A)	3349(14)	5545(8)	2989(6)	62
H(7B)	3933(13)	6855(9)	2026(6)	63
H(7C)	4318(13)	6635(9)	2641(6)	63
H(9A)	7616(13)	5048(8)	2716(6)	51
H(10B)	7542(14)	4806(9)	1846(6)	54
H(12A)	6798(13)	5000(8)	914(6)	54
H(12B)	5695(13)	5560(8)	717(6)	54
H(16A)	3203(14)	2695(9)	489(6)	64
H(18A)	6365(14)	3641(9)	1224(6)	65
H(19A)	1970(13)	4373(10)	-237(6)	68
H(19B)	1873(13)	3459(10)	-237(6)	68
H(20A)	536(14)	2843(10)	280(6)	66
H(21A)	-678(15)	2877(10)	843(6)	78
H(24A)	-731(14)	5500(9)	1268(6)	75
H(24B)	185(14)	5870(9)	955(6)	75
H(25A)	4699(15)	1883(10)	1024(7)	124
H(25B)	5497(15)	2313(10)	1523(7)	124
H(25C)	6022(15)	2133(10)	1012(7)	124
H(26A)	724(15)	4391(10)	3044(6)	110
H(26B)	1524(15)	4977(10)	3446(6)	110
H(26C)	2117(15)	4247(10)	3235(6)	110
H(29A)	8769(13)	10692(9)	485(6)	51
H(31A)	11839(14)	9634(8)	1204(6)	55
H(33A)	12108(13)	8252(8)	962(6)	46
H(33B)	10949(13)	7733(8)	775(6)	46
H(35A)	12757(16)	8233(10)	2813(7)	83
H(36A)	11187(16)	7586(10)	2972(7)	76

H(38A)	9590 (13)	6735 (10)	2713 (7)	71
H(38B)	9209 (13)	6461 (10)	2107 (7)	71
H(40A)	8594 (14)	7828 (9)	3030 (7)	66
H(42A)	5389 (14)	8559 (9)	2204 (6)	67
H(45A)	4516 (14)	7876 (9)	1300 (6)	74
H(45B)	5444 (14)	7494 (9)	998 (6)	74
H(46A)	4409 (15)	9308 (10)	1339 (6)	67
H(47A)	4773 (14)	10480 (9)	1033 (6)	62
H(50A)	7222 (13)	9954 (9)	-148 (6)	58
H(50B)	7301 (13)	9040 (9)	-153 (6)	58
H(51A)	11754 (14)	10998 (9)	1249 (6)	90
H(51B)	10475 (14)	11314 (9)	1281 (6)	90
H(51C)	10933 (14)	11397 (9)	742 (6)	90
H(52A)	7477 (15)	8738 (10)	3457 (6)	113
H(52B)	6082 (15)	8592 (10)	3278 (6)	113
H(52C)	6662 (15)	9321 (10)	3059 (6)	113
H(53A)	6850 (197)	12919 (134)	-518 (96)	195
H(53B)	7507 (204)	13228 (136)	14 (94)	195
H(53C)	5917 (207)	12876 (123)	145 (88)	195
H(54A)	6746 (199)	12024 (135)	-314 (91)	194
H(54B)	8273 (208)	12142 (130)	-31 (88)	194

H(13A) 7975 (456) 12345 (297) 1529 (218) 588
