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Table S1. Crystal data and structure refinement for 1.

Identification code	ST2970
Empirical formula	C_{34} H_{60} Cl Co N_4 O_6
Formula weight	715.24
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Trigonal
Space group	$R\bar{3}$
Unit cell dimensions	a = 31.994(5) Å alpha = 90 deg. b = 31.994(5) Å beta = 90 deg. c = 18.828(3) Å gamma = 120 deg.
Volume	16691(4) Å^3
Z	18
Density (calculated)	1.281 Mg/m^3
Absorption coefficient	0.581 mm^-1
F(000)	6912
Crystal size	0.24 x 0.24 x 0.23 mm
Theta range for data collection	1.27 to 22.50 deg.
Index ranges	-34<=h<=35, -32<=k<=35, -12<=l<=20
Reflections collected	35110
Independent reflections	4836
Absorption correction	SADABS, G. Sheldrick 1994
Max. and min. transmission	0.983 and 0.685
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4569 / 0 / 444
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0731, wR2 = 0.1637
R indices (all data)	R1 = 0.1286, wR2 = 0.1866
Largest diff. peak and hole	2.042 and -0.319 e.A^-3

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Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Co(1)	4775(1)	8702(1)	9613(1)	23(1)
N(1)	4424(2)	8931(2)	10202(3)	23(1)
N(2)	4558(2)	8143(2)	10314(3)	31(2)
N(3)	5330(2)	9072(2)	10266(3)	30(2)
N(4)	4966(2)	9253(2)	9019(3)	22(1)
C(1)	4166(2)	8573(2)	10801(3)	28(2)
C(2)	4098(3)	8086(2)	10589(4)	33(2)
C(3)	4925(3)	8290(3)	10888(4)	37(2)
C(4)	5399(3)	8690(3)	10630(4)	35(2)
C(5)	5203(3)	9344(3)	10798(4)	33(2)
C(6)	4799(2)	9401(2)	10489(3)	27(2)
C(7)	4062(2)	8989(2)	9789(3)	25(2)
C(8)	4221(2)	9263(2)	9091(3)	22(2)
C(9)	4637(2)	9352(2)	8706(3)	21(2)
C(10)	4707(2)	9580(2)	8028(3)	22(2)
C(11)	4359(2)	9678(2)	7774(3)	27(2)
C(12)	3934(2)	9571(2)	8141(4)	25(2)
C(13)	3887(2)	9372(2)	8806(3)	25(2)
C(14)	5154(2)	9709(2)	7560(3)	24(2)
C(15)	5622(2)	10066(2)	7939(4)	31(2)
C(16)	5160(3)	9244(2)	7326(4)	31(2)
C(17)	5155(3)	9966(3)	6857(4)	35(2)
C(18)	3538(2)	9650(3)	7831(4)	35(2)
C(19)	3500(3)	10037(3)	8249(4)	45(2)
C(20)	3646(3)	9817(3)	7047(4)	51(2)
C(21)	3058(3)	9172(3)	7861(4)	50(2)
O(1)	4220(2)	8321(2)	9054(2)	26(1)
O(2)	5168(2)	8527(2)	9084(2)	25(1)
C(22)	4469(3)	7685(2)	9987(4)	38(2)
C(23)	5789(2)	9421(2)	9907(4)	30(2)
C(24)	4207(2)	8103(2)	8476(3)	20(2)
C(25)	4597(2)	8083(2)	8188(3)	23(2)
C(26)	5053(2)	8288(2)	8502(4)	24(2)
C(27)	5459(2)	8225(2)	8167(4)	31(2)
C(28)	5930(3)	8707(3)	8176(4)	43(2)
C(29)	5347(3)	8047(3)	7402(4)	62(3)
C(30)	5523(3)	7867(3)	8628(5)	53(2)
C(31)	3712(2)	7855(2)	8131(3)	25(2)
C(32)	3560(3)	8229(2)	7968(4)	37(2)
C(33)	3349(2)	7472(3)	8654(4)	40(2)
C(34)	3697(2)	7600(3)	7443(4)	40(2)
O(11)	2330(2)	7887(2)	10778(3)	70(2)
O(12)	3082(2)	8593(2)	10927(3)	52(2)
Cl(1X)	2798(1)	8239(1)	10480(2)	33(1)
O(13)	2713(3)	8447(3)	9864(4)	75(3)
O(14)	3035(3)	7964(3)	10254(8)	83(5)
Cl(1Y)	2799(3)	8017(3)	10558(4)	38(2)
O(15)	2885(10)	8092(10)	9835(14)	91(9)
O(16)	2939(6)	7738(6)	10937(9)	51(5)

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Table S3. Bond lengths [Å] and angles [deg] for 1.

Co(1)-O(1)	1.893(4)
Co(1)-O(2)	1.895(4)
Co(1)-N(4)	1.912(6)
Co(1)-N(1)	1.962(5)
Co(1)-N(3)	1.989(6)
Co(1)-N(2)	2.044(6)
N(1)-C(6)	1.479(8)
N(1)-C(7)	1.483(8)
N(1)-C(1)	1.524(8)
N(2)-C(22)	1.481(8)
N(2)-C(2)	1.483(8)
N(2)-C(3)	1.488(9)
N(3)-C(23)	1.491(8)
N(3)-C(4)	1.508(8)
N(3)-C(5)	1.510(8)
N(4)-C(9)	1.376(8)
C(1)-C(2)	1.515(9)
C(3)-C(4)	1.496(10)
C(5)-C(6)	1.512(9)
C(7)-C(8)	1.519(9)
C(8)-C(13)	1.384(9)
C(8)-C(9)	1.415(9)
C(9)-C(10)	1.430(9)
C(10)-C(11)	1.386(9)
C(10)-C(14)	1.547(9)
C(11)-C(12)	1.407(9)
C(12)-C(13)	1.379(9)
C(12)-C(18)	1.524(9)
C(14)-C(15)	1.533(9)
C(14)-C(17)	1.558(9)
C(14)-C(16)	1.561(9)
C(18)-C(19)	1.522(10)
C(18)-C(21)	1.535(10)
C(18)-C(20)	1.549(10)
O(1)-C(24)	1.281(7)
O(2)-C(26)	1.280(7)
C(24)-C(25)	1.394(9)
C(24)-C(31)	1.516(9)
C(25)-C(26)	1.396(9)
C(26)-C(27)	1.544(9)
C(27)-C(29)	1.525(10)
C(27)-C(28)	1.527(10)
C(27)-C(30)	1.530(10)
C(31)-C(34)	1.520(9)
C(31)-C(32)	1.531(9)
C(31)-C(33)	1.548(9)
O(11)-Cl(1Y)	1.406(10)
O(11)-Cl(1X)	1.462(6)
O(12)-Cl(1X)	1.337(6)
O(12)-Cl(1Y)	1.741(9)
Cl(1X)-O(13)	1.430(9)
Cl(1X)-O(14)	1.483(9)
Cl(1Y)-O(16)	1.38(2)
Cl(1Y)-O(15)	1.39(3)
O(1)-Co(1)-O(2)	93.7(2)
O(1)-Co(1)-N(4)	91.8(2)
O(2)-Co(1)-N(4)	90.7(2)
O(1)-Co(1)-N(1)	91.5(2)

O(2)-Co(1)-N(1)	174.7(2)
N(4)-Co(1)-N(1)	88.0(2)
O(1)-Co(1)-N(3)	175.5(2)
O(2)-Co(1)-N(3)	88.6(2)
N(4)-Co(1)-N(3)	92.0(2)
N(1)-Co(1)-N(3)	86.3(2)
O(1)-Co(1)-N(2)	89.8(2)
O(2)-Co(1)-N(2)	93.8(2)
N(4)-Co(1)-N(2)	175.1(2)
N(1)-Co(1)-N(2)	87.4(2)
N(3)-Co(1)-N(2)	86.2(2)
C(6)-N(1)-C(7)	110.6(5)
C(6)-N(1)-C(1)	110.6(5)
C(7)-N(1)-C(1)	108.5(5)
C(6)-N(1)-Co(1)	105.2(4)
C(7)-N(1)-Co(1)	112.3(4)
C(1)-N(1)-Co(1)	109.5(4)
C(22)-N(2)-C(2)	109.6(5)
C(22)-N(2)-C(3)	110.2(5)
C(2)-N(2)-C(3)	111.2(5)
C(22)-N(2)-Co(1)	114.3(4)
C(2)-N(2)-Co(1)	102.5(4)
C(3)-N(2)-Co(1)	108.9(4)
C(23)-N(3)-C(4)	108.9(5)
C(23)-N(3)-C(5)	108.4(5)
C(4)-N(3)-C(5)	110.8(5)
C(23)-N(3)-Co(1)	114.7(4)
C(4)-N(3)-Co(1)	104.3(4)
C(5)-N(3)-Co(1)	109.7(4)
C(9)-N(4)-Co(1)	122.4(4)
C(2)-C(1)-N(1)	108.9(5)
N(2)-C(2)-C(1)	110.0(6)
N(2)-C(3)-C(4)	109.6(6)
C(3)-C(4)-N(3)	110.1(6)
N(3)-C(5)-C(6)	107.9(5)
N(1)-C(6)-C(5)	109.0(5)
N(1)-C(7)-C(8)	118.0(5)
C(13)-C(8)-C(9)	121.1(6)
C(13)-C(8)-C(7)	113.8(6)
C(9)-C(8)-C(7)	124.7(6)
N(4)-C(9)-C(8)	119.1(6)
N(4)-C(9)-C(10)	123.7(6)
C(8)-C(9)-C(10)	117.0(6)
C(11)-C(10)-C(9)	118.8(6)
C(11)-C(10)-C(14)	118.8(6)
C(9)-C(10)-C(14)	122.3(5)
C(10)-C(11)-C(12)	124.5(6)
C(13)-C(12)-C(11)	115.2(6)
C(13)-C(12)-C(18)	121.2(6)
C(11)-C(12)-C(18)	123.6(6)
C(12)-C(13)-C(8)	123.4(6)
C(15)-C(14)-C(10)	111.3(5)
C(15)-C(14)-C(17)	105.0(5)
C(10)-C(14)-C(17)	112.5(5)
C(15)-C(14)-C(16)	111.6(5)
C(10)-C(14)-C(16)	110.8(5)
C(17)-C(14)-C(16)	105.4(5)
C(19)-C(18)-C(12)	110.4(6)
C(19)-C(18)-C(21)	110.1(6)
C(12)-C(18)-C(21)	108.7(6)
C(19)-C(18)-C(20)	107.8(6)
C(12)-C(18)-C(20)	111.2(6)
C(21)-C(18)-C(20)	108.6(6)

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C(24)-O(1)-Co(1)	126.1(4)
C(26)-O(2)-Co(1)	126.4(4)
O(1)-C(24)-C(25)	124.6(6)
O(1)-C(24)-C(31)	113.1(6)
C(25)-C(24)-C(31)	122.3(5)
C(24)-C(25)-C(26)	124.4(6)
O(2)-C(26)-C(25)	124.2(6)
O(2)-C(26)-C(27)	114.8(6)
C(25)-C(26)-C(27)	121.0(6)
C(29)-C(27)-C(28)	108.5(6)
C(29)-C(27)-C(30)	110.6(6)
C(28)-C(27)-C(30)	108.5(6)
C(29)-C(27)-C(26)	112.3(6)
C(28)-C(27)-C(26)	109.4(6)
C(30)-C(27)-C(26)	107.6(6)
C(24)-C(31)-C(34)	113.0(5)
C(24)-C(31)-C(32)	109.5(5)
C(34)-C(31)-C(32)	108.2(6)
C(24)-C(31)-C(33)	108.4(5)
C(34)-C(31)-C(33)	107.8(6)
C(32)-C(31)-C(33)	109.9(6)
O(12)-Cl(1X)-O(13)	108.9(5)
O(12)-Cl(1X)-O(11)	114.3(4)
O(13)-Cl(1X)-O(11)	108.1(5)
O(12)-Cl(1X)-O(14)	110.5(6)
O(13)-Cl(1X)-O(14)	108.4(7)
O(11)-Cl(1X)-O(14)	106.5(5)
O(16)-Cl(1Y)-O(15)	121(2)
O(16)-Cl(1Y)-O(11)	107.5(9)
O(15)-Cl(1Y)-O(11)	115.5(14)
O(16)-Cl(1Y)-O(12)	108.3(8)
O(15)-Cl(1Y)-O(12)	104.7(13)
O(11)-Cl(1Y)-O(12)	96.2(6)

Symmetry transformations used to generate equivalent atoms:

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Table S4. Anisotropic displacement parameters (A^2 x 10^3) for 1. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Co(1)	25(1)	27(1)	15(1)	-1(1)	-1(1)	12(1)
N(1)	29(3)	31(3)	10(3)	0(3)	0(3)	15(3)
N(2)	38(4)	33(4)	23(3)	0(3)	1(3)	19(3)
N(3)	37(4)	32(3)	18(3)	-4(3)	0(3)	16(3)
N(4)	17(3)	30(3)	18(3)	1(3)	5(3)	11(3)
C(1)	30(4)	40(5)	13(4)	2(3)	1(3)	16(4)
C(2)	38(5)	32(4)	20(4)	3(3)	8(4)	11(4)
C(3)	49(5)	35(5)	27(4)	9(4)	1(4)	21(4)
C(4)	48(5)	43(5)	23(4)	-1(4)	-9(4)	30(4)
C(5)	39(5)	31(4)	21(4)	0(4)	3(4)	12(4)
C(6)	37(4)	28(4)	15(4)	-3(3)	0(3)	16(4)
C(7)	26(4)	27(4)	23(4)	-3(3)	4(3)	14(3)
C(8)	22(4)	20(4)	22(4)	-3(3)	-2(3)	9(3)
C(9)	23(4)	22(4)	15(4)	-2(3)	-4(3)	9(3)
C(10)	18(4)	25(4)	26(4)	-3(3)	-2(3)	13(3)
C(11)	36(4)	24(4)	14(4)	0(3)	-1(4)	9(3)
C(12)	32(4)	27(4)	18(4)	-9(3)	-6(3)	16(3)
C(13)	20(4)	29(4)	25(4)	-7(3)	2(3)	11(3)
C(14)	28(4)	34(4)	16(4)	1(3)	2(3)	20(4)
C(15)	24(4)	37(4)	30(4)	8(4)	4(3)	13(4)
C(16)	39(4)	35(4)	23(4)	5(3)	6(4)	21(4)
C(17)	42(5)	40(5)	20(4)	6(4)	8(4)	19(4)
C(18)	30(4)	52(5)	32(4)	-4(4)	-8(4)	28(4)
C(19)	50(5)	58(5)	44(5)	-16(4)	-20(4)	39(5)
C(20)	58(6)	94(7)	29(5)	-4(5)	-15(4)	59(5)
C(21)	34(5)	64(6)	54(6)	-19(5)	-19(4)	26(5)
O(1)	28(3)	26(3)	22(3)	-2(2)	2(2)	12(2)
O(2)	26(3)	31(3)	18(3)	-2(2)	-2(2)	14(2)
C(22)	43(5)	32(4)	29(4)	5(4)	0(4)	12(4)
C(23)	22(4)	40(4)	24(4)	-4(4)	-2(3)	12(4)
C(24)	28(4)	21(4)	8(4)	2(3)	-2(3)	9(3)
C(25)	26(4)	23(4)	14(4)	-5(3)	-1(3)	8(3)
C(26)	32(4)	19(4)	18(4)	1(3)	3(3)	11(3)
C(27)	29(4)	35(4)	25(4)	-7(4)	0(4)	12(4)
C(28)	48(5)	46(5)	38(5)	1(4)	11(4)	25(4)
C(29)	46(5)	94(7)	46(6)	-36(5)	-5(5)	36(5)
C(30)	48(5)	50(5)	71(6)	5(5)	7(5)	31(5)
C(31)	23(4)	32(4)	18(4)	-8(3)	-1(3)	12(3)
C(32)	36(4)	35(5)	38(5)	-7(4)	-17(4)	15(4)
C(33)	28(4)	35(5)	39(5)	-3(4)	-2(4)	3(4)
C(34)	27(4)	49(5)	42(5)	-11(4)	-4(4)	19(4)
O(11)	41(4)	95(5)	73(4)	49(4)	32(3)	34(4)
O(12)	65(4)	68(4)	29(3)	3(3)	12(3)	37(3)
Cl(1X)	30(2)	38(2)	21(2)	0(2)	7(1)	8(2)
O(13)	72(7)	69(7)	31(5)	25(5)	-10(5)	-4(5)
O(14)	26(5)	41(6)	165(13)	-41(7)	48(7)	3(5)

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Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 1.

	x	y	z	U(eq)
H(4)	5144(23)	9257(23)	8730(34)	27
H(1A)	4359(2)	8686(2)	11242(3)	34
H(1B)	3848(2)	8545(2)	10891(3)	34
H(2A)	3991(3)	7868(2)	11006(4)	40
H(2B)	3846(3)	7939(2)	10219(4)	40
H(3A)	4959(3)	8011(3)	11030(4)	44
H(3B)	4819(3)	8398(3)	11309(4)	44
H(4A)	5544(3)	8561(3)	10293(4)	42
H(4B)	5623(3)	8835(3)	11036(4)	42
H(5A)	5488(3)	9665(3)	10892(4)	39
H(5B)	5100(3)	9164(3)	11252(4)	39
H(6A)	4658(2)	9511(2)	10862(3)	32
H(6B)	4925(2)	9646(2)	10106(3)	32
H(7A)	3937(2)	9153(2)	10097(3)	29
H(7B)	3788(2)	8662(2)	9687(3)	29
H(11)	4411(2)	9828(2)	7322(3)	33
H(13)	3613(2)	9306(2)	9082(3)	30
H(15A)	5644(7)	10382(4)	7969(19)	47
H(15B)	5899(2)	10097(11)	7671(12)	47
H(15C)	5624(7)	9948(8)	8418(9)	47
H(16A)	4861(7)	9029(7)	7071(19)	47
H(16B)	5187(15)	9079(8)	7746(4)	47
H(16C)	5437(9)	9333(3)	7012(18)	47
H(17A)	4863(8)	9755(6)	6583(11)	52
H(17B)	5441(8)	10037(13)	6577(11)	52
H(17C)	5160(15)	10268(8)	6969(4)	52
H(19A)	3249(12)	10088(12)	8038(16)	68
H(19B)	3810(6)	10339(5)	8233(21)	68
H(19C)	3416(17)	9933(8)	8743(7)	68
H(20A)	3942(10)	10132(8)	7023(4)	76
H(20B)	3377(8)	9844(17)	6852(8)	76
H(20C)	3688(17)	9581(9)	6771(6)	76
H(21A)	2803(4)	9215(6)	7646(24)	75
H(21B)	2976(9)	9071(9)	8357(5)	75
H(21C)	3089(6)	8924(5)	7600(23)	75
H(22A)	4238(12)	7599(8)	9597(15)	56
H(22B)	4338(15)	7428(4)	10345(7)	56
H(22C)	4773(4)	7724(5)	9802(20)	56
H(23A)	5850(8)	9261(5)	9510(14)	46
H(23B)	6056(3)	9537(11)	10248(7)	46
H(23C)	5763(6)	9695(7)	9729(19)	46
H(25)	4551(2)	7919(2)	7749(3)	28
H(28A)	6190(4)	8665(4)	7980(23)	65
H(28B)	6009(9)	8825(8)	8666(5)	65
H(28C)	5893(6)	8942(5)	7888(20)	65
H(29A)	5076(13)	7714(7)	7395(5)	93
H(29B)	5631(7)	8057(19)	7189(10)	93
H(29C)	5261(19)	8254(12)	7130(8)	93
H(30A)	5767(14)	7807(14)	8416(15)	80
H(30B)	5215(6)	7563(7)	8660(23)	80
H(30C)	5627(18)	8002(8)	9106(9)	80
H(32A)	3522(15)	8365(11)	8414(4)	56
H(32B)	3252(8)	8073(4)	7712(21)	56
H(32C)	3807(8)	8487(8)	7675(19)	56

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H(33A)	3028(4)	7304(11)	8436(10)	60
H(33B)	3337(12)	7631(3)	9092(10)	60
H(33C)	3453(9)	7238(9)	8764(18)	60
H(34A)	3369(4)	7442(14)	7248(13)	59
H(34B)	3791(15)	7356(11)	7537(5)	59
H(34C)	3921(12)	7836(3)	7100(9)	59

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Table S7. Crystal data and structure refinement for 2.

Identification code	ST2760
Empirical formula	C_{82} H_{109} B Mn N_6
Formula weight	1244.50
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 21.101(4) Å alpha = 90 deg. b = 19.209(4) Å beta = 98.14(3) deg. c = 18.070(4) Å gamma = 90 deg.
Volume	7251(3) Å^3
Z	4
Density (calculated)	1.140 Mg/m^3
Absorption coefficient	0.229 mm^-1
F(000)	2692
Crystal size	0.84 x 0.14 x 0.10 mm
Theta range for data collection	1.44 to 20.00 deg.
Index ranges	-14<=h<=23, -21<=k<=21, -20<=l<=19
Reflections collected	19703
Independent reflections	6764
Absorption correction	Not measured
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6354 / 0 / 354
Goodness-of-fit on F^2	0.955
Final R indices [I>2sigma(I)]	R1 = 0.1013, wR2 = 0.2192
R indices (all data)	R1 = 0.1905, wR2 = 0.2521
Largest diff. peak and hole	0.536 and -0.807 e.A^-3

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Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for 2. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mn	7339(1)	9103(1)	4437(1)	17(1)
N(1)	6623(3)	9184(4)	5121(4)	14(2)
N(2)	6601(3)	9359(4)	3605(4)	18(2)
N(3)	6987(4)	8107(4)	4271(5)	22(2)
N(4)	7551(3)	10027(4)	4679(5)	21(2)
N(5)	7866(3)	9042(4)	3686(4)	15(2)
N(6)	7956(3)	8724(4)	5178(5)	22(2)
C(1)	6166(5)	9700(5)	4735(6)	30(3)
C(2)	5998(4)	9526(5)	3939(6)	24(3)
C(3)	6511(5)	8720(5)	3118(6)	27(3)
C(4)	6467(4)	8083(5)	3607(5)	15(3)
C(5)	6734(5)	7898(5)	4967(6)	23(3)
C(6)	6315(4)	8487(4)	5175(6)	22(3)
C(7)	6902(4)	9405(5)	5876(6)	22(3)
C(8)	7348(5)	10027(5)	5975(6)	28(3)
C(9)	7677(5)	10309(5)	5397(6)	26(3)
C(10)	8106(5)	10875(5)	5600(6)	31(3)
C(11)	8196(5)	11110(5)	6330(6)	28(3)
C(12)	7889(5)	10808(5)	6896(6)	33(3)
C(13)	7459(5)	10292(5)	6695(6)	29(3)
C(14)	8469(5)	11236(5)	4991(6)	29(3)
C(15)	8927(5)	10722(5)	4700(6)	30(3)
C(16)	8004(5)	11558(5)	4379(6)	32(3)
C(17)	8893(5)	11831(5)	5353(6)	35(3)
C(18)	8021(5)	11064(5)	7713(7)	38(3)
C(19)	8229(7)	10462(7)	8232(9)	89(5)
C(20)	8537(6)	11602(6)	7863(8)	70(4)
C(21)	7434(6)	11385(7)	7929(8)	81(5)
C(22)	6763(4)	9969(5)	3182(6)	15(3)
C(23)	7411(4)	9989(5)	2893(6)	19(3)
C(24)	7926(4)	9535(5)	3138(6)	17(3)
C(25)	8493(5)	9586(5)	2761(6)	28(3)
C(26)	8526(5)	10120(5)	2272(6)	29(3)
C(27)	8041(5)	10607(5)	2076(6)	28(3)
C(28)	7477(4)	10508(5)	2379(6)	18(3)
C(29)	9039(5)	9051(6)	2941(7)	38(3)
C(30)	9587(5)	9200(6)	2451(6)	44(3)
C(31)	9371(5)	9099(5)	3750(6)	36(3)
C(32)	8807(5)	8316(5)	2723(7)	42(3)
C(33)	8139(5)	11213(5)	1554(6)	33(3)
C(34)	8233(5)	10921(6)	784(6)	44(3)
C(35)	8726(5)	11635(5)	1888(7)	39(3)
C(36)	7562(5)	11690(6)	1415(7)	46(4)
C(37)	7496(4)	7604(5)	4114(6)	26(3)
C(38)	8128(5)	7613(5)	4631(6)	20(3)
C(39)	8329(5)	8137(5)	5155(6)	23(3)
C(40)	8923(5)	8052(5)	5637(6)	23(3)
C(41)	9282(5)	7462(5)	5506(6)	31(3)
C(42)	9126(5)	6968(5)	4957(6)	27(3)
C(43)	8518(4)	7053(5)	4557(6)	22(3)
C(44)	9171(5)	8558(5)	6269(6)	27(3)
C(45)	9312(5)	9280(5)	5961(6)	34(3)
C(46)	9798(5)	8317(5)	6735(6)	40(3)

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C(47)	8670(5)	8630(5)	6830(6)	32(3)
C(48)	9535(5)	6352(5)	4834(7)	34(3)
C(49)	10181(5)	6362(6)	5329(7)	44(3)
C(50)	9673(6)	6333(7)	4037(8)	79(5)
C(51)	9198(5)	5660(6)	4986(7)	58(4)
B(1)	4727(5)	11223(6)	2384(7)	20(3)
C(61)	4805(4)	11608(5)	1592(6)	21(3)
C(62)	4534(5)	11300(5)	905(6)	27(3)
C(63)	4592(5)	11619(5)	219(6)	31(3)
C(64)	4903(5)	12238(5)	175(6)	32(3)
C(65)	5145(5)	12560(5)	835(6)	27(3)
C(66)	5086(5)	12248(5)	1511(6)	27(3)
C(71)	4696(5)	10386(5)	2301(6)	21(3)
C(72)	4347(5)	9944(5)	2694(6)	29(3)
C(73)	4354(5)	9217(5)	2650(6)	34(3)
C(74)	4732(5)	8890(6)	2177(6)	33(3)
C(75)	5114(5)	9309(5)	1799(6)	27(3)
C(76)	5087(5)	10022(5)	1865(6)	26(3)
C(81)	4050(5)	11563(5)	2606(6)	22(3)
C(82)	4054(5)	12175(5)	3046(6)	25(3)
C(83)	3498(5)	12493(5)	3200(6)	29(3)
C(84)	2914(5)	12231(5)	2924(6)	27(3)
C(85)	2888(5)	11642(5)	2500(6)	31(3)
C(86)	3459(5)	11317(5)	2327(6)	31(3)
C(91)	5308(5)	11398(5)	3041(6)	25(3)
C(92)	5925(5)	11645(5)	2944(7)	31(3)
C(93)	6397(5)	11787(5)	3556(6)	31(3)
C(94)	6279(5)	11627(6)	4268(7)	43(3)
C(95)	5711(5)	11364(5)	4385(7)	36(3)
C(96)	5230(5)	11248(5)	3787(6)	33(3)
C(101)	6505(4)	10078(4)	175(6)	90(5)
C(102)	6825(4)	9890(4)	-417(4)	73(5)
C(103)	7295(4)	9379(5)	-319(5)	69(4)
C(104)	7447(4)	9055(4)	371(5)	83(5)
C(105)	7128(4)	9242(4)	963(4)	73(4)
C(106)	6657(4)	9754(4)	865(5)	60(4)
C(107)	6023(7)	10598(7)	57(9)	98(6)

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Table S9. Bond lengths [Å] and angles [deg] for 2.

Mn-N(4)	1.869(8)
Mn-N(5)	1.875(8)
Mn-N(6)	1.878(8)
Mn-N(3)	2.058(8)
Mn-N(2)	2.065(8)
Mn-N(1)	2.090(7)
N(1)-C(7)	1.470(11)
N(1)-C(1)	1.486(11)
N(1)-C(6)	1.497(11)
N(2)-C(22)	1.465(11)
N(2)-C(3)	1.508(11)
N(2)-C(2)	1.517(11)
N(3)-C(5)	1.489(12)
N(3)-C(37)	1.502(11)
N(3)-C(4)	1.509(11)
N(4)-C(9)	1.395(12)
N(5)-C(24)	1.388(11)
N(6)-C(39)	1.379(11)
C(1)-C(2)	1.470(13)
C(3)-C(4)	1.519(12)
C(5)-C(6)	1.516(12)
C(7)-C(8)	1.515(13)
C(8)-C(13)	1.385(14)
C(8)-C(9)	1.440(14)
C(9)-C(10)	1.429(13)
C(10)-C(11)	1.383(14)
C(10)-C(14)	1.59(2)
C(11)-C(12)	1.410(14)
C(12)-C(13)	1.360(13)
C(12)-C(18)	1.54(2)
C(14)-C(16)	1.505(13)
C(14)-C(15)	1.527(13)
C(14)-C(17)	1.538(13)
C(18)-C(21)	1.49(2)
C(18)-C(20)	1.499(14)
C(18)-C(19)	1.51(2)
C(22)-C(23)	1.531(13)
C(23)-C(28)	1.383(12)
C(23)-C(24)	1.416(12)
C(24)-C(25)	1.460(13)
C(25)-C(26)	1.362(13)
C(25)-C(29)	1.543(14)
C(26)-C(27)	1.394(13)
C(27)-C(28)	1.391(13)
C(27)-C(33)	1.531(14)
C(29)-C(32)	1.529(14)
C(29)-C(31)	1.532(14)
C(29)-C(30)	1.580(14)
C(33)-C(36)	1.515(13)
C(33)-C(35)	1.532(13)
C(33)-C(34)	1.54(2)
C(37)-C(38)	1.516(13)
C(38)-C(43)	1.372(12)
C(38)-C(39)	1.407(13)
C(39)-C(40)	1.431(13)
C(40)-C(41)	1.402(13)
C(40)-C(44)	1.533(13)
C(41)-C(42)	1.379(13)
C(42)-C(43)	1.391(12)

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C(42)-C(48)	1.499(13)
C(44)-C(46)	1.537(13)
C(44)-C(45)	1.539(13)
C(44)-C(47)	1.571(14)
C(48)-C(50)	1.51(2)
C(48)-C(49)	1.521(13)
C(48)-C(51)	1.550(14)
B(1)-C(71)	1.614(14)
B(1)-C(91)	1.62(2)
B(1)-C(61)	1.64(2)
B(1)-C(81)	1.67(2)
C(61)-C(66)	1.382(12)
C(61)-C(62)	1.419(13)
C(62)-C(63)	1.404(14)
C(63)-C(64)	1.365(13)
C(64)-C(65)	1.375(13)
C(65)-C(66)	1.383(13)
C(71)-C(72)	1.382(13)
C(71)-C(76)	1.407(13)
C(72)-C(73)	1.400(13)
C(73)-C(74)	1.398(13)
C(74)-C(75)	1.385(13)
C(75)-C(76)	1.377(12)
C(81)-C(86)	1.362(12)
C(81)-C(82)	1.418(13)
C(82)-C(83)	1.386(13)
C(83)-C(84)	1.359(12)
C(84)-C(85)	1.364(13)
C(85)-C(86)	1.431(13)
C(91)-C(96)	1.411(14)
C(91)-C(92)	1.419(13)
C(92)-C(93)	1.406(13)
C(93)-C(94)	1.38(2)
C(94)-C(95)	1.345(13)
C(95)-C(96)	1.391(13)
C(101)-C(102)	1.39
C(101)-C(106)	1.39
C(101)-C(107)	1.420(14)
C(102)-C(103)	1.39
C(103)-C(104)	1.39
C(104)-C(105)	1.39
C(105)-C(106)	1.39

N(4)-Mn-N(5)	94.7(3)
N(4)-Mn-N(6)	94.7(3)
N(5)-Mn-N(6)	94.1(3)
N(4)-Mn-N(3)	170.7(3)
N(5)-Mn-N(3)	94.4(3)
N(6)-Mn-N(3)	86.7(3)
N(4)-Mn-N(2)	94.3(3)
N(5)-Mn-N(2)	87.2(3)
N(6)-Mn-N(2)	170.8(3)
N(3)-Mn-N(2)	84.1(3)
N(4)-Mn-N(1)	87.7(3)
N(5)-Mn-N(1)	170.1(3)
N(6)-Mn-N(1)	95.3(3)
N(3)-Mn-N(1)	83.1(3)
N(2)-Mn-N(1)	83.1(3)
C(7)-N(1)-C(1)	113.1(7)
C(7)-N(1)-C(6)	108.6(7)
C(1)-N(1)-C(6)	111.6(7)
C(7)-N(1)-Mn	110.0(5)
C(1)-N(1)-Mn	104.3(6)

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C(6)-N(1)-Mn	109.1(5)
C(22)-N(2)-C(3)	111.5(8)
C(22)-N(2)-C(2)	108.1(7)
C(3)-N(2)-C(2)	111.2(7)
C(22)-N(2)-Mn	111.2(5)
C(3)-N(2)-Mn	104.5(5)
C(2)-N(2)-Mn	110.4(6)
C(5)-N(3)-C(37)	109.7(7)
C(5)-N(3)-C(4)	110.9(7)
C(37)-N(3)-C(4)	106.8(7)
C(5)-N(3)-Mn	107.1(6)
C(37)-N(3)-Mn	111.9(6)
C(4)-N(3)-Mn	110.5(5)
C(9)-N(4)-Mn	126.5(7)
C(24)-N(5)-Mn	126.7(6)
C(39)-N(6)-Mn	129.5(7)
C(2)-C(1)-N(1)	111.0(8)
C(1)-C(2)-N(2)	109.8(8)
N(2)-C(3)-C(4)	109.2(8)
N(3)-C(4)-C(3)	110.0(7)
N(3)-C(5)-C(6)	107.4(8)
N(1)-C(6)-C(5)	112.2(8)
N(1)-C(7)-C(8)	119.9(9)
C(13)-C(8)-C(9)	120.6(9)
C(13)-C(8)-C(7)	114.8(10)
C(9)-C(8)-C(7)	124.5(10)
N(4)-C(9)-C(10)	124.3(10)
N(4)-C(9)-C(8)	118.8(9)
C(10)-C(9)-C(8)	117.0(10)
C(11)-C(10)-C(9)	119.3(10)
C(11)-C(10)-C(14)	120.4(9)
C(9)-C(10)-C(14)	120.4(10)
C(10)-C(11)-C(12)	123.0(10)
C(13)-C(12)-C(11)	117.6(11)
C(13)-C(12)-C(18)	120.8(10)
C(11)-C(12)-C(18)	121.6(9)
C(12)-C(13)-C(8)	122.4(11)
C(16)-C(14)-C(15)	113.0(9)
C(16)-C(14)-C(17)	106.7(8)
C(15)-C(14)-C(17)	105.6(8)
C(16)-C(14)-C(10)	111.2(8)
C(15)-C(14)-C(10)	110.4(8)
C(17)-C(14)-C(10)	109.8(9)
C(21)-C(18)-C(20)	106.1(10)
C(21)-C(18)-C(19)	109.5(11)
C(20)-C(18)-C(19)	106.0(10)
C(21)-C(18)-C(12)	109.9(10)
C(20)-C(18)-C(12)	114.9(10)
C(19)-C(18)-C(12)	110.3(10)
N(2)-C(22)-C(23)	119.0(8)
C(28)-C(23)-C(24)	120.5(9)
C(28)-C(23)-C(22)	115.3(8)
C(24)-C(23)-C(22)	124.1(9)
N(5)-C(24)-C(23)	119.9(9)
N(5)-C(24)-C(25)	122.9(8)
C(23)-C(24)-C(25)	117.1(10)
C(26)-C(25)-C(24)	118.3(9)
C(26)-C(25)-C(29)	122.1(10)
C(24)-C(25)-C(29)	119.5(10)
C(25)-C(26)-C(27)	124.5(11)
C(28)-C(27)-C(26)	116.5(10)
C(28)-C(27)-C(33)	122.9(9)
C(26)-C(27)-C(33)	120.6(10)

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C(23)-C(28)-C(27)	122.4(9)
C(32)-C(29)-C(31)	112.8(9)
C(32)-C(29)-C(25)	111.1(9)
C(31)-C(29)-C(25)	112.8(9)
C(32)-C(29)-C(30)	104.8(9)
C(31)-C(29)-C(30)	104.5(9)
C(25)-C(29)-C(30)	110.2(9)
C(36)-C(33)-C(27)	112.8(9)
C(36)-C(33)-C(35)	109.4(9)
C(27)-C(33)-C(35)	109.4(9)
C(36)-C(33)-C(34)	105.9(9)
C(27)-C(33)-C(34)	109.0(9)
C(35)-C(33)-C(34)	110.4(9)
N(3)-C(37)-C(38)	117.8(8)
C(43)-C(38)-C(39)	120.0(9)
C(43)-C(38)-C(37)	114.7(9)
C(39)-C(38)-C(37)	125.3(9)
N(6)-C(39)-C(38)	119.1(9)
N(6)-C(39)-C(40)	122.0(9)
C(38)-C(39)-C(40)	118.9(9)
C(41)-C(40)-C(39)	115.9(9)
C(41)-C(40)-C(44)	120.2(9)
C(39)-C(40)-C(44)	123.9(9)
C(42)-C(41)-C(40)	126.8(10)
C(41)-C(42)-C(43)	113.8(9)
C(41)-C(42)-C(48)	124.5(9)
C(43)-C(42)-C(48)	121.5(9)
C(38)-C(43)-C(42)	124.2(10)
C(40)-C(44)-C(46)	113.2(8)
C(40)-C(44)-C(45)	111.4(9)
C(46)-C(44)-C(45)	105.9(8)
C(40)-C(44)-C(47)	110.3(8)
C(46)-C(44)-C(47)	106.2(9)
C(45)-C(44)-C(47)	109.6(8)
C(42)-C(48)-C(50)	110.7(10)
C(42)-C(48)-C(49)	112.9(9)
C(50)-C(48)-C(49)	106.4(10)
C(42)-C(48)-C(51)	111.3(9)
C(50)-C(48)-C(51)	107.6(10)
C(49)-C(48)-C(51)	107.6(9)
C(71)-B(1)-C(91)	107.0(8)
C(71)-B(1)-C(61)	112.1(9)
C(91)-B(1)-C(61)	112.9(8)
C(71)-B(1)-C(81)	112.8(9)
C(91)-B(1)-C(81)	109.1(9)
C(61)-B(1)-C(81)	103.2(8)
C(66)-C(61)-C(62)	113.8(10)
C(66)-C(61)-B(1)	126.2(9)
C(62)-C(61)-B(1)	119.9(8)
C(63)-C(62)-C(61)	121.1(10)
C(64)-C(63)-C(62)	122.2(11)
C(63)-C(64)-C(65)	117.7(11)
C(64)-C(65)-C(66)	120.2(10)
C(61)-C(66)-C(65)	124.9(10)
C(72)-C(71)-C(76)	112.3(9)
C(72)-C(71)-B(1)	125.5(10)
C(76)-C(71)-B(1)	121.8(10)
C(71)-C(72)-C(73)	125.0(11)
C(74)-C(73)-C(72)	119.6(11)
C(75)-C(74)-C(73)	117.6(10)
C(76)-C(75)-C(74)	120.1(10)
C(75)-C(76)-C(71)	125.2(10)
C(86)-C(81)-C(82)	115.3(9)

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C(86)-C(81)-B(1)	122.9(9)
C(82)-C(81)-B(1)	121.5(9)
C(83)-C(82)-C(81)	122.8(10)
C(84)-C(83)-C(82)	120.8(11)
C(83)-C(84)-C(85)	118.4(11)
C(84)-C(85)-C(86)	121.2(10)
C(81)-C(86)-C(85)	121.5(10)
C(96)-C(91)-C(92)	114.9(9)
C(96)-C(91)-B(1)	118.7(9)
C(92)-C(91)-B(1)	126.3(10)
C(93)-C(92)-C(91)	121.8(11)
C(94)-C(93)-C(92)	119.3(11)
C(95)-C(94)-C(93)	120.8(11)
C(94)-C(95)-C(96)	120.5(12)
C(95)-C(96)-C(91)	122.5(11)
C(102)-C(101)-C(106)	120.0
C(102)-C(101)-C(107)	118.7(10)
C(106)-C(101)-C(107)	121.3(10)
C(103)-C(102)-C(101)	120.0
C(102)-C(103)-C(104)	120.0
C(103)-C(104)-C(105)	120.0
C(106)-C(105)-C(104)	120.0
C(105)-C(106)-C(101)	120.0

Symmetry transformations used to generate equivalent atoms:

Table S10. Anisotropic displacement parameters (A^2 x 10^3) for 2. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mn	14(1)	24(1)	16(1)	2(1)	9(1)	0(1)

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Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 2.

	x	y	z	U(eq)
H(4)	7574(3)	10314(4)	4304(5)	26
H(5)	8098(3)	8663(4)	3680(4)	18
H(6)	8015(3)	8955(4)	5603(5)	26
H(1A)	5772(5)	9707(5)	4975(6)	36
H(1B)	6360(5)	10169(5)	4784(6)	36
H(2A)	5774(4)	9924(5)	3670(6)	29
H(2B)	5707(4)	9120(5)	3884(6)	29
H(3A)	6876(5)	8669(5)	2833(6)	32
H(3B)	6114(5)	8765(5)	2756(6)	32
H(4A)	6043(4)	8071(5)	3780(5)	18
H(4B)	6513(4)	7656(5)	3313(5)	18
H(5A)	7091(5)	7814(5)	5374(6)	27
H(5B)	6480(5)	7465(5)	4881(6)	27
H(6A)	5902(4)	8478(4)	4839(6)	26
H(6B)	6225(4)	8416(4)	5693(6)	26
H(7A)	7138(4)	9002(5)	6121(6)	26
H(7B)	6543(4)	9503(5)	6159(6)	26
H(11)	8477(5)	11491(5)	6457(6)	33
H(13)	7225(5)	10105(5)	7062(6)	34
H(15A)	9218(5)	10530(5)	5121(6)	45
H(15B)	9176(5)	10963(5)	4359(6)	45
H(15C)	8682(5)	10344(5)	4432(6)	45
H(16A)	7723(5)	11882(5)	4597(6)	49
H(16B)	7745(5)	11191(5)	4106(6)	49
H(16C)	8240(5)	11810(5)	4034(6)	49
H(17A)	9205(5)	11643(5)	5758(6)	53
H(17B)	8625(5)	12178(5)	5557(6)	53
H(17C)	9119(5)	12049(5)	4976(6)	53
H(19A)	8616(7)	10250(7)	8089(9)	134
H(19B)	7887(7)	10113(7)	8195(9)	134
H(19C)	8319(7)	10632(7)	8747(9)	134
H(20A)	8938(6)	11415(6)	7728(8)	105
H(20B)	8598(6)	11724(6)	8395(8)	105
H(20C)	8414(6)	12018(6)	7563(8)	105
H(21A)	7079(6)	11053(7)	7842(8)	121
H(21B)	7325(6)	11804(7)	7629(8)	121
H(21C)	7509(6)	11510(7)	8460(8)	121
H(22A)	6739(4)	10383(5)	3503(6)	18
H(22B)	6426(4)	10022(5)	2746(6)	18
H(26)	8905(5)	10163(5)	2049(6)	35
H(28)	7125(4)	10807(5)	2226(6)	21
H(30A)	9760(5)	9668(6)	2561(6)	66
H(30B)	9412(5)	9170(6)	1920(6)	66
H(30C)	9929(5)	8856(6)	2567(6)	66
H(31A)	9509(5)	9580(5)	3860(6)	55
H(31B)	9745(5)	8791(5)	3817(6)	55
H(31C)	9072(5)	8958(5)	4090(6)	55
H(32A)	8599(5)	8314(5)	2202(7)	63
H(32B)	8501(5)	8164(5)	3050(7)	63
H(32C)	9173(5)	7997(5)	2776(7)	63
H(34A)	8602(5)	10607(6)	841(6)	65
H(34B)	8307(5)	11305(6)	451(6)	65
H(34C)	7848(5)	10664(6)	571(6)	65
H(35A)	9100(5)	11328(5)	1979(7)	59

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H(35B)	8648(5)	11845(5)	2361(7)	59
H(35C)	8808(5)	12003(5)	1538(7)	59
H(36A)	7649(5)	12067(6)	1079(7)	69
H(36B)	7475(5)	11886(6)	1890(7)	69
H(36C)	7189(5)	11423(6)	1185(7)	69
H(37A)	7587(4)	7691(5)	3599(6)	31
H(37B)	7317(4)	7128(5)	4122(6)	31
H(41)	9674(5)	7396(5)	5829(6)	38
H(43)	8362(4)	6699(5)	4210(6)	26
H(45A)	9469(5)	9591(5)	6376(6)	52
H(45B)	8919(5)	9473(5)	5682(6)	52
H(45C)	9638(5)	9236(5)	5627(6)	52
H(46A)	9932(5)	8660(5)	7128(6)	60
H(46B)	10131(5)	8273(5)	6411(6)	60
H(46C)	9731(5)	7865(5)	6963(6)	60
H(47A)	8834(5)	8955(5)	7230(6)	48
H(47B)	8598(5)	8174(5)	7046(6)	48
H(47C)	8265(5)	8807(5)	6564(6)	48
H(49A)	10427(5)	5950(6)	5226(7)	66
H(49B)	10116(5)	6361(6)	5855(7)	66
H(49C)	10416(5)	6783(6)	5224(7)	66
H(50A)	9940(6)	5928(7)	3968(8)	119
H(50B)	9899(6)	6759(7)	3930(8)	119
H(50C)	9269(6)	6300(7)	3696(8)	119
H(51A)	9476(5)	5268(6)	4902(7)	87
H(51B)	8794(5)	5623(6)	4648(7)	87
H(51C)	9113(5)	5653(6)	5505(7)	87
H(62)	4310(5)	10872(5)	910(6)	32
H(63)	4410(5)	11396(5)	-231(6)	37
H(64)	4950(5)	12439(5)	-294(6)	38
H(65)	5353(5)	12997(5)	825(6)	32
H(66)	5252(5)	12492(5)	1954(6)	33
H(72)	4083(5)	10150(5)	3018(6)	34
H(73)	4104(5)	8947(5)	2941(6)	41
H(74)	4727(5)	8399(6)	2116(6)	39
H(75)	5395(5)	9104(5)	1494(6)	33
H(76)	5355(5)	10290(5)	1593(6)	31
H(82)	4454(5)	12375(5)	3243(6)	30
H(83)	3525(5)	12899(5)	3503(6)	35
H(84)	2533(5)	12453(5)	3024(6)	33
H(85)	2484(5)	11444(5)	2315(6)	37
H(86)	3426(5)	10920(5)	2010(6)	37
H(92)	6021(5)	11716(5)	2452(7)	37
H(93)	6792(5)	11991(5)	3480(6)	38
H(94)	6603(5)	11704(6)	4681(7)	52
H(95)	5637(5)	11257(5)	4879(7)	43
H(96)	4833(5)	11061(5)	3885(6)	40
H(102)	6721(6)	10112(6)	-889(5)	88
H(103)	7513(6)	9251(7)	-724(6)	82
H(104)	7768(5)	8706(5)	438(8)	100
H(105)	7231(6)	9021(6)	1435(5)	88
H(106)	6439(5)	9882(6)	1270(6)	72
H(10A)	5842(7)	10674(7)	521(9)	147
H(10B)	5684(7)	10445(7)	-337(9)	147
H(10C)	6211(7)	11033(7)	-95(9)	147

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Table S13. Crystal data and structure refinement for 3.

Identification code	ST2738
Empirical formula	C_{52} H_{91} Cl_2 Cu N_6 $O_{6.5}$
Formula weight	1038.75
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 13.814(3) Å alpha = 81.48(3) deg. b = 13.869(3) Å beta = 69.13(3) deg. c = 18.171(4) Å gamma = 61.20(3) deg.
Volume	2849.4(11) Å^3
Z	2
Density (calculated)	1.211 Mg/m^3
Absorption coefficient	0.528 mm^-1
F(000)	1120
Crystal size	0.25 x 0.18 x 0.14 mm
Theta range for data collection	1.68 to 25.00 deg.
Index ranges	-21<=h<=14, -21<=k<=20, -27<=l<=27
Reflections collected	22724
Independent reflections	9780
Absorption correction	SADABS, G. M. Sheldrick 1994
Max. and min. transmission	0.946 and 0.696
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8981 / 0 / 671
Goodness-of-fit on F^2	1.040
Final R indices [I>2sigma(I)]	R1 = 0.0689, wR2 = 0.1566
R indices (all data)	R1 = 0.1127, wR2 = 0.1806
Largest diff. peak and hole	0.759 and -0.608 e.A^-3

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Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for 3. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cu(1)	6152(1)	7863(1)	5887(1)	22(1)
N(1)	6296(3)	6331(3)	6252(2)	25(1)
N(2)	7897(3)	7015(3)	5223(2)	26(1)
N(3)	6898(3)	7649(3)	6900(2)	28(1)
N(4)	4372(4)	8590(3)	6342(2)	24(1)
N(5)	5911(4)	7767(3)	4525(2)	24(1)
N(6)	8192(5)	9362(6)	7134(3)	62(2)
Cl(1)	6032(1)	9570(1)	5517(1)	25(1)
C(1)	7171(4)	5620(4)	5537(3)	28(1)
C(2)	8245(4)	5801(4)	5251(3)	32(1)
C(3)	8514(4)	7298(4)	5615(3)	32(1)
C(4)	8184(4)	7132(4)	6504(3)	33(1)
C(5)	6523(4)	6885(4)	7418(3)	30(1)
C(6)	6732(4)	5941(4)	6942(3)	31(1)
C(10)	5144(4)	6354(4)	6442(3)	27(1)
C(11)	4251(4)	7097(4)	7151(3)	24(1)
C(12)	3850(4)	8234(4)	7099(2)	20(1)
C(13)	3036(4)	8950(4)	7749(2)	21(1)
C(14)	2735(4)	8447(4)	8465(3)	24(1)
C(15)	3139(4)	7314(4)	8546(3)	24(1)
C(16)	3883(4)	6657(4)	7871(3)	25(1)
C(17)	2429(4)	10222(4)	7696(3)	24(1)
C(18)	3288(4)	10698(4)	7515(3)	27(1)
C(19)	1816(4)	10550(4)	7074(3)	29(1)
C(20)	1480(4)	10781(4)	8476(3)	33(1)
C(21)	2797(4)	6780(4)	9332(3)	30(1)
C(22)	3900(5)	5931(5)	9519(3)	43(1)
C(23)	2010(5)	7628(4)	10020(3)	40(1)
C(24)	2110(5)	6213(4)	9256(3)	37(1)
C(30)	8192(4)	7394(4)	4385(2)	27(1)
C(31)	7967(4)	6928(4)	3798(2)	23(1)
C(32)	6854(4)	7112(3)	3865(2)	21(1)
C(33)	6711(4)	6639(3)	3293(2)	21(1)
C(34)	7709(4)	6066(3)	2657(2)	24(1)
C(35)	8817(4)	5935(3)	2549(3)	23(1)
C(36)	8929(4)	6357(4)	3136(2)	24(1)
C(37)	5526(4)	6738(4)	3353(3)	26(1)
C(38)	4628(4)	7945(4)	3300(3)	29(1)
C(39)	5066(5)	6202(4)	4116(3)	34(1)
C(40)	5637(4)	6102(4)	2673(3)	32(1)
C(41)	10153(5)	4099(4)	1844(3)	45(1)
C(42)	9530(5)	5797(4)	1060(3)	37(1)
C(43)	10942(4)	5405(4)	1746(3)	37(1)
C(44)	9848(4)	5318(4)	1811(3)	28(1)
C(50)	6405(4)	8728(4)	7294(3)	28(1)
C(51)	6817(4)	8711(4)	7971(3)	27(1)
C(52)	7669(4)	9048(4)	7880(3)	28(1)
C(53)	8008(4)	9019(4)	8536(3)	25(1)
C(54)	7477(4)	8652(3)	9241(3)	22(1)
C(55)	6618(4)	8345(3)	9359(3)	23(1)
C(56)	6297(4)	8399(4)	8706(3)	25(1)
C(57)	6075(4)	7945(4)	10153(3)	25(1)
C(58)	4780(6)	8311(8)	10308(5)	97(3)

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C(59)	6060(9)	8454(7)	10830(3)	96(3)
C(60)	6706(7)	6718(5)	10155(4)	74(2)
C(61)	8931(5)	9377(4)	8484(3)	33(1)
C(62)	8487(5)	10616(5)	8304(4)	51(2)
C(63)	9144(5)	9246(5)	9272(3)	47(2)
C(64)	10111(5)	8676(5)	7868(3)	46(1)
Cl(2)	8633(2)	2465(3)	6300(2)	74(1)
O(21)	8936(9)	2772(8)	5533(6)	195(4)
O(22)	9038(12)	1428(8)	6412(7)	188(6)
O(23)	8904(7)	3241(12)	6520(10)	194(7)
O(24)	7390(6)	3081(7)	6566(5)	152(3)
ClX	8240(6)	2855(5)	6757(4)	53(2)
O(25X)	9324(16)	2318(16)	6695(10)	67(5)
O(26X)	7754(18)	3181(16)	7512(12)	100(6)
O(70)	3198(4)	8372(4)	5403(2)	45(1)
O(80)	7691(7)	3132(7)	4530(5)	55(2)
C(80)	8340(11)	3466(10)	3808(7)	60(4)
C(90)	965(11)	10218(10)	5483(8)	50(3)
O(90)	1485(11)	9998(11)	4717(8)	102(4)
O(95)	113(13)	11137(12)	4238(7)	117(4)

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Table S15. Bond lengths [Å] and angles [deg] for 3.

Cu(1)-N(4)	2.038(4)
Cu(1)-N(1)	2.065(4)
Cu(1)-N(2)	2.066(4)
Cu(1)-Cl(1)	2.3053(13)
Cu(1)-N(3)	2.332(4)
Cu(1)-N(5)	2.641(4)
N(1)-C(10)	1.489(6)
N(1)-C(1)	1.494(6)
N(1)-C(6)	1.500(6)
N(2)-C(3)	1.492(6)
N(2)-C(2)	1.511(6)
N(2)-C(30)	1.512(6)
N(3)-C(5)	1.471(6)
N(3)-C(50)	1.484(6)
N(3)-C(4)	1.484(6)
N(4)-C(12)	1.446(6)
N(5)-C(32)	1.425(6)
N(6)-C(52)	1.408(7)
C(1)-C(2)	1.519(7)
C(3)-C(4)	1.529(7)
C(5)-C(6)	1.530(6)
C(10)-C(11)	1.510(6)
C(11)-C(16)	1.389(6)
C(11)-C(12)	1.397(6)
C(12)-C(13)	1.403(6)
C(13)-C(14)	1.406(6)
C(13)-C(17)	1.552(6)
C(14)-C(15)	1.397(6)
C(15)-C(16)	1.386(6)
C(15)-C(21)	1.535(6)
C(17)-C(20)	1.533(6)
C(17)-C(19)	1.537(6)
C(17)-C(18)	1.539(6)
C(21)-C(22)	1.532(7)
C(21)-C(23)	1.538(7)
C(21)-C(24)	1.542(7)
C(30)-C(31)	1.512(6)
C(31)-C(32)	1.393(6)
C(31)-C(36)	1.404(6)
C(32)-C(33)	1.422(6)
C(33)-C(34)	1.396(6)
C(33)-C(37)	1.541(6)
C(34)-C(35)	1.395(6)
C(35)-C(36)	1.376(6)
C(35)-C(44)	1.537(6)
C(37)-C(40)	1.543(6)
C(37)-C(38)	1.546(7)
C(37)-C(39)	1.550(6)
C(41)-C(44)	1.530(7)
C(42)-C(44)	1.541(7)
C(43)-C(44)	1.536(7)
C(50)-C(51)	1.521(6)
C(51)-C(56)	1.389(6)
C(51)-C(52)	1.414(7)
C(52)-C(53)	1.416(6)
C(53)-C(54)	1.392(6)
C(53)-C(61)	1.546(7)
C(54)-C(55)	1.383(6)
C(55)-C(56)	1.388(6)

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C(55)-C(57)	1.531(6)
C(57)-C(60)	1.492(7)
C(57)-C(59)	1.496(8)
C(57)-C(58)	1.532(8)
C(61)-C(63)	1.531(7)
C(61)-C(64)	1.533(7)
C(61)-C(62)	1.549(7)
Cl(2)-O(22)	1.281(9)
Cl(2)-O(21)	1.371(9)
Cl(2)-O(24)	1.425(7)
Cl(2)-O(23)	1.442(11)
ClX-O(25X)	1.28(2)
ClX-O(26X)	1.33(2)
O(80)-C(80)	1.457(13)
C(90)-O(90)	1.32(2)

N(4)-Cu(1)-N(1)	92.1(2)
N(4)-Cu(1)-N(2)	167.1(2)
N(1)-Cu(1)-N(2)	85.3(2)
N(4)-Cu(1)-Cl(1)	88.99(12)
N(1)-Cu(1)-Cl(1)	177.44(11)
N(2)-Cu(1)-Cl(1)	94.10(12)
N(4)-Cu(1)-N(3)	108.7(2)
N(1)-Cu(1)-N(3)	81.16(14)
N(2)-Cu(1)-N(3)	83.38(14)
Cl(1)-Cu(1)-N(3)	96.30(11)
N(4)-Cu(1)-N(5)	86.7(2)
N(1)-Cu(1)-N(5)	96.17(14)
N(2)-Cu(1)-N(5)	81.08(14)
Cl(1)-Cu(1)-N(5)	86.20(10)
N(3)-Cu(1)-N(5)	164.40(13)
C(10)-N(1)-C(1)	111.1(3)
C(10)-N(1)-C(6)	110.4(4)
C(1)-N(1)-C(6)	110.6(4)
C(10)-N(1)-Cu(1)	109.3(3)
C(1)-N(1)-Cu(1)	102.1(3)
C(6)-N(1)-Cu(1)	113.1(3)
C(3)-N(2)-C(2)	112.2(4)
C(3)-N(2)-C(30)	106.3(3)
C(2)-N(2)-C(30)	111.7(3)
C(3)-N(2)-Cu(1)	104.2(3)
C(2)-N(2)-Cu(1)	108.3(3)
C(30)-N(2)-Cu(1)	114.0(3)
C(5)-N(3)-C(50)	112.9(4)
C(5)-N(3)-C(4)	112.1(4)
C(50)-N(3)-C(4)	113.8(4)
C(5)-N(3)-Cu(1)	102.4(3)
C(50)-N(3)-Cu(1)	110.4(3)
C(4)-N(3)-Cu(1)	104.1(3)
C(12)-N(4)-Cu(1)	117.9(3)
C(32)-N(5)-Cu(1)	123.3(3)
N(1)-C(1)-C(2)	110.1(4)
N(2)-C(2)-C(1)	110.7(4)
N(2)-C(3)-C(4)	114.2(4)
N(3)-C(4)-C(3)	112.1(4)
N(3)-C(5)-C(6)	111.2(4)
N(1)-C(6)-C(5)	112.8(4)
N(1)-C(10)-C(11)	111.1(3)
C(16)-C(11)-C(12)	119.5(4)
C(16)-C(11)-C(10)	120.6(4)
C(12)-C(11)-C(10)	119.8(4)
C(11)-C(12)-C(13)	121.5(4)
C(11)-C(12)-N(4)	114.7(4)

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C(13)-C(12)-N(4)	123.8(4)
C(12)-C(13)-C(14)	116.0(4)
C(12)-C(13)-C(17)	123.6(4)
C(14)-C(13)-C(17)	120.3(4)
C(15)-C(14)-C(13)	124.1(4)
C(16)-C(15)-C(14)	117.0(4)
C(16)-C(15)-C(21)	119.6(4)
C(14)-C(15)-C(21)	123.4(4)
C(15)-C(16)-C(11)	121.8(4)
C(20)-C(17)-C(19)	106.7(4)
C(20)-C(17)-C(18)	105.5(4)
C(19)-C(17)-C(18)	111.2(4)
C(20)-C(17)-C(13)	111.8(4)
C(19)-C(17)-C(13)	109.1(3)
C(18)-C(17)-C(13)	112.3(4)
C(22)-C(21)-C(15)	109.7(4)
C(22)-C(21)-C(23)	108.5(4)
C(15)-C(21)-C(23)	112.3(4)
C(22)-C(21)-C(24)	110.1(4)
C(15)-C(21)-C(24)	108.2(4)
C(23)-C(21)-C(24)	107.9(4)
C(31)-C(30)-N(2)	116.7(4)
C(32)-C(31)-C(36)	120.2(4)
C(32)-C(31)-C(30)	122.9(4)
C(36)-C(31)-C(30)	116.8(4)
C(31)-C(32)-C(33)	119.7(4)
C(31)-C(32)-N(5)	116.8(4)
C(33)-C(32)-N(5)	123.5(4)
C(34)-C(33)-C(32)	116.9(4)
C(34)-C(33)-C(37)	120.1(4)
C(32)-C(33)-C(37)	123.0(4)
C(35)-C(34)-C(33)	124.4(4)
C(36)-C(35)-C(34)	116.8(4)
C(36)-C(35)-C(44)	123.2(4)
C(34)-C(35)-C(44)	120.0(4)
C(35)-C(36)-C(31)	121.8(4)
C(33)-C(37)-C(40)	111.9(4)
C(33)-C(37)-C(38)	111.7(4)
C(40)-C(37)-C(38)	105.8(4)
C(33)-C(37)-C(39)	110.0(4)
C(40)-C(37)-C(39)	105.3(4)
C(38)-C(37)-C(39)	111.9(4)
C(41)-C(44)-C(43)	108.2(4)
C(41)-C(44)-C(35)	109.7(4)
C(43)-C(44)-C(35)	111.8(4)
C(41)-C(44)-C(42)	108.9(4)
C(43)-C(44)-C(42)	107.6(4)
C(35)-C(44)-C(42)	110.5(4)
N(3)-C(50)-C(51)	116.1(4)
C(56)-C(51)-C(52)	119.6(4)
C(56)-C(51)-C(50)	118.4(4)
C(52)-C(51)-C(50)	121.9(4)
N(6)-C(52)-C(51)	119.2(4)
N(6)-C(52)-C(53)	121.7(4)
C(51)-C(52)-C(53)	119.1(4)
C(54)-C(53)-C(52)	117.4(4)
C(54)-C(53)-C(61)	120.4(4)
C(52)-C(53)-C(61)	122.2(4)
C(55)-C(54)-C(53)	125.1(4)
C(54)-C(55)-C(56)	115.8(4)
C(54)-C(55)-C(57)	122.2(4)
C(56)-C(55)-C(57)	122.0(4)
C(55)-C(56)-C(51)	122.9(4)

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C(60)-C(57)-C(59)	111.8(5)
C(60)-C(57)-C(55)	109.5(4)
C(59)-C(57)-C(55)	112.1(4)
C(60)-C(57)-C(58)	108.5(6)
C(59)-C(57)-C(58)	103.5(6)
C(55)-C(57)-C(58)	111.3(4)
C(63)-C(61)-C(64)	107.0(5)
C(63)-C(61)-C(53)	111.2(4)
C(64)-C(61)-C(53)	111.4(4)
C(63)-C(61)-C(62)	105.6(4)
C(64)-C(61)-C(62)	111.0(4)
C(53)-C(61)-C(62)	110.4(4)
O(22)-Cl(2)-O(21)	116.2(8)
O(22)-Cl(2)-O(24)	115.2(7)
O(21)-Cl(2)-O(24)	102.7(6)
O(22)-Cl(2)-O(23)	129.3(9)
O(21)-Cl(2)-O(23)	89.2(9)
O(24)-Cl(2)-O(23)	98.9(6)
O(25X)-ClX-O(26X)	101.2(13)

Symmetry transformations used to generate equivalent atoms:

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Table S16. Anisotropic displacement parameters (A^2 x 10^3) for 3. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cu(1)	23(1)	26(1)	19(1)	-2(1)	-5(1)	-13(1)
N(1)	29(2)	28(2)	16(2)	-5(2)	-4(2)	-13(2)
N(2)	26(2)	33(2)	19(2)	-2(2)	-7(2)	-14(2)
N(3)	28(2)	36(2)	21(2)	-5(2)	-8(2)	-14(2)
N(4)	29(2)	28(2)	20(2)	1(2)	-7(2)	-18(2)
N(5)	25(2)	31(2)	22(2)	-6(2)	-5(2)	-17(2)
N(6)	85(4)	119(5)	28(3)	24(3)	-27(3)	-83(4)
Cl(1)	28(1)	29(1)	23(1)	-1(1)	-7(1)	-17(1)
C(1)	34(3)	28(3)	21(2)	-4(2)	-8(2)	-12(2)
C(2)	30(3)	35(3)	22(3)	-1(2)	-8(2)	-9(2)
C(3)	24(3)	47(3)	28(3)	-8(2)	-7(2)	-17(2)
C(4)	27(3)	41(3)	30(3)	-2(2)	-12(2)	-13(2)
C(5)	34(3)	30(3)	21(2)	-1(2)	-11(2)	-10(2)
C(6)	36(3)	33(3)	20(2)	1(2)	-10(2)	-12(2)
C(10)	36(3)	24(2)	24(2)	-3(2)	-4(2)	-19(2)
C(11)	27(3)	30(3)	21(2)	-5(2)	-7(2)	-17(2)
C(12)	22(2)	29(2)	15(2)	0(2)	-6(2)	-17(2)
C(13)	23(2)	26(2)	21(2)	-3(2)	-5(2)	-16(2)
C(14)	27(3)	30(3)	21(2)	-6(2)	-3(2)	-18(2)
C(15)	26(3)	31(3)	24(2)	-1(2)	-5(2)	-21(2)
C(16)	33(3)	24(2)	23(2)	-2(2)	-5(2)	-20(2)
C(17)	27(3)	25(2)	19(2)	1(2)	-3(2)	-16(2)
C(18)	33(3)	24(2)	29(3)	0(2)	-10(2)	-17(2)
C(19)	31(3)	29(3)	30(3)	0(2)	-6(2)	-18(2)
C(20)	37(3)	25(3)	26(3)	-5(2)	5(2)	-15(2)
C(21)	40(3)	31(3)	20(2)	2(2)	-3(2)	-23(2)
C(22)	51(4)	45(3)	29(3)	7(2)	-9(3)	-22(3)
C(23)	64(4)	39(3)	18(3)	2(2)	-4(3)	-31(3)
C(24)	42(3)	31(3)	34(3)	1(2)	3(2)	-25(3)
C(30)	22(3)	38(3)	19(2)	-6(2)	0(2)	-16(2)
C(31)	27(3)	29(3)	14(2)	-1(2)	-6(2)	-16(2)
C(32)	23(2)	21(2)	15(2)	-2(2)	0(2)	-12(2)
C(33)	25(2)	21(2)	15(2)	-2(2)	0(2)	-13(2)
C(34)	34(3)	20(2)	16(2)	-4(2)	-4(2)	-12(2)
C(35)	25(3)	20(2)	20(2)	2(2)	-5(2)	-9(2)
C(36)	21(2)	27(2)	20(2)	-1(2)	-3(2)	-11(2)
C(37)	33(3)	32(3)	18(2)	-4(2)	-3(2)	-21(2)
C(38)	25(3)	34(3)	28(3)	-7(2)	-4(2)	-15(2)
C(39)	40(3)	40(3)	23(3)	-7(2)	3(2)	-28(3)
C(40)	35(3)	41(3)	25(3)	-10(2)	-3(2)	-24(3)
C(41)	48(4)	30(3)	37(3)	-9(2)	0(3)	-11(3)
C(42)	32(3)	46(3)	23(3)	-7(2)	2(2)	-14(3)
C(43)	29(3)	48(3)	24(3)	-9(2)	2(2)	-15(3)
C(44)	25(3)	29(3)	21(2)	-5(2)	-1(2)	-8(2)
C(50)	31(3)	38(3)	22(2)	-1(2)	-14(2)	-18(2)
C(51)	26(3)	33(3)	23(2)	-6(2)	-8(2)	-12(2)
C(52)	31(3)	33(3)	20(2)	4(2)	-8(2)	-17(2)
C(53)	27(3)	26(2)	23(2)	-2(2)	-6(2)	-13(2)
C(54)	26(3)	16(2)	24(2)	-3(2)	-12(2)	-6(2)
C(55)	25(2)	17(2)	23(2)	-5(2)	-5(2)	-8(2)
C(56)	24(3)	27(2)	27(3)	-4(2)	-9(2)	-13(2)
C(57)	26(3)	24(2)	22(2)	0(2)	-3(2)	-12(2)
C(58)	58(5)	151(8)	80(5)	59(5)	-23(4)	-63(5)

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C(59)	193(10)	102(6)	20(3)	-7(3)	6(4)	-115(7)
C(60)	98(6)	37(3)	36(3)	3(3)	9(4)	-15(4)
C(61)	40(3)	48(3)	25(3)	2(2)	-10(2)	-31(3)
C(62)	59(4)	52(4)	59(4)	4(3)	-16(3)	-41(3)
C(63)	56(4)	71(4)	41(3)	8(3)	-23(3)	-46(3)
C(64)	46(3)	58(4)	49(3)	-3(3)	-8(3)	-39(3)
Cl(2)	57(2)	107(2)	72(2)	48(2)	-36(2)	-50(2)
O(21)	182(9)	159(8)	188(9)	79(7)	-44(7)	-68(7)
O(22)	234(13)	96(7)	163(10)	121(8)	-81(10)	-44(8)
O(23)	35(5)	220(13)	312(17)	-199(13)	-20(7)	-16(7)
O(24)	71(4)	229(9)	180(7)	16(6)	-27(5)	-102(5)
O(70)	41(2)	57(3)	45(2)	-7(2)	-17(2)	-23(2)
O(80)	40(5)	71(6)	53(5)	-25(4)	21(4)	-43(5)
C(80)	51(8)	48(8)	51(8)	-7(6)	10(6)	-16(6)
C(90)	57(8)	51(7)	65(9)	16(6)	-35(7)	-36(7)
O(90)	107(9)	126(10)	124(10)	82(9)	-69(8)	-93(8)
O(95)	160(13)	144(12)	81(8)	10(8)	-39(8)	-98(11)

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Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 3.

	x	y	z	U(eq)
H(4X)	4061(42)	8499(38)	6051(29)	28
H(4Y)	4180(45)	9207(42)	6360(29)	28
H(5X)	5230(45)	7897(38)	4552(28)	29
H(5Y)	5899(44)	8350(41)	4489(29)	29
H(6X)	7932(63)	9554(58)	6801(42)	74
H(6Y)	8544(58)	9883(53)	7107(38)	74
H(1A)	6818(4)	5800(4)	5115(3)	34
H(1B)	7400(4)	4837(4)	5665(3)	34
H(2A)	8711(4)	5443(4)	5610(3)	38
H(2B)	8739(4)	5458(4)	4719(3)	38
H(3A)	8338(4)	8077(4)	5516(3)	39
H(3B)	9368(4)	6840(4)	5371(3)	39
H(4A)	8525(4)	6334(4)	6605(3)	39
H(4B)	8522(4)	7453(4)	6732(3)	39
H(5A)	5681(4)	7289(4)	7724(3)	35
H(5B)	6963(4)	6581(4)	7795(3)	35
H(6A)	7580(4)	5429(4)	6750(3)	37
H(6B)	6333(4)	5529(4)	7291(3)	37
H(10A)	5235(4)	5599(4)	6549(3)	32
H(10B)	4864(4)	6620(4)	5984(3)	32
H(14)	2225(4)	8908(4)	8923(3)	29
H(16)	4149(4)	5885(4)	7901(3)	30
H(18A)	3921(4)	10370(4)	7019(3)	40
H(18B)	3617(4)	10529(4)	7943(3)	40
H(18C)	2875(4)	11498(4)	7468(3)	40
H(19A)	2393(4)	10209(4)	6563(3)	44
H(19B)	1442(4)	11352(4)	7032(3)	44
H(19C)	1221(4)	10297(4)	7230(3)	44
H(20A)	1834(4)	10593(4)	8892(3)	49
H(20B)	889(4)	10525(4)	8617(3)	49
H(20C)	1110(4)	11581(4)	8418(3)	49
H(22A)	3677(5)	5592(5)	10021(3)	65
H(22B)	4337(5)	6296(5)	9557(3)	65
H(22C)	4391(5)	5361(5)	9099(3)	65
H(23A)	1299(5)	8178(4)	9909(3)	60
H(23B)	2433(5)	7993(4)	10084(3)	60
H(23C)	1798(5)	7254(4)	10506(3)	60
H(24A)	1406(5)	6763(4)	9137(3)	55
H(24B)	1884(5)	5866(4)	9754(3)	55
H(24C)	2603(5)	5651(4)	8831(3)	55
H(30A)	7738(4)	8206(4)	4393(2)	32
H(30B)	9030(4)	7207(4)	4191(2)	32
H(34)	7627(4)	5743(3)	2271(2)	29
H(36)	9677(4)	6259(4)	3092(2)	28
H(38A)	3887(4)	7977(4)	3340(3)	44
H(38B)	4927(4)	8239(4)	2794(3)	44
H(38C)	4500(4)	8386(4)	3732(3)	44
H(39A)	4313(5)	6268(4)	4150(3)	50
H(39B)	4966(5)	6577(4)	4575(3)	50
H(39C)	5629(5)	5422(4)	4107(3)	50
H(40A)	4868(4)	6184(4)	2732(3)	47
H(40B)	6180(4)	5321(4)	2688(3)	47
H(40C)	5934(4)	6398(4)	2169(3)	47
H(41A)	9464(5)	4026(4)	1885(3)	67

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H(41B)	10401(5)	3776(4)	2303(3)	67
H(41C)	10790(5)	3713(4)	1363(3)	67
H(42A)	9333(5)	6579(4)	1034(3)	56
H(42B)	8857(5)	5719(4)	1072(3)	56
H(42C)	10199(5)	5400(4)	596(3)	56
H(43A)	10764(4)	6182(4)	1725(3)	56
H(43B)	11576(4)	5013(4)	1266(3)	56
H(43C)	11186(4)	5076(4)	2207(3)	56
H(50A)	5543(4)	9043(4)	7496(3)	34
H(50B)	6601(4)	9230(4)	6893(3)	34
H(54)	7724(4)	8609(3)	9676(3)	27
H(56)	5696(4)	8213(4)	8763(3)	30
H(58A)	4354(6)	9117(8)	10308(5)	145
H(58B)	4455(6)	8050(8)	10821(5)	145
H(58C)	4702(6)	8002(8)	9894(5)	145
H(59A)	5640(9)	9257(7)	10810(3)	144
H(59B)	6865(9)	8226(7)	10799(3)	144
H(59C)	5665(9)	8211(7)	11327(3)	144
H(60A)	6698(7)	6415(5)	9704(4)	111
H(60B)	6317(7)	6459(5)	10645(4)	111
H(60C)	7516(7)	6475(5)	10117(4)	111
H(62A)	8334(5)	10753(5)	7802(4)	77
H(62B)	9082(5)	10830(5)	8270(4)	77
H(62C)	7764(5)	11050(5)	8726(4)	77
H(63A)	8406(5)	9685(5)	9682(3)	71
H(63B)	9712(5)	9502(5)	9227(3)	71
H(63C)	9450(5)	8469(5)	9412(3)	71
H(64A)	10010(5)	8738(5)	7353(3)	69
H(64B)	10408(5)	7904(5)	8022(3)	69
H(64C)	10670(5)	8937(5)	7837(3)	69
H(70X)	2623(54)	8972(50)	5311(35)	55
H(70Y)	2773(53)	7996(48)	5685(35)	55
H(80)	8161(10)	2584(80)	4708(50)	82
H(80A)	8322(65)	4149(40)	3910(14)	91
H(80B)	7983(47)	3586(69)	3401(17)	91
H(80C)	9153(21)	2887(33)	3626(29)	91
H(90A)	406(50)	9921(57)	5689(12)	75
H(90B)	550(57)	11016(10)	5579(9)	75
H(90C)	1554(13)	9878(54)	5749(10)	75
H(90)	1066(94)	9886(186)	4536(26)	152