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Table 1. Crystal data and structure refinement for 1.

Identification code	gr001
Empirical formula	C96 H100 K4 P4
Formula weight	1534.04
Temperature	203(2) K
Wavelength	0.71073 A
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 11.5144(2) A alpha = 67.614(1) deg b = 14.3774(2) A beta = 89.469(1) deg c = 15.1334(2) A gamma = 69.255(1) deg
Volume, Z	2143.32(6) A^3, 1
Density (calculated)	1.189 Mg/m^3
Absorption coefficient	0.327 mm^-1
F(000)	812
Crystal size	0.10 x 0.10 x 0.10 mm
Theta range for data collection	1.47 to 21.00 deg.
Limiting indices	-15<=h<=14, -19<=k<=18, -20<=l<=19
Reflections collected	11533
Independent reflections	4589 [R(int) = 0.0835]
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4589 / 0 / 469
Goodness-of-fit on F^2	1.040
Final R indices [I>2sigma(I)]	R1 = 0.0629, wR2 = 0.1737
R indices (all data)	R1 = 0.0957, wR2 = 0.1920
Largest diff. peak and hole	0.535 and -0.504 e.A^-3

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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^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)
K(1)	-960(2)	11359(1)	520(1)	66(1)
K(2)	2408(1)	9372(1)	2818(1)	49(1)
P(1)	780(1)	8611(1)	1576(1)	35(1)
P(2)	2(1)	11318(1)	2509(1)	40(1)
C(1)	-1175(4)	7981(4)	2323(3)	27(1)
C(2)	-1738(5)	7415(4)	3038(4)	31(1)
C(3)	-1062(5)	6645(4)	3920(4)	33(1)
C(4)	193(5)	6427(4)	4075(3)	30(1)
C(5)	801(5)	6955(4)	3386(3)	29(1)
C(6)	117(5)	7780(4)	2487(3)	27(1)
C(7)	-2076(5)	8517(4)	622(4)	38(1)
C(8)	-2894(5)	9296(5)	-234(4)	43(2)
C(9)	-3613(5)	10337(5)	-327(4)	44(2)
C(10)	-3507(5)	10607(4)	445(4)	42(2)
C(11)	-2714(5)	9858(4)	1301(4)	34(1)
C(12)	-1977(4)	8807(4)	1382(3)	31(1)
C(13)	-1338(6)	7379(4)	688(4)	55(2)
C(14)	-4520(5)	11160(5)	-1245(4)	59(2)
C(15)	-2623(5)	10169(4)	2140(4)	45(2)
C(16)	2615(4)	7059(4)	4195(3)	30(1)
C(17)	3896(5)	6811(4)	4363(4)	40(1)
C(18)	4756(5)	6183(4)	3974(4)	42(2)
C(19)	4311(5)	5766(4)	3421(4)	45(2)
C(20)	3028(5)	5991(4)	3238(3)	34(1)
C(21)	2174(4)	6664(4)	3611(3)	27(1)
C(22)	1703(5)	7748(4)	4641(4)	44(2)
C(23)	6155(5)	5907(5)	4164(5)	61(2)
C(24)	2582(6)	5486(5)	2667(4)	56(2)
C(25)	-1306(5)	13494(4)	2333(3)	30(1)
C(26)	-1387(5)	14358(4)	2562(4)	44(2)
C(27)	-424(6)	14328(5)	3116(4)	48(2)
C(28)	690(5)	13415(4)	3437(4)	43(2)
C(29)	807(5)	12530(4)	3225(3)	31(1)
C(30)	-200(5)	12527(4)	2695(3)	30(1)
C(31)	-2194(5)	13991(4)	648(4)	38(1)
C(32)	-3056(6)	14006(4)	-5(4)	45(2)
C(33)	-4024(6)	13665(4)	283(4)	45(2)
C(34)	-4146(5)	13321(4)	1248(4)	45(2)
C(35)	-3302(5)	13268(4)	1934(4)	38(1)
C(36)	-2298(5)	13591(4)	1639(3)	32(1)
C(37)	-1146(5)	14387(5)	300(4)	58(2)
C(38)	-4947(6)	13702(5)	-456(4)	68(2)
C(39)	-3446(6)	12848(5)	2987(4)	54(2)
C(40)	2278(5)	10671(4)	4401(4)	32(1)
C(41)	3414(5)	9791(4)	4633(4)	37(1)
C(42)	4312(5)	9774(4)	4032(4)	38(1)
C(43)	4066(5)	10658(5)	3162(4)	45(2)
C(44)	2939(5)	11568(4)	2895(4)	37(1)
C(45)	2033(5)	11575(4)	3522(4)	31(1)
C(46)	1321(5)	10678(5)	5093(4)	46(2)

C(47)	5547(5)	8792(5)	4306(5)	56(2)
C(48)	2712(6)	12527(5)	1948(4)	58(2)

Table 3. Bond lengths [A] and angles [deg] for 1.

K(1)-P(1)#1	3.162(2)
K(1)-P(2)	3.189(2)
K(1)-P(1)	3.438(2)
K(1)-K(2)	4.486(2)
K(1)-K(1)#1	4.598(3)
K(2)-P(2)	3.043(2)
K(2)-P(1)	3.365(2)
P(1)-C(6)	1.812(5)
P(1)-K(1)#1	3.162(2)
P(2)-C(30)	1.800(5)
C(1)-C(2)	1.393(7)
C(1)-C(6)	1.417(7)
C(1)-C(12)	1.500(6)
C(2)-C(3)	1.377(7)
C(3)-C(4)	1.369(6)
C(4)-C(5)	1.383(7)
C(5)-C(6)	1.417(6)
C(5)-C(21)	1.491(7)
C(7)-C(12)	1.383(7)
C(7)-C(8)	1.410(7)
C(7)-C(13)	1.518(7)
C(8)-C(9)	1.381(7)
C(9)-C(10)	1.382(7)
C(9)-C(14)	1.524(7)
C(10)-C(11)	1.391(7)
C(11)-C(12)	1.404(7)
C(11)-C(15)	1.513(7)
C(16)-C(17)	1.389(7)
C(16)-C(21)	1.400(7)
C(16)-C(22)	1.516(7)
C(17)-C(18)	1.380(8)
C(18)-C(19)	1.389(8)
C(18)-C(23)	1.517(7)
C(19)-C(20)	1.401(7)
C(20)-C(21)	1.398(7)
C(20)-C(24)	1.512(7)
C(25)-C(26)	1.384(7)
C(25)-C(30)	1.426(7)
C(25)-C(36)	1.492(7)
C(26)-C(27)	1.375(7)
C(27)-C(28)	1.392(7)
C(28)-C(29)	1.388(7)
C(29)-C(30)	1.418(7)
C(29)-C(45)	1.500(7)
C(31)-C(32)	1.396(7)
C(31)-C(36)	1.408(7)
C(31)-C(37)	1.518(7)
C(32)-C(33)	1.374(8)
C(33)-C(34)	1.376(8)
C(33)-C(38)	1.524(7)
C(34)-C(35)	1.390(7)
C(35)-C(36)	1.402(7)
C(35)-C(39)	1.505(7)
C(40)-C(41)	1.390(7)
C(40)-C(45)	1.403(7)
C(40)-C(46)	1.514(7)

C(41)-C(42)	1.371(7)
C(42)-C(43)	1.380(8)
C(42)-C(47)	1.527(7)
C(43)-C(44)	1.401(7)
C(44)-C(45)	1.403(7)
C(44)-C(48)	1.507(7)

P(1)#1-K(1)-P(2)	156.06(7)
P(1)#1-K(1)-P(1)	91.78(5)
P(2)-K(1)-P(1)	83.83(5)
P(1)#1-K(1)-K(2)	120.04(5)
P(2)-K(1)-K(2)	42.67(3)
P(1)-K(1)-K(2)	48.05(3)
P(1)#1-K(1)-K(1)#1	48.36(3)
P(2)-K(1)-K(1)#1	123.24(6)
P(1)-K(1)-K(1)#1	43.42(3)
K(2)-K(1)-K(1)#1	81.05(4)
P(2)-K(2)-P(1)	87.35(4)
P(2)-K(2)-K(1)	45.27(3)
P(1)-K(2)-K(1)	49.45(3)
C(6)-P(1)-K(1)#1	123.8(2)
C(6)-P(1)-K(2)	104.3(2)
K(1)#1-P(1)-K(2)	129.47(6)
C(6)-P(1)-K(1)	117.0(2)
K(1)#1-P(1)-K(1)	88.22(5)
K(2)-P(1)-K(1)	82.51(4)
C(30)-P(2)-K(2)	128.7(2)
C(30)-P(2)-K(1)	123.4(2)
K(2)-P(2)-K(1)	92.06(5)
C(2)-C(1)-C(6)	120.6(4)
C(2)-C(1)-C(12)	118.2(4)
C(6)-C(1)-C(12)	121.2(4)
C(3)-C(2)-C(1)	121.5(5)
C(4)-C(3)-C(2)	118.3(5)
C(3)-C(4)-C(5)	122.6(4)
C(4)-C(5)-C(6)	120.2(5)
C(4)-C(5)-C(21)	119.2(4)
C(6)-C(5)-C(21)	120.6(4)
C(1)-C(6)-C(5)	116.8(4)
C(1)-C(6)-P(1)	119.1(3)
C(5)-C(6)-P(1)	124.1(4)
C(12)-C(7)-C(8)	119.2(5)
C(12)-C(7)-C(13)	121.7(5)
C(8)-C(7)-C(13)	119.1(5)
C(9)-C(8)-C(7)	121.7(5)
C(10)-C(9)-C(8)	118.2(5)
C(10)-C(9)-C(14)	120.7(5)
C(8)-C(9)-C(14)	121.1(5)
C(9)-C(10)-C(11)	121.7(5)
C(10)-C(11)-C(12)	119.6(5)
C(10)-C(11)-C(15)	120.8(5)
C(12)-C(11)-C(15)	119.6(4)
C(7)-C(12)-C(11)	119.6(4)
C(7)-C(12)-C(1)	120.6(4)
C(11)-C(12)-C(1)	119.5(4)
C(17)-C(16)-C(21)	119.3(5)
C(17)-C(16)-C(22)	120.5(5)
C(21)-C(16)-C(22)	120.2(4)
C(18)-C(17)-C(16)	122.3(5)
C(17)-C(18)-C(19)	117.9(5)

C(17)-C(18)-C(23)	122.2(5)
C(19)-C(18)-C(23)	119.9(5)
C(18)-C(19)-C(20)	121.8(5)
C(21)-C(20)-C(19)	119.1(5)
C(21)-C(20)-C(24)	120.6(5)
C(19)-C(20)-C(24)	120.3(5)
C(20)-C(21)-C(16)	119.7(4)
C(20)-C(21)-C(5)	119.9(4)
C(16)-C(21)-C(5)	120.4(4)
C(26)-C(25)-C(30)	119.4(4)
C(26)-C(25)-C(36)	121.3(4)
C(30)-C(25)-C(36)	119.0(4)
C(27)-C(26)-C(25)	122.3(5)
C(26)-C(27)-C(28)	119.3(5)
C(29)-C(28)-C(27)	120.1(5)
C(28)-C(29)-C(30)	121.2(5)
C(28)-C(29)-C(45)	119.9(4)
C(30)-C(29)-C(45)	118.8(4)
C(29)-C(30)-C(25)	117.5(4)
C(29)-C(30)-P(2)	118.3(4)
C(25)-C(30)-P(2)	124.2(4)
C(32)-C(31)-C(36)	119.2(5)
C(32)-C(31)-C(37)	120.7(5)
C(36)-C(31)-C(37)	120.2(5)
C(33)-C(32)-C(31)	122.3(5)
C(32)-C(33)-C(34)	117.9(5)
C(32)-C(33)-C(38)	120.4(6)
C(34)-C(33)-C(38)	121.6(6)
C(33)-C(34)-C(35)	122.3(6)
C(34)-C(35)-C(36)	119.4(5)
C(34)-C(35)-C(39)	120.5(5)
C(36)-C(35)-C(39)	120.0(5)
C(31)-C(36)-C(35)	118.8(5)
C(31)-C(36)-C(25)	118.3(5)
C(35)-C(36)-C(25)	122.8(4)
C(41)-C(40)-C(45)	119.3(5)
C(41)-C(40)-C(46)	121.0(5)
C(45)-C(40)-C(46)	119.8(5)
C(42)-C(41)-C(40)	122.3(5)
C(41)-C(42)-C(43)	118.5(5)
C(41)-C(42)-C(47)	120.9(5)
C(43)-C(42)-C(47)	120.6(5)
C(42)-C(43)-C(44)	121.5(5)
C(43)-C(44)-C(45)	119.2(5)
C(43)-C(44)-C(48)	120.1(5)
C(45)-C(44)-C(48)	120.7(5)
C(40)-C(45)-C(44)	119.3(5)
C(40)-C(45)-C(29)	121.3(5)
C(44)-C(45)-C(29)	119.4(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+2,-z

Table 4. 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
K(1)	113(1)	58(1)	34(1)	-19(1)	9(1)	-41(1)
K(2)	39(1)	34(1)	73(1)	-25(1)	0(1)	-10(1)
P(1)	41(1)	34(1)	32(1)	-11(1)	9(1)	-20(1)
P(2)	38(1)	28(1)	53(1)	-22(1)	-4(1)	-8(1)
C(1)	29(3)	20(3)	34(3)	-12(2)	3(3)	-9(3)
C(2)	24(3)	31(3)	42(3)	-15(3)	8(3)	-12(3)
C(3)	36(4)	25(3)	34(3)	-5(3)	12(3)	-15(3)
C(4)	32(4)	22(3)	28(3)	-5(2)	-1(3)	-9(3)
C(5)	35(3)	25(3)	31(3)	-16(3)	9(3)	-12(3)
C(6)	32(3)	22(3)	29(3)	-14(3)	7(2)	-10(2)
C(7)	41(4)	34(3)	38(3)	-11(3)	2(3)	-17(3)
C(8)	52(4)	41(4)	35(3)	-11(3)	1(3)	-20(3)
C(9)	37(4)	39(4)	39(4)	1(3)	1(3)	-13(3)
C(10)	44(4)	27(3)	47(4)	-8(3)	0(3)	-13(3)
C(11)	37(3)	23(3)	42(3)	-12(3)	3(3)	-13(3)
C(12)	29(3)	28(3)	32(3)	-8(3)	3(2)	-13(3)
C(13)	67(4)	40(4)	51(4)	-22(3)	-5(3)	-10(3)
C(14)	54(4)	52(4)	46(4)	3(3)	-6(3)	-16(3)
C(15)	50(4)	25(3)	57(4)	-18(3)	7(3)	-10(3)
C(16)	23(3)	26(3)	37(3)	-9(3)	6(2)	-8(3)
C(17)	35(4)	40(3)	45(3)	-14(3)	4(3)	-18(3)
C(18)	28(4)	30(3)	55(4)	-4(3)	5(3)	-11(3)
C(19)	35(4)	33(3)	56(4)	-14(3)	17(3)	-5(3)
C(20)	35(4)	28(3)	32(3)	-9(3)	6(3)	-5(3)
C(21)	22(3)	27(3)	30(3)	-8(3)	3(2)	-9(3)
C(22)	41(4)	48(4)	53(4)	-30(3)	6(3)	-16(3)
C(23)	29(4)	46(4)	86(5)	-7(3)	15(3)	-13(3)
C(24)	61(4)	53(4)	65(4)	-38(3)	21(3)	-17(3)
C(25)	35(3)	21(3)	28(3)	-8(2)	5(2)	-8(3)
C(26)	48(4)	25(3)	48(4)	-12(3)	0(3)	-4(3)
C(27)	62(4)	31(4)	58(4)	-27(3)	10(3)	-17(3)
C(28)	52(4)	39(4)	49(4)	-23(3)	1(3)	-24(3)
C(29)	39(3)	27(3)	32(3)	-12(3)	5(3)	-17(3)
C(30)	32(3)	28(3)	35(3)	-15(3)	10(3)	-13(3)
C(31)	40(4)	29(3)	35(3)	-8(3)	7(3)	-8(3)
C(32)	54(4)	36(4)	29(3)	-13(3)	-1(3)	0(3)
C(33)	48(4)	24(3)	45(4)	-10(3)	-17(3)	3(3)
C(34)	34(4)	29(3)	58(4)	-7(3)	-10(3)	-8(3)
C(35)	38(4)	24(3)	42(3)	-7(3)	3(3)	-6(3)
C(36)	31(3)	20(3)	36(3)	-10(3)	2(3)	1(3)
C(37)	55(4)	59(4)	49(4)	-13(3)	19(3)	-19(4)
C(38)	71(5)	45(4)	69(4)	-20(4)	-33(4)	-3(3)
C(39)	55(4)	48(4)	44(4)	-5(3)	7(3)	-17(3)
C(40)	30(3)	32(3)	40(3)	-22(3)	5(3)	-13(3)
C(41)	33(4)	37(4)	44(3)	-19(3)	-2(3)	-15(3)
C(42)	26(3)	42(4)	56(4)	-26(3)	5(3)	-17(3)
C(43)	34(4)	58(4)	62(4)	-37(4)	18(3)	-27(4)
C(44)	32(4)	44(4)	44(3)	-20(3)	10(3)	-22(3)
C(45)	31(3)	31(3)	38(3)	-17(3)	1(3)	-15(3)
C(46)	45(4)	45(4)	42(3)	-15(3)	8(3)	-13(3)

C(47)	31(4)	53(4)	91(5)	-42(4)	6(3)	-10(3)
C(48)	55(4)	72(5)	51(4)	-18(4)	15(3)	-37(4)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

	x	y	z	U(eq)
H(2A)	-2597(5)	7563(4)	2916(4)	37
H(3A)	-1453(5)	6278(4)	4402(4)	40
H(4A)	661(5)	5898(4)	4673(3)	35
H(8A)	-2951(5)	9103(5)	-754(4)	52
H(10A)	-3984(5)	11314(4)	390(4)	51
H(13A)	-1533(6)	7334(4)	87(4)	82
H(13B)	-1561(6)	6858(4)	1215(4)	82
H(13C)	-446(6)	7217(4)	804(4)	82
H(14A)	-4470(5)	10833(5)	-1707(4)	89
H(14B)	-4299(5)	11793(5)	-1521(4)	89
H(14C)	-5369(5)	11377(5)	-1092(4)	89
H(15A)	-2027(5)	9551(4)	2671(4)	67
H(15B)	-3441(5)	10383(4)	2346(4)	67
H(15C)	-2344(5)	10771(4)	1940(4)	67
H(17A)	4186(5)	7080(4)	4756(4)	48
H(19A)	4885(5)	5322(4)	3163(4)	54
H(22A)	855(5)	7838(4)	4450(4)	67
H(22B)	1765(5)	8454(4)	4420(4)	67
H(22C)	1906(5)	7391(4)	5340(4)	67
H(23A)	6596(5)	5461(5)	3828(5)	91
H(23B)	6447(5)	5512(5)	4852(5)	91
H(23C)	6316(5)	6572(5)	3932(5)	91
H(24A)	3295(6)	5049(5)	2465(4)	85
H(24B)	1997(6)	6056(5)	2103(4)	85
H(24C)	2166(6)	5030(5)	3068(4)	85
H(26A)	-2126(5)	14987(4)	2330(4)	53
H(27A)	-517(6)	14919(5)	3277(4)	57
H(28A)	1363(5)	13396(4)	3799(4)	52
H(32A)	-2971(6)	14257(4)	-664(4)	54
H(34A)	-4825(5)	13114(4)	1451(4)	54
H(37A)	-642(5)	14321(5)	847(4)	87
H(37B)	-1504(5)	15142(5)	-154(4)	87
H(37C)	-622(5)	13951(5)	-16(4)	87
H(38A)	-5566(6)	13435(5)	-131(4)	102
H(38B)	-4498(6)	13250(5)	-785(4)	102
H(38C)	-5366(6)	14446(5)	-925(4)	102
H(39A)	-2779(6)	12865(5)	3359(4)	81
H(39B)	-3400(6)	12106(5)	3204(4)	81
H(39C)	-4252(6)	13302(5)	3076(4)	81
H(41A)	3571(5)	9187(4)	5222(4)	44
H(43A)	4670(5)	10650(5)	2740(4)	54
H(46A)	593(5)	11353(5)	4813(4)	69
H(46B)	1688(5)	10615(5)	5698(4)	69
H(46C)	1068(5)	10070(5)	5212(4)	69
H(47A)	6064(5)	8923(5)	3798(5)	83
H(47B)	5376(5)	8152(5)	4388(5)	83
H(47C)	5987(5)	8677(5)	4906(5)	83
H(48A)	1893(6)	13082(5)	1877(4)	87
H(48B)	2742(6)	12296(5)	1421(4)	87
H(48C)	3354(6)	12821(5)	1936(4)	87