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STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{22}\ H_{26}\ Cl_2\ N_4\ O_{10}$
Color; Habit	COLORLESS PRISM
Crystal size (mm)	0.35 X 0.25 X 0.28
Crystal System	Orthorhombic
Space Group	Pnma
Unit Cell Dimensions	$\underline{a}$ = 11.441(2) Å
	$\underline{b}$ = 32.615(7) Å
	$\underline{c}$ = 6.6690(10) Å
Volume	2488.5(10) $Å^3$
Z	4
Formula weight	577.4
Density(calc.)	1.541 Mg/m^3
Absorption Coefficient	0.326 mm^{-1}
F(000)	1200

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
Cl(1)	6115(1)	6114(1)	1361(3)	45(1)
O(1)	1722(4)	3243(1)	3751(7)	45(1)
O(2)	5036(4)	6225(2)	2207(9)	107(3)
O(3)	7040(4)	6275(2)	2544(8)	90(2)
O(4)	6171(6)	5698(1)	1338(12)	158(4)
O(5)	6134(5)	6283(2)	-527(8)	136(3)
N(1)	947(4)	3634(1)	1279(7)	35(2)
N(2)	1684(4)	4040(1)	3854(8)	41(2)
C(1)	839(4)	2888(2)	950(8)	27(2)
C(2)	1200(7)	2500	2091(11)	28(3)
C(5)	1044(6)	2500	-2271(12)	32(3)
C(6)	-284(7)	2500	-2511(13)	40(3)
C(7)	-864(6)	2500	-443(12)	35(3)
C(8)	-507(4)	2886(2)	686(9)	34(2)
C(9)	1426(4)	2886(2)	-1134(8)	32(2)
C(11)	1215(5)	3256(2)	2134(9)	31(2)
C(12)	1153(5)	4010(2)	2078(9)	35(2)
C(13)	799(6)	4367(2)	1124(11)	56(3)
C(14)	994(7)	4736(2)	2035(13)	72(3)
C(15)	1544(6)	4755(2)	3878(12)	66(3)
C(16)	1891(6)	4405(2)	4764(10)	56(3)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

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Table 2. Bond lengths (Å)

Cl(1)-O(2)	1.405 (5)	Cl(1)-O(3)	1.421 (5)
Cl(1)-O(4)	1.358 (5)	Cl(1)-O(5)	1.375 (6)
O(1)-C(11)	1.225 (7)	N(1)-C(11)	1.393 (7)
N(1)-C(12)	1.358 (7)	N(2)-C(12)	1.334 (8)
N(2)-C(16)	1.359 (8)	C(1)-C(2)	1.534 (7)
C(1)-C(8)	1.550 (7)	C(1)-C(9)	1.543 (7)
C(1)-C(11)	1.499 (7)	C(2)-C(1A)	1.534 (7)
C(5)-C(6)	1.527 (11)	C(5)-C(9)	1.532 (7)
C(5)-C(9A)	1.532 (7)	C(6)-C(7)	1.531 (12)
C(7)-C(8)	1.523 (7)	C(7)-C(8A)	1.523 (7)
C(12)-C(13)	1.386 (8)	C(13)-C(14)	1.367 (9)
C(14)-C(15)	1.383 (12)	C(15)-C(16)	1.343 (9)

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Table 3. Bond angles (°)

O(2)-Cl(1)-O(3)	109.7(3)	O(2)-Cl(1)-O(4)	107.6(4)
O(3)-Cl(1)-O(4)	109.9(4)	O(2)-Cl(1)-O(5)	106.2(4)
O(3)-Cl(1)-O(5)	110.4(4)	O(4)-Cl(1)-O(5)	112.9(5)
C(11)-N(1)-C(12)	126.9(5)	C(12)-N(2)-C(16)	122.7(5)
C(2)-C(1)-C(8)	108.7(5)	C(2)-C(1)-C(9)	109.0(4)
C(8)-C(1)-C(9)	109.3(4)	C(2)-C(1)-C(11)	108.7(4)
C(8)-C(1)-C(11)	110.4(4)	C(9)-C(1)-C(11)	110.7(4)
C(1)-C(2)-C(1A)	111.2(6)	C(6)-C(5)-C(9)	109.6(4)
C(6)-C(5)-C(9A)	109.6(4)	C(9)-C(5)-C(9A)	110.3(6)
C(5)-C(6)-C(7)	109.7(7)	C(6)-C(7)-C(8)	109.2(4)
C(6)-C(7)-C(8A)	109.2(4)	C(8)-C(7)-C(8A)	111.6(7)
C(1)-C(8)-C(7)	109.0(5)	C(1)-C(9)-C(5)	109.0(4)
O(1)-C(11)-N(1)	119.6(5)	O(1)-C(11)-C(1)	124.9(5)
N(1)-C(11)-C(1)	115.4(5)	N(1)-C(12)-N(2)	119.5(5)
N(1)-C(12)-C(13)	121.8(5)	N(2)-C(12)-C(13)	118.6(5)
C(12)-C(13)-C(14)	119.2(7)	C(13)-C(14)-C(15)	120.6(6)
C(14)-C(15)-C(16)	119.2(6)	N(2)-C(16)-C(15)	119.7(6)

Table 4. Anisotropic displacement coefficients ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl(1)	44(1)	49(1)	41(1)	2(1)	0(1)	-2(1)
O(1)	65(3)	33(2)	37(3)	3(2)	-24(3)	-4(2)
O(2)	73(4)	167(6)	80(4)	17(4)	26(4)	-34(4)
O(3)	92(4)	79(4)	98(4)	-30(3)	-56(4)	16(3)
O(4)	185(7)	47(3)	241(9)	31(4)	-86(7)	-58(5)
O(5)	86(4)	266(9)	56(3)	-32(5)	-13(4)	69(5)
N(1)	43(3)	32(3)	30(3)	-1(3)	-16(3)	1(3)
N(2)	49(3)	30(3)	44(4)	0(2)	-7(3)	4(3)
C(1)	23(3)	34(3)	23(3)	3(3)	0(3)	1(3)
C(2)	29(4)	31(4)	25(5)	0	1(4)	0
C(5)	25(4)	49(5)	23(4)	0	2(5)	0
C(6)	36(5)	51(6)	32(5)	0	-17(5)	0
C(7)	17(5)	54(5)	35(5)	0	-7(4)	0
C(8)	23(3)	41(3)	39(4)	3(3)	3(3)	4(3)
C(9)	27(3)	39(3)	30(3)	1(3)	0(3)	5(3)
C(11)	24(3)	35(3)	33(4)	1(3)	2(3)	3(3)
C(12)	34(3)	35(4)	35(4)	-1(3)	-3(4)	4(3)
C(13)	73(5)	40(4)	55(5)	3(4)	-24(4)	9(4)
C(14)	92(6)	34(4)	90(7)	6(4)	-40(6)	12(4)
C(15)	85(6)	28(4)	85(7)	-1(4)	-29(5)	-1(4)
C(16)	76(5)	37(4)	55(5)	-5(4)	-27(4)	-3(4)

The anisotropic displacement exponent takes the form:

$-2p^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(1A)	596	3629	71	80
H(2B)	1916	3807	4463	80
H(2C)	2034	2500	2253	80
H(2D)	833	2500	3386	80
H(5B)	1412	2500	-3564	80
H(6A)	-522	2262	-3249	80
H(7B)	-1698	2500	-592	80
H(8A)	-759	3125	-33	80
H(8B)	-872	2887	1982	80
H(9A)	2260	2889	-987	80
H(9B)	1196	3125	-1872	80
H(13A)	428	4353	-166	80
H(14A)	740	4984	1400	80
H(15A)	1674	5013	4526	80
H(16A)	2289	4410	6032	80

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STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{22}\ H_{24}\ Cl_2\ Cu\ N_4\ O_{12}$
Color; Habit	BLUE PRISM
Crystal size (mm)	0.30 X 0.16 X 0.18
Crystal System	Orthorhombic
Space Group	Pbca
Unit Cell Dimensions	$\underline{a}$ = 13.284(3) Å
	$\underline{b}$ = 14.864(2) Å
	$\underline{c}$ = 27.458(3) Å
Volume	5421.5(15) $Å^3$
Z	8
Formula weight	670.9
Density(calc.)	1.644 Mg/m^3
Absorption Coefficient	1.073 mm^{-1}
F(000)	2744

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
Cu(1)	2183(1)	3178(1)	3617(1)	32(1)
Cl(1)	2380(3)	2345(2)	4951(1)	51(1)
Cl(2)	1292(3)	8785(3)	2112(2)	58(2)
O(1)	3290(5)	4024(4)	3629(3)	33(3)
O(2)	3760(5)	7217(4)	3691(3)	37(3)
O(3)	2963(7)	2100(5)	5370(3)	79(4)
O(4)	1665(9)	2950(7)	5111(4)	122(6)
O(5)	2973(8)	2747(7)	4599(4)	94(5)
O(6)	1919(8)	1575(7)	4756(4)	100(5)
O(7)	2193(7)	8275(8)	2106(4)	99(5)
O(8)	1411(9)	9483(8)	2427(5)	162(8)
O(9)	532(7)	8246(9)	2266(5)	152(7)
O(10)	1054(10)	9097(11)	1670(4)	167(8)
N(1)	4585(6)	3045(5)	3559(3)	34(4)
N(2)	3113(6)	2304(6)	3295(3)	29(4)
N(3)	4951(6)	7864(5)	4159(3)	32(3)
N(4)	3746(6)	9004(5)	3986(3)	22(3)
C(1)	4937(8)	4603(6)	3786(4)	22(4)
C(2)	4371(7)	5517(6)	3796(4)	21(4)
C(3)	5111(8)	6266(7)	3945(4)	21(4)
C(4)	5983(7)	6332(6)	3574(4)	32(4)
C(5)	6542(8)	5421(6)	3572(5)	34(4)
C(6)	6939(8)	5190(8)	4073(5)	51(5)
C(7)	6095(8)	5159(8)	4438(5)	45(5)
C(8)	5375(9)	4407(7)	4288(4)	34(4)
C(9)	5808(7)	4677(7)	3410(4)	28(4)
C(10)	5531(9)	6062(7)	4456(4)	35(4)
C(11)	4203(8)	3861(7)	3654(4)	23(4)
C(12)	4122(9)	2331(8)	3337(4)	35(5)
C(13)	4730(9)	1635(7)	3151(4)	43(5)
C(14)	4287(10)	947(8)	2912(5)	54(6)
C(15)	3274(10)	939(8)	2832(4)	46(5)
C(16)	2709(9)	1627(7)	3024(4)	36(4)
C(17)	4549(8)	7154(7)	3928(4)	25(4)
C(18)	4644(7)	8773(7)	4167(3)	25(4)
C(19)	5290(8)	9371(7)	4382(4)	33(4)
C(20)	5015(9)	10275(7)	4398(4)	41(5)
C(21)	4072(9)	10503(7)	4227(4)	42(5)
C(22)	3476(8)	9871(6)	4029(4)	36(4)
W(1)	6668(5)	2512(5)	3719(3)	57(3)
W(2)	1503(5)	3625(5)	2898(3)	50(3)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 2. Bond lengths (Å)

Cu(1)-O(1)	1.934 (7)	Cu(1)-N(2)	1.998 (9)
Cu(1)-W(2)	2.270 (7)	Cu(1)-O(2A)	1.912 (7)
Cu(1)-N(4A)	2.015 (8)	Cl(1)-O(3)	1.434 (10)
Cl(1)-O(4)	1.379 (12)	Cl(1)-O(5)	1.383 (11)
Cl(1)-O(6)	1.404 (11)	Cl(2)-O(7)	1.417 (11)
Cl(2)-O(8)	1.359 (14)	Cl(2)-O(9)	1.356 (12)
Cl(2)-O(10)	1.338 (13)	O(1)-C(11)	1.239 (12)
O(2)-C(17)	1.238 (13)	O(2)-Cu(1A)	1.912 (7)
N(1)-C(11)	1.340 (13)	N(1)-C(12)	1.371 (14)
N(2)-C(12)	1.346 (15)	N(2)-C(16)	1.361 (14)
N(3)-C(17)	1.341 (13)	N(3)-C(18)	1.412 (12)
N(4)-C(18)	1.337 (12)	N(4)-C(22)	1.342 (12)
N(4)-Cu(1A)	2.015 (8)	C(1)-C(2)	1.553 (13)
C(1)-C(8)	1.524 (14)	C(1)-C(9)	1.554 (14)
C(1)-C(11)	1.516 (14)	C(2)-C(3)	1.540 (13)
C(3)-C(4)	1.547 (14)	C(3)-C(10)	1.540 (15)
C(3)-C(17)	1.518 (14)	C(4)-C(5)	1.544 (13)
C(5)-C(6)	1.512 (18)	C(5)-C(9)	1.540 (14)
C(6)-C(7)	1.505 (17)	C(7)-C(8)	1.528 (16)
C(7)-C(10)	1.539 (15)	C(12)-C(13)	1.408 (16)
C(13)-C(14)	1.351 (17)	C(14)-C(15)	1.364 (19)
C(15)-C(16)	1.374 (16)	C(18)-C(19)	1.370 (14)
C(19)-C(20)	1.393 (15)	C(20)-C(21)	1.380 (16)
C(21)-C(22)	1.343 (15)		

Table 3. Bond angles (°)

O(1)-Cu(1)-N(2)	87.8(3)	O(1)-Cu(1)-W(2)	97.3(3)
N(2)-Cu(1)-W(2)	92.9(3)	O(1)-Cu(1)-O(2A)	169.2(3)
N(2)-Cu(1)-O(2A)	88.0(3)	W(2)-Cu(1)-O(2A)	92.9(3)
O(1)-Cu(1)-N(4A)	93.5(3)	N(2)-Cu(1)-N(4A)	175.8(3)
W(2)-Cu(1)-N(4A)	90.9(3)	O(2A)-Cu(1)-N(4A)	90.0(3)
O(3)-Cl(1)-O(4)	106.4(6)	O(3)-Cl(1)-O(5)	111.3(6)
O(4)-Cl(1)-O(5)	109.4(7)	O(3)-Cl(1)-O(6)	109.5(6)
O(4)-Cl(1)-O(6)	110.7(7)	O(5)-Cl(1)-O(6)	109.5(6)
O(7)-Cl(2)-O(8)	108.5(7)	O(7)-Cl(2)-O(9)	108.5(7)
O(8)-Cl(2)-O(9)	109.9(8)	O(7)-Cl(2)-O(10)	112.0(7)
O(8)-Cl(2)-O(10)	109.8(9)	O(9)-Cl(2)-O(10)	108.1(9)
Cu(1)-O(1)-C(11)	128.2(6)	C(17)-O(2)-Cu(1A)	131.8(7)
C(11)-N(1)-C(12)	128.1(9)	Cu(1)-N(2)-C(12)	123.9(7)
Cu(1)-N(2)-C(16)	118.6(7)	C(12)-N(2)-C(16)	117.5(9)
C(17)-N(3)-C(18)	130.2(9)	C(18)-N(4)-C(22)	116.9(8)
C(18)-N(4)-Cu(1A)	125.2(6)	C(22)-N(4)-Cu(1A)	117.7(7)
C(2)-C(1)-C(8)	109.7(8)	C(2)-C(1)-C(9)	108.0(8)
C(8)-C(1)-C(9)	109.2(8)	C(2)-C(1)-C(11)	109.2(8)
C(8)-C(1)-C(11)	108.8(8)	C(9)-C(1)-C(11)	111.9(8)
C(1)-C(2)-C(3)	109.2(8)	C(2)-C(3)-C(4)	110.4(8)
C(2)-C(3)-C(10)	109.4(8)	C(4)-C(3)-C(10)	110.0(8)
C(2)-C(3)-C(17)	107.9(8)	C(4)-C(3)-C(17)	107.0(8)
C(10)-C(3)-C(17)	112.1(8)	C(3)-C(4)-C(5)	107.8(8)
C(4)-C(5)-C(6)	111.4(9)	C(4)-C(5)-C(9)	109.0(8)
C(6)-C(5)-C(9)	108.7(9)	C(5)-C(6)-C(7)	110.7(9)
C(6)-C(7)-C(8)	108.0(10)	C(6)-C(7)-C(10)	110.9(9)
C(8)-C(7)-C(10)	110.0(9)	C(1)-C(8)-C(7)	110.1(9)
C(1)-C(9)-C(5)	109.4(8)	C(3)-C(10)-C(7)	108.6(9)
O(1)-C(11)-N(1)	122.5(9)	O(1)-C(11)-C(1)	120.1(9)
N(1)-C(11)-C(1)	117.4(9)	N(1)-C(12)-N(2)	120.6(10)
N(1)-C(12)-C(13)	118.2(10)	N(2)-C(12)-C(13)	121.2(10)
C(12)-C(13)-C(14)	118.9(11)	C(13)-C(14)-C(15)	121.0(12)
C(14)-C(15)-C(16)	118.1(11)	N(2)-C(16)-C(15)	123.0(11)
O(2)-C(17)-N(3)	121.8(9)	O(2)-C(17)-C(3)	119.8(9)
N(3)-C(17)-C(3)	118.3(9)	N(3)-C(18)-N(4)	119.9(8)
N(3)-C(18)-C(19)	116.5(9)	N(4)-C(18)-C(19)	123.5(9)
C(18)-C(19)-C(20)	118.4(10)	C(19)-C(20)-C(21)	117.6(10)
C(20)-C(21)-C(22)	120.1(10)	N(4)-C(22)-C(21)	123.3(10)

Table 4. Anisotropic displacement coefficients ($Å^2 \times 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu(1)	26(1)	21(1)	49(1)	-3(1)	9(1)	-5(1)
Cl(1)	44(2)	55(2)	54(2)	-3(2)	-14(2)	-1(2)
Cl(2)	38(2)	78(3)	58(3)	-13(2)	-11(2)	9(2)
O(1)	19(4)	20(4)	61(6)	-1(4)	4(5)	-7(5)
O(2)	31(5)	18(4)	61(6)	9(4)	-25(5)	-15(4)
O(3)	67(7)	70(7)	99(8)	-18(6)	-57(6)	24(6)
O(4)	121(10)	125(11)	120(10)	83(9)	-3(8)	-29(8)
O(5)	84(8)	96(8)	102(9)	-30(7)	-4(7)	30(7)
O(6)	92(9)	110(9)	98(8)	-53(7)	-18(7)	-29(7)
O(7)	50(6)	136(9)	110(8)	16(8)	-2(7)	-22(8)
O(8)	125(12)	130(11)	232(16)	23(10)	-71(11)	-105(12)
O(9)	49(7)	145(11)	262(17)	-13(9)	26(9)	95(12)
O(10)	155(13)	276(18)	71(9)	-13(12)	-50(9)	61(11)
N(1)	21(5)	19(6)	62(7)	11(5)	0(6)	-2(6)
N(2)	19(6)	21(6)	47(7)	-9(5)	0(5)	-9(5)
N(3)	24(5)	20(6)	51(7)	5(5)	-8(5)	3(5)
N(4)	20(5)	26(5)	21(5)	-1(5)	1(5)	6(4)
C(1)	20(6)	12(6)	35(8)	-3(6)	3(6)	-1(5)
C(2)	19(6)	15(6)	30(7)	-7(5)	-1(6)	1(5)
C(3)	19(6)	15(6)	28(7)	-1(6)	-9(6)	6(6)
C(4)	28(7)	25(6)	44(8)	-6(6)	15(7)	1(7)
C(5)	21(6)	22(6)	58(9)	2(6)	23(7)	-3(7)
C(6)	27(8)	32(7)	95(12)	10(6)	-28(9)	-9(8)
C(7)	37(8)	37(8)	60(10)	8(7)	-24(8)	-9(7)
C(8)	56(9)	22(7)	25(7)	2(6)	-16(7)	-4(6)
C(9)	27(7)	19(6)	37(8)	0(6)	5(6)	4(6)
C(10)	41(8)	25(7)	39(8)	7(7)	-19(7)	4(6)
C(11)	26(7)	21(6)	23(7)	-5(6)	4(7)	-11(6)
C(12)	39(8)	21(7)	44(9)	-3(7)	13(7)	-1(7)
C(13)	47(8)	20(8)	61(10)	3(7)	4(7)	-12(7)
C(14)	60(10)	25(8)	76(11)	7(8)	8(10)	-11(8)
C(15)	46(9)	30(8)	64(10)	-12(7)	10(8)	-28(7)
C(16)	34(7)	25(7)	48(8)	3(7)	12(7)	-5(6)
C(17)	17(7)	17(6)	40(8)	-6(6)	3(6)	-2(6)
C(18)	26(6)	25(6)	23(6)	-3(6)	-8(5)	-2(6)
C(19)	26(7)	26(7)	47(8)	-3(6)	-6(6)	-10(6)
C(20)	41(8)	32(8)	48(8)	-11(7)	0(7)	-16(6)
C(21)	50(9)	24(7)	53(9)	0(7)	-13(8)	7(7)
C(22)	33(7)	21(6)	55(9)	4(6)	-16(7)	-10(6)
W(1)	36(4)	57(5)	78(7)	23(5)	-6(5)	-2(5)
W(2)	33(5)	63(6)	56(5)	5(5)	-1(4)	10(5)

The anisotropic displacement exponent takes the form:

$-2p^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

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Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(1A)	5224	2955	3657	80
H(3B)	5495	7735	4341	80
H(2A)	3829	5486	4026	80
H(2B)	4094	5647	3480	80
H(4C)	6439	6803	3667	80
H(4D)	5724	6462	3255	80
H(5B)	7091	5442	3345	80
H(6B)	7410	5645	4170	80
H(6C)	7284	4622	4067	80
H(7B)	6357	5034	4757	80
H(8B)	5731	3846	4282	80
H(8C)	4834	4358	4518	80
H(9A)	5536	4816	3095	80
H(9B)	6156	4112	3389	80
H(10A)	5000	6052	4693	80
H(10B)	5997	6529	4544	80
H(13A)	5446	1647	3196	80
H(14A)	4690	453	2798	80
H(15A)	2967	463	2648	80
H(16A)	1997	1638	2963	80
H(19A)	5914	9170	4521	80
H(20A)	5458	10728	4525	80
H(21A)	3843	11114	4246	80
H(22A)	2828	10053	3910	80

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STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{27}\ H_{32}\ N_4\ O_6$
Color; Habit	COLORLESS, IRREGULAR FRAGMENT WITH FISSU
Crystal size (mm)	0.45 X 0.60 X 0.17
Crystal System	Triclinic
Space Group	$P\bar{1}$
Unit Cell Dimensions	a = 10.8300(10) Å
	b = 10.9230(10) Å
	c = 11.2230(10) Å
	a = 76.170(10)°
	b = 81.320(10)°
	c = 85.110(10)°
Volume	1272.7(2) $Å^3$
Z	2
Formula weight	508.6
Density(calc.)	1.327 Mg/m^3
Absorption Coefficient	0.780 mm^{-1}
F(000)	540

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
O(1)	4293(7)	-136(5)	8480(6)	148(4)
O(2)	1614(6)	5237(5)	6814(5)	110(3)
O(3)	2943(6)	2889(6)	3994(5)	116(3)
O(4)	1348(6)	2814(5)	5432(6)	103(3)
O(5)	2138(5)	6224(4)	894(4)	76(2)
O(6)	1124(5)	8052(4)	933(4)	77(2)
N(1)	3214(5)	833(4)	6986(4)	49(2)
N(2)	3265(5)	408(5)	5075(4)	55(2)
N(3)	1554(5)	6240(4)	8371(4)	50(2)
N(4)	870(5)	8241(4)	8554(4)	51(2)
C(1)	3432(5)	1881(5)	8649(5)	47(2)
C(2)	2717(6)	3038(5)	7916(5)	51(2)
C(3)	2535(5)	4105(5)	8617(5)	42(2)
C(4)	1776(5)	3632(5)	9887(6)	51(2)
C(5)	2499(6)	2508(5)	10613(5)	57(2)
C(6)	3758(7)	2920(6)	10765(6)	65(3)
C(7)	4511(6)	3356(6)	9505(6)	56(3)
C(8)	4697(6)	2301(6)	8808(5)	56(2)
C(9)	2671(6)	1440(6)	9932(6)	62(3)
C(10)	3802(5)	4501(5)	8765(5)	50(2)
C(11)	3668(7)	774(6)	8052(6)	64(3)
C(12)	3412(5)	-65(5)	6265(5)	46(2)
C(13)	3714(6)	-1340(5)	6722(6)	54(2)
C(14)	3896(6)	-2116(6)	5919(7)	64(3)
C(15)	3755(7)	-1642(7)	4685(7)	67(3)
C(16)	3425(6)	-393(7)	4316(6)	64(3)
C(17)	1840(6)	5246(6)	7834(6)	57(3)
C(18)	948(5)	7397(5)	7857(5)	48(2)
C(19)	475(6)	7652(6)	6738(5)	55(2)
C(20)	-106(7)	8830(6)	6354(6)	68(3)
C(21)	-165(7)	9707(6)	7044(6)	68(3)
C(22)	327(6)	9392(6)	8135(6)	61(3)
C(23)	2004(10)	3358(9)	4458(8)	96(4)
C(24)	1504(8)	4657(8)	3740(8)	98(4)
C(25)	2362(8)	5631(7)	3492(7)	87(4)
C(26)	1755(7)	6906(6)	2793(6)	72(3)
C(27)	1695(6)	6994(5)	1457(6)	54(2)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

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Table 2. Bond lengths (Å)

O(1)-C(11)	1.197 (9)	O(2)-C(17)	1.210 (9)
O(3)-C(23)	1.202 (11)	O(4)-C(23)	1.257 (10)
O(5)-C(27)	1.196 (8)	O(6)-C(27)	1.314 (7)
N(1)-C(11)	1.346 (9)	N(1)-C(12)	1.398 (8)
N(2)-C(12)	1.340 (7)	N(2)-C(16)	1.344 (9)
N(3)-C(17)	1.355 (8)	N(3)-C(18)	1.409 (7)
N(4)-C(18)	1.334 (8)	N(4)-C(22)	1.350 (7)
C(1)-C(2)	1.550 (8)	C(1)-C(8)	1.529 (9)
C(1)-C(9)	1.537 (8)	C(1)-C(11)	1.503 (10)
C(2)-C(3)	1.539 (9)	C(3)-C(4)	1.530 (7)
C(3)-C(10)	1.517 (9)	C(3)-C(17)	1.551 (8)
C(4)-C(5)	1.528 (8)	C(5)-C(6)	1.518 (11)
C(5)-C(9)	1.525 (10)	C(6)-C(7)	1.513 (8)
C(7)-C(8)	1.524 (10)	C(7)-C(10)	1.541 (8)
C(12)-C(13)	1.393 (8)	C(13)-C(14)	1.361 (10)
C(14)-C(15)	1.384 (10)	C(15)-C(16)	1.361 (10)
C(18)-C(19)	1.386 (9)	C(19)-C(20)	1.384 (9)
C(20)-C(21)	1.361 (10)	C(21)-C(22)	1.366 (10)
C(23)-C(24)	1.552 (12)	C(24)-C(25)	1.423 (12)
C(25)-C(26)	1.570 (10)	C(26)-C(27)	1.491 (10)

Table 3. Bond angles (^{o})

C(11)-N(1)-C(12)	127.0(5)	C(12)-N(2)-C(16)	117.7(5)
C(17)-N(3)-C(18)	126.4(5)	C(18)-N(4)-C(22)	118.4(5)
C(2)-C(1)-C(8)	108.1(5)	C(2)-C(1)-C(9)	108.3(5)
C(8)-C(1)-C(9)	109.1(5)	C(2)-C(1)-C(11)	115.1(5)
C(8)-C(1)-C(11)	108.0(5)	C(9)-C(1)-C(11)	108.1(5)
C(1)-C(2)-C(3)	110.2(5)	C(2)-C(3)-C(4)	109.0(4)
C(2)-C(3)-C(10)	109.4(5)	C(4)-C(3)-C(10)	110.3(5)
C(2)-C(3)-C(17)	108.1(5)	C(4)-C(3)-C(17)	111.1(4)
C(10)-C(3)-C(17)	108.9(5)	C(3)-C(4)-C(5)	108.8(5)
C(4)-C(5)-C(6)	109.3(5)	C(4)-C(5)-C(9)	109.7(5)
C(6)-C(5)-C(9)	110.5(5)	C(5)-C(6)-C(7)	109.6(6)
C(6)-C(7)-C(8)	110.6(5)	C(6)-C(7)-C(10)	108.6(5)
C(8)-C(7)-C(10)	109.6(5)	C(1)-C(8)-C(7)	110.3(5)
C(1)-C(9)-C(5)	109.9(5)	C(3)-C(10)-C(7)	109.0(5)
O(1)-C(11)-N(1)	119.5(7)	O(1)-C(11)-C(1)	121.2(7)
N(1)-C(11)-C(1)	119.2(5)	N(1)-C(12)-N(2)	113.7(5)
N(1)-C(12)-C(13)	124.2(5)	N(2)-C(12)-C(13)	122.2(6)
C(12)-C(13)-C(14)	118.4(6)	C(13)-C(14)-C(15)	120.1(6)
C(14)-C(15)-C(16)	117.9(7)	N(2)-C(16)-C(15)	123.6(6)
O(2)-C(17)-N(3)	124.0(6)	O(2)-C(17)-C(3)	121.3(6)
N(3)-C(17)-C(3)	114.7(5)	N(3)-C(18)-N(4)	113.4(5)
N(3)-C(18)-C(19)	124.1(6)	N(4)-C(18)-C(19)	122.5(5)
C(18)-C(19)-C(20)	117.6(6)	C(19)-C(20)-C(21)	120.3(6)
C(20)-C(21)-C(22)	118.9(6)	N(4)-C(22)-C(21)	122.3(6)
O(3)-C(23)-O(4)	123.9(8)	O(3)-C(23)-C(24)	117.8(7)
O(4)-C(23)-C(24)	118.0(8)	C(23)-C(24)-C(25)	114.2(8)
C(24)-C(25)-C(26)	110.0(7)	C(25)-C(26)-C(27)	114.7(6)
O(5)-C(27)-O(6)	122.6(6)	O(5)-C(27)-C(26)	125.2(6)
O(6)-C(27)-C(26)	112.1(6)		

Table 4. Anisotropic displacement coefficients ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	267(8)	89(4)	127(5)	116(5)	-143(6)	-76(4)
O(2)	191(6)	77(4)	82(4)	74(4)	-83(4)	-46(3)
O(3)	111(5)	106(5)	91(4)	47(4)	15(4)	22(3)
O(4)	119(5)	95(4)	92(4)	14(4)	-28(4)	-15(3)
O(5)	104(4)	61(3)	73(3)	35(3)	-33(3)	-35(3)
O(6)	121(4)	52(3)	60(3)	28(3)	-24(3)	-19(2)
N(1)	68(3)	38(3)	44(3)	15(2)	-14(2)	-17(2)
N(2)	67(4)	57(3)	45(3)	11(3)	-13(3)	-20(3)
N(3)	65(3)	39(3)	47(3)	16(2)	-17(2)	-16(2)
N(4)	64(3)	37(3)	50(3)	8(2)	-5(3)	-12(2)
C(1)	57(4)	46(3)	42(3)	19(3)	-19(3)	-20(3)
C(2)	64(4)	44(3)	53(4)	21(3)	-27(3)	-23(3)
C(3)	49(4)	38(3)	42(3)	12(3)	-14(3)	-16(3)
C(4)	46(4)	42(3)	65(4)	9(3)	-5(3)	-18(3)
C(5)	78(5)	46(4)	41(3)	11(3)	4(3)	-8(3)
C(6)	90(5)	64(4)	50(4)	33(4)	-38(4)	-26(3)
C(7)	46(4)	61(4)	70(4)	13(3)	-23(3)	-31(3)
C(8)	58(4)	61(4)	52(4)	23(3)	-16(3)	-22(3)
C(9)	75(5)	45(4)	63(4)	8(3)	-7(4)	-10(3)
C(10)	47(4)	46(3)	59(4)	-1(3)	-8(3)	-15(3)
C(11)	85(5)	57(4)	62(4)	31(4)	-35(4)	-31(3)
C(12)	45(4)	45(4)	50(4)	0(3)	-4(3)	-20(3)
C(13)	66(4)	40(4)	57(4)	6(3)	-10(3)	-13(3)
C(14)	70(5)	44(4)	82(5)	2(3)	-2(4)	-27(4)
C(15)	73(5)	68(5)	72(5)	-6(4)	0(4)	-42(4)
C(16)	72(5)	76(5)	51(4)	4(4)	-12(3)	-25(4)
C(17)	75(5)	50(4)	54(4)	22(3)	-25(3)	-23(3)
C(18)	53(4)	40(3)	48(4)	9(3)	-4(3)	-9(3)
C(19)	69(4)	50(4)	47(4)	9(3)	-15(3)	-11(3)
C(20)	95(6)	51(4)	49(4)	14(4)	-18(4)	4(3)
C(21)	88(5)	40(4)	64(5)	16(3)	-4(4)	0(3)
C(22)	75(5)	41(4)	61(4)	4(3)	-2(4)	-11(3)
C(23)	114(8)	108(7)	49(5)	13(6)	-6(5)	9(5)
C(24)	93(6)	87(6)	100(7)	11(5)	-16(5)	5(5)
C(25)	108(7)	74(5)	78(5)	4(5)	-23(5)	-12(4)
C(26)	100(6)	52(4)	66(4)	14(4)	-21(4)	-15(3)
C(27)	64(4)	40(4)	61(4)	7(3)	-19(3)	-16(3)

The anisotropic displacement exponent takes the form:

$-2p^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

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Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(24A)	766	4909	4232	80
H(24B)	1265	4572	2975	80
H(25A)	3093	5408	2972	80
H(25B)	2616	5724	4248	80
H(26A)	2215	7591	2869	80
H(26B)	919	7002	3200	80
H(60)	1119	8168	-45	50
H(1N)	2736	1607	6709	50
H(3N)	1504	6219	9225	128
H(2A)	1885	2702	7811	55
H(2B)	3214	3304	6952	101
H(4A)	1603	4330	10414	56
H(4B)	909	3539	9789	49
H(5)	1991	2248	11321	62
H(6A)	4232	2419	11187	54
H(6B)	3644	3692	11168	52
H(7)	5294	3651	9540	89
H(8A)	5035	1601	9282	56
H(8B)	5141	2641	7960	94
H(9A)	3116	897	10400	67
H(9B)	1867	1085	9927	70
H(10A)	3800	5287	9130	58
H(10B)	4419	4855	8046	61
H(13)	3944	-1743	7505	63
H(14)	4275	-2901	6170	89
H(15)	3851	-2103	4020	58
H(16)	3547	110	3358	97
H(19)	502	7045	6151	54
H(20)	-363	8972	5531	74
H(21)	-471	10496	6925	65
H(22)	417	10153	8584	91

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STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{29}\ H_{36}\ N_4\ O_6$
Color; Habit	COLORLESS PLATE
Crystal size (mm)	0.40 X 0.25 X 0.22
Crystal System	Triclinic
Space Group	$P\bar{1}$
Unit Cell Dimensions	a = 11.2630(10) Å
	b = 11.720(2) Å
	c = 12.4110(10) Å
	a = 81.080(10)°
	b = 67.400(10)°
	c = 66.550(10)°
Volume	1387.4(3) $Å^3$
Z	2
Formula weight	536.6
Density(calc.)	1.284 Mg/m^3
Absorption Coefficient	0.742 mm^{-1}
F(000)	572

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Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
O(1)	14295(8)	-2768(7)	1431(10)	131(7)
O(2)	9809(9)	2654(6)	1909(8)	107(6)
O(3)	8873(8)	-544(6)	867(6)	83(5)
O(4)	8989(7)	-282(6)	2563(6)	77(4)
O(5)	2210(7)	3992(6)	3898(6)	72(4)
O(6)	1319(7)	6031(5)	3889(6)	70(4)
N(1)	12102(8)	-2040(7)	1563(8)	59(5)
N(2)	10942(9)	-2780(7)	879(7)	62(5)
N(3)	10213(8)	3745(6)	2950(7)	58(4)
N(4)	9358(8)	5861(7)	3310(7)	55(4)
C(1)	12931(10)	-756(8)	2282(9)	49(5)
C(2)	11804(10)	398(7)	2054(9)	56(6)
C(3)	11626(8)	1551(8)	2675(9)	44(5)
C(4)	12991(10)	1745(9)	2189(12)	84(7)
C(5)	14119(11)	571(10)	2450(15)	99(9)
C(6)	13680(19)	316(12)	3756(17)	124(13)
C(7)	12374(16)	134(11)	4159(12)	102(9)
C(8)	12538(13)	-994(9)	3592(10)	86(7)
C(9)	14277(11)	-549(9)	1832(12)	88(8)
C(10)	11240(11)	1275(8)	3996(9)	70(6)
C(11)	13179(12)	-1921(9)	1726(10)	67(6)
C(12)	12062(11)	-3040(8)	1124(8)	48(5)
C(13)	13112(11)	-4225(9)	940(10)	69(6)
C(14)	12949(14)	-5131(11)	498(10)	80(8)
C(15)	11786(15)	-4901(11)	267(10)	81(8)
C(16)	10845(13)	-3710(12)	438(10)	75(8)
C(17)	10494(11)	2684(9)	2441(11)	68(7)
C(18)	9190(9)	4958(9)	2944(9)	52(5)
C(19)	8086(11)	5153(10)	2573(10)	77(7)
C(20)	7154(11)	6333(10)	2615(10)	73(7)
C(21)	7352(10)	7269(9)	2949(9)	63(6)
C(22)	8462(11)	7000(9)	3274(9)	63(6)
C(23)	8529(10)	111(9)	1752(9)	65(6)
C(24)	7495(10)	1390(10)	1777(10)	76(7)
C(25)	6647(10)	2004(9)	2931(10)	73(6)
C(26)	5545(10)	3300(9)	2894(10)	68(6)
C(27)	4681(10)	3862(9)	4092(9)	70(7)
C(28)	3487(10)	5096(9)	4108(10)	67(6)
C(29)	2273(10)	4999(7)	3969(8)	54(5)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

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Table 2. Bond lengths (Å)

O(1)-C(11)	1.210 (11)	O(2)-C(17)	1.205 (20)
O(3)-C(23)	1.282 (14)	O(4)-C(23)	1.249 (15)
O(5)-C(29)	1.228 (13)	O(6)-C(29)	1.280 (10)
N(1)-C(11)	1.365 (19)	N(1)-C(12)	1.389 (15)
N(2)-C(12)	1.318 (17)	N(2)-C(16)	1.351 (20)
N(3)-C(17)	1.350 (15)	N(3)-C(18)	1.432 (10)
N(4)-C(18)	1.318 (16)	N(4)-C(22)	1.321 (11)
C(1)-C(2)	1.520 (12)	C(1)-C(8)	1.525 (16)
C(1)-C(9)	1.506 (17)	C(1)-C(11)	1.503 (16)
C(2)-C(3)	1.565 (15)	C(3)-C(4)	1.518 (15)
C(3)-C(10)	1.543 (15)	C(3)-C(17)	1.514 (13)
C(4)-C(5)	1.549 (15)	C(5)-C(6)	1.520 (26)
C(5)-C(9)	1.537 (21)	C(6)-C(7)	1.453 (27)
C(7)-C(8)	1.507 (20)	C(7)-C(10)	1.489 (16)
C(12)-C(13)	1.401 (12)	C(13)-C(14)	1.370 (21)
C(14)-C(15)	1.362 (24)	C(15)-C(16)	1.363 (16)
C(18)-C(19)	1.412 (19)	C(19)-C(20)	1.357 (13)
C(20)-C(21)	1.354 (20)	C(21)-C(22)	1.364 (19)
C(23)-C(24)	1.483 (12)	C(24)-C(25)	1.484 (15)
C(25)-C(26)	1.539 (12)	C(26)-C(27)	1.507 (14)
C(27)-C(28)	1.530 (12)	C(28)-C(29)	1.492 (18)

Table 3. Bond angles (°)

C(11)-N(1)-C(12)	129.3(8)	C(12)-N(2)-C(16)	117.1(8)
C(17)-N(3)-C(18)	129.8(11)	C(18)-N(4)-C(22)	116.8(11)
C(2)-C(1)-C(8)	109.3(7)	C(2)-C(1)-C(9)	109.5(8)
C(8)-C(1)-C(9)	108.5(12)	C(2)-C(1)-C(11)	114.4(11)
C(8)-C(1)-C(11)	107.1(8)	C(9)-C(1)-C(11)	107.8(8)
C(1)-C(2)-C(3)	110.2(10)	C(2)-C(3)-C(4)	108.3(7)
C(2)-C(3)-C(10)	108.2(8)	C(4)-C(3)-C(10)	110.3(11)
C(2)-C(3)-C(17)	109.2(10)	C(4)-C(3)-C(17)	110.3(8)
C(10)-C(3)-C(17)	110.6(7)	C(3)-C(4)-C(5)	108.7(9)
C(4)-C(5)-C(6)	109.8(10)	C(4)-C(5)-C(9)	108.8(14)
C(6)-C(5)-C(9)	108.4(11)	C(5)-C(6)-C(7)	109.4(18)
C(6)-C(7)-C(8)	110.6(11)	C(6)-C(7)-C(10)	111.6(11)
C(8)-C(7)-C(10)	112.6(15)	C(1)-C(8)-C(7)	108.1(9)
C(1)-C(9)-C(5)	110.1(8)	C(3)-C(10)-C(7)	107.7(8)
O(1)-C(11)-N(1)	118.6(12)	O(1)-C(11)-C(1)	122.5(14)
N(1)-C(11)-C(1)	118.9(8)	N(1)-C(12)-N(2)	114.1(8)
N(1)-C(12)-C(13)	123.9(12)	N(2)-C(12)-C(13)	122.0(12)
C(12)-C(13)-C(14)	118.1(12)	C(13)-C(14)-C(15)	121.2(10)
C(14)-C(15)-C(16)	116.2(15)	N(2)-C(16)-C(15)	125.3(15)
O(2)-C(17)-N(3)	120.8(9)	O(2)-C(17)-C(3)	123.7(11)
N(3)-C(17)-C(3)	115.3(12)	N(3)-C(18)-N(4)	115.2(10)
N(3)-C(18)-C(19)	121.6(11)	N(4)-C(18)-C(19)	123.2(8)
C(18)-C(19)-C(20)	117.4(13)	C(19)-C(20)-C(21)	119.5(13)
C(20)-C(21)-C(22)	119.2(9)	N(4)-C(22)-C(21)	123.8(12)
O(3)-C(23)-O(4)	123.8(8)	O(3)-C(23)-C(24)	115.3(10)
O(4)-C(23)-C(24)	120.9(10)	C(23)-C(24)-C(25)	117.5(10)
C(24)-C(25)-C(26)	114.5(10)	C(25)-C(26)-C(27)	112.3(9)
C(26)-C(27)-C(28)	114.0(9)	C(27)-C(28)-C(29)	115.6(10)
O(5)-C(29)-O(6)	121.9(11)	O(5)-C(29)-C(28)	122.2(8)
O(6)-C(29)-C(28)	115.9(9)		

Table 4. Anisotropic displacement coefficients ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	63(6)	72(6)	246(13)	13(5)	-53(7)	-80(7)
O(2)	130(8)	56(5)	160(9)	8(5)	-109(7)	-29(5)
O(3)	95(6)	73(5)	71(6)	-20(4)	-24(5)	-17(4)
O(4)	71(5)	54(4)	87(6)	-8(4)	-26(4)	2(4)
O(5)	66(5)	61(4)	91(6)	-14(4)	-39(4)	-3(4)
O(6)	65(5)	40(4)	102(6)	-5(3)	-37(4)	-10(4)
N(1)	58(6)	38(5)	85(7)	-22(4)	-22(5)	-8(4)
N(2)	71(7)	54(5)	62(7)	-24(5)	-24(5)	-5(4)
N(3)	53(5)	33(4)	87(7)	2(4)	-42(5)	-2(4)
N(4)	59(6)	29(4)	67(6)	-2(4)	-22(5)	-16(4)
C(1)	56(7)	33(5)	63(8)	-15(5)	-29(6)	3(5)
C(2)	64(7)	39(6)	71(8)	-13(5)	-36(6)	-1(5)
C(3)	26(5)	44(6)	59(8)	-10(4)	-9(5)	-14(5)
C(4)	48(7)	46(6)	137(12)	-22(6)	2(7)	-24(7)
C(5)	25(6)	63(8)	199(17)	-20(6)	-22(9)	-15(10)
C(6)	144(16)	58(9)	174(19)	21(10)	-111(16)	-29(10)
C(7)	132(13)	61(8)	68(10)	11(9)	-40(10)	8(7)
C(8)	111(10)	38(6)	81(10)	-3(6)	-30(8)	-6(6)
C(9)	63(8)	43(6)	158(14)	-17(6)	-35(8)	-17(7)
C(10)	81(8)	38(6)	60(8)	0(6)	-17(7)	-4(5)
C(11)	54(7)	42(6)	97(10)	-16(6)	-17(7)	-15(6)
C(12)	60(7)	35(5)	39(6)	-16(5)	-11(6)	6(5)
C(13)	58(7)	50(6)	96(10)	-11(6)	-24(7)	-21(6)
C(14)	91(10)	69(8)	75(9)	-41(7)	-4(8)	-25(7)
C(15)	117(11)	71(9)	60(9)	-58(9)	-8(8)	-12(7)
C(16)	92(10)	91(9)	62(9)	-53(8)	-30(7)	7(7)
C(17)	72(8)	52(7)	98(10)	-15(6)	-52(8)	-15(6)
C(18)	36(6)	37(5)	61(7)	3(5)	-19(5)	12(5)
C(19)	57(7)	62(7)	115(11)	-15(6)	-50(8)	15(7)
C(20)	60(8)	54(7)	98(10)	-4(6)	-38(7)	0(7)
C(21)	47(7)	44(6)	74(9)	4(5)	-16(6)	-4(6)
C(22)	64(7)	48(7)	69(8)	-14(6)	-24(6)	6(5)
C(23)	48(6)	58(6)	72(8)	-19(5)	-12(6)	24(5)
C(24)	49(7)	85(8)	89(10)	-28(6)	-19(7)	5(7)
C(25)	50(7)	60(7)	102(10)	-15(6)	-30(7)	13(7)
C(26)	48(6)	64(7)	87(9)	-18(5)	-18(6)	-11(6)
C(27)	69(8)	78(7)	69(9)	-22(6)	-35(7)	-3(6)
C(28)	69(8)	61(7)	73(8)	-18(6)	-28(6)	-17(6)
C(29)	61(7)	38(5)	52(7)	-8(5)	-14(5)	-17(5)

The anisotropic displacement exponent takes the form:

$-2p^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

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Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(2B)	10950	261	2315	80
H(2C)	12070	565	1230	80
H(4B)	12902	2495	2486	80
H(4C)	13263	1808	1355	80
H(5A)	14978	690	2226	80
H(6A)	13555	1014	4159	80
H(6B)	14349	-409	3958	80
H(7A)	12077	-33	4983	80
H(8A)	13242	-1721	3749	80
H(8B)	11694	-1149	3869	80
H(9A)	14481	-320	1023	80
H(9B)	15018	-1295	1903	80
H(10A)	10376	1154	4284	80
H(10B)	11118	1979	4388	80
H(13A)	13897	-4396	1159	80
H(14A)	13686	-5931	317	80
H(15A)	11635	-5547	10	80
H(16A)	10060	-3511	211	80
H(19A)	7994	4468	2321	80
H(20A)	6358	6489	2418	80
H(21A)	6728	8110	2923	80
H(22A)	8620	7673	3474	80
H(24A)	6866	1402	1425	80
H(24B)	7996	1899	1308	80
H(25A)	7253	2086	3261	80
H(25B)	6197	1472	3430	80
H(26A)	4949	3227	2549	80
H(26B)	5991	3847	2419	80
H(27A)	5272	3972	4422	80
H(27B)	4277	3292	4576	80
H(28A)	3864	5556	3447	80
H(28B)	3181	5567	4797	80
H(3N)	10818(73)	3702(62)	3140(66)	44(24)
H(4N)	10519(71)	5719(62)	3676(63)	54(24)
H(2N)	9982(115)	-1987(99)	827(103)	185(48)
H(1N)	11387(83)	-1571(72)	1803(75)	81(29)

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STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{32}\ H_{42}\ N_4\ O_6$
Color; Habit	COLORLESS THIN PLATE WITH INCLUSIONS
Crystal size (mm)	0.65 X 0.28 X 0.10
Crystal System	Monoclinic
Space Group	$P2_1/c$
Unit Cell Dimensions	$\underline{a}$ = 11.5110(10) Å
	$\underline{b}$ = 16.611(2) Å
	$\underline{c}$ = 16.919(2) Å
	b = 104.930(10)°
Volume	3125.9(6) $Å^3$
Z	4
Formula weight	578.7
Density(calc.)	1.230 Mg/m^3
Absorption Coefficient	0.694 mm^{-1}
F(000)	1240

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Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
O(1)	3317(6)	-605(3)	3811(3)	109(3)
O(2)	4618(5)	1660(3)	1505(3)	85(2)
O(3)	1020(5)	2699(4)	3484(3)	96(3)
O(4)	1509(5)	1989(3)	2530(3)	107(3)
O(5)	-2482(6)	5114(3)	-3980(3)	134(3)
O(6)	-2978(5)	5714(4)	-2964(3)	112(3)
N(1)	2617(5)	662(4)	3663(3)	71(3)
N(2)	2273(6)	1629(4)	4557(4)	74(3)
N(3)	3960(5)	1282(3)	174(3)	60(3)
N(4)	4108(5)	1834(4)	-1025(4)	59(3)
C(1)	2698(7)	-96(4)	2443(4)	57(3)
C(2)	3441(6)	561(4)	2155(4)	55(3)
C(3)	3257(6)	527(4)	1227(4)	47(3)
C(4)	3645(6)	-307(4)	982(4)	63(3)
C(5)	2903(7)	-949(4)	1252(5)	72(4)
C(6)	1568(7)	-822(4)	837(4)	74(4)
C(7)	1175(6)	-4(4)	1084(4)	59(3)
C(8)	1356(6)	40(4)	2001(4)	64(3)
C(9)	3079(7)	-920(4)	2189(4)	71(3)
C(10)	1917(6)	651(4)	807(4)	52(3)
C(11)	2903(7)	-52(5)	3360(5)	70(4)
C(12)	2765(7)	913(6)	4481(4)	67(4)
C(13)	3396(8)	470(5)	5140(5)	98(4)
C(14)	3492(10)	790(8)	5905(6)	120(6)
C(15)	3006(10)	1515(7)	5992(6)	110(6)
C(16)	2407(8)	1904(6)	5310(6)	93(4)
C(17)	4027(6)	1200(4)	994(4)	59(3)
C(18)	4472(6)	1875(4)	-213(4)	56(3)
C(19)	5235(6)	2471(4)	194(4)	64(3)
C(20)	5622(7)	3038(5)	-267(5)	72(4)
C(21)	5243(7)	3023(5)	-1101(5)	70(4)
C(22)	4512(7)	2400(5)	-1452(4)	69(3)
C(23)	985(7)	2557(4)	2722(5)	81(4)
C(24)	251(8)	3123(5)	2117(5)	97(4)
C(25)	-225(8)	2797(5)	1260(5)	95(4)
C(26)	-664(8)	3443(5)	602(6)	107(5)
C(27)	-1048(8)	3119(5)	-240(5)	112(5)
C(28)	-1444(9)	3756(6)	-900(5)	137(6)
C(29)	-1795(9)	3408(6)	-1714(6)	188(8)
C(30)	-2494(7)	3944(5)	-2383(5)	175(8)
C(31)	-1787(6)	4572(5)	-2640(6)	164(7)
C(32)	-2488(7)	5138(4)	-3278(4)	103(4)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

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Table 2. Bond lengths (Å)

O(1)-C(11)	1.211 (10)	O(2)-C(17)	1.221 (8)
O(3)-C(23)	1.300 (10)	O(4)-C(23)	1.207 (10)
O(5)-C(32)	1.189 (10)	O(6)-C(32)	1.293 (10)
N(1)-C(11)	1.366 (11)	N(1)-C(12)	1.414 (9)
N(2)-C(12)	1.338 (12)	N(2)-C(16)	1.324 (12)
N(3)-C(17)	1.375 (9)	N(3)-C(18)	1.395 (10)
N(4)-C(18)	1.332 (9)	N(4)-C(22)	1.340 (11)
C(1)-C(2)	1.541 (10)	C(1)-C(8)	1.549 (9)
C(1)-C(9)	1.532 (10)	C(1)-C(11)	1.509 (11)
C(2)-C(3)	1.529 (9)	C(3)-C(4)	1.544 (9)
C(3)-C(10)	1.537 (9)	C(3)-C(17)	1.541 (10)
C(4)-C(5)	1.510 (11)	C(5)-C(6)	1.531 (10)
C(5)-C(9)	1.545 (11)	C(6)-C(7)	1.523 (10)
C(7)-C(8)	1.514 (10)	C(7)-C(10)	1.530 (10)
C(12)-C(13)	1.376 (11)	C(13)-C(14)	1.377 (14)
C(14)-C(15)	1.352 (18)	C(15)-C(16)	1.347 (13)
C(18)-C(19)	1.384 (10)	C(19)-C(20)	1.367 (12)
C(20)-C(21)	1.365 (12)	C(21)-C(22)	1.369 (11)
C(23)-C(24)	1.484 (10)	C(24)-C(25)	1.511 (11)
C(25)-C(26)	1.536 (11)	C(26)-C(27)	1.479 (13)
C(27)-C(28)	1.521 (12)	C(28)-C(29)	1.451 (12)
C(29)-C(30)	1.501 (12)	C(30)-C(31)	1.457 (12)
C(31)-C(32)	1.502 (11)		

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Table 3. Bond angles (^{o})

C(11)-N(1)-C(12)	130.1(6)	C(12)-N(2)-C(16)	116.8(7)
C(17)-N(3)-C(18)	128.4(6)	C(18)-N(4)-C(22)	117.3(6)
C(2)-C(1)-C(8)	108.1(5)	C(2)-C(1)-C(9)	108.7(6)
C(8)-C(1)-C(9)	108.4(5)	C(2)-C(1)-C(11)	109.8(6)
C(8)-C(1)-C(11)	111.2(7)	C(9)-C(1)-C(11)	110.5(6)
C(1)-C(2)-C(3)	110.9(5)	C(2)-C(3)-C(4)	109.6(5)
C(2)-C(3)-C(10)	109.1(6)	C(4)-C(3)-C(10)	108.8(5)
C(2)-C(3)-C(17)	107.4(5)	C(4)-C(3)-C(17)	110.9(6)
C(10)-C(3)-C(17)	111.0(5)	C(3)-C(4)-C(5)	109.1(6)
C(4)-C(5)-C(6)	110.1(6)	C(4)-C(5)-C(9)	110.7(6)
C(6)-C(5)-C(9)	108.5(7)	C(5)-C(6)-C(7)	109.3(5)
C(6)-C(7)-C(8)	110.6(5)	C(6)-C(7)-C(10)	108.8(6)
C(8)-C(7)-C(10)	109.8(5)	C(1)-C(8)-C(7)	110.1(6)
C(1)-C(9)-C(5)	110.1(5)	C(3)-C(10)-C(7)	109.6(5)
O(1)-C(11)-N(1)	121.1(7)	O(1)-C(11)-C(1)	122.9(7)
N(1)-C(11)-C(1)	116.0(6)	N(1)-C(12)-N(2)	114.1(6)
N(1)-C(12)-C(13)	122.8(8)	N(2)-C(12)-C(13)	123.1(7)
C(12)-C(13)-C(14)	116.9(9)	C(13)-C(14)-C(15)	120.7(9)
C(14)-C(15)-C(16)	117.9(10)	N(2)-C(16)-C(15)	124.5(9)
O(2)-C(17)-N(3)	122.0(7)	O(2)-C(17)-C(3)	121.7(7)
N(3)-C(17)-C(3)	116.3(6)	N(3)-C(18)-N(4)	113.0(6)
N(3)-C(18)-C(19)	124.3(6)	N(4)-C(18)-C(19)	122.7(7)
C(18)-C(19)-C(20)	117.9(7)	C(19)-C(20)-C(21)	120.8(7)
C(20)-C(21)-C(22)	117.3(8)	N(4)-C(22)-C(21)	123.8(7)
O(3)-C(23)-O(4)	121.2(7)	O(3)-C(23)-C(24)	115.8(7)
O(4)-C(23)-C(24)	123.0(7)	C(23)-C(24)-C(25)	115.8(7)
C(24)-C(25)-C(26)	114.5(7)	C(25)-C(26)-C(27)	113.9(7)
C(26)-C(27)-C(28)	114.4(7)	C(27)-C(28)-C(29)	112.2(8)
C(28)-C(29)-C(30)	116.3(8)	C(29)-C(30)-C(31)	114.7(7)
C(30)-C(31)-C(32)	115.1(6)	O(5)-C(32)-O(6)	123.5(7)
O(5)-C(32)-C(31)	123.8(8)	O(6)-C(32)-C(31)	112.2(7)

Table 4. Anisotropic displacement coefficients ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	166(6)	81(4)	74(4)	31(4)	22(4)	38(3)
O(2)	105(4)	89(4)	54(3)	-43(4)	13(3)	-11(3)
O(3)	116(5)	95(5)	83(4)	18(4)	38(4)	-14(4)
O(4)	155(5)	85(4)	78(4)	52(4)	24(4)	-8(3)
O(5)	212(7)	112(5)	74(4)	69(5)	33(4)	36(4)
O(6)	149(6)	122(5)	62(4)	39(4)	19(3)	17(4)
N(1)	94(5)	72(5)	43(4)	4(4)	11(3)	13(3)
N(2)	91(5)	85(5)	52(4)	-20(4)	28(4)	-10(4)
N(3)	75(5)	61(4)	48(4)	-16(3)	21(3)	-11(3)
N(4)	65(4)	61(4)	52(4)	-4(4)	18(3)	-7(3)
C(1)	67(6)	48(5)	55(5)	3(4)	12(4)	6(4)
C(2)	54(5)	57(5)	53(4)	9(4)	12(4)	8(4)
C(3)	48(5)	47(4)	46(4)	-3(4)	13(4)	-1(4)
C(4)	68(5)	57(5)	61(5)	2(4)	13(4)	-5(4)
C(5)	85(7)	40(4)	92(6)	8(5)	22(5)	-5(4)
C(6)	84(6)	61(5)	74(5)	-14(5)	18(5)	-7(4)
C(7)	60(5)	55(5)	57(5)	-2(4)	4(4)	-1(4)
C(8)	66(6)	48(4)	78(5)	-10(4)	21(4)	7(4)
C(9)	86(6)	49(5)	74(5)	7(4)	12(5)	16(4)
C(10)	55(5)	47(4)	53(4)	-1(4)	11(4)	0(4)
C(11)	79(6)	61(6)	67(5)	1(5)	17(5)	8(5)
C(12)	75(6)	83(6)	45(5)	-25(5)	15(4)	9(5)
C(13)	129(8)	105(7)	50(6)	-25(6)	6(5)	25(5)
C(14)	143(10)	155(11)	49(7)	-64(9)	3(6)	28(7)
C(15)	127(10)	154(11)	49(6)	-54(9)	23(6)	-20(7)
C(16)	97(7)	115(8)	76(6)	-34(6)	42(6)	-32(7)
C(17)	59(5)	61(5)	58(5)	5(4)	18(4)	-5(4)
C(18)	62(5)	57(5)	52(5)	0(4)	22(4)	-2(4)
C(19)	69(6)	65(5)	65(5)	-13(5)	26(4)	-14(5)
C(20)	77(6)	65(5)	77(6)	-9(5)	28(5)	-10(5)
C(21)	74(6)	53(5)	87(6)	-1(5)	26(5)	6(5)
C(22)	74(6)	77(6)	59(5)	16(5)	25(5)	6(5)
C(23)	106(6)	64(5)	80(5)	-1(5)	39(5)	-12(4)
C(24)	113(7)	65(5)	117(7)	34(5)	40(6)	8(6)
C(25)	105(7)	92(7)	93(6)	20(6)	32(6)	11(6)
C(26)	110(8)	86(7)	129(8)	36(6)	37(7)	22(7)
C(27)	83(7)	130(9)	117(8)	23(6)	18(6)	29(8)
C(28)	159(10)	126(9)	132(9)	67(8)	50(8)	64(8)
C(29)	193(13)	229(15)	160(11)	135(11)	78(10)	135(12)
C(30)	145(11)	158(11)	224(14)	2(10)	51(10)	-16(10)
C(31)	153(11)	153(10)	200(13)	41(9)	71(10)	75(10)
C(32)	121(8)	109(7)	67(5)	31(6)	6(5)	44(5)

The anisotropic displacement exponent takes the form:

$-2p^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

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Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(30)	1520(71)	2278(46)	3804(48)	121(33)
H(60)	-3387(77)	6370(55)	-3421(54)	144(34)
H(1A)	2279	1032	3285	80
H(3B)	3523	909	-160	80
H(2B)	4276	465	2410	80
H(2C)	3228	1081	2320	80
H(4B)	4477	-382	1261	80
H(4C)	3568	-333	404	80
H(5A)	3148	-1468	1104	80
H(6A)	1108	-1235	1015	80
H(6B)	1431	-868	255	80
H(7A)	339	71	818	80
H(8A)	1117	558	2155	80
H(8B)	883	-362	2183	80
H(9A)	2618	-1332	2366	80
H(9B)	3912	-1001	2461	80
H(10A)	1786	663	223	80
H(10B)	1680	1163	978	80
H(13A)	3731	-46	5069	80
H(14A)	3927	512	6388	80
H(15A)	3059	1738	6524	80
H(16A)	2064	2421	5366	80
H(19A)	5472	2477	781	80
H(20A)	6148	3459	2	80
H(21A)	5480	3430	-1431	80
H(22A)	4282	2368	-2038	80
H(24A)	772	3566	2081	80
H(24B)	-406	3328	2311	80
H(25A)	-907	2463	1256	80
H(25B)	383	2470	1123	80
H(26A)	4	3796	626	80
H(26B)	-1309	3751	715	80
H(27A)	-1721	2770	-264	80
H(27B)	-406	2805	-349	80
H(28A)	-765	4094	-892	80
H(28B)	-2070	4080	-783	80
H(29A)	-2366	2994	-1687	80
H(29B)	-1130	3162	-1868	80
H(30A)	-3104	4239	-2213	80
H(30B)	-2864	3645	-2869	80
H(31A)	-1223	4286	-2866	80
H(31B)	-1358	4829	-2142	80

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STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{27}\ H_{30}\ N_4\ O_7$
Color; Habit	COLORLESS THIN PLATE
Crystal size (mm)	0.40 X 0.50 X 0.08
Crystal System	Triclinic
Space Group	$P\bar{1}$
Unit Cell Dimensions	a = 10.525(5) Å
	b = 10.730(2) Å
	c = 13.732(4) Å
	a = 88.17(2)°
	b = 67.84(3)°
	c = 65.33(2)°
Volume	1290.5(8) $Å^3$
Z	2
Formula weight	522.6
Density(calc.)	1.345 Mg/m^3
Absorption Coefficient	0.816 mm^{-1}
F(000)	552

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Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
O(1)	1282(4)	-3571(3)	-519(2)	121(3)
O(2)	2416(3)	-3244(2)	3652(2)	86(2)
O(3)	3755(3)	-836(2)	1165(2)	59(1)
O(4)	1400(3)	-481(2)	2236(2)	62(1)
O(5)	2389(3)	2161(2)	4314(2)	78(2)
O(6)	3036(3)	1533(2)	5670(2)	66(2)
O(7)	4382(3)	-910(3)	2906(2)	68(1)
N(1)	1885(3)	-2249(3)	293(2)	48(2)
N(2)	2813(3)	-662(3)	-342(2)	44(1)
N(3)	2674(3)	-5240(3)	4334(2)	45(1)
N(4)	3324(3)	-6109(3)	5719(2)	44(1)
C(1)	1745(3)	-4347(3)	1025(2)	43(2)
C(2)	2035(4)	-3868(3)	1929(2)	46(2)
C(3)	2185(3)	-4939(3)	2711(2)	37(2)
C(4)	702(3)	-5122(3)	3167(2)	44(2)
C(5)	430(4)	-5613(3)	2264(2)	47(2)
C(6)	1765(4)	-7002(3)	1667(3)	55(2)
C(7)	3231(4)	-6825(3)	1192(2)	55(2)
C(8)	3091(4)	-5760(3)	422(2)	58(2)
C(9)	275(3)	-4543(3)	1501(2)	47(2)
C(10)	3534(3)	-6335(3)	2087(2)	50(2)
C(11)	1595(4)	-3356(4)	207(3)	60(2)
C(12)	2039(3)	-1340(3)	-445(2)	41(2)
C(13)	1466(4)	-1124(3)	-1230(2)	50(2)
C(14)	1758(4)	-222(3)	-1920(2)	56(2)
C(15)	2600(4)	435(3)	-1839(3)	58(2)
C(16)	3095(4)	213(3)	-1026(2)	54(2)
C(17)	2432(4)	-4383(3)	3596(2)	47(2)
C(18)	2977(3)	-5010(3)	5209(2)	41(2)
C(19)	2943(4)	-3769(3)	5526(2)	53(2)
C(20)	3282(4)	-3692(4)	6392(3)	60(2)
C(21)	3641(4)	-4815(4)	6919(3)	57(2)
C(22)	3642(4)	-5994(3)	6564(2)	51(2)
C(23)	2667(4)	-614(3)	2088(2)	42(2)
C(24)	3077(4)	-545(3)	3036(2)	42(2)
C(25)	1776(4)	-63(3)	4105(2)	49(2)
C(26)	2227(4)	141(3)	5000(2)	57(2)
C(27)	2569(4)	1370(3)	4948(2)	48(2)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

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Table 2. Bond lengths (Å)

O(1)-C(11)	1.218 (6)	O(2)-C(17)	1.219 (5)
O(3)-C(23)	1.292 (4)	O(4)-C(23)	1.216 (5)
O(5)-C(27)	1.208 (4)	O(6)-C(27)	1.306 (5)
O(7)-C(24)	1.201 (5)	N(1)-C(11)	1.362 (6)
N(1)-C(12)	1.396 (4)	N(2)-C(12)	1.341 (5)
N(2)-C(16)	1.349 (4)	N(3)-C(17)	1.370 (4)
N(3)-C(18)	1.408 (5)	N(4)-C(18)	1.340 (4)
N(4)-C(22)	1.346 (5)	C(1)-C(2)	1.535 (5)
C(1)-C(8)	1.547 (4)	C(1)-C(9)	1.538 (5)
C(1)-C(11)	1.528 (5)	C(2)-C(3)	1.547 (4)
C(3)-C(4)	1.542 (5)	C(3)-C(10)	1.544 (3)
C(3)-C(17)	1.522 (5)	C(4)-C(5)	1.529 (5)
C(5)-C(6)	1.526 (4)	C(5)-C(9)	1.528 (4)
C(6)-C(7)	1.524 (6)	C(7)-C(8)	1.531 (5)
C(7)-C(10)	1.538 (6)	C(12)-C(13)	1.391 (5)
C(13)-C(14)	1.379 (5)	C(14)-C(15)	1.376 (7)
C(15)-C(16)	1.375 (6)	C(18)-C(19)	1.396 (5)
C(19)-C(20)	1.378 (6)	C(20)-C(21)	1.374 (5)
C(21)-C(22)	1.370 (6)	C(23)-C(24)	1.531 (6)
C(24)-C(25)	1.496 (4)	C(25)-C(26)	1.526 (6)
C(26)-C(27)	1.498 (6)		

Table 3. Bond angles (^{o})

C(11)-N(1)-C(12)	127.1(3)	C(12)-N(2)-C(16)	120.2(3)
C(17)-N(3)-C(18)	127.9(3)	C(18)-N(4)-C(22)	118.1(3)
C(2)-C(1)-C(8)	108.9(3)	C(2)-C(1)-C(9)	109.2(2)
C(8)-C(1)-C(9)	108.4(3)	C(2)-C(1)-C(11)	114.5(3)
C(8)-C(1)-C(11)	107.2(2)	C(9)-C(1)-C(11)	108.4(3)
C(1)-C(2)-C(3)	110.9(3)	C(2)-C(3)-C(4)	108.7(3)
C(2)-C(3)-C(10)	108.3(2)	C(4)-C(3)-C(10)	109.2(3)
C(2)-C(3)-C(17)	108.0(3)	C(4)-C(3)-C(17)	110.5(2)
C(10)-C(3)-C(17)	112.1(3)	C(3)-C(4)-C(5)	109.8(2)
C(4)-C(5)-C(6)	109.3(3)	C(4)-C(5)-C(9)	110.1(3)
C(6)-C(5)-C(9)	109.9(2)	C(5)-C(6)-C(7)	109.5(3)
C(6)-C(7)-C(8)	109.9(3)	C(6)-C(7)-C(10)	109.6(3)
C(8)-C(7)-C(10)	109.7(3)	C(1)-C(8)-C(7)	109.6(2)
C(1)-C(9)-C(5)	109.9(3)	C(3)-C(10)-C(7)	109.5(3)
O(1)-C(11)-N(1)	121.0(3)	O(1)-C(11)-C(1)	121.4(4)
N(1)-C(11)-C(1)	117.6(4)	N(1)-C(12)-N(2)	113.8(3)
N(1)-C(12)-C(13)	125.0(4)	N(2)-C(12)-C(13)	121.2(3)
C(12)-C(13)-C(14)	117.9(4)	C(13)-C(14)-C(15)	121.0(4)
C(14)-C(15)-C(16)	118.5(3)	N(2)-C(16)-C(15)	121.2(4)
O(2)-C(17)-N(3)	121.6(4)	O(2)-C(17)-C(3)	122.4(3)
N(3)-C(17)-C(3)	115.9(3)	N(3)-C(18)-N(4)	113.6(3)
N(3)-C(18)-C(19)	124.2(3)	N(4)-C(18)-C(19)	122.2(3)
C(18)-C(19)-C(20)	118.0(3)	C(19)-C(20)-C(21)	120.3(4)
C(20)-C(21)-C(22)	118.2(4)	N(4)-C(22)-C(21)	123.2(3)
O(3)-C(23)-O(4)	125.0(4)	O(3)-C(23)-C(24)	115.0(4)
O(4)-C(23)-C(24)	120.0(3)	O(7)-C(24)-C(23)	120.5(2)
O(7)-C(24)-C(25)	123.5(3)	C(23)-C(24)-C(25)	115.9(3)
C(24)-C(25)-C(26)	113.3(3)	C(25)-C(26)-C(27)	112.4(3)
O(5)-C(27)-O(6)	122.9(4)	O(5)-C(27)-C(26)	123.0(4)
O(6)-C(27)-C(26)	114.0(3)		

Table 4. Anisotropic displacement coefficients ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	260(4)	132(3)	84(2)	-146(3)	-118(3)	66(2)
O(2)	171(3)	58(2)	84(2)	-69(2)	-87(2)	34(1)
O(3)	52(2)	85(2)	38(1)	-30(1)	-18(1)	7(1)
O(4)	59(2)	91(2)	52(1)	-45(1)	-26(1)	13(1)
O(5)	151(3)	61(2)	79(2)	-68(2)	-81(2)	39(1)
O(6)	111(2)	61(2)	63(2)	-49(2)	-60(2)	25(1)
O(7)	54(2)	101(2)	56(1)	-34(2)	-29(1)	16(1)
N(1)	70(2)	56(2)	37(2)	-40(2)	-29(1)	21(1)
N(2)	48(2)	52(2)	34(1)	-25(1)	-16(1)	13(1)
N(3)	65(2)	40(2)	43(2)	-30(1)	-29(1)	11(1)
N(4)	49(2)	51(2)	41(1)	-25(1)	-23(1)	11(1)
C(1)	57(2)	48(2)	30(2)	-29(2)	-18(2)	8(1)
C(2)	67(2)	49(2)	38(2)	-37(2)	-24(2)	14(1)
C(3)	47(2)	34(2)	35(2)	-22(2)	-18(2)	7(1)
C(4)	45(2)	46(2)	38(2)	-20(2)	-14(2)	9(1)
C(5)	51(2)	54(2)	49(2)	-32(2)	-23(2)	16(2)
C(6)	73(3)	40(2)	61(2)	-28(2)	-34(2)	8(2)
C(7)	55(2)	43(2)	48(2)	-6(2)	-17(2)	-11(2)
C(8)	55(2)	72(2)	39(2)	-28(2)	-10(2)	-3(2)
C(9)	53(2)	48(2)	46(2)	-22(2)	-25(2)	10(2)
C(10)	42(2)	51(2)	51(2)	-13(2)	-20(2)	1(2)
C(11)	97(3)	69(2)	38(2)	-53(2)	-34(2)	17(2)
C(12)	43(2)	45(2)	32(2)	-17(2)	-14(2)	9(1)
C(13)	55(2)	61(2)	40(2)	-27(2)	-24(2)	13(2)
C(14)	58(2)	68(2)	43(2)	-21(2)	-29(2)	21(2)
C(15)	61(2)	64(2)	50(2)	-28(2)	-24(2)	28(2)
C(16)	57(2)	59(2)	46(2)	-28(2)	-18(2)	22(2)
C(17)	67(2)	40(2)	45(2)	-29(2)	-29(2)	13(2)
C(18)	47(2)	45(2)	35(2)	-22(2)	-17(2)	4(1)
C(19)	70(2)	51(2)	47(2)	-35(2)	-22(2)	5(2)
C(20)	73(3)	66(2)	51(2)	-40(2)	-24(2)	-2(2)
C(21)	53(2)	79(3)	43(2)	-32(2)	-19(2)	2(2)
C(22)	51(2)	64(2)	43(2)	-26(2)	-24(2)	11(2)
C(23)	49(2)	39(2)	43(2)	-20(2)	-22(2)	8(1)
C(24)	53(2)	41(2)	41(2)	-27(2)	-22(2)	11(1)
C(25)	66(2)	52(2)	37(2)	-36(2)	-19(2)	8(1)
C(26)	92(3)	53(2)	42(2)	-43(2)	-31(2)	16(2)
C(27)	70(2)	44(2)	40(2)	-27(2)	-27(2)	11(2)

The anisotropic displacement exponent takes the form:

$-2p^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

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Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(2B)	1202	-2992	2307	80
H(2C)	2953	-3746	1635	80
H(4B)	-138	-4254	3555	80
H(4C)	779	-5790	3650	80
H(5A)	-494	-5727	2556	80
H(6A)	1591	-7337	1112	80
H(6B)	1856	-7670	2150	80
H(7A)	4065	-7700	812	80
H(8A)	4016	-5650	121	80
H(8B)	2925	-6073	-147	80
H(9A)	85	-4844	941	80
H(9B)	-570	-3672	1877	80
H(10A)	3656	-7017	2557	80
H(10B)	4458	-6223	1789	80
H(13A)	877	-1584	-1279	80
H(14A)	1378	-54	-2469	80
H(15A)	2834	1035	-2337	80
H(16A)	3643	697	-941	80
H(19A)	2683	-2995	5150	80
H(20A)	3273	-2855	6628	80
H(21A)	3878	-4771	7524	80
H(22A)	3882	-6779	6932	80
H(25A)	1366	-730	4250	80
H(25B)	990	804	4087	80
H(26A)	3120	-678	4945	80
H(26B)	1427	254	5678	80
H(3N)	2706(35)	-6090(32)	4256(23)	62(10)
H(1N)	2077(38)	-2152(33)	850(25)	73(12)
H(60)	3216(42)	2388(39)	5643(27)	99(13)
H(4X)	3260(44)	-775(38)	450(32)	123(14)

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STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{26}\ H_{30}\ N_4\ O_6$
Color; Habit	COLORLESS PRISM
Crystal size (mm)	0.16 X 0.25 X 0.50
Crystal System	Monoclinic
Space Group	$P2_1/n$
Unit Cell Dimensions	$\underline{a}$ = 12.1490(10) Å
	$\underline{b}$ = 15.7680(10) Å
	$\underline{c}$ = 13.682(2) Å
	b = 107.720(10)^o
Volume	2496.6(4) Å^3
Z	4
Formula weight	494.5
Density(calc.)	1.316 Mg/m^3
Absorption Coefficient	0.781 mm^{-1}
F(000)	1048

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
O(1)	411(11)	4584(9)	6400(16)	234(11)
O(2)	-3732(11)	4110(11)	5247(16)	291(13)
O(3)	829(11)	6967(9)	8471(16)	215(11)
O(4)	2681(11)	6723(8)	8854(16)	213(11)
O(5)	754(11)	3955(8)	9158(15)	228(11)
O(6)	-1114(10)	4211(10)	8535(14)	198(10)
N(1)	1726(12)	3583(8)	6417(15)	167(10)
N(2)	3715(13)	3594(9)	6735(15)	176(10)
N(3)	-4568(13)	2889(11)	4545(16)	192(11)
N(4)	-6434(11)	2422(12)	3938(15)	182(10)
C(1)	-338(9)	3112(12)	5766(13)	93(8)
C(2)	-1489(12)	3596(11)	5579(18)	197(13)
C(3)	-2476(12)	2942(11)	5126(15)	107(9)
C(4)	-2339(14)	2263(14)	5972(19)	206(16)
C(5)	-1185(12)	1637(13)	6222(18)	188(13)
C(6)	-955(15)	1668(15)	5268(19)	223(18)
C(7)	-1147(14)	2100(14)	4417(20)	195(14)
C(8)	-136(13)	2879(13)	4782(10)	125(10)
C(9)	-164(12)	2492(10)	6573(17)	170(12)
C(10)	-2306(12)	2558(11)	4150(16)	170(12)
C(11)	639(17)	3866(12)	6182(21)	213(14)
C(12)	2793(17)	4029(11)	6698(19)	180(13)
C(13)	2860(19)	4863(13)	6938(25)	272(22)
C(14)	3962(23)	5223(15)	7250(32)	425(36)
C(15)	4901(21)	4759(15)	7310(27)	290(23)
C(16)	4706(19)	3963(15)	7089(22)	225(18)
C(17)	-3631(15)	3403(15)	4960(23)	248(17)
C(18)	-5761(16)	3085(14)	4259(21)	209(14)
C(19)	-6152(15)	3918(13)	4262(18)	194(14)
C(20)	-7320(16)	4033(17)	3945(22)	276(20)
C(21)	-8048(16)	3366(16)	3653(18)	199(15)
C(22)	-7583(14)	2589(15)	3610(19)	235(17)
C(23)	1747(18)	6461(13)	8744(24)	209(16)
C(24)	1427(14)	5583(12)	8942(23)	284(23)
C(25)	173(13)	5332(11)	8534(18)	173(13)
C(26)	-18(18)	4442(15)	8796(25)	226(18)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

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Table 2. Bond lengths (Å)

O(1)-C(11)	1.224 (25)	O(2)-C(17)	1.201 (30)
O(3)-C(23)	1.329 (24)	O(4)-C(23)	1.173 (26)
O(5)-C(26)	1.197 (25)	O(6)-C(26)	1.320 (24)
N(1)-C(11)	1.338 (24)	N(1)-C(12)	1.422 (24)
N(2)-C(12)	1.302 (26)	N(2)-C(16)	1.292 (26)
N(3)-C(17)	1.372 (25)	N(3)-C(18)	1.415 (24)
N(4)-C(18)	1.317 (26)	N(4)-C(22)	1.356 (21)
C(1)-C(2)	1.544 (21)	C(1)-C(8)	1.486 (24)
C(1)-C(9)	1.442 (27)	C(1)-C(11)	1.654 (24)
C(2)-C(3)	1.559 (22)	C(3)-C(4)	1.549 (31)
C(3)-C(10)	1.536 (30)	C(3)-C(17)	1.533 (25)
C(4)-C(5)	1.662 (25)	C(5)-C(6)	1.418 (37)
C(5)-C(9)	1.796 (24)	C(6)-C(7)	1.306 (36)
C(7)-C(8)	1.701 (27)	C(7)-C(10)	1.525 (24)
C(12)-C(13)	1.352 (28)	C(13)-C(14)	1.397 (34)
C(14)-C(15)	1.337 (38)	C(15)-C(16)	1.296 (34)
C(18)-C(19)	1.398 (30)	C(19)-C(20)	1.364 (26)
C(20)-C(21)	1.355 (33)	C(21)-C(22)	1.357 (34)
C(23)-C(24)	1.486 (30)	C(24)-C(25)	1.507 (23)
C(25)-C(26)	1.485 (31)		

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Table 3. Bond angles (^{o})

C(11)-N(1)-C(12)	130.7(15)	C(12)-N(2)-C(16)	118.0(18)
C(17)-N(3)-C(18)	129.6(19)	C(18)-N(4)-C(22)	115.4(18)
C(2)-C(1)-C(8)	111.3(14)	C(2)-C(1)-C(9)	112.1(15)
C(8)-C(1)-C(9)	120.0(17)	C(2)-C(1)-C(11)	102.8(14)
C(8)-C(1)-C(11)	101.0(15)	C(9)-C(1)-C(11)	107.5(13)
C(1)-C(2)-C(3)	106.7(14)	C(2)-C(3)-C(4)	105.4(14)
C(2)-C(3)-C(10)	108.4(16)	C(4)-C(3)-C(10)	111.4(16)
C(2)-C(3)-C(17)	107.7(15)	C(4)-C(3)-C(17)	108.9(18)
C(10)-C(3)-C(17)	114.6(16)	C(3)-C(4)-C(5)	117.2(18)
C(4)-C(5)-C(6)	100.4(17)	C(4)-C(5)-C(9)	94.6(13)
C(6)-C(5)-C(9)	84.6(15)	C(5)-C(6)-C(7)	143.8(22)
C(6)-C(7)-C(8)	101.4(16)	C(6)-C(7)-C(10)	111.2(21)
C(8)-C(7)-C(10)	105.0(16)	C(1)-C(8)-C(7)	98.1(15)
C(1)-C(9)-C(5)	112.1(14)	C(3)-C(10)-C(7)	109.7(15)
O(1)-C(11)-N(1)	122.0(17)	O(1)-C(11)-C(1)	123.9(17)
N(1)-C(11)-C(1)	113.3(15)	N(1)-C(12)-N(2)	116.9(16)
N(1)-C(12)-C(13)	122.0(19)	N(2)-C(12)-C(13)	121.1(19)
C(12)-C(13)-C(14)	116.8(22)	C(13)-C(14)-C(15)	121.2(22)
C(14)-C(15)-C(16)	115.1(23)	N(2)-C(16)-C(15)	127.4(22)
O(2)-C(17)-N(3)	121.9(18)	O(2)-C(17)-C(3)	124.8(17)
N(3)-C(17)-C(3)	112.9(18)	N(3)-C(18)-N(4)	113.5(19)
N(3)-C(18)-C(19)	121.6(18)	N(4)-C(18)-C(19)	124.7(17)
C(18)-C(19)-C(20)	116.5(19)	C(19)-C(20)-C(21)	120.8(23)
C(20)-C(21)-C(22)	118.1(18)	N(4)-C(22)-C(21)	124.1(19)
O(3)-C(23)-O(4)	121.4(19)	O(3)-C(23)-C(24)	111.5(18)
O(4)-C(23)-C(24)	127.0(18)	C(23)-C(24)-C(25)	117.9(16)
C(24)-C(25)-C(26)	111.9(15)	O(5)-C(26)-O(6)	122.4(22)
O(5)-C(26)-C(25)	123.1(19)	O(6)-C(26)-C(25)	114.4(17)