Electronic Supplementary Material (ESI) for Dalton Transactions

Zinc and Cobalt Complexes Based on Tripodal Ligands: Synthesis, Structure and Reactivity toward Lactide

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General considerations. NMR spectra were recorded on a Bruker Avance 300, Avance 400 or AM-500 MHz spectrometer (at the Ecole Nationale Supérieure de Chimie de Paris and at University of Caen). Chemical shifts are reported in ppm and coupling constants *J* in hertz. NMR spectra were calibrated using residual ^{1}H and ^{13}C resonances of deuterated solvents. The paramagnetic spectrum sequence was as followed: a π/6 pulse followed by a 550 ms acquisition and a 2 s delay for a spectrum width of 220 ppm with 64 k points. After the FFT, a 0.3 Hz filter is applied. For the T_1 measurements, the inversion-recovery sequence was used: π pulse, variable delay τ, π/2 pulse and acquisition. The paramagnetic COSY 45 used an acquisition time of 32 ms and a delay of 1 s with TD1 = 512, TD2 = 2048 with an accumulation of 64 scans. UV-visible spectra were recorded on a Safas-Monaco spectrometer from 250 nm to 1000 nm with 2 nm steps. Molar conductivities of freshly prepared 10^{-3} mol/L solutions of cobalt complexes in DMF were measured on a CDM 210 conductivity meter.

Procedure for measuring the magnetic susceptibility by solution NMR

A solution with a known concentration *C* (expressed in $mol.mL^{-1}$) of the complex was freshly prepared (typically less than $1.0*10^{-5}$ $mol.mL^{-1}$). The tube with the complex to measure was locked and shimmed, the receiver gain was determined and a spectrum could be recorded. A tube with the pure solvent was then locked in the NMR magnet. Then, the analyzed tube was sent back in the magnet and the NMR spectrum was recorded. The residual peak solvent was shifted by Δν. At 293 K and for a 300 MHz spectrometer, the magnetic susceptibility (expressed in μ_B) follows the equation:

$$\mu_{eff} = 1{,}36.10^{-3}\sqrt{\frac{\Delta\nu}{C}}$$

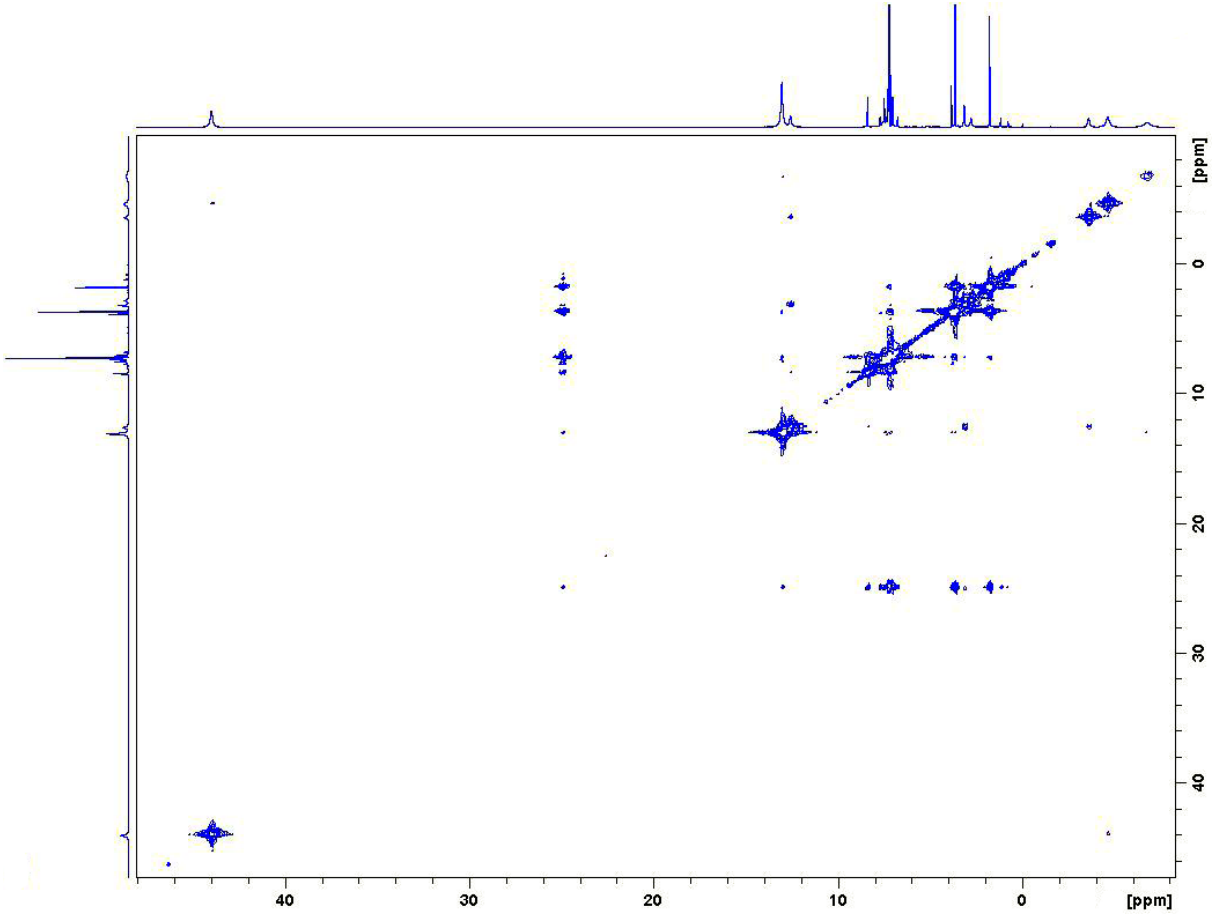


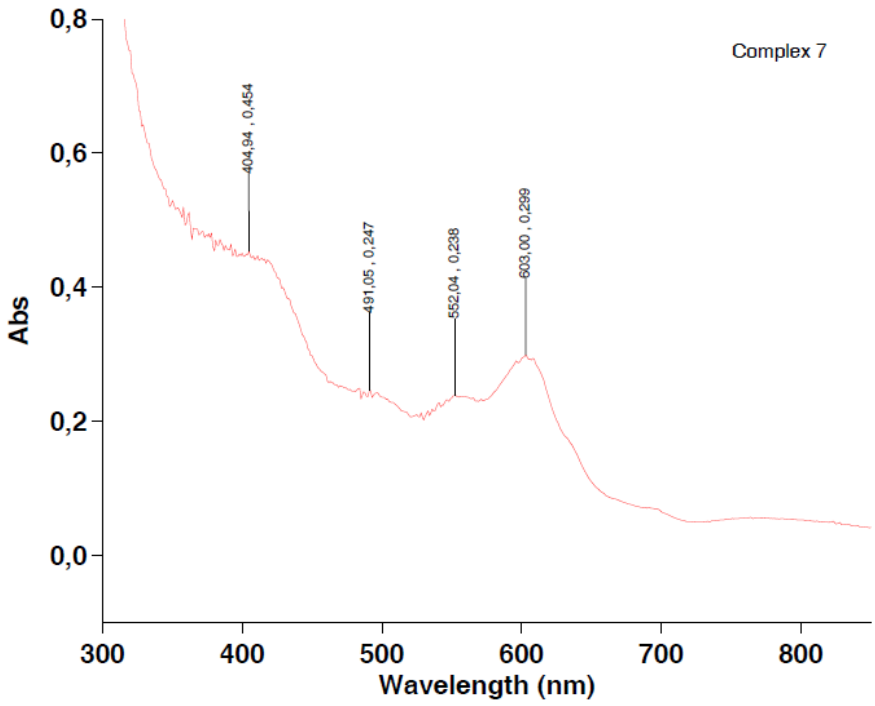
Figure 1S. 2D COSY NMR spectrum of complex **12** ($CDCl_3$, 25°C, 400 MHz).

Molar conductivities

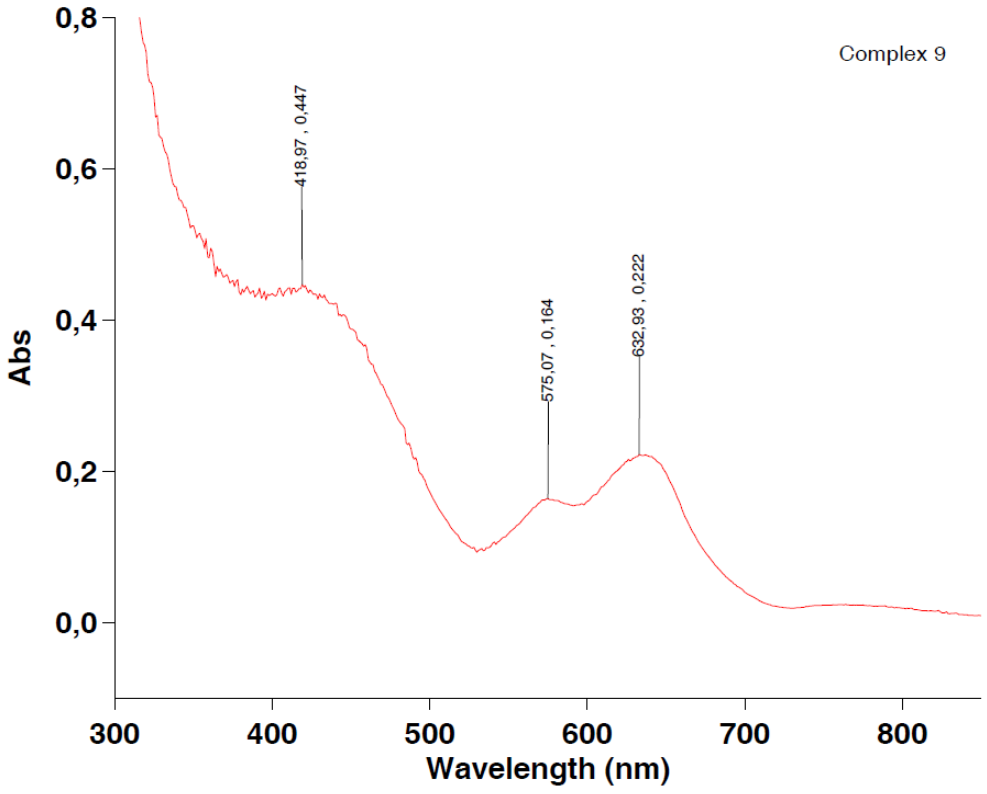
C = 10^{-3} mol/L in DMF, 20°C.

Complex	Color	Conductivity µS/cm
1	colorless	13.4
2	colorless	51.0
3	colorless	40.0
4	colorless	19.7
5	colorless	23.8
6	colorless	40.5
7	brown	37.8
9	green	37.5
10	pale green	114.5
11	blue	101.0

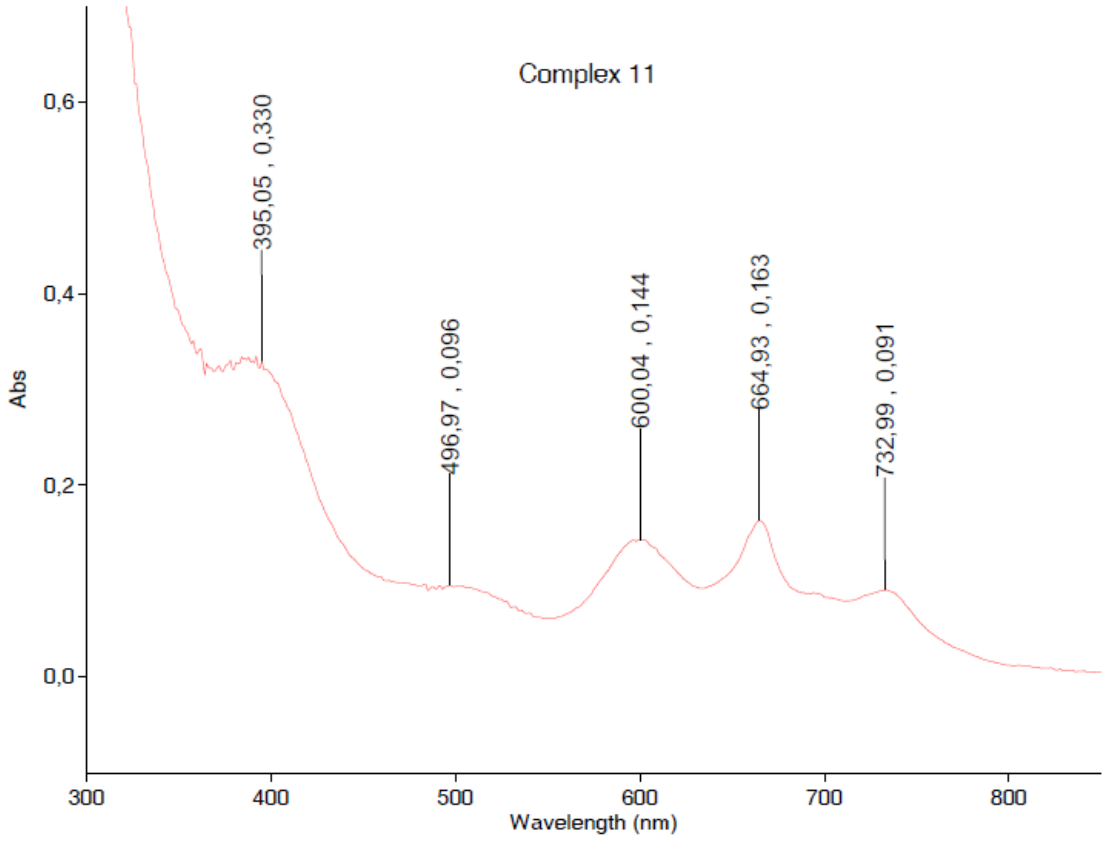
UV-vis spectrum of complex 7



UV-vis spectrum of complex 9



UV-vis spectrum of complex 11



[L^1]H: Crystal structure report

X-ray crystallographic study

(C_{27} H_{35} N_3 O); *M* = 417.58. APEXII, Bruker-AXS diffractometer, Mo-Kα radiation (λ = 0.71073 Å), *T* = 100(2) K; monoclinic $P2_1/n$ (I.T.#14), a = 10.052(2), b = 24.616(6), c = 10.268(2) Å, β = 110.971(12) °, *V* = 2372.4(9) Å^3, *Z* = 4, *d* = 1.169 g.cm^{-3}, μ = 0.071 mm^{-1}. The structure was solved by direct methods using the *SIR97* program [1], and then refined with full-matrix least-square methods based on F^2 (*SHELXL-97*) [2] with the aid of the *WINGX* [3] program. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 5268 unique intensities and 282 parameters converged at $\omega R(F^2)$ = 0.1496 ($R(F)$ = 0.0672) for 3419 observed reflections with $I > 2\sigma(I)$.

[1] A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, J. Appl. Cryst. (1999) 32, 115-119

[2] Sheldrick G.M., Acta Cryst. A64 (2008), 112-122

[3] L. J. Farrugia, J. Appl. Cryst., 1999, 32, 837-838

Structural data

Empirical formula	C_{27} H_{35} N_3 O
Formula weight	417.58
Temperature	100(2) *K*
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, $P\ 2_1/n$
Unit cell dimensions	a = 10.052(2) Å, α = 90 °
	b = 24.616(6) Å, β = 110.971(12) °
	c = 10.268(2) Å, γ = 90 °
Volume	2372.4(9) Å^3
Z, Calculated density	4 , 1.169 (g.cm^{-3})
Absorption coefficient	0.071 mm^{-1}
F(000)	904
Crystal size	0.55 x 0.5 x 0.43 mm
Crystal color	colorless
Theta range for data collection	2.57 to 27.61 °
h_min, h_max	-13 , 11
k_min, k_max	-32 , 31
l_min, l_max	-13 , 12
Reflections collected / unique	17275 / 5268 [R(int) = 0.069]
Completeness to theta_max	0.957
Absorption correction type	multi-scan
Max. and min. transmission	0.970 , 0.952
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	5268 / 0 / 282
Goodness-of-fit	1.013
Final *R* indices [I>2σ]	$R1^a$ = 0.0672, $wR2^b$ = 0.1496
R indices (all data)	$R1^a$ = 0.107, $wR2^b$ = 0.1663
Largest diff. peak and hole	0.28 and -0.262 e.Å^{-3}

$^a R1 = \sum \; | \; |F_o| - |F_c| \; | \; / \sum |F_o|$

$^b wR2 = \{\sum \; [w(F_o^2 - F_c^2)^2] \; / \sum \; [w(F_o^2)^2]\}^{1/2}$

Atomic coordinates, site occupancy (%) and equivalent isotropic displacement parameters (Å^2 x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	occ.	U(eq)
N1	0.79856(18)	0.24382(7)	0.96323(18)	1	0.0210(4)
C1	0.7629(2)	0.24212(9)	1.0892(2)	1	0.0249(5)
H1A	0.7499	0.2798	1.1165	1	0.03
H1B	0.8439	0.226	1.1658	1	0.03
C2	0.6296(2)	0.20982(9)	1.0721(2)	1	0.0246(5)
C3	0.5201(2)	0.20368(9)	0.9442(3)	1	0.0288(5)
H3	0.5282	0.2185	0.8619	1	0.035
C4	0.3991(3)	0.17560(10)	0.9385(3)	1	0.0362(6)
H4	0.3226	0.1707	0.8522	1	0.043
C5	0.3913(3)	0.15477(10)	1.0603(3)	1	0.0376(6)
H5	0.3093	0.1355	1.0599	1	0.045
C6	0.5055(3)	0.16258(10)	1.1828(3)	1	0.0359(6)
H6	0.4995	0.148	1.2662	1	0.043
N7	0.6241(2)	0.18942(8)	1.1918(2)	1	0.0308(5)
C11	0.8517(2)	0.19051(9)	0.9384(2)	1	0.0240(5)
H11A	0.7853	0.1619	0.9455	1	0.029
H11B	0.9455	0.1836	1.0121	1	0.029
C12	0.8668(2)	0.18653(8)	0.7974(2)	1	0.0221(5)
C13	0.9743(3)	0.15542(10)	0.7801(3)	1	0.0326(6)
H13	1.0419	0.1376	0.8579	1	0.039
C14	0.9826(3)	0.15040(10)	0.6491(3)	1	0.0387(6)
H14	1.0548	0.1288	0.6352	1	0.046
C15	0.8842(3)	0.17737(10)	0.5391(3)	1	0.0347(6)
H15	0.8868	0.1748	0.4477	1	0.042
C16	0.7818(2)	0.20810(10)	0.5650(3)	1	0.0324(6)
H16	0.715	0.2271	0.4891	1	0.039
N17	0.77089(19)	0.21283(8)	0.6910(2)	1	0.0287(5)
C21	0.9094(2)	0.28542(8)	0.9792(2)	1	0.0226(5)
H21A	0.942	0.2831	0.8991	1	0.027
H21B	0.9922	0.2778	1.0651	1	0.027
C22	0.8560(2)	0.34195(8)	0.9872(2)	1	0.0212(5)
C23	0.9295(2)	0.37562(8)	1.0989(2)	1	0.0225(5)
H23	1.0125	0.3622	1.17	1	0.027
C24	0.8845(2)	0.42799(9)	1.1087(2)	1	0.0237(5)
C24A	0.9596(2)	0.46593(9)	1.2318(2)	1	0.0267(5)
C24B	1.1003(2)	0.44179(10)	1.3298(3)	1	0.0313(6)
H24A	1.0818	0.4069	1.3659	1	0.047
H24B	1.1443	0.4668	1.4077	1	0.047

H24C	1.1648	0.4363	1.2785	1	0.047
C24C	0.8608(3)	0.47533(11)	1.3143(3)	1	0.0380(6)
H24D	0.8403	0.4405	1.3493	1	0.057
H24E	0.7716	0.4918	1.2532	1	0.057
H24F	0.9076	0.4997	1.393	1	0.057
C24D	0.9924(3)	0.52075(10)	1.1805(3)	1	0.0405(7)
H24G	0.9038	0.5371	1.1177	1	0.061
H24H	1.0581	0.5155	1.1305	1	0.061
H24I	1.0363	0.5448	1.2605	1	0.061
C25	0.7624(2)	0.44591(9)	0.9997(2)	1	0.0236(5)
H25	0.7295	0.4817	1.0055	1	0.028
C26	0.6864(2)	0.41482(9)	0.8838(2)	1	0.0216(5)
C26A	0.5592(2)	0.43867(8)	0.7636(2)	1	0.0221(5)
C26B	0.5843(2)	0.43383(9)	0.6249(2)	1	0.0278(5)
H26A	0.5023	0.4488	0.5494	1	0.042
H26B	0.5963	0.3955	0.6058	1	0.042
H26C	0.6704	0.4541	0.6312	1	0.042
C26C	0.5373(2)	0.49923(9)	0.7849(3)	1	0.0281(5)
H26D	0.5207	0.5042	0.8726	1	0.042
H26E	0.4547	0.5126	0.7072	1	0.042
H26F	0.6224	0.5195	0.7887	1	0.042
C26D	0.4210(2)	0.40862(9)	0.7520(2)	1	0.0274(5)
H26G	0.405	0.4117	0.8404	1	0.041
H26H	0.4295	0.3702	0.7311	1	0.041
H26I	0.3405	0.4248	0.677	1	0.041
C27	0.7338(2)	0.36121(8)	0.8806(2)	1	0.0203(5)
O27	0.66058(15)	0.32764(6)	0.77081(16)	1	0.0270(4)
H27	0.6876	0.2954	0.791	1	0.04

Anisotropic displacement parameters ($Å^2$)

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

Atom	U11	U22	U33	U23	U13	U12
N1	0.0216(9)	0.0220(9)	0.0209(10)	0.0001(8)	0.0096(8)	-0.0004(7)
C1	0.0246(11)	0.0264(12)	0.0238(12)	-0.0004(9)	0.0087(10)	-0.0001(9)
C2	0.0254(11)	0.0249(11)	0.0268(13)	0.0009(10)	0.0134(10)	0.0029(9)
C3	0.0238(11)	0.0343(13)	0.0289(13)	0.0044(10)	0.0102(11)	0.0009(9)
C4	0.0247(12)	0.0440(15)	0.0390(16)	0.0040(12)	0.0103(12)	-0.0009(10)
C5	0.0324(13)	0.0393(15)	0.0501(18)	-0.0019(12)	0.0259(13)	-0.0063(11)
C6	0.0452(15)	0.0298(13)	0.0428(16)	0.0020(11)	0.0281(14)	-0.0027(11)
N7	0.0374(11)	0.0292(11)	0.0308(12)	0.0015(9)	0.0182(10)	-0.0002(8)
C11	0.0212(10)	0.0239(11)	0.0255(12)	0.0009(9)	0.0066(10)	0.0014(8)
C12	0.0184(10)	0.0231(11)	0.0241(12)	-0.0006(9)	0.0067(10)	-0.0015(8)
C13	0.0315(12)	0.0352(14)	0.0336(14)	0.0043(11)	0.0148(12)	0.0089(10)
C14	0.0456(15)	0.0355(14)	0.0438(17)	0.0029(12)	0.0268(14)	0.0126(11)
C15	0.0412(14)	0.0364(14)	0.0307(14)	-0.0051(11)	0.0182(12)	-0.0049(11)
C16	0.0240(11)	0.0488(16)	0.0242(13)	0.0016(11)	0.0086(11)	-0.0007(10)

N17	0.0209(9)	0.0422(12)	0.0219(11)	0.0024(9)	0.0063(8)	0.0048(8)
C21	0.0164(9)	0.0246(11)	0.0232(12)	0.0005(9)	0.0025(9)	-0.0004(8)
C22	0.0178(9)	0.0252(11)	0.0216(12)	0.0007(9)	0.0083(9)	-0.0004(8)
C23	0.0184(10)	0.0273(12)	0.0223(12)	0.0002(9)	0.0077(10)	-0.0010(8)
C24	0.0198(10)	0.0275(12)	0.0255(12)	-0.0015(9)	0.0100(10)	-0.0020(8)
C24A	0.0224(11)	0.0285(12)	0.0266(13)	-0.0029(10)	0.0056(10)	0.0018(9)
C24B	0.0218(11)	0.0394(14)	0.0289(13)	-0.0100(11)	0.0043(11)	-0.0001(10)
C24C	0.0289(12)	0.0537(17)	0.0281(14)	-0.0125(12)	0.0063(12)	0.0057(11)
C24D	0.0414(15)	0.0334(14)	0.0359(15)	-0.0072(11)	0.0008(13)	-0.0091(11)
C25	0.0214(10)	0.0242(11)	0.0267(12)	-0.0026(9)	0.0105(10)	-0.0001(8)
C26	0.0174(10)	0.0269(12)	0.0214(12)	0.0010(9)	0.0082(9)	-0.0008(8)
C26A	0.0186(10)	0.0249(11)	0.0219(12)	-0.0007(9)	0.0061(9)	0.0004(8)
C26B	0.0220(11)	0.0299(13)	0.0303(13)	0.0017(10)	0.0079(10)	0.0000(9)
C26C	0.0231(11)	0.0282(12)	0.0300(13)	0.0016(10)	0.0058(11)	0.0038(9)
C26D	0.0201(10)	0.0329(13)	0.0272(13)	0.0018(10)	0.0060(10)	-0.0013(9)
C27	0.0178(9)	0.0233(11)	0.0188(11)	-0.0016(9)	0.0051(9)	-0.0033(8)
O27	0.0242(8)	0.0225(8)	0.0274(9)	-0.0026(7)	0.0010(7)	0.0010(6)

Bond lengths [Å]

N1	- C1	=	1.461(3)
N1	- C11	=	1.473(3)
N1	- C21	=	1.479(3)
C1	- C2	=	1.513(3)
C1	- H1A	=	0.99
C1	- H1B	=	0.99
C2	- N7	=	1.346(3)
C2	- C3	=	1.387(3)
C3	- C4	=	1.382(3)
C3	- H3	=	0.95
C4	- C5	=	1.380(4)
C4	- H4	=	0.95
C5	- C6	=	1.380(4)
C5	- H5	=	0.95
C6	- N7	=	1.337(3)
C6	- H6	=	0.95
C11	- C12	=	1.512(3)
C11	- H11A	=	0.99
C11	- H11B	=	0.99
C12	- N17	=	1.338(3)
C12	- C13	=	1.387(3)
C13	- C14	=	1.383(3)
C13	- H13	=	0.95
C14	- C15	=	1.377(4)
C14	- H14	=	0.95
C15	- C16	=	1.378(3)
C15	- H15	=	0.95
C16	- N17	=	1.342(3)
C16	- H16	=	0.95
C21	- C22	=	1.504(3)
C21	- H21A	=	0.99
C21	- H21B	=	0.99
C22	- C23	=	1.393(3)

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C22  - C27      = 1.404(3)
C23  - C24      = 1.382(3)
C23  - H23      = 0.95
C24  - C25      = 1.404(3)
C24  - C24A     = 1.535(3)
C24A - C24D     = 1.527(3)
C24A - C24B     = 1.532(3)
C24A - C24C     = 1.535(3)
C24B - H24A     = 0.98
C24B - H24B     = 0.98
C24B - H24C     = 0.98
C24C - H24D     = 0.98
C24C - H24E     = 0.98
C24C - H24F     = 0.98
C24D - H24G     = 0.98
C24D - H24H     = 0.98
C24D - H24I     = 0.98
C25  - C26      = 1.391(3)
C25  - H25      = 0.95
C26  - C27      = 1.407(3)
C26  - C26A     = 1.541(3)
C26A - C26C     = 1.534(3)
C26A - C26B     = 1.537(3)
C26A - C26D     = 1.541(3)
C26B - H26A     = 0.98
C26B - H26B     = 0.98
C26B - H26C     = 0.98
C26C - H26D     = 0.98
C26C - H26E     = 0.98
C26C - H26F     = 0.98
C26D - H26G     = 0.98
C26D - H26H     = 0.98
C26D - H26I     = 0.98
C27  - O27      = 1.379(2)
O27  - H27      = 0.84
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Angles [°]

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C1       - N1       - C11      = 110.28(17)
C1       - N1       - C21      = 109.59(17)
C11      - N1       - C21      = 109.32(17)
N1       - C1       - C2       = 113.57(18)
N1       - C1       - H1A      = 108.9
C2       - C1       - H1A      = 108.9
N1       - C1       - H1B      = 108.9
C2       - C1       - H1B      = 108.9
H1A      - C1       - H1B      = 107.7
N7       - C2       - C3       = 123.0(2)
N7       - C2       - C1       = 114.5(2)
C3       - C2       - C1       = 122.4(2)
C4       - C3       - C2       = 118.9(2)
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C4	- C3	- H3	= 120.6
C2	- C3	- H3	= 120.6
C5	- C4	- C3	= 118.8(2)
C5	- C4	- H4	= 120.6
C3	- C4	- H4	= 120.6
C6	- C5	- C4	= 118.4(2)
C6	- C5	- H5	= 120.8
C4	- C5	- H5	= 120.8
N7	- C6	- C5	= 124.2(2)
N7	- C6	- H6	= 117.9
C5	- C6	- H6	= 117.9
C6	- N7	- C2	= 116.6(2)
N1	- C11	- C12	= 112.98(18)
N1	- C11	- H11A	= 109
C12	- C11	- H11A	= 109
N1	- C11	- H11B	= 109
C12	- C11	- H11B	= 109
H11A	- C11	- H11B	= 107.8
N17	- C12	- C13	= 122.0(2)
N17	- C12	- C11	= 117.40(19)
C13	- C12	- C11	= 120.6(2)
C14	- C13	- C12	= 119.7(2)
C14	- C13	- H13	= 120.2
C12	- C13	- H13	= 120.2
C15	- C14	- C13	= 118.6(2)
C15	- C14	- H14	= 120.7
C13	- C14	- H14	= 120.7
C16	- C15	- C14	= 118.2(2)
C16	- C15	- H15	= 120.9
C14	- C15	- H15	= 120.9
N17	- C16	- C15	= 124.0(2)
N17	- C16	- H16	= 118
C15	- C16	- H16	= 118
C12	- N17	- C16	= 117.5(2)
N1	- C21	- C22	= 112.18(17)
N1	- C21	- H21A	= 109.2
C22	- C21	- H21A	= 109.2
N1	- C21	- H21B	= 109.2
C22	- C21	- H21B	= 109.2
H21A	- C21	- H21B	= 107.9
C23	- C22	- C27	= 119.93(19)
C23	- C22	- C21	= 120.06(18)
C27	- C22	- C21	= 120.00(19)
C24	- C23	- C22	= 121.6(2)
C24	- C23	- H23	= 119.2
C22	- C23	- H23	= 119.2
C23	- C24	- C25	= 116.8(2)
C23	- C24	- C24A	= 123.4(2)
C25	- C24	- C24A	= 119.83(19)
C24D	- C24A	- C24B	= 107.9(2)
C24D	- C24A	- C24C	= 108.6(2)
C24B	- C24A	- C24C	= 108.9(2)
C24D	- C24A	- C24	= 110.88(19)
C24B	- C24A	- C24	= 111.78(18)
C24C	- C24A	- C24	= 108.76(18)
C24A	- C24B	- H24A	= 109.5
C24A	- C24B	- H24B	= 109.5
H24A	- C24B	- H24B	= 109.5

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C24A     - C24B     - H24C     = 109.5
H24A     - C24B     - H24C     = 109.5
H24B     - C24B     - H24C     = 109.5
C24A     - C24C     - H24D     = 109.5
C24A     - C24C     - H24E     = 109.5
H24D     - C24C     - H24E     = 109.5
C24A     - C24C     - H24F     = 109.5
H24D     - C24C     - H24F     = 109.5
H24E     - C24C     - H24F     = 109.5
C24A     - C24D     - H24G     = 109.5
C24A     - C24D     - H24H     = 109.5
H24G     - C24D     - H24H     = 109.5
C24A     - C24D     - H24I     = 109.5
H24G     - C24D     - H24I     = 109.5
H24H     - C24D     - H24I     = 109.5
C26      - C25      - C24      = 124.4(2)
C26      - C25      - H25      = 117.8
C24      - C25      - H25      = 117.8
C25      - C26      - C27      = 116.68(19)
C25      - C26      - C26A     = 121.36(19)
C27      - C26      - C26A     = 121.94(19)
C26C     - C26A     - C26B     = 106.71(18)
C26C     - C26A     - C26D     = 107.81(18)
C26B     - C26A     - C26D     = 109.50(18)
C26C     - C26A     - C26      = 112.08(17)
C26B     - C26A     - C26      = 110.41(17)
C26D     - C26A     - C26      = 110.22(18)
C26A     - C26B     - H26A     = 109.5
C26A     - C26B     - H26B     = 109.5
H26A     - C26B     - H26B     = 109.5
C26A     - C26B     - H26C     = 109.5
H26A     - C26B     - H26C     = 109.5
H26B     - C26B     - H26C     = 109.5
C26A     - C26C     - H26D     = 109.5
C26A     - C26C     - H26E     = 109.5
H26D     - C26C     - H26E     = 109.5
C26A     - C26C     - H26F     = 109.5
H26D     - C26C     - H26F     = 109.5
H26E     - C26C     - H26F     = 109.5
C26A     - C26D     - H26G     = 109.5
C26A     - C26D     - H26H     = 109.5
H26G     - C26D     - H26H     = 109.5
C26A     - C26D     - H26I     = 109.5
H26G     - C26D     - H26I     = 109.5
H26H     - C26D     - H26I     = 109.5
O27      - C27      - C22      = 119.81(18)
O27      - C27      - C26      = 119.67(18)
C22      - C27      - C26      = 120.51(19)
C27      - O27      - H27      = 109.5
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Torsion angles [°]

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C11      - N1       - C1       - C2       = -72.0(2)
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C21	- N1	- C1	- C2	= 167.65(17)
N1	- C1	- C2	- N7	= 154.96(19)
N1	- C1	- C2	- C3	= -27.4(3)
N7	- C2	- C3	- C4	= 0.3(3)
C1	- C2	- C3	- C4	= -177.1(2)
C2	- C3	- C4	- C5	= 0.1(4)
C3	- C4	- C5	- C6	= -0.4(4)
C4	- C5	- C6	- N7	= 0.3(4)
C5	- C6	- N7	- C2	= 0.2(4)
C3	- C2	- N7	- C6	= -0.5(3)
C1	- C2	- N7	- C6	= 177.1(2)
C1	- N1	- C11	- C12	= 170.23(17)
C21	- N1	- C11	- C12	= -69.2(2)
N1	- C11	- C12	- N17	= -35.0(3)
N1	- C11	- C12	- C13	= 146.8(2)
N17	- C12	- C13	- C14	= -1.0(4)
C11	- C12	- C13	- C14	= 177.2(2)
C12	- C13	- C14	- C15	= 1.0(4)
C13	- C14	- C15	- C16	= -0.1(4)
C14	- C15	- C16	- N17	= -0.9(4)
C13	- C12	- N17	- C16	= 0.1(3)
C11	- C12	- N17	- C16	= -178.2(2)
C15	- C16	- N17	- C12	= 0.9(4)
C1	- N1	- C21	- C22	= -66.1(2)
C11	- N1	- C21	- C22	= 172.93(18)
N1	- C21	- C22	- C23	= 126.0(2)
N1	- C21	- C22	- C27	= -55.3(3)
C27	- C22	- C23	- C24	= 0.5(3)
C21	- C22	- C23	- C24	= 179.2(2)
C22	- C23	- C24	- C25	= -0.9(3)
C22	- C23	- C24	- C24A	= 178.2(2)
C23	- C24	- C24A	- C24D	= 128.6(2)
C25	- C24	- C24A	- C24D	= -52.4(3)
C23	- C24	- C24A	- C24B	= 8.2(3)
C25	- C24	- C24A	- C24B	= -172.8(2)
C23	- C24	- C24A	- C24C	= -112.1(2)
C25	- C24	- C24A	- C24C	= 67.0(3)
C23	- C24	- C25	- C26	= -0.7(3)
C24A	- C24	- C25	- C26	= -179.8(2)
C24	- C25	- C26	- C27	= 2.6(3)
C24	- C25	- C26	- C26A	= -175.8(2)
C25	- C26	- C26A	- C26C	= 3.8(3)
C27	- C26	- C26A	- C26C	= -174.5(2)
C25	- C26	- C26A	- C26B	= 122.6(2)
C27	- C26	- C26A	- C26B	= -55.7(3)
C25	- C26	- C26A	- C26D	= -116.3(2)
C27	- C26	- C26A	- C26D	= 65.4(3)
C23	- C22	- C27	- O27	= -179.45(18)
C21	- C22	- C27	- O27	= 1.8(3)
C23	- C22	- C27	- C26	= 1.5(3)
C21	- C22	- C27	- C26	= -177.2(2)
C25	- C26	- C27	- O27	= 178.02(19)
C26A	- C26	- C27	- O27	= -3.6(3)
C25	- C26	- C27	- C22	= -2.9(3)
C26A	- C26	- C27	- C22	= 175.5(2)

[L²]H: Crystal structure report

X-ray crystallographic study

(C_{39} H_{35} N_3 O); *M* = 561.7. APEXII, Bruker-AXS diffractometer, Mo-Kα radiation (λ = 0.71073 Å), *T* = 100(2) K; triclinic *P*-1 (I.T.#2), a = 10.9042(6), b = 13.0721(6), c = 14.7332(7) Å, α = 112.417(2), β = 91.203(2), γ = 104.786(2) °, *V* = 1860.58(16) $Å^3$, *Z* = 2, *d* = 1.003 $g.cm^{-3}$, μ = 0.060 mm^{-1}. The structure was solved by direct methods using the *SIR97* program [1], and then refined with full-matrix least-square methods based on F^2 (*SHELXL-97*) [2] with the aid of the *WINGX* [3] program. The contribution of the disordered solvents to the calculated structure factors was estimated following the *BYPASS* algorithm [4], implemented as the *SQUEEZE* option in *PLATON* [5]. A new data set, free of solvent contribution, was then used in the final refinement. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 8390 unique intensities and 391 parameters converged at $\omega R(F^2)$ = 0.1518 ($R(F)$ = 0.0524) for 5717 observed reflections with $I > 2\sigma(I)$.

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[2] Sheldrick G.M., Acta Cryst. A64 (2008), 112-122

[3] L. J. Farrugia, J. Appl. Cryst., 1999, 32, 837-838

[4] P. v.d. Sluis and A.L. Spek, Acta Cryst. (1990) A46, 194-201

[5] A. L. Spek, J. Appl. Cryst. (2003), 36, 7-13

Structural data

Empirical formula	C_{39} H_{35} N_3 O
Formula weight	561.7
Temperature	100(2) *K*
Wavelength	0.71073 Å
Crystal system, space group	triclinic, *P -1*
Unit cell dimensions	a = 10.9042(6) Å, α = 112.417(2) °
	b = 13.0721(6) Å, β = 91.203(2) °
	c = 14.7332(7) Å, γ = 104.786(2) °
Volume	1860.58(16) $Å^3$
Z, Calculated density	2 , 1.003 ($g.cm^{-3}$)
Absorption coefficient	0.060 mm^{-1}
F(000)	596
Crystal size	0.55 x 0.32 x 0.18 mm
Crystal color	colorless
Theta range for data collection	1.76 to 27.57 °

h_min, h_max	-14 , 14
k_min, k_max	-16 , 16
l_min, l_max	-19 , 19
Reflections collected / unique	34702 / 8390 [R(int) = 0.0481]
Completeness to theta_max	0.975
Absorption correction type	multi-scan
Max. and min. transmission	0.989 , 0.958
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8390 / 0 / 391
Goodness-of-fit	1.093
Final *R* indices [I>2σ]	$R1^a$ = 0.0524, $wR2^b$ = 0.1518
R indices (all data)	$R1^a$ = 0.0744, $wR2^b$ = 0.1591
Largest diff. peak and hole	0.243 and -0.235 e.Å^{-3}

$^a R1 = \sum \; | \; |F_o| - |F_c| \; | \; / \sum |F_o|$

$^b wR2 = \{\sum \; [w(F_o^2 - F_c^2)^2] \; / \sum \; [w(F_o^2)^2]\}^{1/2}$

Atomic coordinates, site occupancy (%) and equivalent isotropic displacement parameters (Å^2 x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	occ.	U(eq)
C1	0.21219(13)	0.50520(11)	0.15735(10)	1	0.0194(3)
C2	0.13186(13)	0.37724(11)	0.10359(10)	1	0.0197(3)
C3	0.09920(14)	0.32248(11)	0.00111(10)	1	0.0214(3)
H3	0.1294	0.3651	-0.0377	1	0.026
C4	0.02462(14)	0.20855(11)	-0.04731(11)	1	0.0236(3)
C5	-0.02193(15)	0.14822(12)	0.01033(11)	1	0.0262(3)
H5	-0.0736	0.0705	-0.0212	1	0.031
C6	0.00501(14)	0.19844(11)	0.11243(11)	1	0.0240(3)
C7	0.08157(14)	0.31360(11)	0.16021(11)	1	0.0214(3)
O7	0.11004(10)	0.36560(8)	0.26025(7)	1	0.0241(2)
H7	0.0707	0.321	0.2854	1	0.036
C8	-0.00320(17)	0.15294(13)	-0.15831(11)	1	0.0312(4)
H8A	0.0625	0.115	-0.1853	1	0.047
H8B	-0.0029	0.212	-0.184	1	0.047
H8C	-0.0873	0.0955	-0.1781	1	0.047
C9	-0.04381(16)	0.12887(12)	0.17259(11)	1	0.0301(4)
H9A	-0.1139	0.0598	0.1311	1	0.036
H9B	0.0261	0.102	0.1911	1	0.036
C11	0.25248(13)	0.55800(11)	0.08060(10)	1	0.0189(3)
C12	0.33488(14)	0.51413(12)	0.01495(11)	1	0.0224(3)
H12	0.3652	0.4538	0.019	1	0.027
C13	0.37354(15)	0.55653(13)	-0.05614(11)	1	0.0256(3)
H13	0.428	0.5241	-0.1011	1	0.031
C14	0.33235(14)	0.64656(13)	-0.06132(12)	1	0.0277(4)
H14	0.3587	0.6764	-0.1096	1	0.033
C15	0.25300(15)	0.69218(12)	0.00422(11)	1	0.0268(4)
H15	0.2257	0.7545	0.0015	1	0.032
C16	0.21222(14)	0.64815(11)	0.07442(11)	1	0.0227(3)
H16	0.1565	0.68	0.1184	1	0.027
C21	0.33951(14)	0.51773(12)	0.21451(10)	1	0.0210(3)

C22	0.37367(15)	0.42516(12)	0.22268(11)	1	0.0242(3)
H22	0.3164	0.3496	0.1922	1	0.029
C23	0.48969(16)	0.44190(15)	0.27445(12)	1	0.0324(4)
H23	0.51	0.3781	0.2804	1	0.039
C24	0.57671(17)	0.55130(16)	0.31776(12)	1	0.0366(4)
H24	0.6557	0.5628	0.354	1	0.044
C25	0.54626(16)	0.64304(15)	0.30717(12)	1	0.0347(4)
H25	0.6056	0.7178	0.3347	1	0.042
C26	0.42962(15)	0.62592(13)	0.25665(11)	1	0.0268(3)
H26	0.4101	0.6899	0.2504	1	0.032
C31	0.12603(14)	0.56925(11)	0.22622(10)	1	0.0204(3)
C32	0.16751(16)	0.64833(13)	0.32308(11)	1	0.0271(3)
H32	0.2528	0.6635	0.3512	1	0.032
C33	0.08657(17)	0.70595(14)	0.38003(12)	1	0.0343(4)
H33	0.1176	0.7608	0.4459	1	0.041
C34	-0.03828(17)	0.68393(13)	0.34148(12)	1	0.0318(4)
H34	-0.0937	0.7227	0.3806	1	0.038
C35	-0.08136(16)	0.60519(13)	0.24572(12)	1	0.0288(4)
H35	-0.1672	0.5895	0.2185	1	0.035
C36	-0.00067(14)	0.54848(12)	0.18850(11)	1	0.0231(3)
H36	-0.0321	0.4945	0.1224	1	0.028
N41	-0.09087(12)	0.19459(10)	0.26282(9)	1	0.0256(3)
C51	-0.10986(16)	0.13267(12)	0.32884(12)	1	0.0298(4)
H51A	-0.1618	0.0519	0.2908	1	0.036
H51B	-0.1575	0.1695	0.3824	1	0.036
C52	0.01612(16)	0.13334(12)	0.37379(11)	1	0.0277(4)
C53	0.02710(18)	0.03996(13)	0.39384(12)	1	0.0341(4)
H53	-0.0448	-0.0254	0.3794	1	0.041
C54	0.14339(19)	0.04353(14)	0.43483(13)	1	0.0396(4)
H54	0.1528	-0.0192	0.4493	1	0.048
C55	0.24628(18)	0.13936(14)	0.45465(13)	1	0.0390(4)
H55	0.3281	0.1439	0.4821	1	0.047
C56	0.22660(18)	0.22845(14)	0.43329(15)	1	0.0421(5)
H56	0.2968	0.2952	0.4479	1	0.051
N57	0.11435(14)	0.22614(11)	0.39320(11)	1	0.0380(4)
C61	-0.20686(16)	0.22286(13)	0.24045(12)	1	0.0303(4)
H61A	-0.2791	0.1515	0.2118	1	0.036
H61B	-0.1929	0.2576	0.1911	1	0.036
C62	-0.23921(15)	0.30663(12)	0.33392(11)	1	0.0255(3)
C63	-0.15426(16)	0.41514(12)	0.38589(12)	1	0.0281(4)
H63	-0.0779	0.4399	0.3607	1	0.034
C64	-0.18225(17)	0.48668(13)	0.47466(12)	1	0.0328(4)
H64	-0.1254	0.5612	0.5117	1	0.039
C65	-0.29480(17)	0.44759(14)	0.50860(12)	1	0.0345(4)
H65	-0.3158	0.4941	0.5701	1	0.041
C66	-0.37566(17)	0.34007(15)	0.45144(12)	1	0.0342(4)
H66	-0.4541	0.3149	0.474	1	0.041
N67	-0.34960(13)	0.26912(11)	0.36562(10)	1	0.0322(3)

Anisotropic displacement parameters ($Å^2$)

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

Atom	U11	U22	U33	U23	U13	U12
C1	0.0220(8)	0.0177(6)	0.0199(8)	0.0084(6)	0.0034(6)	0.0066(5)
C2	0.0212(8)	0.0186(6)	0.0213(8)	0.0081(6)	0.0055(6)	0.0082(5)
C3	0.0240(8)	0.0213(6)	0.0215(8)	0.0088(6)	0.0051(6)	0.0100(6)
C4	0.0270(9)	0.0231(7)	0.0215(8)	0.0068(6)	0.0044(6)	0.0116(6)
C5	0.0274(9)	0.0195(6)	0.0258(9)	0.0036(6)	0.0067(7)	0.0055(6)
C6	0.0284(9)	0.0193(6)	0.0235(8)	0.0072(6)	0.0083(7)	0.0071(6)
C7	0.0255(8)	0.0193(6)	0.0197(8)	0.0063(6)	0.0067(6)	0.0090(6)
O7	0.0333(6)	0.0189(5)	0.0184(6)	0.0080(4)	0.0063(5)	0.0034(4)
C8	0.0428(10)	0.0244(7)	0.0223(9)	0.0045(6)	0.0018(7)	0.0106(7)
C9	0.0410(10)	0.0191(7)	0.0279(9)	0.0077(6)	0.0134(7)	0.0068(6)
C11	0.0191(8)	0.0194(6)	0.0171(7)	0.0074(6)	-0.0008(6)	0.0038(5)
C12	0.0240(8)	0.0244(7)	0.0207(8)	0.0099(6)	0.0032(6)	0.0087(6)
C13	0.0229(8)	0.0321(7)	0.0237(8)	0.0121(7)	0.0053(6)	0.0094(6)
C14	0.0249(9)	0.0350(8)	0.0294(9)	0.0216(7)	0.0036(7)	0.0054(7)
C15	0.0281(9)	0.0284(7)	0.0304(9)	0.0172(7)	0.0044(7)	0.0098(6)
C16	0.0216(8)	0.0229(6)	0.0257(8)	0.0112(6)	0.0046(6)	0.0075(6)
C21	0.0227(8)	0.0273(7)	0.0164(8)	0.0104(6)	0.0061(6)	0.0098(6)
C22	0.0289(9)	0.0297(7)	0.0219(8)	0.0147(6)	0.0099(7)	0.0144(6)
C23	0.0329(10)	0.0534(10)	0.0289(9)	0.0266(8)	0.0132(7)	0.0257(8)
C24	0.0256(9)	0.0646(11)	0.0277(9)	0.0247(9)	0.0040(7)	0.0167(8)
C25	0.0266(9)	0.0443(9)	0.0265(9)	0.0128(8)	-0.0014(7)	0.0017(7)
C26	0.0268(9)	0.0305(7)	0.0246(8)	0.0130(7)	0.0015(7)	0.0081(6)
C31	0.0272(9)	0.0177(6)	0.0209(8)	0.0106(6)	0.0066(6)	0.0092(6)
C32	0.0301(9)	0.0313(7)	0.0224(8)	0.0091(7)	0.0032(7)	0.0154(7)
C33	0.0489(11)	0.0361(8)	0.0214(9)	0.0082(7)	0.0074(8)	0.0228(8)
C34	0.0403(10)	0.0367(8)	0.0319(10)	0.0190(8)	0.0176(8)	0.0242(7)
C35	0.0284(9)	0.0316(8)	0.0359(10)	0.0202(7)	0.0108(7)	0.0133(7)
C36	0.0260(9)	0.0210(6)	0.0229(8)	0.0094(6)	0.0046(6)	0.0066(6)
N41	0.0349(8)	0.0206(6)	0.0236(7)	0.0098(5)	0.0118(6)	0.0096(5)
C51	0.0395(10)	0.0214(7)	0.0299(9)	0.0131(7)	0.0133(7)	0.0059(6)
C52	0.0384(10)	0.0197(7)	0.0229(8)	0.0059(6)	0.0117(7)	0.0084(6)
C53	0.0515(12)	0.0244(7)	0.0247(9)	0.0112(7)	0.0080(8)	0.0055(7)
C54	0.0590(13)	0.0328(8)	0.0335(10)	0.0164(8)	0.0099(9)	0.0189(8)
C55	0.0456(11)	0.0352(8)	0.0370(10)	0.0111(8)	0.0091(8)	0.0176(8)
C56	0.0367(11)	0.0309(8)	0.0581(12)	0.0152(8)	0.0119(9)	0.0119(7)
N57	0.0370(9)	0.0243(6)	0.0527(10)	0.0138(7)	0.0115(7)	0.0110(6)
C61	0.0318(10)	0.0300(8)	0.0258(9)	0.0101(7)	0.0053(7)	0.0048(7)
C62	0.0277(9)	0.0298(7)	0.0221(8)	0.0121(6)	0.0047(7)	0.0108(6)
C63	0.0300(9)	0.0261(7)	0.0314(9)	0.0128(7)	0.0063(7)	0.0111(6)
C64	0.0425(11)	0.0277(7)	0.0321(10)	0.0121(7)	0.0032(8)	0.0164(7)
C65	0.0478(11)	0.0413(9)	0.0271(9)	0.0164(8)	0.0112(8)	0.0288(8)
C66	0.0335(10)	0.0483(10)	0.0328(10)	0.0231(8)	0.0132(8)	0.0201(8)
N67	0.0292(8)	0.0386(7)	0.0292(8)	0.0150(6)	0.0044(6)	0.0079(6)

Bond lengths [Å]

C1 - C21 = 1.547(2)
C1 - C2 = 1.5509(18)

```
C1   - C31      = 1.5514(19)
C1   - C11      = 1.5521(18)
C2   - C3       = 1.394(2)
C2   - C7       = 1.4157(18)
C3   - C4       = 1.3912(19)
C3   - H3       = 0.95
C4   - C5       = 1.388(2)
C4   - C8       = 1.502(2)
C5   - C6       = 1.382(2)
C5   - H5       = 0.95
C6   - C7       = 1.4087(19)
C6   - C9       = 1.5111(19)
C7   - O7       = 1.3563(17)
O7   - H7       = 0.84
C8   - H8A      = 0.98
C8   - H8B      = 0.98
C8   - H8C      = 0.98
C9   - N41      = 1.4667(19)
C9   - H9A      = 0.99
C9   - H9B      = 0.99
C11  - C16      = 1.3906(18)
C11  - C12      = 1.396(2)
C12  - C13      = 1.387(2)
C12  - H12      = 0.95
C13  - C14      = 1.389(2)
C13  - H13      = 0.95
C14  - C15      = 1.377(2)
C14  - H14      = 0.95
C15  - C16      = 1.393(2)
C15  - H15      = 0.95
C16  - H16      = 0.95
C21  - C26      = 1.395(2)
C21  - C22      = 1.3989(18)
C22  - C23      = 1.386(2)
C22  - H22      = 0.95
C23  - C24      = 1.392(3)
C23  - H23      = 0.95
C24  - C25      = 1.384(2)
C24  - H24      = 0.95
C25  - C26      = 1.382(2)
C25  - H25      = 0.95
C26  - H26      = 0.95
C31  - C32      = 1.385(2)
C31  - C36      = 1.397(2)
C32  - C33      = 1.392(2)
C32  - H32      = 0.95
C33  - C34      = 1.379(2)
C33  - H33      = 0.95
C34  - C35      = 1.374(2)
C34  - H34      = 0.95
C35  - C36      = 1.386(2)
C35  - H35      = 0.95
C36  - H36      = 0.95
N41  - C61      = 1.469(2)
N41  - C51      = 1.4721(18)
C51  - C52      = 1.509(2)
C51  - H51A     = 0.99
C51  - H51B     = 0.99
```

C52	- N57	= 1.327(2)
C52	- C53	= 1.393(2)
C53	- C54	= 1.375(3)
C53	- H53	= 0.95
C54	- C55	= 1.380(2)
C54	- H54	= 0.95
C55	- C56	= 1.380(2)
C55	- H55	= 0.95
C56	- N57	= 1.336(2)
C56	- H56	= 0.95
C61	- C62	= 1.512(2)
C61	- H61A	= 0.99
C61	- H61B	= 0.99
C62	- N67	= 1.343(2)
C62	- C63	= 1.388(2)
C63	- C64	= 1.381(2)
C63	- H63	= 0.95
C64	- C65	= 1.385(2)
C64	- H64	= 0.95
C65	- C66	= 1.377(2)
C65	- H65	= 0.95
C66	- N67	= 1.340(2)
C66	- H66	= 0.95

Angles [°]

C21	- C1	- C2	= 112.10(10)
C21	- C1	- C31	= 112.42(11)
C2	- C1	- C31	= 106.71(11)
C21	- C1	- C11	= 104.92(11)
C2	- C1	- C11	= 110.13(11)
C31	- C1	- C11	= 110.62(10)
C3	- C2	- C7	= 117.37(12)
C3	- C2	- C1	= 123.09(11)
C7	- C2	- C1	= 119.41(12)
C4	- C3	- C2	= 123.34(13)
C4	- C3	- H3	= 118.3
C2	- C3	- H3	= 118.3
C5	- C4	- C3	= 117.78(13)
C5	- C4	- C8	= 121.38(13)
C3	- C4	- C8	= 120.84(13)
C6	- C5	- C4	= 121.62(13)
C6	- C5	- H5	= 119.2
C4	- C5	- H5	= 119.2
C5	- C6	- C7	= 119.85(13)
C5	- C6	- C9	= 120.14(12)
C7	- C6	- C9	= 119.98(13)
O7	- C7	- C6	= 121.45(12)
O7	- C7	- C2	= 118.55(12)
C6	- C7	- C2	= 120.00(13)
C7	- O7	- H7	= 109.5

C4	- C8	- H8A	= 109.5
C4	- C8	- H8B	= 109.5
H8A	- C8	- H8B	= 109.5
C4	- C8	- H8C	= 109.5
H8A	- C8	- H8C	= 109.5
H8B	- C8	- H8C	= 109.5
N41	- C9	- C6	= 112.91(11)
N41	- C9	- H9A	= 109
C6	- C9	- H9A	= 109
N41	- C9	- H9B	= 109
C6	- C9	- H9B	= 109
H9A	- C9	- H9B	= 107.8
C16	- C11	- C12	= 117.92(12)
C16	- C11	- C1	= 123.50(12)
C12	- C11	- C1	= 118.57(11)
C13	- C12	- C11	= 121.52(12)
C13	- C12	- H12	= 119.2
C11	- C12	- H12	= 119.2
C12	- C13	- C14	= 119.77(14)
C12	- C13	- H13	= 120.1
C14	- C13	- H13	= 120.1
C15	- C14	- C13	= 119.33(13)
C15	- C14	- H14	= 120.3
C13	- C14	- H14	= 120.3
C14	- C15	- C16	= 120.90(13)
C14	- C15	- H15	= 119.6
C16	- C15	- H15	= 119.6
C11	- C16	- C15	= 120.53(13)
C11	- C16	- H16	= 119.7
C15	- C16	- H16	= 119.7
C26	- C21	- C22	= 117.04(13)
C26	- C21	- C1	= 119.05(11)
C22	- C21	- C1	= 123.82(13)
C23	- C22	- C21	= 121.08(15)
C23	- C22	- H22	= 119.5
C21	- C22	- H22	= 119.5
C22	- C23	- C24	= 120.66(14)
C22	- C23	- H23	= 119.7
C24	- C23	- H23	= 119.7
C25	- C24	- C23	= 118.91(15)
C25	- C24	- H24	= 120.5
C23	- C24	- H24	= 120.5
C26	- C25	- C24	= 120.05(15)
C26	- C25	- H25	= 120
C24	- C25	- H25	= 120
C25	- C26	- C21	= 122.18(14)
C25	- C26	- H26	= 118.9
C21	- C26	- H26	= 118.9
C32	- C31	- C36	= 117.35(13)
C32	- C31	- C1	= 124.03(13)
C36	- C31	- C1	= 118.60(12)
C31	- C32	- C33	= 121.24(15)
C31	- C32	- H32	= 119.4
C33	- C32	- H32	= 119.4
C34	- C33	- C32	= 120.48(15)
C34	- C33	- H33	= 119.8
C32	- C33	- H33	= 119.8
C35	- C34	- C33	= 119.09(14)

C35	- C34	- H34	= 120.5
C33	- C34	- H34	= 120.5
C34	- C35	- C36	= 120.59(15)
C34	- C35	- H35	= 119.7
C36	- C35	- H35	= 119.7
C35	- C36	- C31	= 121.24(14)
C35	- C36	- H36	= 119.4
C31	- C36	- H36	= 119.4
C9	- N41	- C61	= 111.98(12)
C9	- N41	- C51	= 110.36(11)
C61	- N41	- C51	= 112.11(12)
N41	- C51	- C52	= 111.46(12)
N41	- C51	- H51A	= 109.3
C52	- C51	- H51A	= 109.3
N41	- C51	- H51B	= 109.3
C52	- C51	- H51B	= 109.3
H51A	- C51	- H51B	= 108
N57	- C52	- C53	= 122.12(16)
N57	- C52	- C51	= 117.15(13)
C53	- C52	- C51	= 120.74(14)
C54	- C53	- C52	= 119.16(15)
C54	- C53	- H53	= 120.4
C52	- C53	- H53	= 120.4
C53	- C54	- C55	= 119.11(15)
C53	- C54	- H54	= 120.4
C55	- C54	- H54	= 120.4
C54	- C55	- C56	= 117.89(17)
C54	- C55	- H55	= 121.1
C56	- C55	- H55	= 121.1
N57	- C56	- C55	= 123.70(16)
N57	- C56	- H56	= 118.1
C55	- C56	- H56	= 118.1
C52	- N57	- C56	= 118.01(14)
N41	- C61	- C62	= 110.03(12)
N41	- C61	- H61A	= 109.7
C62	- C61	- H61A	= 109.7
N41	- C61	- H61B	= 109.7
C62	- C61	- H61B	= 109.7
H61A	- C61	- H61B	= 108.2
N67	- C62	- C63	= 122.45(14)
N67	- C62	- C61	= 117.04(13)
C63	- C62	- C61	= 120.44(14)
C64	- C63	- C62	= 119.12(15)
C64	- C63	- H63	= 120.4
C62	- C63	- H63	= 120.4
C63	- C64	- C65	= 118.66(15)
C63	- C64	- H64	= 120.7
C65	- C64	- H64	= 120.7
C66	- C65	- C64	= 118.69(15)
C66	- C65	- H65	= 120.7
C64	- C65	- H65	= 120.7
N67	- C66	- C65	= 123.47(16)
N67	- C66	- H66	= 118.3
C65	- C66	- H66	= 118.3
C66	- N67	- C62	= 117.57(14)

L^4: Crystal structure report

X-ray crystallographic study

(C_{44} H_{38} N_2 P_2); M = 656.7. APEXII, Bruker-AXS diffractometer, Mo-Kα radiation (λ = 0.71073 Å), T = 150(2) K; monoclinic $P2_1/c$ (I.T.#14), a = 14.0718(9), b = 13.5580(8), c = 19.6384(9) Å, β = 98.664(2) °, V = 3704.0(4) Å^3, Z = 4, d = 1.178 g.cm^{-3}, μ = 0.150 mm^{-1}. The structure was solved by direct methods using the *SIR97* program [1], and then refined with full-matrix least-square methods based on F^2 (*SHELXL-97*) [2] with the aid of the *WINGX* [3] program. The contribution of the disordered solvents to the calculated structure factors was estimated following the *BYPASS* algorithm [4], implemented as the *SQUEEZE* option in *PLATON* [5]. A new data set, free of solvent contribution, was then used in the final refinement. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 8432 unique intensities and 433 parameters converged at $\omega R(F^2)$ = 0.122 ($R(F)$ = 0.0451) for 6300 observed reflections with $I > 2\sigma(I)$.

[1] A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, J. Appl. Cryst. (1999) 32, 115-119

[2] Sheldrick G.M., Acta Cryst. A64 (2008), 112-122

[3] L. J. Farrugia, J. Appl. Cryst., 1999, 32, 837-838

[4] P. v.d. Sluis and A.L. Spek, Acta Cryst. (1990) A46, 194-201

[5] A. L. Spek, J. Appl. Cryst. (2003), 36, 7-13

Structural data

Empirical formula	C_{44} H_{38} N_2 P_2
Formula weight	656.7
Temperature	150(2) *K*
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, *P* $2_1/c$
Unit cell dimensions	a = 14.0718(9) Å, alpha = 90 °
	b = 13.5580(8) Å, beta = 98.664(2) °
	c = 19.6384(9) Å, gamma = 90 °
Volume	3704.0(4) Å^3
Z, Calculated density	4 , 1.178 (g.cm^{-3})
Absorption coefficient	0.150 mm^{-1}
F(000)	1384
Crystal size	0.27 x 0.18 x 0.11 mm
Crystal color	colourless
Theta range for data collection	2.93 to 27.5 °
h_min, h_max	-18 , 17

k_min, k_max	-17 , 14
l_min, l_max	-15 , 25
Reflections collected / unique	30098 / 8432 [R(int) = 0.0504]
Completeness to theta_max	0.991
Absorption correction type	multi-scan
Max. and min. transmission	0.984 , 0.726
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8432 / 0 / 433
Goodness-of-fit	1.055
Final *R* indices [I>2σ]	$R1^a$ = 0.0451, $wR2^b$ = 0.122
R indices (all data)	$R1^a$ = 0.0638, $wR2^b$ = 0.1312
Largest diff. peak and hole	0.32 and -0.259 e.Å^{-3}

$^a R1 = \sum \; | \; |F_o| - |F_c| \; | \; / \sum |F_o|$

$^b wR2 = \{\sum \; [w(F_o^2 - F_c^2)^2] \; / \sum \; [w(F_o^2)^2]\}^{1/2}$

Atomic coordinates and equivalent isotropic displacement parameters (Å^2 x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
P1	0.31206(3)	1.02606(3)	0.17199(2)	0.02335(12)
C1	0.40166(11)	0.95419(12)	0.13513(8)	0.0250(4)
C2	0.47474(12)	0.89972(12)	0.17347(9)	0.0284(4)
H2	0.4842	0.9039	0.2223	0.034
C3	0.53387(13)	0.83950(14)	0.14123(10)	0.0371(4)
H3	0.5829	0.802	0.1681	0.044
C4	0.52201(14)	0.83365(15)	0.07019(11)	0.0415(5)
H4	0.5623	0.7918	0.0483	0.05
C5	0.45139(15)	0.88881(15)	0.03130(10)	0.0415(5)
H5	0.4443	0.8866	-0.0176	0.05
C6	0.39073(13)	0.94758(13)	0.06346(9)	0.0337(4)
H6	0.341	0.9838	0.0363	0.04
C7	0.34615(11)	1.15296(12)	0.15440(8)	0.0257(3)
C8	0.43026(12)	1.18101(13)	0.12955(9)	0.0299(4)
H8	0.4758	1.1323	0.1214	0.036
C9	0.44760(13)	1.27966(14)	0.11680(9)	0.0358(4)
H9	0.5043	1.2977	0.0991	0.043
C10	0.38353(15)	1.35157(14)	0.12955(10)	0.0420(5)
H10	0.3964	1.4189	0.1212	0.05
C11	0.30025(15)	1.32537(14)	0.15462(11)	0.0430(5)
H11	0.256	1.3747	0.1639	0.052
C12	0.28180(13)	1.22694(13)	0.16616(9)	0.0351(4)
H12	0.2239	1.2094	0.1825	0.042
C13	0.35505(11)	1.01871(11)	0.26523(8)	0.0228(3)
C14	0.42972(12)	1.07719(12)	0.29810(9)	0.0280(4)
H14	0.4621	1.1209	0.2715	0.034
C15	0.45765(12)	1.07264(13)	0.36898(9)	0.0320(4)
H15	0.5087	1.1129	0.3906	0.038
C16	0.41083(13)	1.00920(13)	0.40782(9)	0.0328(4)
H16	0.4292	1.0061	0.4563	0.039
C17	0.33711(12)	0.95010(12)	0.37592(8)	0.0279(4)
H17	0.3055	0.9063	0.4029	0.033
C18	0.30843(11)	0.95374(11)	0.30497(8)	0.0225(3)

C19	0.22671(11)	0.88906(12)	0.27267(8)	0.0236(3)
H19A	0.2001	0.8529	0.3093	0.028
H19B	0.1749	0.9309	0.2481	0.028
P2	0.04059(3)	0.58441(3)	0.17445(2)	0.02546(12)
C21	0.01216(11)	0.45397(13)	0.15967(8)	0.0267(4)
C22	0.04917(12)	0.38891(14)	0.21203(10)	0.0345(4)
H22	0.0878	0.4135	0.2523	0.041
C23	0.03011(13)	0.28875(15)	0.20580(11)	0.0419(5)
H23	0.0563	0.245	0.2415	0.05
C24	-0.02669(13)	0.25240(14)	0.14801(11)	0.0412(5)
H24	-0.0395	0.1837	0.1439	0.049
C25	-0.06518(13)	0.31583(13)	0.09589(10)	0.0367(4)
H25	-0.1051	0.2909	0.0563	0.044
C26	-0.04517(12)	0.41610(13)	0.10166(9)	0.0293(4)
H26	-0.071	0.4594	0.0655	0.035
C27	-0.05845(11)	0.64483(12)	0.11783(9)	0.0260(4)
C28	-0.14862(12)	0.64739(14)	0.13958(10)	0.0352(4)
H28	-0.1566	0.6176	0.1821	0.042
C29	-0.22596(13)	0.69220(15)	0.10052(12)	0.0453(5)
H29	-0.2866	0.6929	0.1162	0.054
C30	-0.21575(14)	0.73642(16)	0.03822(12)	0.0468(5)
H30	-0.269	0.7677	0.0113	0.056
C31	-0.12786(14)	0.73440(17)	0.01594(12)	0.0515(6)
H31	-0.1203	0.764	-0.0268	0.062
C32	-0.04994(13)	0.68922(15)	0.05572(10)	0.0403(5)
H32	0.0106	0.6888	0.0398	0.048
C33	0.14036(11)	0.60437(12)	0.12522(8)	0.0222(3)
C34	0.16495(11)	0.53580(12)	0.07763(8)	0.0248(3)
H34	0.1304	0.4755	0.0711	0.03
C35	0.23848(12)	0.55390(13)	0.03976(8)	0.0275(4)
H35	0.2553	0.5057	0.0085	0.033
C36	0.28754(11)	0.64336(13)	0.04781(8)	0.0279(4)
H36	0.3364	0.6574	0.0207	0.034
C37	0.26517(11)	0.71136(13)	0.09498(8)	0.0269(4)
H37	0.2994	0.772	0.1003	0.032
C38	0.19320(11)	0.69301(12)	0.13515(8)	0.0230(3)
C39	0.17218(11)	0.76819(12)	0.18771(8)	0.0263(4)
H39A	0.1281	0.8187	0.1642	0.032
H39B	0.1385	0.7349	0.2221	0.032
N41	0.25798(9)	0.81791(10)	0.22406(6)	0.0229(3)
C42	0.33291(11)	0.74960(12)	0.25636(8)	0.0255(4)
H42A	0.3832	0.789	0.2849	0.031
H42B	0.3631	0.7186	0.2193	0.031
C43	0.30209(11)	0.66810(13)	0.30098(9)	0.0285(4)
N44	0.27803(11)	0.69472(11)	0.36184(8)	0.0368(4)
C45	0.24938(14)	0.62315(16)	0.40101(11)	0.0472(5)
H45	0.2305	0.6414	0.4437	0.057
C46	0.24545(15)	0.52496(16)	0.38356(13)	0.0516(6)
H46	0.2249	0.477	0.4134	0.062
C47	0.27218(15)	0.49811(15)	0.32159(12)	0.0473(5)
H47	0.2712	0.4308	0.3081	0.057
C48	0.30041(13)	0.57025(13)	0.27939(10)	0.0382(5)
H48	0.3185	0.5534	0.2362	0.046

Anisotropic displacement parameters ($Å^2$)

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

Atom	U11	U22	U33	U23	U13	U12
P1	0.0233(2)	0.0232(2)	0.0246(2)	-0.00015(17)	0.00695(17)	-0.00141(17
C1	0.0276(8)	0.0206(8)	0.0294(8)	-0.0019(7)	0.0121(7)	-0.0057(7)
C2	0.0273(9)	0.0255(9)	0.0339(9)	-0.0017(7)	0.0095(7)	-0.0032(7)
C3	0.0305(9)	0.0280(10)	0.0550(12)	-0.0014(9)	0.0141(9)	0.0009(8)
C4	0.0392(11)	0.0353(11)	0.0564(12)	-0.0072(10)	0.0279(9)	-0.0014(9)
C5	0.0529(12)	0.0414(12)	0.0356(10)	-0.0057(9)	0.0238(9)	-0.0038(9)
C6	0.0416(10)	0.0310(10)	0.0312(9)	0.0010(8)	0.0142(8)	0.0000(8)
C7	0.0273(8)	0.0240(9)	0.0257(8)	0.0026(7)	0.0044(7)	0.0016(7)
C8	0.0293(9)	0.0269(10)	0.0337(9)	0.0028(7)	0.0060(7)	-0.0015(7)
C9	0.0376(10)	0.0333(10)	0.0356(9)	0.0073(8)	0.0022(8)	-0.0104(8)
C10	0.0546(12)	0.0256(10)	0.0432(11)	0.0079(8)	-0.0015(9)	-0.0067(9)
C11	0.0497(12)	0.0265(10)	0.0529(12)	0.0025(9)	0.0076(10)	0.0079(9)
C12	0.0353(10)	0.0315(10)	0.0404(10)	0.0041(8)	0.0120(8)	0.0036(8)
C13	0.0223(8)	0.0206(8)	0.0267(8)	-0.0023(7)	0.0074(6)	0.0023(6)
C14	0.0263(8)	0.0233(9)	0.0352(9)	-0.0024(7)	0.0074(7)	-0.0026(7)
C15	0.0288(9)	0.0284(10)	0.0367(9)	-0.0084(8)	-0.0015(8)	-0.0004(7)
C16	0.0379(10)	0.0327(10)	0.0263(8)	-0.0058(8)	-0.0003(8)	0.0069(8)
C17	0.0342(9)	0.0255(9)	0.0254(8)	-0.0010(7)	0.0094(7)	0.0028(7)
C18	0.0250(8)	0.0192(8)	0.0243(8)	-0.0032(6)	0.0074(7)	0.0024(6)
C19	0.0249(8)	0.0214(8)	0.0265(8)	-0.0012(7)	0.0100(7)	-0.0006(6)
P2	0.0256(2)	0.0277(2)	0.0246(2)	-0.00363(18)	0.00878(17)	-0.00413(18
C21	0.0259(8)	0.0299(9)	0.0271(8)	0.0012(7)	0.0133(7)	-0.0011(7)
C22	0.0264(9)	0.0397(11)	0.0386(10)	0.0098(8)	0.0087(8)	-0.0037(8)
C23	0.0314(10)	0.0385(11)	0.0584(13)	0.0203(10)	0.0158(9)	0.0036(8)
C24	0.0410(11)	0.0246(10)	0.0642(13)	0.0029(9)	0.0284(10)	-0.0008(8)
C25	0.0408(10)	0.0308(10)	0.0422(10)	-0.0071(8)	0.0181(9)	-0.0082(8)
C26	0.0338(9)	0.0280(9)	0.0276(8)	-0.0005(7)	0.0098(7)	-0.0031(7)
C27	0.0224(8)	0.0221(9)	0.0348(9)	-0.0060(7)	0.0085(7)	-0.0050(6)
C28	0.0276(9)	0.0326(10)	0.0484(11)	-0.0036(8)	0.0152(8)	-0.0046(8)
C29	0.0236(9)	0.0436(12)	0.0707(14)	-0.0111(11)	0.0135(9)	-0.0021(8)
C30	0.0284(10)	0.0450(12)	0.0651(14)	-0.0004(11)	0.0012(9)	0.0051(9)
C31	0.0378(11)	0.0640(15)	0.0532(12)	0.0185(11)	0.0087(10)	0.0098(10)
C32	0.0263(9)	0.0553(13)	0.0410(10)	0.0081(10)	0.0109(8)	0.0066(9)
C33	0.0223(8)	0.0238(8)	0.0205(7)	-0.0008(6)	0.0038(6)	-0.0006(6)
C34	0.0260(8)	0.0238(9)	0.0250(8)	-0.0028(7)	0.0053(7)	-0.0016(7)
C35	0.0296(9)	0.0292(9)	0.0248(8)	-0.0055(7)	0.0079(7)	0.0019(7)
C36	0.0248(8)	0.0370(10)	0.0237(8)	0.0005(7)	0.0092(7)	-0.0020(7)
C37	0.0248(8)	0.0291(9)	0.0270(8)	-0.0028(7)	0.0049(7)	-0.0055(7)
C38	0.0231(8)	0.0253(9)	0.0205(7)	-0.0009(6)	0.0028(6)	0.0001(6)
C39	0.0208(8)	0.0270(9)	0.0315(8)	-0.0068(7)	0.0054(7)	-0.0025(7)
N41	0.0215(7)	0.0233(7)	0.0247(7)	-0.0054(6)	0.0055(5)	-0.0016(5)
C42	0.0233(8)	0.0240(9)	0.0300(8)	-0.0048(7)	0.0066(7)	-0.0001(7)
C43	0.0216(8)	0.0272(9)	0.0358(9)	-0.0009(8)	0.0013(7)	0.0026(7)
N44	0.0402(9)	0.0331(9)	0.0394(8)	0.0072(7)	0.0131(7)	0.0052(7)
C45	0.0460(12)	0.0473(13)	0.0505(12)	0.0184(10)	0.0147(10)	0.0086(10)
C46	0.0418(12)	0.0423(13)	0.0681(15)	0.0262(11)	0.0002(11)	0.0004(9)
C47	0.0423(12)	0.0266(10)	0.0668(14)	0.0079(10)	-0.0116(11)	0.0002(9)
C48	0.0359(10)	0.0270(10)	0.0481(11)	-0.0005(9)	-0.0048(9)	0.0034(8)

Bond lengths [Å]

P1 - C1 = 1.8271(17)
P1 - C7 = 1.8329(17)
P1 - C13 = 1.8425(16)
C1 - C2 = 1.392(2)
C1 - C6 = 1.395(2)
C2 - C3 = 1.385(2)
C2 - H2 = 0.95
C3 - C4 = 1.382(3)
C3 - H3 = 0.95
C4 - C5 = 1.379(3)
C4 - H4 = 0.95
C5 - C6 = 1.387(3)
C5 - H5 = 0.95
C6 - H6 = 0.95
C7 - C12 = 1.394(2)
C7 - C8 = 1.399(2)
C8 - C9 = 1.389(2)
C8 - H8 = 0.95
C9 - C10 = 1.376(3)
C9 - H9 = 0.95
C10 - C11 = 1.384(3)
C10 - H10 = 0.95
C11 - C12 = 1.385(3)
C11 - H11 = 0.95
C12 - H12 = 0.95
C13 - C14 = 1.395(2)
C13 - C18 = 1.403(2)
C14 - C15 = 1.390(2)
C14 - H14 = 0.95
C15 - C16 = 1.381(3)
C15 - H15 = 0.95
C16 - C17 = 1.384(2)
C16 - H16 = 0.95
C17 - C18 = 1.392(2)
C17 - H17 = 0.95
C18 - C19 = 1.508(2)
C19 - N41 = 1.4703(19)
C19 - H19A = 0.99
C19 - H19B = 0.99
P2 - C21 = 1.8268(18)
P2 - C27 = 1.8393(17)
P2 - C33 = 1.8407(16)
C21 - C26 = 1.391(2)
C21 - C22 = 1.395(2)
C22 - C23 = 1.386(3)
C22 - H22 = 0.95
C23 - C24 = 1.377(3)
C23 - H23 = 0.95
C24 - C25 = 1.383(3)
C24 - H24 = 0.95
C25 - C26 = 1.389(2)
C25 - H25 = 0.95
C26 - H26 = 0.95
C27 - C32 = 1.382(2)
C27 - C28 = 1.399(2)

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C28  - C29  = 1.375(3)
C28  - H28  = 0.95
C29  - C30  = 1.389(3)
C29  - H29  = 0.95
C30  - C31  = 1.373(3)
C30  - H30  = 0.95
C31  - C32  = 1.389(3)
C31  - H31  = 0.95
C32  - H32  = 0.95
C33  - C34  = 1.398(2)
C33  - C38  = 1.411(2)
C34  - C35  = 1.384(2)
C34  - H34  = 0.95
C35  - C36  = 1.393(2)
C35  - H35  = 0.95
C36  - C37  = 1.377(2)
C36  - H36  = 0.95
C37  - C38  = 1.397(2)
C37  - H37  = 0.95
C38  - C39  = 1.511(2)
C39  - N41  = 1.4704(19)
C39  - H39A = 0.99
C39  - H39B = 0.99
N41  - C42  = 1.473(2)
C42  - C43  = 1.514(2)
C42  - H42A = 0.99
C42  - H42B = 0.99
C43  - N44  = 1.340(2)
C43  - C48  = 1.392(2)
N44  - C45  = 1.338(2)
C45  - C46  = 1.374(3)
C45  - H45  = 0.95
C46  - C47  = 1.376(3)
C46  - H46  = 0.95
C47  - C48  = 1.379(3)
C47  - H47  = 0.95
C48  - H48  = 0.95
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Angles [°]

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C1   - P1   - C7   = 102.13(7)
C1   - P1   - C13  = 102.83(7)
C7   - P1   - C13  = 100.48(7)
C2   - C1   - C6   = 118.16(15)
C2   - C1   - P1   = 124.50(12)
C6   - C1   - P1   = 117.13(13)
C3   - C2   - C1   = 120.75(16)
C3   - C2   - H2   = 119.6
C1   - C2   - H2   = 119.6
C4   - C3   - C2   = 120.38(18)
C4   - C3   - H3   = 119.8
C2   - C3   - H3   = 119.8
C5   - C4   - C3   = 119.69(17)
C5   - C4   - H4   = 120.2
C3   - C4   - H4   = 120.2
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C4   - C5   - C6   = 120.05(17)
C4   - C5   - H5   = 120
C6   - C5   - H5   = 120
C5   - C6   - C1   = 120.94(17)
C5   - C6   - H6   = 119.5
C1   - C6   - H6   = 119.5
C12  - C7   - C8   = 117.84(16)
C12  - C7   - P1   = 116.70(13)
C8   - C7   - P1   = 125.45(13)
C9   - C8   - C7   = 120.35(17)
C9   - C8   - H8   = 119.8
C7   - C8   - H8   = 119.8
C10  - C9   - C8   = 120.77(17)
C10  - C9   - H9   = 119.6
C8   - C9   - H9   = 119.6
C9   - C10  - C11  = 119.73(18)
C9   - C10  - H10  = 120.1
C11  - C10  - H10  = 120.1
C10  - C11  - C12  = 119.68(18)
C10  - C11  - H11  = 120.2
C12  - C11  - H11  = 120.2
C11  - C12  - C7   = 121.60(17)
C11  - C12  - H12  = 119.2
C7   - C12  - H12  = 119.2
C14  - C13  - C18  = 118.83(15)
C14  - C13  - P1   = 122.75(12)
C18  - C13  - P1   = 118.39(11)
C15  - C14  - C13  = 121.20(16)
C15  - C14  - H14  = 119.4
C13  - C14  - H14  = 119.4
C16  - C15  - C14  = 119.64(16)
C16  - C15  - H15  = 120.2
C14  - C15  - H15  = 120.2
C15  - C16  - C17  = 119.87(16)
C15  - C16  - H16  = 120.1
C17  - C16  - H16  = 120.1
C16  - C17  - C18  = 121.14(16)
C16  - C17  - H17  = 119.4
C18  - C17  - H17  = 119.4
C17  - C18  - C13  = 119.31(15)
C17  - C18  - C19  = 119.22(14)
C13  - C18  - C19  = 121.46(13)
N41  - C19  - C18  = 111.76(12)
N41  - C19  - H19A = 109.3
C18  - C19  - H19A = 109.3
N41  - C19  - H19B = 109.3
C18  - C19  - H19B = 109.3
H19A - C19  - H19B = 107.9
C21  - P2   - C27  = 101.96(7)
C21  - P2   - C33  = 103.00(7)
C27  - P2   - C33  = 100.69(7)
C26  - C21  - C22  = 118.45(16)
C26  - C21  - P2   = 124.99(13)
C22  - C21  - P2   = 116.52(13)
C23  - C22  - C21  = 120.58(18)
C23  - C22  - H22  = 119.7
C21  - C22  - H22  = 119.7
C24  - C23  - C22  = 120.27(18)
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C24  - C23  - H23  = 119.9
C22  - C23  - H23  = 119.9
C23  - C24  - C25  = 120.08(18)
C23  - C24  - H24  = 120
C25  - C24  - H24  = 120
C24  - C25  - C26  = 119.73(18)
C24  - C25  - H25  = 120.1
C26  - C25  - H25  = 120.1
C25  - C26  - C21  = 120.88(17)
C25  - C26  - H26  = 119.6
C21  - C26  - H26  = 119.6
C32  - C27  - C28  = 117.52(16)
C32  - C27  - P2   = 124.69(13)
C28  - C27  - P2   = 117.78(13)
C29  - C28  - C27  = 121.26(18)
C29  - C28  - H28  = 119.4
C27  - C28  - H28  = 119.4
C28  - C29  - C30  = 120.25(17)
C28  - C29  - H29  = 119.9
C30  - C29  - H29  = 119.9
C31  - C30  - C29  = 119.33(19)
C31  - C30  - H30  = 120.3
C29  - C30  - H30  = 120.3
C30  - C31  - C32  = 120.1(2)
C30  - C31  - H31  = 119.9
C32  - C31  - H31  = 119.9
C27  - C32  - C31  = 121.50(17)
C27  - C32  - H32  = 119.2
C31  - C32  - H32  = 119.2
C34  - C33  - C38  = 118.71(14)
C34  - C33  - P2   = 122.58(12)
C38  - C33  - P2   = 118.70(11)
C35  - C34  - C33  = 121.43(15)
C35  - C34  - H34  = 119.3
C33  - C34  - H34  = 119.3
C34  - C35  - C36  = 119.43(15)
C34  - C35  - H35  = 120.3
C36  - C35  - H35  = 120.3
C37  - C36  - C35  = 119.99(15)
C37  - C36  - H36  = 120
C35  - C36  - H36  = 120
C36  - C37  - C38  = 121.30(15)
C36  - C37  - H37  = 119.4
C38  - C37  - H37  = 119.4
C37  - C38  - C33  = 119.04(14)
C37  - C38  - C39  = 119.92(14)
C33  - C38  - C39  = 121.03(14)
N41  - C39  - C38  = 114.20(12)
N41  - C39  - H39A = 108.7
C38  - C39  - H39A = 108.7
N41  - C39  - H39B = 108.7
C38  - C39  - H39B = 108.7
H39A - C39  - H39B = 107.6
C19  - N41  - C39  = 108.17(11)
C19  - N41  - C42  = 113.44(12)
C39  - N41  - C42  = 113.76(12)
N41  - C42  - C43  = 117.34(13)
N41  - C42  - H42A = 108
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C43 - C42 - H42A = 108
N41 - C42 - H42B = 108
C43 - C42 - H42B = 108
H42A - C42 - H42B = 107.2
N44 - C43 - C48 = 122.24(17)
N44 - C43 - C42 = 116.92(15)
C48 - C43 - C42 = 120.84(16)
C45 - N44 - C43 = 117.15(17)
N44 - C45 - C46 = 124.3(2)
N44 - C45 - H45 = 117.8
C46 - C45 - H45 = 117.8
C45 - C46 - C47 = 118.1(2)
C45 - C46 - H46 = 121
C47 - C46 - H46 = 121
C46 - C47 - C48 = 119.1(2)
C46 - C47 - H47 = 120.5
C48 - C47 - H47 = 120.5
C47 - C48 - C43 = 119.10(19)
C47 - C48 - H48 = 120.5
C43 - C48 - H48 = 120.5

Torsion angles [°]

C7 - P1 - C1 - C2 = 110.94(14)
C13 - P1 - C1 - C2 = 7.07(16)
C7 - P1 - C1 - C6 = -74.44(14)
C13 - P1 - C1 - C6 = -178.32(13)
C6 - C1 - C2 - C3 = -1.0(2)
P1 - C1 - C2 - C3 = 173.57(13)
C1 - C2 - C3 - C4 = 0.9(3)
C2 - C3 - C4 - C5 = 0.6(3)
C3 - C4 - C5 - C6 = -1.9(3)
C4 - C5 - C6 - C1 = 1.9(3)
C2 - C1 - C6 - C5 = -0.4(3)
P1 - C1 - C6 - C5 = -175.35(14)
C1 - P1 - C7 - C12 = 169.72(13)
C13 - P1 - C7 - C12 = -84.57(14)
C1 - P1 - C7 - C8 = -9.44(16)
C13 - P1 - C7 - C8 = 96.27(15)
C12 - C7 - C8 - C9 = -0.5(2)
P1 - C7 - C8 - C9 = 178.69(13)
C7 - C8 - C9 - C10 = 1.2(3)
C8 - C9 - C10 - C11 = -0.8(3)
C9 - C10 - C11 - C12 = -0.5(3)
C10 - C11 - C12 - C7 = 1.3(3)
C8 - C7 - C12 - C11 = -0.8(3)
P1 - C7 - C12 - C11 = 179.99(15)
C1 - P1 - C13 - C14 = 79.44(14)
C7 - P1 - C13 - C14 = -25.71(15)
C1 - P1 - C13 - C18 = -102.68(13)
C7 - P1 - C13 - C18 = 152.17(13)
C18 - C13 - C14 - C15 = -0.6(2)
P1 - C13 - C14 - C15 = 177.28(13)
C13 - C14 - C15 - C16 = 0.0(3)
C14 - C15 - C16 - C17 = 0.5(3)

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C15  - C16  - C17  - C18  = -0.5(3)
C16  - C17  - C18  - C13  = -0.2(2)
C16  - C17  - C18  - C19  = -179.06(15)
C14  - C13  - C18  - C17  = 0.7(2)
P1   - C13  - C18  - C17  = -177.30(12)
C14  - C13  - C18  - C19  = 179.54(14)
P1   - C13  - C18  - C19  = 1.6(2)
C17  - C18  - C19  - N41  = -117.62(16)
C13  - C18  - C19  - N41  = 63.51(19)
C27  - P2   - C21  - C26  = 22.07(16)
C33  - P2   - C21  - C26  = -82.02(15)
C27  - P2   - C21  - C22  = -155.99(13)
C33  - P2   - C21  - C22  = 99.92(13)
C26  - C21  - C22  - C23  = 0.8(3)
P2   - C21  - C22  - C23  = 179.01(14)
C21  - C22  - C23  - C24  = -0.8(3)
C22  - C23  - C24  - C25  = -0.1(3)
C23  - C24  - C25  - C26  = 0.9(3)
C24  - C25  - C26  - C21  = -0.9(3)
C22  - C21  - C26  - C25  = 0.0(3)
P2   - C21  - C26  - C25  = -178.04(13)
C21  - P2   - C27  - C32  = -105.10(16)
C33  - P2   - C27  - C32  = 0.80(17)
C21  - P2   - C27  - C28  = 75.89(14)
C33  - P2   - C27  - C28  = -178.21(13)
C32  - C27  - C28  - C29  = 0.2(3)
P2   - C27  - C28  - C29  = 179.24(14)
C27  - C28  - C29  - C30  = -0.2(3)
C28  - C29  - C30  - C31  = 0.4(3)
C29  - C30  - C31  - C32  = -0.5(3)
C28  - C27  - C32  - C31  = -0.3(3)
P2   - C27  - C32  - C31  = -179.33(17)
C30  - C31  - C32  - C27  = 0.5(3)
C21  - P2   - C33  - C34  = 12.76(15)
C27  - P2   - C33  - C34  = -92.32(14)
C21  - P2   - C33  - C38  = -168.21(12)
C27  - P2   - C33  - C38  = 86.72(13)
C38  - C33  - C34  - C35  = -1.0(2)
P2   - C33  - C34  - C35  = 178.05(12)
C33  - C34  - C35  - C36  = -1.7(2)
C34  - C35  - C36  - C37  = 2.4(2)
C35  - C36  - C37  - C38  = -0.5(2)
C36  - C37  - C38  - C33  = -2.2(2)
C36  - C37  - C38  - C39  = 178.47(15)
C34  - C33  - C38  - C37  = 2.9(2)
P2   - C33  - C38  - C37  = -176.15(12)
C34  - C33  - C38  - C39  = -177.80(14)
P2   - C33  - C38  - C39  = 3.1(2)
C37  - C38  - C39  - N41  = -37.9(2)
C33  - C38  - C39  - N41  = 142.88(15)
C18  - C19  - N41  - C39  = -171.87(13)
C18  - C19  - N41  - C42  = 60.95(17)
C38  - C39  - N41  - C19  = 179.47(13)
C38  - C39  - N41  - C42  = -53.53(18)
C19  - N41  - C42  - C43  = 74.37(17)
C39  - N41  - C42  - C43  = -49.83(18)
N41  - C42  - C43  - N44  = -71.30(19)
N41  - C42  - C43  - C48  = 109.49(17)
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C48  - C43  - N44  - C45  = -1.8(2)
C42  - C43  - N44  - C45  = 179.03(15)
C43  - N44  - C45  - C46  = 1.6(3)
N44  - C45  - C46  - C47  = -0.4(3)
C45  - C46  - C47  - C48  = -0.8(3)
C46  - C47  - C48  - C43  = 0.7(3)
N44  - C43  - C48  - C47  = 0.6(3)
C42  - C43  - C48  - C47  = 179.81(15)
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L^5: Crystal structure report

X-ray crystallographic study

(2(C_{57} H_{48} N P_3)); *M* = 1679.75. APEXII, Bruker-AXS diffractometer, Mo-Kα radiation (λ = 0.71073 Å), *T* = 150(2) K; triclinic *P*-1 (I.T.#2), a = 15.6653(16), b = 18.0030(18), c = 18.1172(19) Å, α = 98.534(4), ß = 112.551(4), γ = 92.618(4) °, *V* = 4637.0(8) Å^3, *Z* = 2, *d* = 1.203 g.cm^{-3}, μ = 0.167 mm^{-1}. The structure was solved by direct methods using the *SIR97* program [1], and then refined with full-matrix least-square methods based on F^2 (*SHELXL-97*) [2] with the aid of the *WINGX* [3] program. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 20787 unique intensities and 1099 parameters converged at $\omega R(F^2)$ = 0.1132 ($R(F)$ = 0.0488) for 15461 observed reflections with $I > 2\sigma(I)$.

[1] A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, J. Appl. Cryst. (1999) 32, 115-119

[2] Sheldrick G.M., Acta Cryst. A64 (2008), 112-122

[3] L. J. Farrugia, J. Appl. Cryst., 1999, 32, 837-838

Structural data

Empirical formula	C_{114} H_{96} N_2 P_6
Extended formula	2(C_{57} H_{48} N P_3)
Formula weight	1679.75
Temperature	150(2) *K*
Wavelength	0.71073 Å
Crystal system, space group	triclinic, *P -1*
Unit cell dimensions	a = 15.6653(16) Å, α = 98.534(4) ° b = 18.0030(18) Å, β = 112.551(4) ° c = 18.1172(19) Å, γ = 92.618(4) °
Volume	4637.0(8) Å^3
Z, Calculated density	2 , 1.203 (g.cm^{-3})
Absorption coefficient	0.167 mm^{-1}
F(000)	1768
Crystal size	0.56 x 0.39 x 0.25 mm
Crystal color	colourless
Theta range for data collection	2.91 to 27.48 °
h_min, h_max	-14 , 20
k_min, k_max	-23 , 23
l_min, l_max	-23 , 21
Reflections collected / unique	65501 / 20787 [R(int) = 0.0637]
Completeness to theta_max	0.976
Absorption correction type	multi-scan
Max. and min. transmission	0.959 , 0.876
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	20787 / 0 / 1099
Goodness-of-fit	1.038
Final *R* indices [I>2σ]	$R1^a$ = 0.0488, $wR2^b$ = 0.1132
R indices (all data)	$R1^a$ = 0.0714, $wR2^b$ = 0.1261

Largest diff. peak and hole 0.356 and -0.34 e.Å^{-3}

$^{a}R1 = \sum \; | \; |F_o| - |F_c| \; | \; / \sum |F_o|$

$^{b}wR2 = \{\sum \; [w(F_o^2 - F_c^2)^2] \; / \sum \; [w(F_o^2)^2]\}^{1/2}$

Atomic coordinates and equivalent isotropic displacement parameters (Å^2 x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
N1	0.28365(10)	0.26589(7)	0.72405(8)	0.0221(3)
P1	0.46191(3)	0.22248(3)	0.95512(3)	0.02600(11)
C1	0.48733(13)	0.31183(10)	1.02792(10)	0.0263(4)
C2	0.41986(14)	0.33160(11)	1.05707(12)	0.0330(4)
H2	0.3643	0.2985	1.0403	0.04
C3	0.43225(16)	0.39883(12)	1.11022(13)	0.0416(5)
H3	0.3852	0.4114	1.1294	0.05
C4	0.51181(17)	0.44718(12)	1.13526(13)	0.0453(6)
H4	0.5203	0.493	1.172	0.054
C5	0.57992(17)	0.42921(12)	1.10696(14)	0.0472(6)
H5	0.6354	0.4627	1.1244	0.057
C6	0.56724(14)	0.36217(11)	1.05302(12)	0.0368(5)
H6	0.6138	0.3506	1.033	0.044
C7	0.55291(13)	0.16450(10)	1.00450(11)	0.0278(4)
C8	0.63243(14)	0.18788(11)	1.07493(12)	0.0348(5)
H8	0.6423	0.2383	1.1036	0.042
C9	0.69754(15)	0.13806(12)	1.10370(13)	0.0421(5)
H9	0.7522	0.1548	1.1514	0.051
C10	0.68315(16)	0.06462(12)	1.06347(12)	0.0413(5)
H10	0.7273	0.0305	1.084	0.05
C11	0.60509(17)	0.04050(11)	0.99376(13)	0.0450(6)
H11	0.5955	-0.0101	0.9656	0.054
C12	0.54027(16)	0.09005(11)	0.96455(12)	0.0413(5)
H12	0.4862	0.0729	0.9164	0.05
C13	0.50482(12)	0.25418(9)	0.88194(10)	0.0225(4)
C14	0.59356(13)	0.24359(10)	0.88408(11)	0.0278(4)
H14	0.6334	0.2175	0.9234	0.033
C15	0.62435(13)	0.27048(10)	0.82987(11)	0.0307(4)
H15	0.6843	0.2617	0.8314	0.037
C16	0.56824(14)	0.31001(10)	0.77364(11)	0.0314(4)
H16	0.5905	0.3307	0.7382	0.038
C17	0.47944(13)	0.31928(9)	0.76923(10)	0.0281(4)
H17	0.4406	0.3459	0.7299	0.034
C18	0.44563(12)	0.29031(9)	0.82135(10)	0.0223(4)
C19	0.34575(12)	0.29752(9)	0.80874(10)	0.0244(4)
H19A	0.3295	0.2703	0.846	0.029
H19B	0.3375	0.3515	0.8214	0.029
P2	0.20684(3)	0.01548(2)	0.64129(3)	0.02225(11)
C21	0.32754(12)	-0.00448(9)	0.69085(10)	0.0256(4)
C22	0.34421(15)	-0.05522(10)	0.74509(12)	0.0397(5)
H22	0.2934	-0.0783	0.753	0.048
C23	0.43257(16)	-0.07238(12)	0.78711(13)	0.0474(6)
H23	0.4421	-0.1075	0.823	0.057
C24	0.50734(16)	-0.03866(12)	0.77721(12)	0.0440(6)

H24	0.5684	-0.0505	0.8061	0.053
C25	0.49264(14)	0.01227(12)	0.72505(12)	0.0430(5)
H25	0.5441	0.036	0.7185	0.052
C26	0.40346(13)	0.02946(11)	0.68179(11)	0.0321(4)
H26	0.3944	0.0646	0.6459	0.039
C27	0.15361(12)	-0.07101(9)	0.56591(10)	0.0232(4)
C28	0.20216(13)	-0.11855(10)	0.53274(11)	0.0301(4)
H28	0.2679	-0.1088	0.5521	0.036
C29	0.15581(14)	-0.17991(10)	0.47183(12)	0.0375(5)
H29	0.1898	-0.2115	0.4491	0.045
C30	0.06050(14)	-0.19540(11)	0.44400(13)	0.0444(6)
H30	0.0288	-0.2374	0.402	0.053
C31	0.01134(14)	-0.14959(11)	0.47735(14)	0.0448(6)
H31	-0.0542	-0.1603	0.4588	0.054
C32	0.05782(13)	-0.08778(10)	0.53808(12)	0.0328(4)
H32	0.0237	-0.0565	0.5609	0.039
C33	0.21647(11)	0.08186(9)	0.57650(10)	0.0198(3)
C34	0.18501(12)	0.06127(9)	0.49175(10)	0.0243(4)
H34	0.1601	0.0105	0.4667	0.029
C35	0.18949(13)	0.11330(10)	0.44379(11)	0.0275(4)
H35	0.1663	0.0984	0.3864	0.033
C36	0.22778(13)	0.18680(10)	0.47958(11)	0.0277(4)
H36	0.2322	0.2225	0.4471	0.033
C37	0.25984(12)	0.20821(9)	0.56332(10)	0.0259(4)
H37	0.2872	0.2586	0.5877	0.031
C38	0.25287(12)	0.15782(9)	0.61239(10)	0.0220(4)
C39	0.28704(13)	0.18431(9)	0.70350(10)	0.0261(4)
H39A	0.248	0.1565	0.7247	0.031
H39B	0.3518	0.1726	0.7301	0.031
P3	0.14937(3)	0.37639(2)	0.84927(3)	0.02245(11)
C41	0.15716(12)	0.46332(9)	0.91918(10)	0.0234(4)
C42	0.08105(14)	0.49720(10)	0.92389(11)	0.0302(4)
H42	0.0199	0.4756	0.8884	0.036
C43	0.09401(15)	0.56285(10)	0.98043(12)	0.0373(5)
H43	0.0416	0.5854	0.9837	0.045
C44	0.18207(16)	0.59506(10)	1.03131(12)	0.0384(5)
H44	0.1904	0.6402	1.0691	0.046
C45	0.25892(15)	0.56192(10)	1.02769(12)	0.0362(5)
H45	0.3199	0.5842	1.0629	0.043
C46	0.24613(13)	0.49595(10)	0.97239(11)	0.0286(4)
H46	0.2988	0.4727	0.9708	0.034
C47	0.02420(12)	0.34473(9)	0.80416(10)	0.0226(4)
C48	-0.03806(12)	0.36179(9)	0.73143(10)	0.0245(4)
H48	-0.0162	0.3923	0.7024	0.029
C49	-0.13124(13)	0.33474(10)	0.70113(11)	0.0285(4)
H49	-0.1727	0.3466	0.6513	0.034
C50	-0.16454(14)	0.29073(10)	0.74254(12)	0.0334(4)
H50	-0.2287	0.2726	0.7217	0.04
C51	-0.10329(15)	0.27314(11)	0.81510(13)	0.0397(5)
H51	-0.1257	0.2429	0.8441	0.048
C52	-0.01020(14)	0.29937(11)	0.84510(12)	0.0345(5)
H52	0.0312	0.2864	0.8943	0.041
C53	0.16442(12)	0.41498(9)	0.76578(10)	0.0224(4)
C54	0.16318(13)	0.49184(10)	0.76077(11)	0.0269(4)
H54	0.152	0.5257	0.8007	0.032
C55	0.17798(14)	0.51938(11)	0.69881(12)	0.0341(5)
H55	0.1775	0.5718	0.6968	0.041
C56	0.19350(15)	0.47071(11)	0.63985(12)	0.0379(5)

H56	0.2033	0.4894	0.597	0.046
C57	0.19460(14)	0.39476(11)	0.64366(11)	0.0335(5)
H57	0.2046	0.3613	0.6027	0.04
C58	0.18135(12)	0.36604(9)	0.70607(10)	0.0232(4)
C59	0.18831(12)	0.28267(9)	0.70723(11)	0.0264(4)
H59A	0.1689	0.268	0.7495	0.032
H59B	0.146	0.2529	0.654	0.032
N11	0.28523(10)	0.23771(7)	0.24049(8)	0.0210(3)
P11	0.47167(3)	0.21706(3)	0.47932(3)	0.02383(11)
C101	0.50626(13)	0.31104(9)	0.54540(10)	0.0248(4)
C102	0.43598(14)	0.35164(11)	0.55378(11)	0.0328(4)
H102	0.3731	0.3295	0.5281	0.039
C103	0.45699(17)	0.42438(11)	0.59953(13)	0.0429(5)
H103	0.4085	0.4517	0.6048	0.051
C104	0.54778(18)	0.45669(11)	0.63708(13)	0.0446(6)
H104	0.562	0.5062	0.6686	0.053
C105	0.61853(16)	0.41750(11)	0.62916(12)	0.0390(5)
H105	0.6813	0.4399	0.6552	0.047
C106	0.59751(13)	0.34524(10)	0.58299(11)	0.0302(4)
H106	0.6462	0.3187	0.577	0.036
C107	0.55667(12)	0.15737(10)	0.53411(10)	0.0250(4)
C108	0.60027(14)	0.16928(10)	0.61858(11)	0.0332(4)
H108	0.5929	0.2139	0.6498	0.04
C109	0.65417(15)	0.11693(11)	0.65760(12)	0.0404(5)
H109	0.6837	0.1261	0.7152	0.048
C110	0.66547(14)	0.05163(11)	0.61377(13)	0.0373(5)
H110	0.703	0.0161	0.6408	0.045
C111	0.62178(14)	0.03840(11)	0.53020(13)	0.0373(5)
H111	0.629	-0.0067	0.4995	0.045
C112	0.56754(14)	0.09038(10)	0.49080(12)	0.0330(4)
H112	0.5372	0.0802	0.4332	0.04
C113	0.51250(12)	0.23919(9)	0.40121(10)	0.0226(4)
C114	0.60335(12)	0.23278(10)	0.40735(11)	0.0276(4)
H114	0.646	0.2145	0.4524	0.033
C115	0.63238(13)	0.25254(11)	0.34902(12)	0.0337(5)
H115	0.6942	0.2469	0.3537	0.04
C116	0.57133(14)	0.28050(11)	0.28384(12)	0.0360(5)
H116	0.5913	0.2951	0.2442	0.043
C117	0.48133(14)	0.28698(10)	0.27694(11)	0.0317(4)
H117	0.4396	0.3062	0.2322	0.038
C118	0.44995(12)	0.26594(9)	0.33409(10)	0.0228(4)
C119	0.35034(12)	0.27374(10)	0.32238(10)	0.0240(4)
H11A	0.3363	0.2502	0.3631	0.029
H11B	0.3419	0.328	0.3314	0.029
P12	0.19062(3)	-0.01413(2)	0.16463(3)	0.02231(11)
C121	0.09442(12)	0.01251(9)	0.19296(10)	0.0240(4)
C122	0.07299(14)	-0.02844(10)	0.24516(11)	0.0304(4)
H122	0.1074	-0.0689	0.2634	0.036
C123	0.00238(14)	-0.01036(11)	0.27006(11)	0.0377(5)
H123	-0.0129	-0.0396	0.3037	0.045
C124	-0.04616(14)	0.04986(11)	0.24644(12)	0.0381(5)
H124	-0.0936	0.0629	0.2649	0.046
C125	-0.02533(14)	0.09106(11)	0.19585(12)	0.0350(5)
H125	-0.0584	0.1328	0.1798	0.042
C126	0.04340(13)	0.07213(9)	0.16836(11)	0.0282(4)
H126	0.0558	0.1001	0.1324	0.034
C127	0.13649(12)	-0.10053(9)	0.08875(10)	0.0221(4)
C128	0.19396(13)	-0.14263(9)	0.06059(12)	0.0299(4)

H128	0.2589	-0.1271	0.082	0.036
C129	0.15682(14)	-0.20714(10)	0.00140(12)	0.0345(5)
H129	0.1964	-0.235	-0.0181	0.041
C130	0.06282(14)	-0.23114(10)	-0.02937(11)	0.0322(4)
H130	0.0377	-0.2753	-0.0698	0.039
C131	0.00583(13)	-0.19065(9)	-0.00108(10)	0.0280(4)
H131	-0.0588	-0.2073	-0.0217	0.034
C132	0.04208(12)	-0.12556(9)	0.05753(10)	0.0246(4)
H132	0.002	-0.0979	0.0764	0.029
C133	0.19811(11)	0.05313(9)	0.09938(10)	0.0205(4)
C134	0.16277(12)	0.03179(9)	0.01464(10)	0.0239(4)
H134	0.1263	-0.0157	-0.01	0.029
C135	0.17964(13)	0.07807(9)	-0.03418(10)	0.0255(4)
H135	0.154	0.0626	-0.0915	0.031
C136	0.23368(13)	0.14656(10)	0.00080(11)	0.0290(4)
H136	0.2476	0.1777	-0.032	0.035
C137	0.26768(13)	0.16964(9)	0.08451(11)	0.0270(4)
H137	0.3042	0.2172	0.1083	0.032
C138	0.24954(12)	0.12488(9)	0.13445(10)	0.0212(4)
C139	0.28783(12)	0.15531(9)	0.22543(10)	0.0231(4)
H13A	0.2503	0.1305	0.25	0.028
H13B	0.3527	0.1436	0.2511	0.028
P13	0.15362(3)	0.36666(2)	0.36171(3)	0.02350(11)
C141	0.03186(13)	0.32676(9)	0.32538(11)	0.0282(4)
C142	0.00585(16)	0.28784(10)	0.37599(13)	0.0401(5)
H142	0.0515	0.2815	0.4267	0.048
C143	-0.08570(17)	0.25837(11)	0.35328(16)	0.0480(6)
H143	-0.1026	0.2329	0.3888	0.058
C144	-0.15214(17)	0.26597(12)	0.27932(16)	0.0499(6)
H144	-0.215	0.2462	0.2641	0.06
C145	-0.12746(15)	0.30213(12)	0.22750(14)	0.0444(5)
H145	-0.1731	0.306	0.1759	0.053
C146	-0.03624(14)	0.33300(10)	0.25011(12)	0.0333(4)
H146	-0.0201	0.3585	0.2142	0.04
C147	0.15325(13)	0.46057(9)	0.41722(10)	0.0234(4)
C148	0.07427(13)	0.49077(10)	0.42003(11)	0.0278(4)
H148	0.015	0.462	0.3923	0.033
C149	0.08174(15)	0.56323(10)	0.46352(11)	0.0337(5)
H149	0.0276	0.5835	0.4657	0.04
C150	0.16728(16)	0.60563(10)	0.50338(11)	0.0358(5)
H150	0.1717	0.6553	0.5321	0.043
C151	0.24642(15)	0.57635(10)	0.50182(11)	0.0340(5)
H151	0.3054	0.6055	0.5296	0.041
C152	0.23951(13)	0.50379(10)	0.45936(11)	0.0286(4)
H152	0.2942	0.4833	0.459	0.034
C153	0.16022(12)	0.39140(9)	0.26869(10)	0.0210(4)
C154	0.15109(12)	0.46466(9)	0.25146(10)	0.0236(4)
H154	0.1374	0.502	0.287	0.028
C155	0.16150(13)	0.48384(9)	0.18397(11)	0.0267(4)
H155	0.1558	0.5341	0.174	0.032
C156	0.18024(13)	0.42997(10)	0.13094(11)	0.0287(4)
H156	0.1871	0.4426	0.0843	0.034
C157	0.18885(12)	0.35707(10)	0.14717(10)	0.0263(4)
H157	0.2013	0.3199	0.1107	0.032
C158	0.17980(11)	0.33681(9)	0.21511(10)	0.0200(4)
C159	0.19067(12)	0.25558(9)	0.22678(10)	0.0215(4)
H15A	0.1764	0.2473	0.2739	0.026
H15B	0.1458	0.2212	0.178	0.026

Anisotropic displacement parameters ($Å^2$)

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

Atom	U11	U22	U33	U23	U13	U12
N1	0.0241(8)	0.0188(7)	0.0192(7)	-0.0014(6)	0.0057(6)	0.0022(6)
P1	0.0240(3)	0.0289(2)	0.0262(2)	0.00779(19)	0.0104(2)	-0.0001(2)
C1	0.0292(10)	0.0298(9)	0.0243(9)	0.0110(7)	0.0129(8)	0.0051(8)
C2	0.0343(11)	0.0367(10)	0.0358(11)	0.0128(9)	0.0200(9)	0.0056(9)
C3	0.0494(14)	0.0480(12)	0.0418(12)	0.0120(10)	0.0310(11)	0.0165(11)
C4	0.0628(16)	0.0359(11)	0.0415(12)	0.0010(9)	0.0275(12)	0.0064(11)
C5	0.0543(15)	0.0392(11)	0.0494(13)	-0.0021(10)	0.0268(12)	-0.0077(11)
C6	0.0347(12)	0.0397(11)	0.0399(11)	0.0010(9)	0.0217(10)	-0.0026(9)
C7	0.0312(11)	0.0282(9)	0.0277(9)	0.0086(8)	0.0145(8)	0.0021(8)
C8	0.0363(12)	0.0330(10)	0.0328(10)	0.0065(8)	0.0108(9)	0.0065(9)
C9	0.0375(13)	0.0465(12)	0.0366(11)	0.0075(10)	0.0077(10)	0.0106(10)
C10	0.0503(14)	0.0448(12)	0.0385(12)	0.0153(10)	0.0235(11)	0.0205(11)
C11	0.0628(16)	0.0319(10)	0.0399(12)	0.0052(9)	0.0194(11)	0.0133(11)
C12	0.0476(14)	0.0342(10)	0.0335(11)	0.0054(9)	0.0070(10)	0.0030(10)
C13	0.0254(10)	0.0202(8)	0.0205(8)	0.0004(7)	0.0090(7)	-0.0011(7)
C14	0.0252(10)	0.0312(9)	0.0268(9)	0.0045(8)	0.0103(8)	0.0027(8)
C15	0.0275(10)	0.0357(10)	0.0304(10)	-0.0016(8)	0.0162(8)	-0.0011(8)
C16	0.0430(12)	0.0301(9)	0.0264(10)	0.0031(8)	0.0209(9)	-0.0022(9)
C17	0.0365(11)	0.0269(9)	0.0210(9)	0.0037(7)	0.0115(8)	0.0036(8)
C18	0.0260(10)	0.0196(8)	0.0178(8)	-0.0023(7)	0.0073(7)	0.0002(7)
C19	0.0269(10)	0.0238(8)	0.0190(8)	0.0001(7)	0.0065(7)	0.0051(7)
P2	0.0226(2)	0.0192(2)	0.0252(2)	0.00168(17)	0.01072(19)	0.00106(18
C21	0.0261(10)	0.0216(8)	0.0235(9)	-0.0033(7)	0.0065(8)	0.0022(7)
C22	0.0360(12)	0.0328(10)	0.0397(11)	0.0112(9)	0.0025(9)	-0.0037(9)
C23	0.0459(14)	0.0367(11)	0.0427(12)	0.0100(10)	-0.0022(11)	0.0071(10)
C24	0.0366(13)	0.0506(12)	0.0323(11)	-0.0047(10)	0.0026(10)	0.0214(11)
C25	0.0286(12)	0.0632(14)	0.0361(11)	0.0000(11)	0.0146(9)	0.0085(10)
C26	0.0282(11)	0.0404(10)	0.0300(10)	0.0059(8)	0.0136(8)	0.0089(9)
C27	0.0233(9)	0.0187(8)	0.0266(9)	0.0027(7)	0.0094(8)	0.0022(7)
C28	0.0204(10)	0.0285(9)	0.0375(10)	-0.0005(8)	0.0097(8)	0.0014(8)
C29	0.0297(11)	0.0318(10)	0.0432(12)	-0.0078(9)	0.0106(9)	0.0078(9)
C30	0.0302(12)	0.0310(10)	0.0504(13)	-0.0153(9)	0.0007(10)	0.0028(9)
C31	0.0192(10)	0.0390(11)	0.0586(14)	-0.0135(10)	0.0046(10)	0.0002(9)
C32	0.0235(10)	0.0262(9)	0.0439(11)	-0.0028(8)	0.0113(9)	0.0051(8)
C33	0.0165(9)	0.0203(8)	0.0238(8)	0.0019(7)	0.0099(7)	0.0041(7)
C34	0.0237(10)	0.0217(8)	0.0248(9)	-0.0022(7)	0.0091(8)	0.0018(7)
C35	0.0296(10)	0.0314(9)	0.0202(9)	0.0007(7)	0.0099(8)	0.0043(8)
C36	0.0301(10)	0.0290(9)	0.0275(9)	0.0066(8)	0.0147(8)	0.0034(8)
C37	0.0288(10)	0.0219(8)	0.0269(9)	-0.0001(7)	0.0130(8)	-0.0016(7)
C38	0.0235(9)	0.0206(8)	0.0213(8)	0.0008(7)	0.0094(7)	0.0029(7)
C39	0.0330(11)	0.0206(8)	0.0226(9)	0.0005(7)	0.0103(8)	0.0014(8)
P3	0.0249(3)	0.0238(2)	0.0212(2)	0.00716(18)	0.01047(19)	0.00572(19
C41	0.0287(10)	0.0246(8)	0.0210(8)	0.0088(7)	0.0124(8)	0.0038(7)

C42	0.0318(11)	0.0287(9)	0.0314(10)	0.0055(8)	0.0135(9)	0.0067(8)
C43	0.0461(13)	0.0290(10)	0.0452(12)	0.0063(9)	0.0267(10)	0.0110(9)
C44	0.0565(15)	0.0231(9)	0.0382(11)	0.0013(8)	0.0236(11)	-0.0014(9)
C45	0.0385(12)	0.0335(10)	0.0339(11)	0.0027(8)	0.0138(9)	-0.0079(9)
C46	0.0287(10)	0.0320(9)	0.0283(10)	0.0079(8)	0.0140(8)	0.0014(8)
C47	0.0275(10)	0.0194(8)	0.0240(9)	0.0051(7)	0.0129(8)	0.0041(7)
C48	0.0302(10)	0.0223(8)	0.0242(9)	0.0063(7)	0.0134(8)	0.0045(8)
C49	0.0294(10)	0.0277(9)	0.0262(9)	0.0047(8)	0.0083(8)	0.0048(8)
C50	0.0261(10)	0.0315(10)	0.0420(11)	0.0055(9)	0.0137(9)	-0.0015(8)
C51	0.0388(12)	0.0408(11)	0.0471(12)	0.0219(10)	0.0209(10)	-0.0014(10)
C52	0.0344(12)	0.0390(10)	0.0335(10)	0.0179(9)	0.0133(9)	0.0029(9)
C53	0.0187(9)	0.0285(9)	0.0225(9)	0.0089(7)	0.0090(7)	0.0058(7)
C54	0.0319(11)	0.0278(9)	0.0266(9)	0.0103(7)	0.0152(8)	0.0094(8)
C55	0.0396(12)	0.0318(10)	0.0399(11)	0.0178(9)	0.0203(10)	0.0128(9)
C56	0.0461(13)	0.0480(12)	0.0355(11)	0.0242(9)	0.0260(10)	0.0176(10)
C57	0.0407(12)	0.0436(11)	0.0239(9)	0.0112(8)	0.0180(9)	0.0162(9)
C58	0.0186(9)	0.0299(9)	0.0203(8)	0.0050(7)	0.0062(7)	0.0055(7)
C59	0.0257(10)	0.0278(9)	0.0222(9)	-0.0005(7)	0.0079(8)	-0.0012(8)
N11	0.0206(8)	0.0187(6)	0.0212(7)	0.0013(6)	0.0062(6)	0.0041(6)
P11	0.0185(2)	0.0305(2)	0.0231(2)	0.00537(19)	0.00879(19)	0.00165(19
C101	0.0290(10)	0.0294(9)	0.0206(8)	0.0088(7)	0.0131(8)	0.0042(8)
C102	0.0331(11)	0.0396(10)	0.0312(10)	0.0085(8)	0.0175(9)	0.0084(9)
C103	0.0561(15)	0.0403(11)	0.0403(12)	0.0089(10)	0.0258(11)	0.0187(11)
C104	0.0694(17)	0.0299(10)	0.0370(12)	0.0033(9)	0.0250(12)	0.0031(11)
C105	0.0452(13)	0.0383(11)	0.0331(11)	0.0033(9)	0.0176(10)	-0.0106(10)
C106	0.0302(11)	0.0364(10)	0.0267(9)	0.0068(8)	0.0142(8)	0.0006(8)
C107	0.0212(9)	0.0292(9)	0.0262(9)	0.0080(7)	0.0102(8)	0.0006(7)
C108	0.0426(12)	0.0286(9)	0.0266(10)	0.0066(8)	0.0111(9)	0.0030(9)
C109	0.0477(13)	0.0385(11)	0.0276(10)	0.0129(9)	0.0045(9)	0.0026(10)
C110	0.0334(12)	0.0350(10)	0.0447(12)	0.0171(9)	0.0127(10)	0.0071(9)
C111	0.0382(12)	0.0345(10)	0.0433(12)	0.0091(9)	0.0189(10)	0.0117(9)
C112	0.0344(11)	0.0373(10)	0.0273(10)	0.0043(8)	0.0124(9)	0.0061(9)
C113	0.0211(9)	0.0244(8)	0.0202(8)	0.0000(7)	0.0075(7)	-0.0005(7)
C114	0.0203(9)	0.0361(10)	0.0250(9)	0.0034(8)	0.0082(8)	0.0020(8)
C115	0.0208(10)	0.0447(11)	0.0341(10)	-0.0038(9)	0.0136(8)	-0.0025(8)
C116	0.0344(12)	0.0483(12)	0.0288(10)	0.0041(9)	0.0182(9)	-0.0040(9)
C117	0.0340(11)	0.0387(10)	0.0224(9)	0.0073(8)	0.0104(8)	0.0032(9)
C118	0.0224(9)	0.0236(8)	0.0188(8)	-0.0011(7)	0.0061(7)	0.0008(7)
C119	0.0235(9)	0.0279(9)	0.0177(8)	0.0010(7)	0.0057(7)	0.0051(7)
P12	0.0225(2)	0.0200(2)	0.0231(2)	0.00567(17)	0.00685(19)	0.00351(18
C121	0.0259(10)	0.0221(8)	0.0209(8)	-0.0005(7)	0.0079(7)	-0.0016(7)
C122	0.0379(12)	0.0296(9)	0.0239(9)	0.0050(8)	0.0127(9)	0.0003(8)
C123	0.0450(13)	0.0438(11)	0.0279(10)	0.0034(9)	0.0208(10)	-0.0074(10)
C124	0.0344(12)	0.0459(12)	0.0357(11)	-0.0056(9)	0.0210(10)	-0.0025(10)
C125	0.0301(11)	0.0330(10)	0.0432(12)	0.0027(9)	0.0171(9)	0.0056(9)
C126	0.0289(10)	0.0255(9)	0.0316(10)	0.0055(8)	0.0137(8)	0.0010(8)
C127	0.0246(9)	0.0182(8)	0.0246(9)	0.0085(7)	0.0090(7)	0.0042(7)
C128	0.0285(10)	0.0244(9)	0.0401(11)	0.0069(8)	0.0167(9)	0.0042(8)
C129	0.0406(12)	0.0255(9)	0.0424(11)	0.0032(8)	0.0225(10)	0.0071(9)
C130	0.0447(12)	0.0222(9)	0.0270(10)	0.0021(7)	0.0123(9)	0.0013(8)
C131	0.0267(10)	0.0278(9)	0.0255(9)	0.0078(7)	0.0054(8)	-0.0004(8)
C132	0.0263(10)	0.0239(8)	0.0243(9)	0.0084(7)	0.0088(8)	0.0072(7)
C133	0.0181(9)	0.0200(8)	0.0242(9)	0.0045(7)	0.0086(7)	0.0067(7)
C134	0.0228(9)	0.0202(8)	0.0264(9)	0.0029(7)	0.0075(8)	0.0036(7)
C135	0.0298(10)	0.0273(9)	0.0203(8)	0.0033(7)	0.0106(8)	0.0070(8)
C136	0.0384(11)	0.0272(9)	0.0284(10)	0.0079(8)	0.0197(9)	0.0034(8)
C137	0.0333(11)	0.0210(8)	0.0293(9)	0.0024(7)	0.0164(8)	-0.0011(8)
C138	0.0205(9)	0.0212(8)	0.0231(8)	0.0022(7)	0.0103(7)	0.0049(7)

C139	0.0244(9)	0.0200(8)	0.0242(9)	0.0020(7)	0.0093(7)	0.0042(7)
P13	0.0296(3)	0.0220(2)	0.0239(2)	0.00783(18)	0.0141(2)	0.00749(19
C141	0.0365(11)	0.0190(8)	0.0358(10)	0.0015(7)	0.0227(9)	0.0040(8)
C142	0.0512(14)	0.0315(10)	0.0486(13)	0.0103(9)	0.0305(11)	0.0053(10)
C143	0.0622(16)	0.0327(11)	0.0700(17)	0.0032(11)	0.0518(15)	-0.0037(11)
C144	0.0445(14)	0.0443(12)	0.0651(16)	-0.0177(12)	0.0381(13)	-0.0124(11)
C145	0.0358(12)	0.0509(13)	0.0435(12)	-0.0106(10)	0.0207(10)	-0.0073(10)
C146	0.0327(11)	0.0342(10)	0.0329(10)	-0.0032(8)	0.0168(9)	-0.0021(9)
C147	0.0312(10)	0.0244(8)	0.0192(8)	0.0079(7)	0.0132(8)	0.0058(8)
C148	0.0309(11)	0.0277(9)	0.0254(9)	0.0054(7)	0.0110(8)	0.0078(8)
C149	0.0463(13)	0.0300(9)	0.0314(10)	0.0087(8)	0.0203(10)	0.0150(9)
C150	0.0594(15)	0.0239(9)	0.0285(10)	0.0056(8)	0.0220(10)	0.0043(9)
C151	0.0443(13)	0.0314(10)	0.0280(10)	0.0040(8)	0.0176(9)	-0.0053(9)
C152	0.0312(11)	0.0324(9)	0.0268(9)	0.0079(8)	0.0156(8)	0.0028(8)
C153	0.0185(9)	0.0236(8)	0.0213(8)	0.0056(7)	0.0076(7)	0.0037(7)
C154	0.0264(10)	0.0225(8)	0.0251(9)	0.0062(7)	0.0123(8)	0.0074(7)
C155	0.0299(10)	0.0226(8)	0.0295(9)	0.0103(7)	0.0114(8)	0.0054(8)
C156	0.0313(11)	0.0342(10)	0.0249(9)	0.0118(8)	0.0134(8)	0.0052(8)
C157	0.0269(10)	0.0295(9)	0.0231(9)	0.0029(7)	0.0112(8)	0.0053(8)
C158	0.0133(8)	0.0222(8)	0.0214(8)	0.0035(7)	0.0036(7)	0.0018(7)
C159	0.0199(9)	0.0218(8)	0.0217(8)	0.0029(7)	0.0072(7)	0.0023(7)

Bond lengths [Å]

N1 - C59 = 1.461(2)
N1 - C39 = 1.469(2)
N1 - C19 = 1.473(2)
P1 - C7 = 1.8322(19)
P1 - C1 = 1.8424(18)
P1 - C13 = 1.8463(18)
C1 - C2 = 1.389(3)
C1 - C6 = 1.390(3)
C2 - C3 = 1.385(3)
C2 - H2 = 0.95
C3 - C4 = 1.366(3)
C3 - H3 = 0.95
C4 - C5 = 1.381(3)
C4 - H4 = 0.95
C5 - C6 = 1.389(3)
C5 - H5 = 0.95
C6 - H6 = 0.95
C7 - C8 = 1.390(3)
C7 - C12 = 1.392(3)
C8 - C9 = 1.390(3)
C8 - H8 = 0.95
C9 - C10 = 1.375(3)
C9 - H9 = 0.95
C10 - C11 = 1.372(3)
C10 - H10 = 0.95
C11 - C12 = 1.385(3)
C11 - H11 = 0.95
C12 - H12 = 0.95
C13 - C14 = 1.398(2)
C13 - C18 = 1.405(2)
C14 - C15 = 1.384(3)
C14 - H14 = 0.95
C15 - C16 = 1.379(3)

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C15  - H15  = 0.95
C16  - C17  = 1.382(3)
C16  - H16  = 0.95
C17  - C18  = 1.396(2)
C17  - H17  = 0.95
C18  - C19  = 1.507(2)
C19  - H19A = 0.99
C19  - H19B = 0.99
P2   - C27  = 1.8336(16)
P2   - C33  = 1.8342(17)
P2   - C21  = 1.8347(18)
C21  - C26  = 1.388(3)
C21  - C22  = 1.400(3)
C22  - C23  = 1.375(3)
C22  - H22  = 0.95
C23  - C24  = 1.379(3)
C23  - H23  = 0.95
C24  - C25  = 1.377(3)
C24  - H24  = 0.95
C25  - C26  = 1.390(3)
C25  - H25  = 0.95
C26  - H26  = 0.95
C27  - C28  = 1.389(2)
C27  - C32  = 1.389(2)
C28  - C29  = 1.384(2)
C28  - H28  = 0.95
C29  - C30  = 1.380(3)
C29  - H29  = 0.95
C30  - C31  = 1.380(3)
C30  - H30  = 0.95
C31  - C32  = 1.388(3)
C31  - H31  = 0.95
C32  - H32  = 0.95
C33  - C34  = 1.404(2)
C33  - C38  = 1.414(2)
C34  - C35  = 1.385(2)
C34  - H34  = 0.95
C35  - C36  = 1.380(2)
C35  - H35  = 0.95
C36  - C37  = 1.388(2)
C36  - H36  = 0.95
C37  - C38  = 1.389(2)
C37  - H37  = 0.95
C38  - C39  = 1.518(2)
C39  - H39A = 0.99
C39  - H39B = 0.99
P3   - C41  = 1.8288(17)
P3   - C47  = 1.8352(18)
P3   - C53  = 1.8430(17)
C41  - C42  = 1.389(2)
C41  - C46  = 1.394(2)
C42  - C43  = 1.395(2)
C42  - H42  = 0.95
C43  - C44  = 1.372(3)
C43  - H43  = 0.95
C44  - C45  = 1.387(3)
C44  - H44  = 0.95
C45  - C46  = 1.388(2)
```

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C45  - H45  = 0.95
C46  - H46  = 0.95
C47  - C48  = 1.394(2)
C47  - C52  = 1.398(2)
C48  - C49  = 1.382(2)
C48  - H48  = 0.95
C49  - C50  = 1.379(3)
C49  - H49  = 0.95
C50  - C51  = 1.390(3)
C50  - H50  = 0.95
C51  - C52  = 1.378(3)
C51  - H51  = 0.95
C52  - H52  = 0.95
C53  - C54  = 1.401(2)
C53  - C58  = 1.405(2)
C54  - C55  = 1.384(3)
C54  - H54  = 0.95
C55  - C56  = 1.382(3)
C55  - H55  = 0.95
C56  - C57  = 1.380(3)
C56  - H56  = 0.95
C57  - C58  = 1.390(3)
C57  - H57  = 0.95
C58  - C59  = 1.513(2)
C59  - H59A = 0.99
C59  - H59B = 0.99
N11  - C159 = 1.464(2)
N11  - C119 = 1.468(2)
N11  - C139 = 1.4732(19)
P11  - C107 = 1.8294(18)
P11  - C101 = 1.8459(17)
P11  - C113 = 1.8462(18)
C101 - C106 = 1.391(2)
C101 - C102 = 1.392(3)
C102 - C103 = 1.393(3)
C102 - H102 = 0.95
C103 - C104 = 1.374(3)
C103 - H103 = 0.95
C104 - C105 = 1.382(3)
C104 - H104 = 0.95
C105 - C106 = 1.388(3)
C105 - H105 = 0.95
C106 - H106 = 0.95
C107 - C112 = 1.393(2)
C107 - C108 = 1.393(2)
C108 - C109 = 1.383(3)
C108 - H108 = 0.95
C109 - C110 = 1.376(3)
C109 - H109 = 0.95
C110 - C111 = 1.379(3)
C110 - H110 = 0.95
C111 - C112 = 1.383(3)
C111 - H111 = 0.95
C112 - H112 = 0.95
C113 - C114 = 1.396(2)
C113 - C118 = 1.405(2)
C114 - C115 = 1.384(3)
C114 - H114 = 0.95
```

```
C115 - C116 = 1.385(3)
C115 - H115 = 0.95
C116 - C117 = 1.379(3)
C116 - H116 = 0.95
C117 - C118 = 1.395(3)
C117 - H117 = 0.95
C118 - C119 = 1.508(2)
C119 - H11A = 0.99
C119 - H11B = 0.99
P12  - C121 = 1.8306(18)
P12  - C127 = 1.8383(16)
P12  - C133 = 1.8427(17)
C121 - C126 = 1.392(2)
C121 - C122 = 1.407(2)
C122 - C123 = 1.380(3)
C122 - H122 = 0.95
C123 - C124 = 1.379(3)
C123 - H123 = 0.95
C124 - C125 = 1.380(3)
C124 - H124 = 0.95
C125 - C126 = 1.385(3)
C125 - H125 = 0.95
C126 - H126 = 0.95
C127 - C132 = 1.390(2)
C127 - C128 = 1.395(2)
C128 - C129 = 1.388(2)
C128 - H128 = 0.95
C129 - C130 = 1.381(3)
C129 - H129 = 0.95
C130 - C131 = 1.375(3)
C130 - H130 = 0.95
C131 - C132 = 1.390(2)
C131 - H131 = 0.95
C132 - H132 = 0.95
C133 - C134 = 1.402(2)
C133 - C138 = 1.411(2)
C134 - C135 = 1.387(2)
C134 - H134 = 0.95
C135 - C136 = 1.378(2)
C135 - H135 = 0.95
C136 - C137 = 1.389(2)
C136 - H136 = 0.95
C137 - C138 = 1.393(2)
C137 - H137 = 0.95
C138 - C139 = 1.523(2)
C139 - H13A = 0.99
C139 - H13B = 0.99
P13  - C141 = 1.833(2)
P13  - C147 = 1.8359(17)
P13  - C153 = 1.8443(17)
C141 - C142 = 1.396(3)
C141 - C146 = 1.397(3)
C142 - C143 = 1.386(3)
C142 - H142 = 0.95
C143 - C144 = 1.377(3)
C143 - H143 = 0.95
C144 - C145 = 1.375(3)
C144 - H144 = 0.95
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C145 - C146 = 1.389(3)
C145 - H145 = 0.95
C146 - H146 = 0.95
C147 - C148 = 1.390(2)
C147 - C152 = 1.397(2)
C148 - C149 = 1.395(2)
C148 - H148 = 0.95
C149 - C150 = 1.379(3)
C149 - H149 = 0.95
C150 - C151 = 1.378(3)
C150 - H150 = 0.95
C151 - C152 = 1.391(2)
C151 - H151 = 0.95
C152 - H152 = 0.95
C153 - C154 = 1.401(2)
C153 - C158 = 1.406(2)
C154 - C155 = 1.384(2)
C154 - H154 = 0.95
C155 - C156 = 1.384(2)
C155 - H155 = 0.95
C156 - C157 = 1.388(2)
C156 - H156 = 0.95
C157 - C158 = 1.389(2)
C157 - H157 = 0.95
C158 - C159 = 1.516(2)
C159 - H15A = 0.99
C159 - H15B = 0.99

Angles [°]

C59 - N1 - C39 = 110.94(13)
C59 - N1 - C19 = 111.06(13)
C39 - N1 - C19 = 112.22(13)
C7 - P1 - C1 = 105.19(8)
C7 - P1 - C13 = 100.48(8)
C1 - P1 - C13 = 99.40(8)
C2 - C1 - C6 = 117.82(17)
C2 - C1 - P1 = 117.40(14)
C6 - C1 - P1 = 124.73(14)
C3 - C2 - C1 = 121.13(19)
C3 - C2 - H2 = 119.4
C1 - C2 - H2 = 119.4
C4 - C3 - C2 = 120.33(19)
C4 - C3 - H3 = 119.8
C2 - C3 - H3 = 119.8
C3 - C4 - C5 = 119.83(19)
C3 - C4 - H4 = 120.1
C5 - C4 - H4 = 120.1
C4 - C5 - C6 = 119.9(2)
C4 - C5 - H5 = 120
C6 - C5 - H5 = 120
C5 - C6 - C1 = 120.93(19)
C5 - C6 - H6 = 119.5
C1 - C6 - H6 = 119.5
C8 - C7 - C12 = 118.16(18)

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C8   - C7   - P1   = 126.84(14)
C12  - C7   - P1   = 114.97(14)
C7   - C8   - C9   = 120.45(18)
C7   - C8   - H8   = 119.8
C9   - C8   - H8   = 119.8
C10  - C9   - C8   = 120.3(2)
C10  - C9   - H9   = 119.9
C8   - C9   - H9   = 119.9
C11  - C10  - C9   = 120.1(2)
C11  - C10  - H10  = 120
C9   - C10  - H10  = 120
C10  - C11  - C12  = 119.84(19)
C10  - C11  - H11  = 120.1
C12  - C11  - H11  = 120.1
C11  - C12  - C7   = 121.15(19)
C11  - C12  - H12  = 119.4
C7   - C12  - H12  = 119.4
C14  - C13  - C18  = 118.61(16)
C14  - C13  - P1   = 122.84(13)
C18  - C13  - P1   = 118.55(13)
C15  - C14  - C13  = 121.10(17)
C15  - C14  - H14  = 119.4
C13  - C14  - H14  = 119.4
C16  - C15  - C14  = 120.16(18)
C16  - C15  - H15  = 119.9
C14  - C15  - H15  = 119.9
C15  - C16  - C17  = 119.49(17)
C15  - C16  - H16  = 120.3
C17  - C16  - H16  = 120.3
C16  - C17  - C18  = 121.34(17)
C16  - C17  - H17  = 119.3
C18  - C17  - H17  = 119.3
C17  - C18  - C13  = 119.11(17)
C17  - C18  - C19  = 118.24(15)
C13  - C18  - C19  = 122.63(16)
N1   - C19  - C18  = 110.25(13)
N1   - C19  - H19A = 109.6
C18  - C19  - H19A = 109.6
N1   - C19  - H19B = 109.6
C18  - C19  - H19B = 109.6
H19A - C19  - H19B = 108.1
C27  - P2   - C33  = 101.19(7)
C27  - P2   - C21  = 102.19(7)
C33  - P2   - C21  = 102.38(8)
C26  - C21  - C22  = 117.90(17)
C26  - C21  - P2   = 125.19(14)
C22  - C21  - P2   = 116.83(15)
C23  - C22  - C21  = 121.4(2)
C23  - C22  - H22  = 119.3
C21  - C22  - H22  = 119.3
C22  - C23  - C24  = 120.1(2)
C22  - C23  - H23  = 119.9
C24  - C23  - H23  = 119.9
C25  - C24  - C23  = 119.4(2)
C25  - C24  - H24  = 120.3
C23  - C24  - H24  = 120.3
C24  - C25  - C26  = 120.9(2)
C24  - C25  - H25  = 119.6
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C26  - C25  - H25  = 119.6
C21  - C26  - C25  = 120.28(19)
C21  - C26  - H26  = 119.9
C25  - C26  - H26  = 119.9
C28  - C27  - C32  = 118.40(15)
C28  - C27  - P2   = 124.29(13)
C32  - C27  - P2   = 117.26(13)
C29  - C28  - C27  = 120.73(17)
C29  - C28  - H28  = 119.6
C27  - C28  - H28  = 119.6
C30  - C29  - C28  = 120.28(18)
C30  - C29  - H29  = 119.9
C28  - C29  - H29  = 119.9
C29  - C30  - C31  = 119.76(17)
C29  - C30  - H30  = 120.1
C31  - C30  - H30  = 120.1
C30  - C31  - C32  = 119.91(18)
C30  - C31  - H31  = 120
C32  - C31  - H31  = 120
C31  - C32  - C27  = 120.90(17)
C31  - C32  - H32  = 119.6
C27  - C32  - H32  = 119.6
C34  - C33  - C38  = 118.25(15)
C34  - C33  - P2   = 122.65(12)
C38  - C33  - P2   = 119.03(12)
C35  - C34  - C33  = 121.53(15)
C35  - C34  - H34  = 119.2
C33  - C34  - H34  = 119.2
C36  - C35  - C34  = 119.82(16)
C36  - C35  - H35  = 120.1
C34  - C35  - H35  = 120.1
C35  - C36  - C37  = 119.56(17)
C35  - C36  - H36  = 120.2
C37  - C36  - H36  = 120.2
C36  - C37  - C38  = 121.68(15)
C36  - C37  - H37  = 119.2
C38  - C37  - H37  = 119.2
C37  - C38  - C33  = 119.07(15)
C37  - C38  - C39  = 119.77(14)
C33  - C38  - C39  = 121.13(15)
N1   - C39  - C38  = 111.65(14)
N1   - C39  - H39A = 109.3
C38  - C39  - H39A = 109.3
N1   - C39  - H39B = 109.3
C38  - C39  - H39B = 109.3
H39A - C39  - H39B = 108
C41  - P3   - C47  = 102.66(8)
C41  - P3   - C53  = 101.00(8)
C47  - P3   - C53  = 101.27(8)
C42  - C41  - C46  = 118.62(16)
C42  - C41  - P3   = 124.51(14)
C46  - C41  - P3   = 116.84(13)
C41  - C42  - C43  = 120.34(18)
C41  - C42  - H42  = 119.8
C43  - C42  - H42  = 119.8
C44  - C43  - C42  = 120.32(19)
C44  - C43  - H43  = 119.8
C42  - C43  - H43  = 119.8
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C43  - C44  - C45  = 120.17(17)
C43  - C44  - H44  = 119.9
C45  - C44  - H44  = 119.9
C44  - C45  - C46  = 119.59(19)
C44  - C45  - H45  = 120.2
C46  - C45  - H45  = 120.2
C45  - C46  - C41  = 120.94(18)
C45  - C46  - H46  = 119.5
C41  - C46  - H46  = 119.5
C48  - C47  - C52  = 118.17(17)
C48  - C47  - P3   = 124.40(13)
C52  - C47  - P3   = 117.43(14)
C49  - C48  - C47  = 120.68(16)
C49  - C48  - H48  = 119.7
C47  - C48  - H48  = 119.7
C50  - C49  - C48  = 120.62(17)
C50  - C49  - H49  = 119.7
C48  - C49  - H49  = 119.7
C49  - C50  - C51  = 119.38(18)
C49  - C50  - H50  = 120.3
C51  - C50  - H50  = 120.3
C52  - C51  - C50  = 120.18(18)
C52  - C51  - H51  = 119.9
C50  - C51  - H51  = 119.9
C51  - C52  - C47  = 120.97(18)
C51  - C52  - H52  = 119.5
C47  - C52  - H52  = 119.5
C54  - C53  - C58  = 118.27(16)
C54  - C53  - P3   = 122.76(13)
C58  - C53  - P3   = 118.93(13)
C55  - C54  - C53  = 121.29(16)
C55  - C54  - H54  = 119.4
C53  - C54  - H54  = 119.4
C56  - C55  - C54  = 120.04(17)
C56  - C55  - H55  = 120
C54  - C55  - H55  = 120
C57  - C56  - C55  = 119.45(18)
C57  - C56  - H56  = 120.3
C55  - C56  - H56  = 120.3
C56  - C57  - C58  = 121.48(17)
C56  - C57  - H57  = 119.3
C58  - C57  - H57  = 119.3
C57  - C58  - C53  = 119.46(16)
C57  - C58  - C59  = 117.58(15)
C53  - C58  - C59  = 122.95(15)
N1   - C59  - C58  = 110.41(14)
N1   - C59  - H59A = 109.6
C58  - C59  - H59A = 109.6
N1   - C59  - H59B = 109.6
C58  - C59  - H59B = 109.6
H59A - C59  - H59B = 108.1
C159 - N11  - C119 = 110.38(13)
C159 - N11  - C139 = 110.73(13)
C119 - N11  - C139 = 112.32(13)
C107 - P11  - C101 = 104.76(8)
C107 - P11  - C113 = 103.34(8)
C101 - P11  - C113 = 97.55(7)
C106 - C101 - C102 = 118.39(16)
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C106 - C101 - P11  = 123.78(14)
C102 - C101 - P11  = 117.71(14)
C101 - C102 - C103 = 120.60(19)
C101 - C102 - H102 = 119.7
C103 - C102 - H102 = 119.7
C104 - C103 - C102 = 120.0(2)
C104 - C103 - H103 = 120
C102 - C103 - H103 = 120
C103 - C104 - C105 = 120.27(19)
C103 - C104 - H104 = 119.9
C105 - C104 - H104 = 119.9
C104 - C105 - C106 = 119.7(2)
C104 - C105 - H105 = 120.2
C106 - C105 - H105 = 120.2
C105 - C106 - C101 = 121.00(18)
C105 - C106 - H106 = 119.5
C101 - C106 - H106 = 119.5
C112 - C107 - C108 = 117.72(17)
C112 - C107 - P11  = 118.45(14)
C108 - C107 - P11  = 123.04(14)
C109 - C108 - C107 = 120.85(17)
C109 - C108 - H108 = 119.6
C107 - C108 - H108 = 119.6
C110 - C109 - C108 = 120.65(18)
C110 - C109 - H109 = 119.7
C108 - C109 - H109 = 119.7
C109 - C110 - C111 = 119.31(18)
C109 - C110 - H110 = 120.3
C111 - C110 - H110 = 120.3
C110 - C111 - C112 = 120.35(18)
C110 - C111 - H111 = 119.8
C112 - C111 - H111 = 119.8
C111 - C112 - C107 = 121.10(18)
C111 - C112 - H112 = 119.4
C107 - C112 - H112 = 119.4
C114 - C113 - C118 = 118.81(16)
C114 - C113 - P11  = 122.87(13)
C118 - C113 - P11  = 118.29(13)
C115 - C114 - C113 = 121.22(17)
C115 - C114 - H114 = 119.4
C113 - C114 - H114 = 119.4
C114 - C115 - C116 = 119.96(18)
C114 - C115 - H115 = 120
C116 - C115 - H115 = 120
C117 - C116 - C115 = 119.41(18)
C117 - C116 - H116 = 120.3
C115 - C116 - H116 = 120.3
C116 - C117 - C118 = 121.64(17)
C116 - C117 - H117 = 119.2
C118 - C117 - H117 = 119.2
C117 - C118 - C113 = 118.93(17)
C117 - C118 - C119 = 118.89(15)
C113 - C118 - C119 = 122.17(16)
N11  - C119 - C118 = 111.60(13)
N11  - C119 - H11A = 109.3
C118 - C119 - H11A = 109.3
N11  - C119 - H11B = 109.3
C118 - C119 - H11B = 109.3
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H11A - C119 - H11B = 108
C121 - P12  - C127 = 101.54(8)
C121 - P12  - C133 = 104.36(8)
C127 - P12  - C133 = 101.08(7)
C126 - C121 - C122 = 118.10(17)
C126 - C121 - P12  = 124.19(14)
C122 - C121 - P12  = 117.67(13)
C123 - C122 - C121 = 120.61(18)
C123 - C122 - H122 = 119.7
C121 - C122 - H122 = 119.7
C124 - C123 - C122 = 120.49(19)
C124 - C123 - H123 = 119.8
C122 - C123 - H123 = 119.8
C123 - C124 - C125 = 119.55(18)
C123 - C124 - H124 = 120.2
C125 - C124 - H124 = 120.2
C124 - C125 - C126 = 120.59(18)
C124 - C125 - H125 = 119.7
C126 - C125 - H125 = 119.7
C125 - C126 - C121 = 120.62(18)
C125 - C126 - H126 = 119.7
C121 - C126 - H126 = 119.7
C132 - C127 - C128 = 118.54(15)
C132 - C127 - P12  = 123.87(13)
C128 - C127 - P12  = 117.59(13)
C129 - C128 - C127 = 120.37(18)
C129 - C128 - H128 = 119.8
C127 - C128 - H128 = 119.8
C130 - C129 - C128 = 120.47(18)
C130 - C129 - H129 = 119.8
C128 - C129 - H129 = 119.8
C131 - C130 - C129 = 119.58(16)
C131 - C130 - H130 = 120.2
C129 - C130 - H130 = 120.2
C130 - C131 - C132 = 120.46(17)
C130 - C131 - H131 = 119.8
C132 - C131 - H131 = 119.8
C131 - C132 - C127 = 120.58(16)
C131 - C132 - H132 = 119.7
C127 - C132 - H132 = 119.7
C134 - C133 - C138 = 118.09(15)
C134 - C133 - P12  = 121.35(12)
C138 - C133 - P12  = 120.14(12)
C135 - C134 - C133 = 121.79(15)
C135 - C134 - H134 = 119.1
C133 - C134 - H134 = 119.1
C136 - C135 - C134 = 119.79(16)
C136 - C135 - H135 = 120.1
C134 - C135 - H135 = 120.1
C135 - C136 - C137 = 119.40(16)
C135 - C136 - H136 = 120.3
C137 - C136 - H136 = 120.3
C136 - C137 - C138 = 121.70(16)
C136 - C137 - H137 = 119.1
C138 - C137 - H137 = 119.1
C137 - C138 - C133 = 119.12(15)
C137 - C138 - C139 = 118.22(14)
C133 - C138 - C139 = 122.66(15)
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N11  - C139 - C138 = 110.24(13)
N11  - C139 - H13A = 109.6
C138 - C139 - H13A = 109.6
N11  - C139 - H13B = 109.6
C138 - C139 - H13B = 109.6
H13A - C139 - H13B = 108.1
C141 - P13  - C147 = 102.21(8)
C141 - P13  - C153 = 102.10(8)
C147 - P13  - C153 = 100.85(7)
C142 - C141 - C146 = 118.21(19)
C142 - C141 - P13  = 117.96(16)
C146 - C141 - P13  = 123.83(15)
C143 - C142 - C141 = 120.9(2)
C143 - C142 - H142 = 119.6
C141 - C142 - H142 = 119.6
C144 - C143 - C142 = 120.1(2)
C144 - C143 - H143 = 120
C142 - C143 - H143 = 120
C145 - C144 - C143 = 120.0(2)
C145 - C144 - H144 = 120
C143 - C144 - H144 = 120
C144 - C145 - C146 = 120.5(2)
C144 - C145 - H145 = 119.8
C146 - C145 - H145 = 119.8
C145 - C146 - C141 = 120.3(2)
C145 - C146 - H146 = 119.8
C141 - C146 - H146 = 119.8
C148 - C147 - C152 = 118.67(16)
C148 - C147 - P13  = 124.82(14)
C152 - C147 - P13  = 116.50(13)
C147 - C148 - C149 = 120.14(18)
C147 - C148 - H148 = 119.9
C149 - C148 - H148 = 119.9
C150 - C149 - C148 = 120.34(19)
C150 - C149 - H149 = 119.8
C148 - C149 - H149 = 119.8
C151 - C150 - C149 = 120.30(17)
C151 - C150 - H150 = 119.8
C149 - C150 - H150 = 119.8
C150 - C151 - C152 = 119.60(19)
C150 - C151 - H151 = 120.2
C152 - C151 - H151 = 120.2
C151 - C152 - C147 = 120.93(18)
C151 - C152 - H152 = 119.5
C147 - C152 - H152 = 119.5
C154 - C153 - C158 = 118.32(15)
C154 - C153 - P13  = 121.92(12)
C158 - C153 - P13  = 119.67(12)
C155 - C154 - C153 = 121.55(16)
C155 - C154 - H154 = 119.2
C153 - C154 - H154 = 119.2
C154 - C155 - C156 = 120.13(16)
C154 - C155 - H155 = 119.9
C156 - C155 - H155 = 119.9
C155 - C156 - C157 = 118.79(17)
C155 - C156 - H156 = 120.6
C157 - C156 - H156 = 120.6
C156 - C157 - C158 = 122.04(16)
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C156 - C157 - H157 = 119
C158 - C157 - H157 = 119
C157 - C158 - C153 = 119.16(15)
C157 - C158 - C159 = 117.50(14)
C153 - C158 - C159 = 123.33(15)
N11 - C159 - C158 = 111.24(13)
N11 - C159 - H15A = 109.4
C158 - C159 - H15A = 109.4
N11 - C159 - H15B = 109.4
C158 - C159 - H15B = 109.4
H15A - C159 - H15B = 108

Torsion angles [°]

C7 - P1 - C1 - C2 = -119.21(15)
C13 - P1 - C1 - C2 = 137.14(15)
C7 - P1 - C1 - C6 = 63.61(18)
C13 - P1 - C1 - C6 = -40.04(18)
C6 - C1 - C2 - C3 = -0.8(3)
P1 - C1 - C2 - C3 = -178.18(15)
C1 - C2 - C3 - C4 = -0.2(3)
C2 - C3 - C4 - C5 = 0.5(3)
C3 - C4 - C5 - C6 = 0.2(3)
C4 - C5 - C6 - C1 = -1.1(3)
C2 - C1 - C6 - C5 = 1.4(3)
P1 - C1 - C6 - C5 = 178.61(16)
C1 - P1 - C7 - C8 = -10.0(2)
C13 - P1 - C7 - C8 = 92.85(18)
C1 - P1 - C7 - C12 = 171.88(15)
C13 - P1 - C7 - C12 = -85.28(16)
C12 - C7 - C8 - C9 = 0.6(3)
P1 - C7 - C8 - C9 = -177.44(16)
C7 - C8 - C9 - C10 = -1.1(3)
C8 - C9 - C10 - C11 = 1.2(3)
C9 - C10 - C11 - C12 = -0.8(3)
C10 - C11 - C12 - C7 = 0.3(3)
C8 - C7 - C12 - C11 = -0.2(3)
P1 - C7 - C12 - C11 = 178.07(18)
C7 - P1 - C13 - C14 = -10.68(16)
C1 - P1 - C13 - C14 = 96.82(15)
C7 - P1 - C13 - C18 = 169.13(13)
C1 - P1 - C13 - C18 = -83.38(14)
C18 - C13 - C14 - C15 = 2.4(2)
P1 - C13 - C14 - C15 = -177.76(13)
C13 - C14 - C15 - C16 = 1.5(3)
C14 - C15 - C16 - C17 = -3.2(3)
C15 - C16 - C17 - C18 = 0.9(3)
C16 - C17 - C18 - C13 = 3.1(2)
C16 - C17 - C18 - C19 = -175.45(15)
C14 - C13 - C18 - C17 = -4.7(2)
P1 - C13 - C18 - C17 = 175.53(12)
C14 - C13 - C18 - C19 = 173.79(15)
P1 - C13 - C18 - C19 = -6.0(2)
C59 - N1 - C19 - C18 = -171.25(14)
C39 - N1 - C19 - C18 = 63.93(18)

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C17  - C18  - C19  - N1   = 53.60(19)
C13  - C18  - C19  - N1   = -124.86(16)
C27  - P2   - C21  - C26  = 108.49(15)
C33  - P2   - C21  - C26  = 3.97(16)
C27  - P2   - C21  - C22  = -74.88(15)
C33  - P2   - C21  - C22  = -179.40(13)
C26  - C21  - C22  - C23  = -1.3(3)
P2   - C21  - C22  - C23  = -178.16(16)
C21  - C22  - C23  - C24  = 0.9(3)
C22  - C23  - C24  - C25  = 0.1(3)
C23  - C24  - C25  - C26  = -0.7(3)
C22  - C21  - C26  - C25  = 0.7(3)
P2   - C21  - C26  - C25  = 177.29(14)
C24  - C25  - C26  - C21  = 0.3(3)
C33  - P2   - C27  - C28  = 79.54(16)
C21  - P2   - C27  - C28  = -25.90(18)
C33  - P2   - C27  - C32  = -97.61(15)
C21  - P2   - C27  - C32  = 156.95(15)
C32  - C27  - C28  - C29  = 1.8(3)
P2   - C27  - C28  - C29  = -175.33(15)
C27  - C28  - C29  - C30  = -1.0(3)
C28  - C29  - C30  - C31  = -0.2(3)
C29  - C30  - C31  - C32  = 0.7(4)
C30  - C31  - C32  - C27  = 0.2(3)
C28  - C27  - C32  - C31  = -1.4(3)
P2   - C27  - C32  - C31  = 175.95(17)
C27  - P2   - C33  - C34  = 1.30(16)
C21  - P2   - C33  - C34  = 106.59(15)
C27  - P2   - C33  - C38  = 178.18(13)
C21  - P2   - C33  - C38  = -76.53(14)
C38  - C33  - C34  - C35  = 0.3(3)
P2   - C33  - C34  - C35  = 177.23(13)
C33  - C34  - C35  - C36  = 1.7(3)
C34  - C35  - C36  - C37  = -1.2(3)
C35  - C36  - C37  - C38  = -1.2(3)
C36  - C37  - C38  - C33  = 3.2(3)
C36  - C37  - C38  - C39  = -178.69(16)
C34  - C33  - C38  - C37  = -2.7(2)
P2   - C33  - C38  - C37  = -179.74(13)
C34  - C33  - C38  - C39  = 179.23(16)
P2   - C33  - C38  - C39  = 2.2(2)
C59  - N1   - C39  - C38  = 75.87(18)
C19  - N1   - C39  - C38  = -159.24(15)
C37  - C38  - C39  - N1   = 26.5(2)
C33  - C38  - C39  - N1   = -155.51(16)
C47  - P3   - C41  - C42  = -7.43(17)
C53  - P3   - C41  - C42  = 96.92(16)
C47  - P3   - C41  - C46  = 170.84(13)
C53  - P3   - C41  - C46  = -84.82(14)
C46  - C41  - C42  - C43  = 0.5(3)
P3   - C41  - C42  - C43  = 178.74(14)
C41  - C42  - C43  - C44  = 0.7(3)
C42  - C43  - C44  - C45  = -1.0(3)
C43  - C44  - C45  - C46  = -0.1(3)
C44  - C45  - C46  - C41  = 1.4(3)
C42  - C41  - C46  - C45  = -1.6(3)
P3   - C41  - C46  - C45  = -179.93(14)
C41  - P3   - C47  - C48  = 93.91(15)
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C53  - P3   - C47  - C48  = -10.23(16)
C41  - P3   - C47  - C52  = -87.28(15)
C53  - P3   - C47  - C52  = 168.58(14)
C52  - C47  - C48  - C49  = 0.3(2)
P3   - C47  - C48  - C49  = 179.10(13)
C47  - C48  - C49  - C50  = 0.4(3)
C48  - C49  - C50  - C51  = -0.5(3)
C49  - C50  - C51  - C52  = -0.1(3)
C50  - C51  - C52  - C47  = 0.9(3)
C48  - C47  - C52  - C51  = -0.9(3)
P3   - C47  - C52  - C51  = -179.83(15)
C41  - P3   - C53  - C54  = -10.16(17)
C47  - P3   - C53  - C54  = 95.29(16)
C41  - P3   - C53  - C58  = 167.38(14)
C47  - P3   - C53  - C58  = -87.17(14)
C58  - C53  - C54  - C55  = 0.1(3)
P3   - C53  - C54  - C55  = 177.68(14)
C53  - C54  - C55  - C56  = 0.6(3)
C54  - C55  - C56  - C57  = -0.4(3)
C55  - C56  - C57  - C58  = -0.7(3)
C56  - C57  - C58  - C53  = 1.4(3)
C56  - C57  - C58  - C59  = -177.16(18)
C54  - C53  - C58  - C57  = -1.1(3)
P3   - C53  - C58  - C57  = -178.77(14)
C54  - C53  - C58  - C59  = 177.36(16)
P3   - C53  - C58  - C59  = -0.3(2)
C39  - N1   - C59  - C58  = -164.37(13)
C19  - N1   - C59  - C58  = 70.08(17)
C57  - C58  - C59  - N1   = 67.2(2)
C53  - C58  - C59  - N1   = -111.32(18)
C107 - P11  - C101 - C106 = 45.35(16)
C113 - P11  - C101 - C106 = -60.65(16)
C107 - P11  - C101 - C102 = -138.74(14)
C113 - P11  - C101 - C102 = 115.26(15)
C106 - C101 - C102 - C103 = -0.7(3)
P11  - C101 - C102 - C103 = -176.85(15)
C101 - C102 - C103 - C104 = -0.2(3)
C102 - C103 - C104 - C105 = 0.5(3)
C103 - C104 - C105 - C106 = 0.0(3)
C104 - C105 - C106 - C101 = -0.9(3)
C102 - C101 - C106 - C105 = 1.3(3)
P11  - C101 - C106 - C105 = 177.15(14)
C101 - P11  - C107 - C112 = -160.70(15)
C113 - P11  - C107 - C112 = -59.04(16)
C101 - P11  - C107 - C108 = 29.76(18)
C113 - P11  - C107 - C108 = 131.42(16)
C112 - C107 - C108 - C109 = 1.5(3)
P11  - C107 - C108 - C109 = 171.07(16)
C107 - C108 - C109 - C110 = -0.4(3)
C108 - C109 - C110 - C111 = -0.5(3)
C109 - C110 - C111 - C112 = 0.3(3)
C110 - C111 - C112 - C107 = 0.8(3)
C108 - C107 - C112 - C111 = -1.7(3)
P11  - C107 - C112 - C111 = -171.78(16)
C107 - P11  - C113 - C114 = -19.91(16)
C101 - P11  - C113 - C114 = 87.28(15)
C107 - P11  - C113 - C118 = 162.20(13)
C101 - P11  - C113 - C118 = -90.61(14)
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C118 - C113 - C114 - C115 = 0.3(3)
P11  - C113 - C114 - C115 = -177.59(13)
C113 - C114 - C115 - C116 = 1.2(3)
C114 - C115 - C116 - C117 = -1.3(3)
C115 - C116 - C117 - C118 = -0.1(3)
C116 - C117 - C118 - C113 = 1.5(3)
C116 - C117 - C118 - C119 = -179.37(16)
C114 - C113 - C118 - C117 = -1.6(2)
P11  - C113 - C118 - C117 = 176.39(13)
C114 - C113 - C118 - C119 = 179.31(15)
P11  - C113 - C118 - C119 = -2.7(2)
C159 - N11  - C119 - C118 = -171.69(14)
C139 - N11  - C119 - C118 = 64.21(18)
C117 - C118 - C119 - N11  = 51.2(2)
C113 - C118 - C119 - N11  = -129.65(16)
C127 - P12  - C121 - C126 = -105.58(15)
C133 - P12  - C121 - C126 = -0.82(16)
C127 - P12  - C121 - C122 = 76.66(14)
C133 - P12  - C121 - C122 = -178.58(13)
C126 - C121 - C122 - C123 = 0.9(3)
P12  - C121 - C122 - C123 = 178.82(14)
C121 - C122 - C123 - C124 = -2.3(3)
C122 - C123 - C124 - C125 = 1.6(3)
C123 - C124 - C125 - C126 = 0.4(3)
C124 - C125 - C126 - C121 = -1.7(3)
C122 - C121 - C126 - C125 = 1.1(3)
P12  - C121 - C126 - C125 = -176.68(14)
C121 - P12  - C127 - C132 = 8.67(16)
C133 - P12  - C127 - C132 = -98.67(15)
C121 - P12  - C127 - C128 = -172.03(14)
C133 - P12  - C127 - C128 = 80.63(14)
C132 - C127 - C128 - C129 = 1.4(3)
P12  - C127 - C128 - C129 = -177.97(14)
C127 - C128 - C129 - C130 = -1.1(3)
C128 - C129 - C130 - C131 = 0.1(3)
C129 - C130 - C131 - C132 = 0.6(3)
C130 - C131 - C132 - C127 = -0.3(3)
C128 - C127 - C132 - C131 = -0.7(2)
P12  - C127 - C132 - C131 = 178.60(13)
C121 - P12  - C133 - C134 = -102.54(14)
C127 - P12  - C133 - C134 = 2.56(16)
C121 - P12  - C133 - C138 = 84.98(14)
C127 - P12  - C133 - C138 = -169.91(13)
C138 - C133 - C134 - C135 = 2.0(2)
P12  - C133 - C134 - C135 = -170.58(13)
C133 - C134 - C135 - C136 = 1.0(3)
C134 - C135 - C136 - C137 = -2.4(3)
C135 - C136 - C137 - C138 = 0.8(3)
C136 - C137 - C138 - C133 = 2.3(3)
C136 - C137 - C138 - C139 = -178.72(16)
C134 - C133 - C138 - C137 = -3.6(2)
P12  - C133 - C138 - C137 = 169.09(13)
C134 - C133 - C138 - C139 = 177.43(15)
P12  - C133 - C138 - C139 = -9.9(2)
C159 - N11  - C139 - C138 = 77.26(17)
C119 - N11  - C139 - C138 = -158.83(14)
C137 - C138 - C139 - N11  = 35.7(2)
C133 - C138 - C139 - N11  = -145.32(16)
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C147 - P13  - C141 - C142 = -88.47(15)
C153 - P13  - C141 - C142 = 167.44(14)
C147 - P13  - C141 - C146 = 91.57(16)
C153 - P13  - C141 - C146 = -12.51(16)
C146 - C141 - C142 - C143 = -2.1(3)
P13  - C141 - C142 - C143 = 177.94(14)
C141 - C142 - C143 - C144 = 1.3(3)
C142 - C143 - C144 - C145 = 0.7(3)
C143 - C144 - C145 - C146 = -1.8(3)
C144 - C145 - C146 - C141 = 0.9(3)
C142 - C141 - C146 - C145 = 1.0(3)
P13  - C141 - C146 - C145 = -179.01(14)
C141 - P13  - C147 - C148 = -5.51(17)
C153 - P13  - C147 - C148 = 99.54(16)
C141 - P13  - C147 - C152 = 174.40(13)
C153 - P13  - C147 - C152 = -80.54(14)
C152 - C147 - C148 - C149 = 0.7(3)
P13  - C147 - C148 - C149 = -179.36(14)
C147 - C148 - C149 - C150 = 0.6(3)
C148 - C149 - C150 - C151 = -1.1(3)
C149 - C150 - C151 - C152 = 0.4(3)
C150 - C151 - C152 - C147 = 1.0(3)
C148 - C147 - C152 - C151 = -1.5(3)
P13  - C147 - C152 - C151 = 178.57(14)
C141 - P13  - C153 - C154 = 96.56(15)
C147 - P13  - C153 - C154 = -8.59(16)
C141 - P13  - C153 - C158 = -86.87(14)
C147 - P13  - C153 - C158 = 167.98(14)
C158 - C153 - C154 - C155 = -0.4(3)
P13  - C153 - C154 - C155 = 176.19(13)
C153 - C154 - C155 - C156 = 0.8(3)
C154 - C155 - C156 - C157 = -0.4(3)
C155 - C156 - C157 - C158 = -0.4(3)
C156 - C157 - C158 - C153 = 0.8(3)
C156 - C157 - C158 - C159 = -179.93(16)
C154 - C153 - C158 - C157 = -0.4(2)
P13  - C153 - C158 - C157 = -177.05(13)
C154 - C153 - C158 - C159 = -179.60(15)
P13  - C153 - C158 - C159 = 3.7(2)
C119 - N11  - C159 - C158 = 73.36(17)
C139 - N11  - C159 - C158 = -161.63(13)
C157 - C158 - C159 - N11  = 64.73(19)
C153 - C158 - C159 - N11  = -116.02(17)
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$L^5 \cdot HCl$: Crystal structure report

X-ray crystallographic study

(C_{60} H_{52} Cl_{10} N P_3); M = 1234.44. APEXII, Bruker-AXS diffractometer, Mo-Kα radiation (λ = 0.71073 Å), T = 150(2) K; triclinic P-1 (I.T.#2), a = 10.8501(19), b = 13.843(2), c = 20.392(3) Å, α = 93.544(6), ß = 95.702(6), &gamma = 96.184(7) °, V = 3021.8(8) $Å^3$, Z = 2, d = 1.357 $g.cm^{-3}$, μ = 0.579 mm^{-1}. The structure was solved by direct methods using the *SIR97* program [1], and then refined with full-matrix least-square methods based on F^2 (*SHELXL-97*) [2] with the aid of the *WINGX* [3] program. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 13664 unique intensities and 671 parameters converged at $\omega R(F^2)$ = 0.1481 ($R(F)$ = 0.0631) for 10236 observed reflections with $I > 2\sigma(I)$.

[1] A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, J. Appl. Cryst. (1999) 32, 115-119

[2] Sheldrick G.M., Acta Cryst. A64 (2008), 112-122

[3] L. J. Farrugia, J. Appl. Cryst., 1999, 32, 837-838

[4] P. v.d. Sluis and A.L. Spek, Acta Cryst. (1990) A46, 194-201

[5] A. L. Spek, J. Appl. Cryst. (2003), 36, 7-13

Structural data

Empirical formula	C_{60} H_{52} Cl_{10} N P_3
Formula weight	1234.44
Temperature	150(2) *K*
Wavelength	0.71073 Å
Crystal system, space group	triclinic, *P -1*
Unit cell dimensions	a = 10.8501(19) Å, alpha = 93.544(6) °
	b = 13.843(2) Å, beta = 95.702(6) °
	c = 20.392(3) Å, gamma = 96.184(7) °
Volume	3021.8(8) $Å^3$
Z, Calculated density	2 , 1.357 ($g.cm^{-3}$)
Absorption coefficient	0.579 mm^{-1}
F(000)	1268
Crystal size	0.57 x 0.51 x 0.42 mm
Crystal color	colourless
Theta range for data collection	2.91 to 27.49 °
h_min, h_max	-14 , 14
k_min, k_max	-17 , 17
l_min, l_max	-16 , 26
Reflections collected / unique	44988 / 13664 [R(int) = 0.0554]
Completeness to theta_max	0.987
Absorption correction type	multi-scan

Max. and min. transmission	0.784 , 0.645
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13664 / 0 / 671
Goodness-of-fit	1.052
Final *R* indices [I>2σ]	$R1^a$ = 0.0631, $wR2^b$ = 0.1481
R indices (all data)	$R1^a$ = 0.087, $wR2^b$ = 0.1619
Largest diff. peak and hole	1.563 and -1.534 e.Å^{-3}

$^a R1 = \sum \; | \; |F_o| - |F_c| \; | \; / \sum |F_o|$

$^b wR2 = \{\sum \; [w(F_o^2 - F_c^2)^2] \; / \sum \; [w(F_o^2)^2]\}^{1/2}$

Atomic coordinates and equivalent isotropic displacement parameters (Å^2 x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U(eq)
N1	0.2988(2)	0.12728(16)	0.74664(11)	0.0188(5)
H1	0.3452	0.1879	0.7472	0.023
P1	0.24071(7)	0.36305(5)	0.74830(3)	0.02101(16)
P2	0.49906(7)	0.23703(5)	0.65324(4)	0.02327(16)
P3	0.50664(7)	0.26127(5)	0.86947(4)	0.02480(17)
C1	0.1626(2)	0.1418(2)	0.74501(13)	0.0216(6)
H1A	0.1382	0.1743	0.7046	0.026
H1B	0.1129	0.0771	0.7418	0.026
C2	0.1296(2)	0.2010(2)	0.80397(13)	0.0208(5)
C3	0.0690(3)	0.1527(2)	0.85129(15)	0.0268(6)
H3	0.0552	0.0836	0.8476	0.032
C4	0.0281(3)	0.2040(2)	0.90390(15)	0.0315(7)
H4	-0.0121	0.1699	0.9363	0.038
C5	0.0458(3)	0.3043(2)	0.90920(15)	0.0312(7)
H5	0.0159	0.3396	0.9446	0.037
C6	0.1079(3)	0.3540(2)	0.86234(14)	0.0268(6)
H6	0.1208	0.4231	0.8664	0.032
C7	0.1513(2)	0.3032(2)	0.80943(13)	0.0216(6)
C8	0.2807(3)	0.4874(2)	0.78534(14)	0.0249(6)
C9	0.2070(3)	0.5618(2)	0.77380(16)	0.0366(8)
H9	0.1292	0.5483	0.7473	0.044
C10	0.2469(4)	0.6561(3)	0.80101(19)	0.0479(10)
H10	0.1967	0.707	0.7925	0.057
C11	0.3583(4)	0.6757(3)	0.8401(2)	0.0515(10)
H11	0.3847	0.74	0.8588	0.062
C12	0.4322(4)	0.6023(3)	0.8523(2)	0.0513(10)
H12	0.5089	0.6159	0.8799	0.062
C13	0.3943(3)	0.5087(2)	0.82434(18)	0.0380(8)
H13	0.4463	0.4586	0.8318	0.046
C14	0.1196(3)	0.3777(2)	0.68157(14)	0.0238(6)
C15	0.1600(3)	0.4006(2)	0.62130(15)	0.0343(7)
H15	0.2467	0.408	0.6167	0.041
C16	0.0745(4)	0.4127(3)	0.56737(16)	0.0422(8)
H16	0.103	0.4284	0.5263	0.051
C17	-0.0505(4)	0.4020(3)	0.57378(18)	0.0460(9)
H17	-0.109	0.4091	0.537	0.055
C18	-0.0911(4)	0.3811(4)	0.6335(2)	0.0638(13)
H18	-0.1778	0.3757	0.6381	0.077

C19	-0.0066(3)	0.3677(3)	0.68754(18)	0.0495(10)
H19	-0.036	0.3517	0.7283	0.059
C21	0.3192(3)	0.0668(2)	0.68458(13)	0.0216(6)
H21A	0.4087	0.0579	0.6857	0.026
H21B	0.2715	0.0016	0.6841	0.026
C22	0.2793(3)	0.1136(2)	0.62203(13)	0.0228(6)
C23	0.1647(3)	0.0794(2)	0.58673(14)	0.0268(6)
H23	0.1149	0.026	0.6014	0.032
C24	0.1224(3)	0.1226(2)	0.53028(15)	0.0324(7)
H24	0.0432	0.1	0.5071	0.039
C25	0.1967(3)	0.1987(2)	0.50810(15)	0.0332(7)
H25	0.1688	0.2283	0.4694	0.04
C26	0.3121(3)	0.2318(2)	0.54243(14)	0.0298(7)
H26	0.3627	0.2837	0.5265	0.036
C27	0.3552(3)	0.1904(2)	0.59987(13)	0.0227(6)
C28	0.5484(3)	0.3519(2)	0.61911(15)	0.0262(6)
C29	0.5982(3)	0.3602(2)	0.55919(16)	0.0325(7)
H29	0.6085	0.3033	0.5328	0.039
C30	0.6326(3)	0.4511(3)	0.53796(18)	0.0402(8)
H30	0.6662	0.4566	0.4969	0.048
C31	0.6183(3)	0.5342(3)	0.5766(2)	0.0463(9)
H31	0.642	0.5966	0.5619	0.056
C32	0.5700(3)	0.5268(3)	0.6362(2)	0.0439(9)
H32	0.5605	0.584	0.6625	0.053
C33	0.5351(3)	0.4359(2)	0.65765(17)	0.0337(7)
H33	0.502	0.4309	0.6989	0.04
C34	0.6116(3)	0.1556(2)	0.62872(14)	0.0252(6)
C35	0.7223(4)	0.1620(3)	0.6692(2)	0.0548(11)
H35	0.7375	0.2089	0.706	0.066
C36	0.8114(4)	0.1007(4)	0.6569(2)	0.0652(13)
H36	0.8879	0.1069	0.6847	0.078
C37	0.7902(3)	0.0317(3)	0.60519(19)	0.0429(8)
H37	0.8516	-0.0102	0.5968	0.051
C38	0.6812(4)	0.0234(4)	0.5661(2)	0.0697(15)
H38	0.6653	-0.0256	0.5306	0.084
C39	0.5915(4)	0.0858(3)	0.5771(2)	0.0623(13)
H39	0.5159	0.0799	0.5485	0.075
C41	0.3430(3)	0.0781(2)	0.80781(13)	0.0219(6)
H41A	0.3223	0.1154	0.8475	0.026
H41B	0.2978	0.0118	0.8062	0.026
C42	0.4814(3)	0.0709(2)	0.81409(13)	0.0226(6)
C43	0.5228(3)	-0.0162(2)	0.79295(15)	0.0285(6)
H43	0.4641	-0.0696	0.7753	0.034
C44	0.6497(3)	-0.0257(2)	0.79754(17)	0.0367(8)
H44	0.6777	-0.0847	0.7817	0.044
C45	0.7342(3)	0.0506(3)	0.82510(19)	0.0410(8)
H45	0.8208	0.0439	0.8287	0.049
C46	0.6946(3)	0.1370(2)	0.84766(17)	0.0359(7)
H46	0.7541	0.1889	0.867	0.043
C47	0.5681(3)	0.1487(2)	0.84233(14)	0.0239(6)
C48	0.4553(3)	0.2292(2)	0.94921(14)	0.0254(6)
C49	0.3609(3)	0.2779(2)	0.97243(16)	0.0333(7)
H49	0.3291	0.328	0.9483	0.04
C50	0.3129(3)	0.2539(3)	1.03022(17)	0.0394(8)
H50	0.2492	0.2884	1.0458	0.047
C51	0.3561(3)	0.1808(3)	1.06540(17)	0.0393(8)
H51	0.322	0.1643	1.1049	0.047
C52	0.4496(3)	0.1314(2)	1.04293(16)	0.0371(8)

H52	0.4797	0.0806	1.067	0.045
C53	0.4995(3)	0.1558(2)	0.98530(15)	0.0317(7)
H53	0.5644	0.122	0.9704	0.038
C54	0.6456(3)	0.3484(2)	0.89215(16)	0.0291(6)
C55	0.6851(3)	0.3856(2)	0.95698(18)	0.0388(8)
H55	0.6452	0.3599	0.9926	0.047
C56	0.7825(4)	0.4599(3)	0.9692(2)	0.0520(10)
H56	0.8084	0.4854	1.0134	0.062
C57	0.8421(4)	0.4971(3)	0.9184(2)	0.0538(11)
H57	0.9093	0.5476	0.9275	0.065
C58	0.8040(3)	0.4605(3)	0.8538(2)	0.0483(9)
H58	0.8453	0.4858	0.8185	0.058
C59	0.7062(3)	0.3876(2)	0.84092(18)	0.0386(8)
H59	0.6795	0.3636	0.7966	0.046
C101	0.1505(4)	0.2671(3)	0.2809(2)	0.0540(10)
H101	0.0779	0.2169	0.2667	0.065
C111	0.25929(13)	0.21588(8)	0.33303(5)	0.0647(3)
C112	0.09806(12)	0.36572(11)	0.32211(9)	0.0977(6)
C113	0.2206(2)	0.30222(11)	0.21092(7)	0.1104(6)
C201	0.7421(4)	0.2269(3)	0.3774(2)	0.0610(12)
H201	0.7871	0.2025	0.3404	0.073
C121	0.7708(3)	0.35400(11)	0.38523(8)	0.1423(10)
C122	0.8088(2)	0.18747(14)	0.44992(9)	0.1298(8)
C123	0.5884(3)	0.2144(3)	0.35135(18)	0.0923(9)
C128	0.5901(3)	0.1536(3)	0.38149(18)	0.0923(9)
C301	0.1110(3)	0.8743(3)	0.91254(18)	0.0416(8)
H301	0.1209	0.8672	0.8643	0.05
C131	0.13465(12)	0.76374(8)	0.94754(6)	0.0635(3)
C132	-0.03924(8)	0.90512(8)	0.92245(5)	0.0524(3)
C133	0.22306(9)	0.96776(8)	0.95105(5)	0.0534(3)
C14	0.11239(8)	0.88469(6)	0.74534(4)	0.03676(19)

Anisotropic displacement parameters (Å^2)

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

Atom	U11	U22	U33	U23	U13	U12
N1	0.0171(11)	0.0179(11)	0.0212(11)	0.0020(8)	0.0017(9)	0.0014(9)
P1	0.0214(4)	0.0201(3)	0.0213(3)	0.0016(3)	0.0010(3)	0.0027(3)
P2	0.0211(4)	0.0244(4)	0.0240(3)	0.0036(3)	0.0008(3)	0.0019(3)
P3	0.0221(4)	0.0236(4)	0.0283(4)	0.0027(3)	-0.0031(3)	0.0057(3)
C1	0.0158(13)	0.0221(14)	0.0260(13)	0.0010(11)	-0.0010(10)	0.0021(10)
C2	0.0154(13)	0.0249(14)	0.0221(13)	0.0026(10)	-0.0006(10)	0.0052(11)
C3	0.0205(14)	0.0287(15)	0.0328(15)	0.0089(12)	0.0038(12)	0.0053(12)
C4	0.0219(15)	0.0462(19)	0.0290(15)	0.0119(14)	0.0079(12)	0.0064(13)
C5	0.0273(16)	0.0434(19)	0.0250(14)	0.0010(13)	0.0058(12)	0.0114(14)
C6	0.0280(15)	0.0282(15)	0.0246(14)	-0.0013(11)	0.0014(11)	0.0086(12)
C7	0.0171(13)	0.0256(14)	0.0225(13)	0.0036(11)	-0.0002(10)	0.0051(11)
C8	0.0282(15)	0.0209(14)	0.0246(14)	-0.0005(11)	0.0010(11)	0.0009(11)

C9	0.0424(19)	0.0303(17)	0.0354(17)	-0.0036(13)	-0.0065(14)	0.0098(14)
C10	0.070(3)	0.0263(17)	0.048(2)	-0.0046(15)	-0.0012(19)	0.0171(17)
C11	0.068(3)	0.0286(19)	0.053(2)	-0.0129(16)	0.002(2)	-0.0053(18)
C12	0.044(2)	0.044(2)	0.059(2)	-0.0120(18)	-0.0109(18)	-0.0064(17)
C13	0.0305(17)	0.0345(18)	0.0464(19)	-0.0014(15)	-0.0065(14)	0.0037(14)
C14	0.0258(15)	0.0193(13)	0.0254(14)	0.0007(11)	-0.0012(11)	0.0026(11)
C15	0.0359(18)	0.0383(18)	0.0303(16)	0.0075(13)	0.0035(13)	0.0088(14)
C16	0.056(2)	0.047(2)	0.0252(16)	0.0092(14)	0.0005(15)	0.0157(18)
C17	0.050(2)	0.045(2)	0.0378(19)	0.0116(16)	-0.0185(16)	0.0014(17)
C18	0.0268(19)	0.104(4)	0.058(3)	0.036(2)	-0.0125(17)	-0.004(2)
C19	0.0299(18)	0.080(3)	0.0375(19)	0.0257(19)	-0.0036(15)	-0.0028(18)
C21	0.0237(14)	0.0195(13)	0.0217(13)	0.0006(10)	0.0035(11)	0.0031(11)
C22	0.0239(14)	0.0244(14)	0.0203(13)	-0.0022(11)	0.0019(11)	0.0069(11)
C23	0.0243(15)	0.0271(15)	0.0277(14)	-0.0031(11)	0.0026(11)	0.0000(12)
C24	0.0263(16)	0.0397(18)	0.0287(15)	-0.0083(13)	-0.0057(12)	0.0058(14)
C25	0.0354(18)	0.0390(18)	0.0245(14)	0.0023(13)	-0.0070(13)	0.0104(14)
C26	0.0309(16)	0.0311(16)	0.0277(15)	0.0078(12)	0.0010(12)	0.0037(13)
C27	0.0238(14)	0.0233(14)	0.0216(13)	0.0010(11)	0.0022(11)	0.0068(11)
C28	0.0180(14)	0.0267(15)	0.0330(15)	0.0065(12)	-0.0020(11)	-0.0001(11)
C29	0.0263(16)	0.0379(18)	0.0337(16)	0.0090(13)	0.0015(13)	0.0030(13)
C30	0.0260(17)	0.053(2)	0.0405(18)	0.0206(16)	-0.0024(14)	-0.0050(15)
C31	0.039(2)	0.037(2)	0.058(2)	0.0205(17)	-0.0152(17)	-0.0099(15)
C32	0.041(2)	0.0269(17)	0.059(2)	0.0029(16)	-0.0077(17)	-0.0029(15)
C33	0.0267(16)	0.0303(17)	0.0423(18)	0.0010(14)	0.0002(13)	-0.0009(13)
C34	0.0232(15)	0.0239(14)	0.0291(14)	0.0079(11)	0.0029(11)	0.0023(11)
C35	0.038(2)	0.059(3)	0.063(3)	-0.024(2)	-0.0130(18)	0.0190(19)
C36	0.032(2)	0.083(3)	0.077(3)	-0.020(2)	-0.018(2)	0.026(2)
C37	0.0328(19)	0.040(2)	0.059(2)	0.0036(17)	0.0080(16)	0.0136(15)
C38	0.046(2)	0.077(3)	0.080(3)	-0.046(3)	-0.013(2)	0.029(2)
C39	0.039(2)	0.081(3)	0.061(3)	-0.037(2)	-0.0203(19)	0.028(2)
C41	0.0208(14)	0.0231(14)	0.0219(13)	0.0045(11)	0.0025(10)	0.0014(11)
C42	0.0217(14)	0.0261(14)	0.0210(13)	0.0061(11)	0.0017(10)	0.0057(11)
C43	0.0315(16)	0.0258(15)	0.0284(15)	0.0028(12)	0.0016(12)	0.0054(12)
C44	0.0363(18)	0.0337(18)	0.0434(18)	0.0020(14)	0.0056(15)	0.0180(15)
C45	0.0234(16)	0.043(2)	0.059(2)	0.0035(17)	0.0031(15)	0.0149(15)
C46	0.0223(16)	0.0347(18)	0.050(2)	0.0022(15)	-0.0024(14)	0.0050(13)
C47	0.0222(14)	0.0242(14)	0.0264(14)	0.0058(11)	0.0005(11)	0.0077(11)
C48	0.0219(14)	0.0247(14)	0.0279(14)	0.0003(11)	-0.0031(11)	0.0011(11)
C49	0.0259(16)	0.0381(18)	0.0364(17)	0.0017(14)	-0.0018(13)	0.0109(13)
C50	0.0290(17)	0.053(2)	0.0372(18)	-0.0034(15)	0.0036(14)	0.0108(15)
C51	0.0359(19)	0.047(2)	0.0324(17)	-0.0002(15)	0.0050(14)	-0.0061(16)
C52	0.045(2)	0.0306(17)	0.0342(17)	0.0038(13)	-0.0019(14)	0.0007(15)
C53	0.0334(17)	0.0304(16)	0.0320(16)	0.0034(13)	0.0002(13)	0.0092(13)
C54	0.0247(15)	0.0208(14)	0.0416(17)	0.0035(12)	-0.0023(13)	0.0059(12)
C55	0.0347(18)	0.0341(18)	0.0450(19)	-0.0015(15)	-0.0032(15)	0.0014(14)
C56	0.045(2)	0.039(2)	0.065(3)	-0.0154(18)	-0.0078(19)	-0.0026(17)
C57	0.037(2)	0.0283(19)	0.093(3)	-0.002(2)	0.005(2)	-0.0036(16)
C58	0.036(2)	0.035(2)	0.076(3)	0.0149(19)	0.0121(19)	0.0040(16)
C59	0.0388(19)	0.0319(17)	0.0462(19)	0.0085(15)	0.0033(15)	0.0069(15)
C101	0.059(3)	0.038(2)	0.059(2)	-0.0059(18)	-0.006(2)	-0.0053(18)
C111	0.0917(9)	0.0527(6)	0.0518(6)	0.0033(5)	0.0031(6)	0.0221(6)
C112	0.0530(7)	0.0848(9)	0.1451(14)	-0.0495(9)	-0.0256(8)	0.0280(7)
C113	0.205(2)	0.0670(9)	0.0598(8)	0.0217(7)	0.0199(10)	0.0016(10)
C201	0.072(3)	0.056(3)	0.058(3)	-0.014(2)	0.012(2)	0.023(2)
C121	0.310(3)	0.0608(9)	0.0770(10)	0.0134(7)	0.0852(14)	0.0513(13)
C122	0.200(2)	0.1167(14)	0.0883(11)	0.0079(10)	0.0041(12)	0.1004(15)
C123	0.0625(10)	0.108(2)	0.099(2)	-0.0396(15)	0.0015(13)	0.0096(16)
C128	0.0625(10)	0.108(2)	0.099(2)	-0.0396(15)	0.0015(13)	0.0096(16)

C301	0.042(2)	0.050(2)	0.0373(18)	0.0151(16)	0.0138(15)	0.0117(17)
C131	0.0903(8)	0.0507(6)	0.0629(6)	0.0196(5)	0.0397(6)	0.0305(6)
C132	0.0314(5)	0.0675(6)	0.0611(6)	0.0199(5)	0.0076(4)	0.0074(4)
C133	0.0371(5)	0.0651(6)	0.0573(6)	0.0187(5)	-0.0047(4)	0.0038(4)
C14	0.0480(5)	0.0238(4)	0.0372(4)	-0.0013(3)	0.0108(3)	-0.0056(3)

Bond lengths [Å]

N1	- C1	= 1.510(3)			
N1	- C41	= 1.518(3)			
N1	- C21	= 1.522(3)			
N1	- H1	= 0.93			
P1	- C8	= 1.826(3)			
P1	- C14	= 1.832(3)			
P1	- C7	= 1.837(3)			
P2	- C28	= 1.823(3)			
P2	- C34	= 1.833(3)			
P2	- C27	= 1.843(3)			
P3	- C54	= 1.829(3)			
P3	- C48	= 1.835(3)			
P3	- C47	= 1.836(3)			
C1	- C2	= 1.508(4)			
C1	- H1A	= 0.99			
C1	- H1B	= 0.99			
C2	- C3	= 1.387(4)			
C2	- C7	= 1.405(4)			
C3	- C4	= 1.385(4)			
C3	- H3	= 0.95			
C4	- C5	= 1.378(5)			
C4	- H4	= 0.95			
C5	- C6	= 1.396(4)			
C5	- H5	= 0.95			
C6	- C7	= 1.400(4)			
C6	- H6	= 0.95			
C8	- C9	= 1.387(4)			
C8	- C13	= 1.392(4)			
C9	- C10	= 1.394(5)			
C9	- H9	= 0.95			
C10	- C11	= 1.372(6)			
C10	- H10	= 0.95			
C11	- C12	= 1.380(6)			
C11	- H11	= 0.95			
C12	- C13	= 1.387(5)			
C12	- H12	= 0.95			
C13	- H13	= 0.95			
C14	- C19	= 1.379(5)			
C14	- C15	= 1.389(4)			
C15	- C16	= 1.398(4)			
C15	- H15	= 0.95			
C16	- C17	= 1.368(5)			
C16	- H16	= 0.95			
C17	- C18	= 1.372(6)			
C17	- H17	= 0.95			
C18	- C19	= 1.397(5)			
C18	- H18	= 0.95			
C19	- H19	= 0.95			
C21	- C22	= 1.512(4)			

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C21  - H21A = 0.99
C21  - H21B = 0.99
C22  - C23  = 1.393(4)
C22  - C27  = 1.399(4)
C23  - C24  = 1.390(4)
C23  - H23  = 0.95
C24  - C25  = 1.383(5)
C24  - H24  = 0.95
C25  - C26  = 1.389(4)
C25  - H25  = 0.95
C26  - C27  = 1.397(4)
C26  - H26  = 0.95
C28  - C29  = 1.391(4)
C28  - C33  = 1.392(4)
C29  - C30  = 1.381(5)
C29  - H29  = 0.95
C30  - C31  = 1.385(6)
C30  - H30  = 0.95
C31  - C32  = 1.374(6)
C31  - H31  = 0.95
C32  - C33  = 1.385(5)
C32  - H32  = 0.95
C33  - H33  = 0.95
C34  - C39  = 1.369(5)
C34  - C35  = 1.380(5)
C35  - C36  = 1.384(5)
C35  - H35  = 0.95
C36  - C37  = 1.364(6)
C36  - H36  = 0.95
C37  - C38  = 1.349(5)
C37  - H37  = 0.95
C38  - C39  = 1.395(5)
C38  - H38  = 0.95
C39  - H39  = 0.95
C41  - C42  = 1.509(4)
C41  - H41A = 0.99
C41  - H41B = 0.99
C42  - C43  = 1.390(4)
C42  - C47  = 1.406(4)
C43  - C44  = 1.391(4)
C43  - H43  = 0.95
C44  - C45  = 1.375(5)
C44  - H44  = 0.95
C45  - C46  = 1.381(5)
C45  - H45  = 0.95
C46  - C47  = 1.393(4)
C46  - H46  = 0.95
C48  - C53  = 1.390(4)
C48  - C49  = 1.391(4)
C49  - C50  = 1.379(5)
C49  - H49  = 0.95
C50  - C51  = 1.372(5)
C50  - H50  = 0.95
C51  - C52  = 1.382(5)
C51  - H51  = 0.95
C52  - C53  = 1.388(5)
C52  - H52  = 0.95
C53  - H53  = 0.95
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```
C54  - C59  = 1.395(5)
C54  - C55  = 1.397(5)
C55  - C56  = 1.386(5)
C55  - H55  = 0.95
C56  - C57  = 1.372(6)
C56  - H56  = 0.95
C57  - C58  = 1.389(6)
C57  - H57  = 0.95
C58  - C59  = 1.376(5)
C58  - H58  = 0.95
C59  - H59  = 0.95
C101 - Cl12 = 1.736(4)
C101 - Cl11 = 1.747(4)
C101 - Cl13 = 1.753(5)
C101 - H101 = 1
C201 - Cl23 = 1.686(6)
C201 - Cl22 = 1.726(5)
C201 - Cl21 = 1.748(5)
C201 - Cl28 = 1.853(6)
C201 - H201 = 1
C301 - Cl32 = 1.756(4)
C301 - Cl31 = 1.761(4)
C301 - Cl33 = 1.765(4)
C301 - H301 = 1
```

Angles [°]

```
C1   - N1   - C41  = 111.4(2)
C1   - N1   - C21  = 109.4(2)
C41  - N1   - C21  = 110.2(2)
C1   - N1   - H1   = 108.6
C41  - N1   - H1   = 108.6
C21  - N1   - H1   = 108.6
C8   - P1   - C14  = 102.45(13)
C8   - P1   - C7   = 103.11(13)
C14  - P1   - C7   = 102.68(13)
C28  - P2   - C34  = 104.25(13)
C28  - P2   - C27  = 103.26(13)
C34  - P2   - C27  = 103.35(13)
C54  - P3   - C48  = 103.88(14)
C54  - P3   - C47  = 104.24(13)
C48  - P3   - C47  = 100.92(13)
C2   - C1   - N1   = 114.8(2)
C2   - C1   - H1A  = 108.6
N1   - C1   - H1A  = 108.6
C2   - C1   - H1B  = 108.6
N1   - C1   - H1B  = 108.6
H1A  - C1   - H1B  = 107.5
C3   - C2   - C7   = 119.9(3)
C3   - C2   - C1   = 118.4(3)
C7   - C2   - C1   = 121.6(2)
C4   - C3   - C2   = 120.9(3)
C4   - C3   - H3   = 119.6
C2   - C3   - H3   = 119.6
C5   - C4   - C3   = 120.0(3)
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```
C5   - C4   - H4   = 120
C3   - C4   - H4   = 120
C4   - C5   - C6   = 119.7(3)
C4   - C5   - H5   = 120.1
C6   - C5   - H5   = 120.1
C5   - C6   - C7   = 120.9(3)
C5   - C6   - H6   = 119.6
C7   - C6   - H6   = 119.6
C6   - C7   - C2   = 118.5(3)
C6   - C7   - P1   = 123.4(2)
C2   - C7   - P1   = 118.1(2)
C9   - C8   - C13  = 118.9(3)
C9   - C8   - P1   = 123.4(2)
C13  - C8   - P1   = 117.5(2)
C8   - C9   - C10  = 120.2(3)
C8   - C9   - H9   = 119.9
C10  - C9   - H9   = 119.9
C11  - C10  - C9   = 120.2(3)
C11  - C10  - H10  = 119.9
C9   - C10  - H10  = 119.9
C10  - C11  - C12  = 120.3(3)
C10  - C11  - H11  = 119.8
C12  - C11  - H11  = 119.8
C11  - C12  - C13  = 119.8(3)
C11  - C12  - H12  = 120.1
C13  - C12  - H12  = 120.1
C12  - C13  - C8   = 120.6(3)
C12  - C13  - H13  = 119.7
C8   - C13  - H13  = 119.7
C19  - C14  - C15  = 118.9(3)
C19  - C14  - P1   = 124.6(2)
C15  - C14  - P1   = 116.5(2)
C14  - C15  - C16  = 120.7(3)
C14  - C15  - H15  = 119.7
C16  - C15  - H15  = 119.7
C17  - C16  - C15  = 119.9(3)
C17  - C16  - H16  = 120.1
C15  - C16  - H16  = 120.1
C16  - C17  - C18  = 119.8(3)
C16  - C17  - H17  = 120.1
C18  - C17  - H17  = 120.1
C17  - C18  - C19  = 120.8(4)
C17  - C18  - H18  = 119.6
C19  - C18  - H18  = 119.6
C14  - C19  - C18  = 119.9(3)
C14  - C19  - H19  = 120.1
C18  - C19  - H19  = 120.1
C22  - C21  - N1   = 112.5(2)
C22  - C21  - H21A = 109.1
N1   - C21  - H21A = 109.1
C22  - C21  - H21B = 109.1
N1   - C21  - H21B = 109.1
H21A - C21  - H21B = 107.8
C23  - C22  - C27  = 120.2(3)
C23  - C22  - C21  = 118.9(3)
C27  - C22  - C21  = 120.9(2)
C24  - C23  - C22  = 120.8(3)
C24  - C23  - H23  = 119.6
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C22  - C23  - H23  = 119.6
C25  - C24  - C23  = 119.4(3)
C25  - C24  - H24  = 120.3
C23  - C24  - H24  = 120.3
C24  - C25  - C26  = 120.0(3)
C24  - C25  - H25  = 120
C26  - C25  - H25  = 120
C25  - C26  - C27  = 121.4(3)
C25  - C26  - H26  = 119.3
C27  - C26  - H26  = 119.3
C26  - C27  - C22  = 118.2(3)
C26  - C27  - P2   = 124.5(2)
C22  - C27  - P2   = 117.0(2)
C29  - C28  - C33  = 119.3(3)
C29  - C28  - P2   = 124.9(2)
C33  - C28  - P2   = 115.8(2)
C30  - C29  - C28  = 120.2(3)
C30  - C29  - H29  = 119.9
C28  - C29  - H29  = 119.9
C29  - C30  - C31  = 119.9(3)
C29  - C30  - H30  = 120
C31  - C30  - H30  = 120
C32  - C31  - C30  = 120.4(3)
C32  - C31  - H31  = 119.8
C30  - C31  - H31  = 119.8
C31  - C32  - C33  = 119.9(3)
C31  - C32  - H32  = 120.1
C33  - C32  - H32  = 120.1
C32  - C33  - C28  = 120.3(3)
C32  - C33  - H33  = 119.9
C28  - C33  - H33  = 119.9
C39  - C34  - C35  = 118.2(3)
C39  - C34  - P2   = 125.7(2)
C35  - C34  - P2   = 116.0(2)
C34  - C35  - C36  = 120.7(4)
C34  - C35  - H35  = 119.7
C36  - C35  - H35  = 119.7
C37  - C36  - C35  = 120.5(4)
C37  - C36  - H36  = 119.8
C35  - C36  - H36  = 119.8
C38  - C37  - C36  = 119.3(3)
C38  - C37  - H37  = 120.3
C36  - C37  - H37  = 120.3
C37  - C38  - C39  = 120.9(4)
C37  - C38  - H38  = 119.6
C39  - C38  - H38  = 119.6
C34  - C39  - C38  = 120.4(3)
C34  - C39  - H39  = 119.8
C38  - C39  - H39  = 119.8
C42  - C41  - N1   = 112.7(2)
C42  - C41  - H41A = 109.1
N1   - C41  - H41A = 109.1
C42  - C41  - H41B = 109.1
N1   - C41  - H41B = 109.1
H41A - C41  - H41B = 107.8
C43  - C42  - C47  = 119.7(3)
C43  - C42  - C41  = 118.7(3)
C47  - C42  - C41  = 121.6(2)
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C42  - C43  - C44  = 120.5(3)
C42  - C43  - H43  = 119.8
C44  - C43  - H43  = 119.8
C45  - C44  - C43  = 119.6(3)
C45  - C44  - H44  = 120.2
C43  - C44  - H44  = 120.2
C44  - C45  - C46  = 120.7(3)
C44  - C45  - H45  = 119.6
C46  - C45  - H45  = 119.6
C45  - C46  - C47  = 120.6(3)
C45  - C46  - H46  = 119.7
C47  - C46  - H46  = 119.7
C46  - C47  - C42  = 118.9(3)
C46  - C47  - P3   = 123.8(2)
C42  - C47  - P3   = 117.3(2)
C53  - C48  - C49  = 118.5(3)
C53  - C48  - P3   = 124.1(2)
C49  - C48  - P3   = 117.3(2)
C50  - C49  - C48  = 120.5(3)
C50  - C49  - H49  = 119.7
C48  - C49  - H49  = 119.7
C51  - C50  - C49  = 120.8(3)
C51  - C50  - H50  = 119.6
C49  - C50  - H50  = 119.6
C50  - C51  - C52  = 119.5(3)
C50  - C51  - H51  = 120.2
C52  - C51  - H51  = 120.2
C51  - C52  - C53  = 120.2(3)
C51  - C52  - H52  = 119.9
C53  - C52  - H52  = 119.9
C52  - C53  - C48  = 120.5(3)
C52  - C53  - H53  = 119.8
C48  - C53  - H53  = 119.8
C59  - C54  - C55  = 118.7(3)
C59  - C54  - P3   = 117.5(2)
C55  - C54  - P3   = 123.4(3)
C56  - C55  - C54  = 119.9(4)
C56  - C55  - H55  = 120.1
C54  - C55  - H55  = 120.1
C57  - C56  - C55  = 120.8(4)
C57  - C56  - H56  = 119.6
C55  - C56  - H56  = 119.6
C56  - C57  - C58  = 119.8(4)
C56  - C57  - H57  = 120.1
C58  - C57  - H57  = 120.1
C59  - C58  - C57  = 119.9(4)
C59  - C58  - H58  = 120.1
C57  - C58  - H58  = 120.1
C58  - C59  - C54  = 120.9(4)
C58  - C59  - H59  = 119.5
C54  - C59  - H59  = 119.5
Cl12 - C101 - Cl11 = 110.3(2)
Cl12 - C101 - Cl13 = 111.2(2)
Cl11 - C101 - Cl13 = 108.6(3)
Cl12 - C101 - H101 = 108.9
Cl11 - C101 - H101 = 108.9
Cl13 - C101 - H101 = 108.9
Cl23 - C201 - Cl22 = 125.8(3)
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C123 - C201 - C121 = 99.4(3)
C122 - C201 - C121 = 106.0(3)
C122 - C201 - C128 = 93.7(3)
C121 - C201 - C128 = 126.2(3)
C123 - C201 - H201 = 108.1
C122 - C201 - H201 = 108.1
C121 - C201 - H201 = 108.1
C128 - C201 - H201 = 112.4
C132 - C301 - C131 = 110.8(2)
C132 - C301 - C133 = 109.5(2)
C131 - C301 - C133 = 109.4(2)
C132 - C301 - H301 = 109.1
C131 - C301 - H301 = 109.1
C133 - C301 - H301 = 109.1
```

Torsion angles [°]

```
C41  - N1   - C1   - C2   = 57.9(3)
C21  - N1   - C1   - C2   = -179.9(2)
N1   - C1   - C2   - C3   = -104.7(3)
N1   - C1   - C2   - C7   = 79.7(3)
C7   - C2   - C3   - C4   = 0.6(4)
C1   - C2   - C3   - C4   = -175.1(3)
C2   - C3   - C4   - C5   = 1.0(4)
C3   - C4   - C5   - C6   = -1.7(4)
C4   - C5   - C6   - C7   = 0.7(4)
C5   - C6   - C7   - C2   = 0.8(4)
C5   - C6   - C7   - P1   = -176.7(2)
C3   - C2   - C7   - C6   = -1.5(4)
C1   - C2   - C7   - C6   = 174.1(2)
C3   - C2   - C7   - P1   = 176.2(2)
C1   - C2   - C7   - P1   = -8.2(3)
C8   - P1   - C7   - C6   = 11.7(3)
C14  - P1   - C7   - C6   = -94.5(2)
C8   - P1   - C7   - C2   = -165.8(2)
C14  - P1   - C7   - C2   = 87.9(2)
C14  - P1   - C8   - C9   = 15.5(3)
C7   - P1   - C8   - C9   = -90.9(3)
C14  - P1   - C8   - C13  = -161.1(3)
C7   - P1   - C8   - C13  = 92.5(3)
C13  - C8   - C9   - C10  = 0.0(5)
P1   - C8   - C9   - C10  = -176.5(3)
C8   - C9   - C10  - C11  = -0.9(6)
C9   - C10  - C11  - C12  = 0.5(6)
C10  - C11  - C12  - C13  = 0.8(7)
C11  - C12  - C13  - C8   = -1.7(6)
C9   - C8   - C13  - C12  = 1.3(5)
P1   - C8   - C13  - C12  = 178.0(3)
C8   - P1   - C14  - C19  = -92.3(3)
C7   - P1   - C14  - C19  = 14.4(3)
C8   - P1   - C14  - C15  = 87.7(3)
C7   - P1   - C14  - C15  = -165.6(2)
C19  - C14  - C15  - C16  = -0.3(5)
P1   - C14  - C15  - C16  = 179.7(3)
C14  - C15  - C16  - C17  = 0.0(5)
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```
C15  - C16  - C17  - C18  = 1.2(6)
C16  - C17  - C18  - C19  = -1.9(7)
C15  - C14  - C19  - C18  = -0.4(6)
P1   - C14  - C19  - C18  = 179.6(3)
C17  - C18  - C19  - C14  = 1.5(7)
C1   - N1   - C21  - C22  = 58.4(3)
C41  - N1   - C21  - C22  = -178.8(2)
N1   - C21  - C22  - C23  = -100.8(3)
N1   - C21  - C22  - C27  = 78.6(3)
C27  - C22  - C23  - C24  = -1.8(4)
C21  - C22  - C23  - C24  = 177.7(3)
C22  - C23  - C24  - C25  = 1.6(4)
C23  - C24  - C25  - C26  = -0.4(5)
C24  - C25  - C26  - C27  = -0.6(5)
C25  - C26  - C27  - C22  = 0.5(4)
C25  - C26  - C27  - P2   = -173.6(2)
C23  - C22  - C27  - C26  = 0.7(4)
C21  - C22  - C27  - C26  = -178.8(3)
C23  - C22  - C27  - P2   = 175.2(2)
C21  - C22  - C27  - P2   = -4.3(3)
C28  - P2   - C27  - C26  = 7.9(3)
C34  - P2   - C27  - C26  = -100.5(3)
C28  - P2   - C27  - C22  = -166.2(2)
C34  - P2   - C27  - C22  = 85.4(2)
C34  - P2   - C28  - C29  = 35.8(3)
C27  - P2   - C28  - C29  = -72.0(3)
C34  - P2   - C28  - C33  = -143.5(2)
C27  - P2   - C28  - C33  = 108.8(2)
C33  - C28  - C29  - C30  = -0.7(4)
P2   - C28  - C29  - C30  = -179.9(2)
C28  - C29  - C30  - C31  = 0.4(5)
C29  - C30  - C31  - C32  = 0.1(5)
C30  - C31  - C32  - C33  = -0.1(5)
C31  - C32  - C33  - C28  = -0.2(5)
C29  - C28  - C33  - C32  = 0.7(5)
P2   - C28  - C33  - C32  = 180.0(3)
C28  - P2   - C34  - C39  = -100.7(4)
C27  - P2   - C34  - C39  = 6.9(4)
C28  - P2   - C34  - C35  = 84.0(3)
C27  - P2   - C34  - C35  = -168.4(3)
C39  - C34  - C35  - C36  = 1.4(7)
P2   - C34  - C35  - C36  = 177.1(4)
C34  - C35  - C36  - C37  = -1.3(8)
C35  - C36  - C37  - C38  = -0.1(8)
C36  - C37  - C38  - C39  = 1.4(8)
C35  - C34  - C39  - C38  = -0.1(7)
P2   - C34  - C39  - C38  = -175.3(4)
C37  - C38  - C39  - C34  = -1.3(8)
C1   - N1   - C41  - C42  = -174.8(2)
C21  - N1   - C41  - C42  = 63.6(3)
N1   - C41  - C42  - C43  = -98.2(3)
N1   - C41  - C42  - C47  = 83.7(3)
C47  - C42  - C43  - C44  = -2.2(4)
C41  - C42  - C43  - C44  = 179.6(3)
C42  - C43  - C44  - C45  = 2.1(5)
C43  - C44  - C45  - C46  = -0.7(5)
C44  - C45  - C46  - C47  = -0.6(6)
C45  - C46  - C47  - C42  = 0.5(5)
```

```
C45  - C46  - C47  - P3   = -178.9(3)
C43  - C42  - C47  - C46  = 0.9(4)
C41  - C42  - C47  - C46  = 179.0(3)
C43  - C42  - C47  - P3   = -179.7(2)
C41  - C42  - C47  - P3   = -1.6(4)
C54  - P3   - C47  - C46  = 6.8(3)
C48  - P3   - C47  - C46  = -100.7(3)
C54  - P3   - C47  - C42  = -172.5(2)
C48  - P3   - C47  - C42  = 79.9(2)
C54  - P3   - C48  - C53  = -86.6(3)
C47  - P3   - C48  - C53  = 21.3(3)
C54  - P3   - C48  - C49  = 97.5(3)
C47  - P3   - C48  - C49  = -154.6(2)
C53  - C48  - C49  - C50  = 0.4(5)
P3   - C48  - C49  - C50  = 176.5(3)
C48  - C49  - C50  - C51  = -0.9(5)
C49  - C50  - C51  - C52  = 0.6(5)
C50  - C51  - C52  - C53  = 0.2(5)
C51  - C52  - C53  - C48  = -0.7(5)
C49  - C48  - C53  - C52  = 0.4(5)
P3   - C48  - C53  - C52  = -175.4(2)
C48  - P3   - C54  - C59  = -179.3(2)
C47  - P3   - C54  - C59  = 75.4(3)
C48  - P3   - C54  - C55  = -6.9(3)
C47  - P3   - C54  - C55  = -112.2(3)
C59  - C54  - C55  - C56  = 0.1(5)
P3   - C54  - C55  - C56  = -172.3(3)
C54  - C55  - C56  - C57  = -0.7(6)
C55  - C56  - C57  - C58  = 0.5(6)
C56  - C57  - C58  - C59  = 0.4(6)
C57  - C58  - C59  - C54  = -1.1(5)
C55  - C54  - C59  - C58  = 0.8(5)
P3   - C54  - C59  - C58  = 173.7(3)
```

Complex 2: Crystal structure

report

X-ray crystallographic study

(C_{39} H_{34} Cl N_3 O Zn, C_6 H_6); *M* = 739.62. APEXII, Bruker-AXS diffractometer, Mo-Kα radiation (λ = 0.71073 Å), *T* = 150(2) K; monoclinic $P2_1/n$ (I.T.#14), a = 9.1363(15), b = 22.025(5), c = 19.679(4) Å, β = 91.470(11) °, *V* = 3958.6(14) $Å^3$, *Z* = 4, *d* = 1.241 $g.cm^{-3}$, μ = 0.725 mm^{-1}. The structure was solved by direct methods using the *SIR97* program [1], and then refined with full-matrix least-square methods based on F^2 (*SHELXL-97*) [2] with the aid of the *WINGX* [3] program. The contribution of the disordered solvents to the calculated structure factors was estimated following the *BYPASS* algorithm [4], implemented as the *SQUEEZE* option in *PLATON* [5]. A new data set, free of solvent contribution, was then used in the final refinement. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 8975 unique intensities and 407 parameters converged at $\omega R(F^2)$ = 0.2197 ($R(F)$ = 0.0986) for 3230 observed reflections with $I > 2\sigma(I)$.

[1] A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, J. Appl. Cryst. (1999) 32, 115-119

[2] Sheldrick G.M., Acta Cryst. A64 (2008), 112-122

[3] L. J. Farrugia, J. Appl. Cryst., 1999, 32, 837-838

[4] P. v.d. Sluis and A.L. Spek, Acta Cryst. (1990) A46, 194-201

[5] A. L. Spek, J. Appl. Cryst. (2003), 36, 7-13

Structural data

Empirical formula	C_{45} H_{40} Cl N_3 O Zn
Extended formula	C_{39} H_{34} Cl N_3 O Zn, C_6 H_6
Formula weight	739.62
Temperature	150(2) *K*
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, $P\ 2_1/n$
Unit cell dimensions	a = 9.1363(15) Å, α = 90 °
	b = 22.025(5) Å, β = 91.470(11) °
	c = 19.679(4) Å, γ = 90 °
Volume	3958.6(14) $Å^3$
Z, Calculated density	4 , 1.241 ($g.cm^{-3}$)
Absorption coefficient	0.725 mm^{-1}
F(000)	1544

Crystal size	0.1 x 0.1 x 0.1 mm
Crystal color	colorless
Theta range for data collection	1.39 to 27.6 °
h_min, h_max	-11 , 11
k_min, k_max	-28 , 27
l_min, l_max	-25 , 25
Reflections collected / unique	42068 / 8975 [R(int) = 0.2219]
Completeness to theta_max	0.978
Absorption correction type	multi-scan
Max. and min. transmission	0.930 , 0.921
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8975 / 0 / 407
Goodness-of-fit	0.912
Final *R* indices [I>2σ]	$R1^a$ = 0.0986, $wR2^b$ = 0.2197
R indices (all data)	$R1^a$ = 0.2295, $wR2^b$ = 0.2549
Largest diff. peak and hole	0.798 and -1.086 e.Å^{-3}

$^a R1 = \sum \; | \; |F_o| - |F_c| \; | \; / \sum |F_o|$

$^b wR2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}$

Atomic coordinates, site occupancy (%) and equivalent isotropic displacement parameters (Å^2 x 10^3). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	occ.	U(eq)
Zn1	0.11039(9)	0.24654(4)	0.73454(4)	1	0.0196(3)
Cl1	-0.0382(2)	0.27199(12)	0.64585(12)	1	0.0537(7)
N1	0.0424(6)	0.1543(3)	0.7469(3)	1	0.0167(14)
C2	-0.0892(9)	0.1331(4)	0.7255(4)	1	0.0304(10)
H2	-0.1582	0.1604	0.7055	1	0.036
C3	-0.1267(9)	0.0719(4)	0.7322(4)	1	0.0304(10)
H3	-0.2188	0.0576	0.7154	1	0.036
C4	-0.0303(8)	0.0332(4)	0.7626(4)	1	0.0304(10)
H4	-0.0544	-0.0085	0.7681	1	0.036
C5	0.1031(8)	0.0552(4)	0.7856(4)	1	0.0304(10)
H5	0.1715	0.029	0.808	1	0.036
C6	0.1367(9)	0.1155(4)	0.7756(4)	1	0.0304(10)
C7	0.2855(7)	0.1406(3)	0.7937(4)	1	0.0174(17)
H7A	0.327	0.1184	0.8334	1	0.021
H7B	0.3514	0.1344	0.7551	1	0.021
N11	0.3151(6)	0.2544(3)	0.6866(3)	1	0.0219(14)
C12	0.3250(9)	0.2654(3)	0.6207(4)	1	0.028(2)
H12	0.2379	0.2725	0.5945	1	0.033
C13	0.4582(9)	0.2668(4)	0.5886(4)	1	0.034(2)
H13	0.4616	0.2728	0.5409	1	0.04
C14	0.5846(8)	0.2595(4)	0.6263(4)	1	0.027(2)
H14	0.6774	0.2616	0.6058	1	0.032
C15	0.5738(8)	0.2489(4)	0.6950(4)	1	0.0285(18)
H15	0.6604	0.2435	0.7221	1	0.034
C16	0.4394(7)	0.2460(3)	0.7250(3)	1	0.0170(16)
C17	0.4193(7)	0.2358(3)	0.7992(3)	1	0.0188(18)
H17A	0.4999	0.2101	0.8177	1	0.023

H17B	0.4221	0.2751	0.8235	1	0.023
N18	0.2776(6)	0.2056(3)	0.8097(3)	1	0.0168(14)
O21	0.0555(5)	0.3035(2)	0.8037(2)	1	0.0156(11)
C22	0.1285(7)	0.3193(3)	0.8601(3)	1	0.0155(7)
C23	0.1263(7)	0.3824(3)	0.8812(3)	1	0.0155(7)
C24	0.1915(7)	0.3966(3)	0.9437(3)	1	0.0155(7)
H24	0.1858	0.4374	0.9589	1	0.019
C25	0.2640(7)	0.3553(3)	0.9852(3)	1	0.0155(7)
C26	0.2748(7)	0.2963(3)	0.9621(3)	1	0.0155(7)
H26	0.3289	0.2676	0.9886	1	0.019
C27	0.2084(7)	0.2779(3)	0.9012(3)	1	0.0155(7)
C28	0.3364(7)	0.3751(4)	1.0512(3)	1	0.0238(19)
H28A	0.3449	0.4195	1.0519	1	0.036
H28B	0.4342	0.357	1.0554	1	0.036
H28C	0.2772	0.3618	1.0893	1	0.036
C29	0.2224(7)	0.2125(3)	0.8806(3)	1	0.0174(17)
H29A	0.1256	0.1926	0.8833	1	0.021
H29B	0.2904	0.1916	0.9128	1	0.021
C40	0.0446(7)	0.4300(3)	0.8376(3)	1	0.0159(17)
C41	0.0918(7)	0.4949(3)	0.8617(3)	1	0.0147(17)
C42	0.0001(8)	0.5410(4)	0.8806(4)	1	0.0231(19)
H42	-0.1025	0.534	0.8792	1	0.028
C43	0.0514(8)	0.5969(4)	0.9016(4)	1	0.028(2)
H43	-0.0155	0.6271	0.9158	1	0.033
C44	0.1979(9)	0.6092(4)	0.9020(4)	1	0.029(2)
H44	0.233	0.6478	0.9166	1	0.035
C45	0.2965(9)	0.5646(4)	0.8809(4)	1	0.028(2)
H45	0.3986	0.5728	0.8803	1	0.034
C46	0.2432(8)	0.5093(3)	0.8614(4)	1	0.0221(18)
H46	0.3101	0.4791	0.8471	1	0.027
C51	-0.1192(7)	0.4191(3)	0.8464(3)	1	0.0152(17)
C52	-0.2076(7)	0.3949(3)	0.7948(4)	1	0.0169(17)
H52	-0.1669	0.3847	0.7523	1	0.02
C53	-0.3551(8)	0.3855(4)	0.8051(4)	1	0.0247(19)
H53	-0.4158	0.3709	0.7688	1	0.03
C54	-0.4152(7)	0.3969(4)	0.8671(4)	1	0.0221(19)
H54	-0.5165	0.3897	0.8734	1	0.026
C55	-0.3298(7)	0.4185(4)	0.9196(4)	1	0.027(2)
H55	-0.3711	0.427	0.9624	1	0.033
C56	-0.1793(8)	0.4280(4)	0.9095(4)	1	0.0250(19)
H56	-0.1181	0.4407	0.9466	1	0.03
C61	0.0923(7)	0.4309(3)	0.7616(3)	1	0.0169(17)
C62	0.2170(7)	0.4011(3)	0.7404(4)	1	0.0195(18)
H62	0.2728	0.3769	0.7716	1	0.023
C63	0.2603(8)	0.4068(4)	0.6733(4)	1	0.0256(19)
H63	0.3476	0.3872	0.6599	1	0.031
C64	0.1808(9)	0.4398(4)	0.6257(4)	1	0.031(2)
H64	0.2092	0.4414	0.5796	1	0.037
C65	0.0568(9)	0.4710(4)	0.6475(4)	1	0.039(2)
H65	0.0009	0.4948	0.616	1	0.046
C66	0.0147(7)	0.4672(4)	0.7152(4)	1	0.0235(19)
H66	-0.0675	0.4897	0.7298	1	0.028
C101	0.8151(9)	0.2103(5)	0.8762(5)	1	0.045(3)
H101	0.8859	0.2177	0.8426	1	0.054
C102	0.7708(9)	0.1502(4)	0.8923(5)	1	0.043(2)
H102	0.8126	0.1171	0.8687	1	0.052
C103	0.6690(9)	0.1387(4)	0.9410(4)	1	0.042(2)
H103	0.6411	0.0982	0.9511	1	0.051

C104	0.6079(9)	0.1872(5)	0.9752(4)	1	0.043(3)
H104	0.5366	0.1804	1.0087	1	0.051
C105	0.6515(8)	0.2451(5)	0.9601(4)	1	0.038(2)
H105	0.6111	0.2781	0.9845	1	0.046
C106	0.7523(8)	0.2571(4)	0.9106(4)	1	0.036(2)
H106	0.778	0.2979	0.9006	1	0.043

Anisotropic displacement parameters ($Å^2$)

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

Atom	U11	U22	U33	U23	U13	U12
Zn1	0.0206(5)	0.0188(5)	0.0195(4)	-0.0017(5)	0.0054(3)	-0.0030(4)
Cl1	0.0418(14)	0.076(2)	0.0433(14)	-0.0025(13)	0.0019(11)	-0.0063(13)
N1	0.015(3)	0.021(4)	0.014(3)	0.000(3)	0.003(2)	-0.001(3)
C2	0.040(2)	0.029(3)	0.023(2)	-0.0099(19)	0.0120(17)	-0.0106(19)
C3	0.040(2)	0.029(3)	0.023(2)	-0.0099(19)	0.0120(17)	-0.0106(19)
C4	0.040(2)	0.029(3)	0.023(2)	-0.0099(19)	0.0120(17)	-0.0106(19)
C5	0.040(2)	0.029(3)	0.023(2)	-0.0099(19)	0.0120(17)	-0.0106(19)
C6	0.040(2)	0.029(3)	0.023(2)	-0.0099(19)	0.0120(17)	-0.0106(19)
C7	0.019(4)	0.014(5)	0.019(4)	-0.002(3)	-0.002(3)	0.002(3)
N11	0.026(3)	0.022(4)	0.019(3)	-0.007(3)	0.004(3)	-0.002(3)
C12	0.037(5)	0.025(6)	0.022(4)	-0.003(4)	0.003(4)	-0.009(4)
C13	0.045(6)	0.034(6)	0.023(4)	-0.007(4)	0.015(4)	-0.006(4)
C14	0.026(4)	0.024(6)	0.030(4)	-0.007(4)	0.016(4)	-0.003(4)
C15	0.031(5)	0.021(5)	0.034(4)	0.000(4)	0.010(4)	0.005(4)
C16	0.017(4)	0.015(4)	0.019(4)	0.000(4)	0.006(3)	-0.003(4)
C17	0.016(4)	0.021(5)	0.019(4)	-0.005(3)	-0.001(3)	0.003(3)
N18	0.013(3)	0.026(4)	0.012(3)	0.003(3)	0.007(2)	0.002(3)
O21	0.020(3)	0.011(3)	0.016(3)	-0.002(2)	0.001(2)	-0.001(2)
C22	0.0100(15)	0.0175(18)	0.0192(15)	0.0012(14)	0.0060(11)	0.0032(13)
C23	0.0100(15)	0.0175(18)	0.0192(15)	0.0012(14)	0.0060(11)	0.0032(13)
C24	0.0100(15)	0.0175(18)	0.0192(15)	0.0012(14)	0.0060(11)	0.0032(13)
C25	0.0100(15)	0.0175(18)	0.0192(15)	0.0012(14)	0.0060(11)	0.0032(13)
C26	0.0100(15)	0.0175(18)	0.0192(15)	0.0012(14)	0.0060(11)	0.0032(13)
C27	0.0100(15)	0.0175(18)	0.0192(15)	0.0012(14)	0.0060(11)	0.0032(13)
C28	0.017(4)	0.042(6)	0.012(4)	0.007(4)	-0.002(3)	0.006(4)
C29	0.022(4)	0.017(5)	0.013(4)	0.007(3)	0.006(3)	0.007(3)
C40	0.021(4)	0.012(4)	0.014(4)	-0.003(3)	0.007(3)	-0.002(3)
C41	0.010(4)	0.022(5)	0.012(4)	0.004(3)	0.001(3)	-0.001(3)
C42	0.017(4)	0.027(5)	0.024(4)	-0.010(4)	-0.004(3)	0.007(4)
C43	0.026(5)	0.018(5)	0.039(5)	-0.006(4)	0.006(4)	0.007(4)
C44	0.051(6)	0.011(5)	0.025(5)	0.009(4)	-0.004(4)	-0.007(4)
C45	0.039(5)	0.019(5)	0.026(5)	-0.003(4)	0.007(4)	-0.006(4)
C46	0.025(5)	0.018(5)	0.023(4)	-0.003(4)	0.003(3)	0.003(4)
C51	0.011(4)	0.016(4)	0.019(4)	0.002(3)	0.005(3)	0.003(3)
C52	0.008(4)	0.017(5)	0.026(4)	0.005(3)	0.000(3)	0.003(3)
C53	0.028(5)	0.027(5)	0.019(4)	0.008(4)	-0.008(3)	-0.003(4)

C54	0.004(4)	0.034(5)	0.029(5)	-0.003(4)	-0.001(3)	0.009(3)
C55	0.013(4)	0.038(6)	0.031(5)	0.005(4)	0.007(3)	0.001(4)
C56	0.022(5)	0.031(5)	0.023(4)	0.003(4)	0.003(3)	0.003(4)
C61	0.023(4)	0.016(5)	0.012(4)	-0.004(3)	0.002(3)	-0.015(3)
C62	0.020(4)	0.013(5)	0.025(4)	0.006(3)	0.002(3)	-0.005(3)
C63	0.031(5)	0.022(5)	0.024(5)	-0.007(4)	0.008(4)	-0.009(4)
C64	0.042(6)	0.038(6)	0.012(4)	0.006(4)	0.005(4)	-0.013(4)
C65	0.036(5)	0.058(7)	0.022(5)	0.006(4)	-0.004(4)	0.004(5)
C66	0.016(4)	0.035(6)	0.019(4)	0.008(4)	-0.003(3)	0.003(4)
C101	0.041(6)	0.059(8)	0.035(6)	0.004(5)	0.009(4)	0.008(5)
C102	0.047(6)	0.037(7)	0.046(6)	-0.007(5)	0.014(5)	0.003(5)
C103	0.049(6)	0.037(6)	0.042(6)	0.006(5)	0.012(5)	-0.016(5)
C104	0.037(6)	0.062(8)	0.028(5)	-0.006(5)	0.010(4)	-0.013(5)
C105	0.032(5)	0.046(7)	0.037(5)	-0.023(5)	-0.006(4)	0.014(5)
C106	0.033(5)	0.044(7)	0.032(5)	-0.002(5)	0.007(4)	-0.013(5)

Bond lengths [Å]

Zn1	-	O21	=	1.927(5)
Zn1	-	N11	=	2.123(6)
Zn1	-	N1	=	2.141(6)
Zn1	-	Cl1	=	2.254(3)
Zn1	-	N18	=	2.285(5)
N1	-	C6	=	1.329(9)
N1	-	C2	=	1.346(9)
C2	-	C3	=	1.398(10)
C2	-	H2	=	0.95
C3	-	C4	=	1.354(11)
C3	-	H3	=	0.95
C4	-	C5	=	1.377(10)
C4	-	H4	=	0.95
C5	-	C6	=	1.379(11)
C5	-	H5	=	0.95
C6	-	C7	=	1.501(10)
C7	-	N18	=	1.469(9)
C7	-	H7A	=	0.99
C7	-	H7B	=	0.99
N11	-	C12	=	1.326(9)
N11	-	C16	=	1.360(8)
C12	-	C13	=	1.385(10)
C12	-	H12	=	0.95
C13	-	C14	=	1.366(10)
C13	-	H13	=	0.95
C14	-	C15	=	1.377(10)
C14	-	H14	=	0.95
C15	-	C16	=	1.377(9)
C15	-	H15	=	0.95
C16	-	C17	=	1.494(9)
C17	-	N18	=	1.475(8)
C17	-	H17A	=	0.99
C17	-	H17B	=	0.99
N18	-	C29	=	1.503(8)
O21	-	C22	=	1.328(8)

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C22  - C27      = 1.410(9)
C22  - C23      = 1.450(10)
C23  - C24      = 1.388(9)
C23  - C40      = 1.537(9)
C24  - C25      = 1.381(9)
C24  - H24      = 0.95
C25  - C26      = 1.381(9)
C25  - C28      = 1.507(9)
C26  - C27      = 1.391(9)
C26  - H26      = 0.95
C27  - C29      = 1.502(10)
C28  - H28A     = 0.98
C28  - H28B     = 0.98
C28  - H28C     = 0.98
C29  - H29A     = 0.99
C29  - H29B     = 0.99
C40  - C51      = 1.530(9)
C40  - C41      = 1.563(10)
C40  - C61      = 1.569(9)
C41  - C42      = 1.373(10)
C41  - C46      = 1.419(9)
C42  - C43      = 1.379(10)
C42  - H42      = 0.95
C43  - C44      = 1.365(10)
C43  - H43      = 0.95
C44  - C45      = 1.403(11)
C44  - H44      = 0.95
C45  - C46      = 1.363(10)
C45  - H45      = 0.95
C46  - H46      = 0.95
C51  - C56      = 1.386(9)
C51  - C52      = 1.388(9)
C52  - C53      = 1.383(9)
C52  - H52      = 0.95
C53  - C54      = 1.373(10)
C53  - H53      = 0.95
C54  - C55      = 1.365(10)
C54  - H54      = 0.95
C55  - C56      = 1.410(10)
C55  - H55      = 0.95
C56  - H56      = 0.95
C61  - C62      = 1.388(10)
C61  - C66      = 1.393(9)
C62  - C63      = 1.395(10)
C62  - H62      = 0.95
C63  - C64      = 1.377(10)
C63  - H63      = 0.95
C64  - C65      = 1.401(11)
C64  - H64      = 0.95
C65  - C66      = 1.400(10)
C65  - H65      = 0.95
C66  - H66      = 0.95
C101 - C106     = 1.368(12)
C101 - C102     = 1.422(12)
C101 - H101     = 0.95
C102 - C103     = 1.377(11)
C102 - H102     = 0.95
C103 - C104     = 1.388(12)
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C103	- H103	= 0.95
C104	- C105	= 1.371(12)
C104	- H104	= 0.95
C105	- C106	= 1.383(11)
C105	- H105	= 0.95
C106	- H106	= 0.95

Angles [°]

O21	- Zn1	- N11	= 120.6(2)
O21	- Zn1	- N1	= 117.2(2)
N11	- Zn1	- N1	= 112.9(2)
O21	- Zn1	- Cl1	= 102.84(15)
N11	- Zn1	- Cl1	= 98.96(17)
N1	- Zn1	- Cl1	= 98.80(16)
O21	- Zn1	- N18	= 88.95(19)
N11	- Zn1	- N18	= 74.8(2)
N1	- Zn1	- N18	= 75.1(2)
Cl1	- Zn1	- N18	= 168.21(16)
C6	- N1	- C2	= 118.3(7)
C6	- N1	- Zn1	= 118.1(5)
C2	- N1	- Zn1	= 123.6(5)
N1	- C2	- C3	= 121.6(8)
N1	- C2	- H2	= 119.2
C3	- C2	- H2	= 119.2
C4	- C3	- C2	= 119.4(8)
C4	- C3	- H3	= 120.3
C2	- C3	- H3	= 120.3
C3	- C4	- C5	= 118.9(8)
C3	- C4	- H4	= 120.5
C5	- C4	- H4	= 120.5
C4	- C5	- C6	= 119.4(8)
C4	- C5	- H5	= 120.3
C6	- C5	- H5	= 120.3
N1	- C6	- C5	= 122.4(7)
N1	- C6	- C7	= 116.0(7)
C5	- C6	- C7	= 121.6(8)
N18	- C7	- C6	= 111.1(6)
N18	- C7	- H7A	= 109.4
C6	- C7	- H7A	= 109.4
N18	- C7	- H7B	= 109.4
C6	- C7	- H7B	= 109.4
H7A	- C7	- H7B	= 108
C12	- N11	- C16	= 119.4(6)
C12	- N11	- Zn1	= 122.2(5)
C16	- N11	- Zn1	= 118.4(4)
N11	- C12	- C13	= 122.2(7)
N11	- C12	- H12	= 118.9
C13	- C12	- H12	= 118.9
C14	- C13	- C12	= 119.4(7)
C14	- C13	- H13	= 120.3

C12	- C13	- H13	= 120.3
C13	- C14	- C15	= 118.2(7)
C13	- C14	- H14	= 120.9
C15	- C14	- H14	= 120.9
C16	- C15	- C14	= 121.0(7)
C16	- C15	- H15	= 119.5
C14	- C15	- H15	= 119.5
N11	- C16	- C15	= 119.8(6)
N11	- C16	- C17	= 116.2(6)
C15	- C16	- C17	= 124.0(6)
N18	- C17	- C16	= 109.6(5)
N18	- C17	- H17A	= 109.7
C16	- C17	- H17A	= 109.7
N18	- C17	- H17B	= 109.7
C16	- C17	- H17B	= 109.7
H17A	- C17	- H17B	= 108.2
C7	- N18	- C17	= 111.2(5)
C7	- N18	- C29	= 108.5(5)
C17	- N18	- C29	= 113.7(5)
C7	- N18	- Zn1	= 106.3(4)
C17	- N18	- Zn1	= 107.8(4)
C29	- N18	- Zn1	= 109.0(4)
C22	- O21	- Zn1	= 128.9(4)
O21	- C22	- C27	= 123.4(7)
O21	- C22	- C23	= 118.7(6)
C27	- C22	- C23	= 117.9(6)
C24	- C23	- C22	= 117.4(6)
C24	- C23	- C40	= 122.2(6)
C22	- C23	- C40	= 120.3(6)
C25	- C24	- C23	= 124.4(7)
C25	- C24	- H24	= 117.8
C23	- C24	- H24	= 117.8
C24	- C25	- C26	= 117.5(6)
C24	- C25	- C28	= 120.9(7)
C26	- C25	- C28	= 121.5(6)
C25	- C26	- C27	= 121.7(7)
C25	- C26	- H26	= 119.1
C27	- C26	- H26	= 119.1
C26	- C27	- C22	= 120.8(7)
C26	- C27	- C29	= 118.3(6)
C22	- C27	- C29	= 120.8(6)
C25	- C28	- H28A	= 109.5
C25	- C28	- H28B	= 109.5
H28A	- C28	- H28B	= 109.5
C25	- C28	- H28C	= 109.5
H28A	- C28	- H28C	= 109.5
H28B	- C28	- H28C	= 109.5
C27	- C29	- N18	= 112.3(6)
C27	- C29	- H29A	= 109.1
N18	- C29	- H29A	= 109.1
C27	- C29	- H29B	= 109.1
N18	- C29	- H29B	= 109.1
H29A	- C29	- H29B	= 107.9
C51	- C40	- C23	= 107.0(5)
C51	- C40	- C41	= 111.9(5)
C23	- C40	- C41	= 109.2(5)
C51	- C40	- C61	= 114.0(5)
C23	- C40	- C61	= 113.5(6)

C41	- C40	- C61	= 101.4(5)
C42	- C41	- C46	= 116.0(7)
C42	- C41	- C40	= 126.3(6)
C46	- C41	- C40	= 117.6(6)
C41	- C42	- C43	= 122.5(7)
C41	- C42	- H42	= 118.8
C43	- C42	- H42	= 118.8
C44	- C43	- C42	= 120.3(7)
C44	- C43	- H43	= 119.9
C42	- C43	- H43	= 119.9
C43	- C44	- C45	= 119.8(8)
C43	- C44	- H44	= 120.1
C45	- C44	- H44	= 120.1
C46	- C45	- C44	= 118.8(8)
C46	- C45	- H45	= 120.6
C44	- C45	- H45	= 120.6
C45	- C46	- C41	= 122.6(7)
C45	- C46	- H46	= 118.7
C41	- C46	- H46	= 118.7
C56	- C51	- C52	= 118.3(6)
C56	- C51	- C40	= 119.4(6)
C52	- C51	- C40	= 122.0(6)
C53	- C52	- C51	= 120.0(7)
C53	- C52	- H52	= 120
C51	- C52	- H52	= 120
C54	- C53	- C52	= 121.2(7)
C54	- C53	- H53	= 119.4
C52	- C53	- H53	= 119.4
C55	- C54	- C53	= 120.1(7)
C55	- C54	- H54	= 119.9
C53	- C54	- H54	= 119.9
C54	- C55	- C56	= 119.1(7)
C54	- C55	- H55	= 120.4
C56	- C55	- H55	= 120.4
C51	- C56	- C55	= 121.0(7)
C51	- C56	- H56	= 119.5
C55	- C56	- H56	= 119.5
C62	- C61	- C66	= 118.9(7)
C62	- C61	- C40	= 122.0(6)
C66	- C61	- C40	= 118.8(6)
C61	- C62	- C63	= 119.7(7)
C61	- C62	- H62	= 120.1
C63	- C62	- H62	= 120.1
C64	- C63	- C62	= 122.3(7)
C64	- C63	- H63	= 118.9
C62	- C63	- H63	= 118.9
C63	- C64	- C65	= 117.9(7)
C63	- C64	- H64	= 121.1
C65	- C64	- H64	= 121.1
C66	- C65	- C64	= 120.4(8)
C66	- C65	- H65	= 119.8
C64	- C65	- H65	= 119.8
C61	- C66	- C65	= 120.6(7)
C61	- C66	- H66	= 119.7
C65	- C66	- H66	= 119.7
C106	- C101	- C102	= 117.7(9)
C106	- C101	- H101	= 121.1
C102	- C101	- H101	= 121.1

C103	- C102	- C101	= 121.9(9)
C103	- C102	- H102	= 119
C101	- C102	- H102	= 119
C102	- C103	- C104	= 118.8(9)
C102	- C103	- H103	= 120.6
C104	- C103	- H103	= 120.6
C105	- C104	- C103	= 119.3(8)
C105	- C104	- H104	= 120.3
C103	- C104	- H104	= 120.3
C104	- C105	- C106	= 122.2(8)
C104	- C105	- H105	= 118.9
C106	- C105	- H105	= 118.9
C101	- C106	- C105	= 120.0(9)
C101	- C106	- H106	= 120
C105	- C106	- H106	= 120

Torsion angles [°]

O21	- Zn1	- N1	- C6	= -95.9(5)
N11	- Zn1	- N1	- C6	= 51.0(6)
Cl1	- Zn1	- N1	- C6	= 154.7(5)
N18	- Zn1	- N1	- C6	= -15.0(5)
O21	- Zn1	- N1	- C2	= 85.9(6)
N11	- Zn1	- N1	- C2	= -127.2(5)
Cl1	- Zn1	- N1	- C2	= -23.5(5)
N18	- Zn1	- N1	- C2	= 166.8(6)
C6	- N1	- C2	- C3	= -0.9(10)
Zn1	- N1	- C2	- C3	= 177.3(5)
N1	- C2	- C3	- C4	= 2.1(11)
C2	- C3	- C4	- C5	= -0.8(11)
C3	- C4	- C5	- C6	= -1.5(11)
C2	- N1	- C6	- C5	= -1.6(10)
Zn1	- N1	- C6	- C5	= -179.9(6)
C2	- N1	- C6	- C7	= 175.7(6)
Zn1	- N1	- C6	- C7	= -2.6(8)
C4	- C5	- C6	- N1	= 2.8(11)
C4	- C5	- C6	- C7	= -174.3(7)
N1	- C6	- C7	- N18	= 29.7(9)
C5	- C6	- C7	- N18	= -153.0(7)
O21	- Zn1	- N11	- C12	= -116.7(6)
N1	- Zn1	- N11	- C12	= 97.6(6)
Cl1	- Zn1	- N11	- C12	= -5.9(6)
N18	- Zn1	- N11	- C12	= 163.8(6)
O21	- Zn1	- N11	- C16	= 65.4(6)
N1	- Zn1	- N11	- C16	= -80.3(6)
Cl1	- Zn1	- N11	- C16	= 176.1(5)
N18	- Zn1	- N11	- C16	= -14.1(5)
C16	- N11	- C12	- C13	= 2.0(11)
Zn1	- N11	- C12	- C13	= -175.9(6)
N11	- C12	- C13	- C14	= -3.1(12)
C12	- C13	- C14	- C15	= 2.1(12)
C13	- C14	- C15	- C16	= -0.3(12)
C12	- N11	- C16	- C15	= -0.1(11)

Zn1	- N11	- C16	- C15	= 177.9(5)
C12	- N11	- C16	- C17	= 178.2(7)
Zn1	- N11	- C16	- C17	= -3.8(9)
C14	- C15	- C16	- N11	= -0.8(12)
C14	- C15	- C16	- C17	= -178.9(7)
N11	- C16	- C17	- N18	= 29.9(9)
C15	- C16	- C17	- N18	= -151.9(7)
C6	- C7	- N18	- C17	= -156.0(6)
C6	- C7	- N18	- C29	= 78.2(7)
C6	- C7	- N18	- Zn1	= -38.9(6)
C16	- C17	- N18	- C7	= 77.4(7)
C16	- C17	- N18	- C29	= -159.8(6)
C16	- C17	- N18	- Zn1	= -38.8(6)
O21	- Zn1	- N18	- C7	= 147.2(4)
N11	- Zn1	- N18	- C7	= -90.6(4)
N1	- Zn1	- N18	- C7	= 28.7(4)
Cl1	- Zn1	- N18	- C7	= -31.4(10)
O21	- Zn1	- N18	- C17	= -93.4(4)
N11	- Zn1	- N18	- C17	= 28.7(4)
N1	- Zn1	- N18	- C17	= 148.1(5)
Cl1	- Zn1	- N18	- C17	= 88.0(9)
O21	- Zn1	- N18	- C29	= 30.4(4)
N11	- Zn1	- N18	- C29	= 152.6(5)
N1	- Zn1	- N18	- C29	= -88.1(4)
Cl1	- Zn1	- N18	- C29	= -148.2(7)
N11	- Zn1	- O21	- C22	= -53.5(6)
N1	- Zn1	- O21	- C22	= 90.7(6)
Cl1	- Zn1	- O21	- C22	= -162.2(5)
N18	- Zn1	- O21	- C22	= 18.1(6)
Zn1	- O21	- C22	- C27	= -39.2(9)
Zn1	- O21	- C22	- C23	= 140.9(5)
O21	- C22	- C23	- C24	= 173.9(6)
C27	- C22	- C23	- C24	= -6.0(9)
O21	- C22	- C23	- C40	= -1.8(9)
C27	- C22	- C23	- C40	= 178.3(6)
C22	- C23	- C24	- C25	= 3.4(10)
C40	- C23	- C24	- C25	= 178.9(6)
C23	- C24	- C25	- C26	= 1.4(10)
C23	- C24	- C25	- C28	= 177.8(6)
C24	- C25	- C26	- C27	= -3.5(9)
C28	- C25	- C26	- C27	= -179.8(6)
C25	- C26	- C27	- C22	= 0.7(10)
C25	- C26	- C27	- C29	= -178.5(6)
O21	- C22	- C27	- C26	= -175.7(6)
C23	- C22	- C27	- C26	= 4.2(9)
O21	- C22	- C27	- C29	= 3.4(10)
C23	- C22	- C27	- C29	= -176.6(6)
C26	- C27	- C29	- N18	= -127.9(6)
C22	- C27	- C29	- N18	= 52.9(8)
C7	- N18	- C29	- C27	= -179.1(5)
C17	- N18	- C29	- C27	= 56.6(7)
Zn1	- N18	- C29	- C27	= -63.7(6)
C24	- C23	- C40	- C51	= -102.7(7)
C22	- C23	- C40	- C51	= 72.7(7)
C24	- C23	- C40	- C41	= 18.5(8)
C22	- C23	- C40	- C41	= -166.1(6)
C24	- C23	- C40	- C61	= 130.8(7)
C22	- C23	- C40	- C61	= -53.8(8)

C51	- C40	- C41	- C42	= -8.0(10)
C23	- C40	- C41	- C42	= -126.2(7)
C61	- C40	- C41	- C42	= 113.8(7)
C51	- C40	- C41	- C46	= 175.0(6)
C23	- C40	- C41	- C46	= 56.8(8)
C61	- C40	- C41	- C46	= -63.2(7)
C46	- C41	- C42	- C43	= -3.2(11)
C40	- C41	- C42	- C43	= 179.7(7)
C41	- C42	- C43	- C44	= 2.2(12)
C42	- C43	- C44	- C45	= 0.1(11)
C43	- C44	- C45	- C46	= -1.1(11)
C44	- C45	- C46	- C41	= -0.1(11)
C42	- C41	- C46	- C45	= 2.2(10)
C40	- C41	- C46	- C45	= 179.5(7)
C23	- C40	- C51	- C56	= 65.2(8)
C41	- C40	- C51	- C56	= -54.3(8)
C61	- C40	- C51	- C56	= -168.6(6)
C23	- C40	- C51	- C52	= -108.5(7)
C41	- C40	- C51	- C52	= 132.0(7)
C61	- C40	- C51	- C52	= 17.7(9)
C56	- C51	- C52	- C53	= 5.9(10)
C40	- C51	- C52	- C53	= 179.7(6)
C51	- C52	- C53	- C54	= -3.3(11)
C52	- C53	- C54	- C55	= 0.7(12)
C53	- C54	- C55	- C56	= -0.9(12)
C52	- C51	- C56	- C55	= -6.2(11)
C40	- C51	- C56	- C55	= 179.9(7)
C54	- C55	- C56	- C51	= 3.7(11)
C51	- C40	- C61	- C62	= -136.0(7)
C23	- C40	- C61	- C62	= -13.3(9)
C41	- C40	- C61	- C62	= 103.6(7)
C51	- C40	- C61	- C66	= 50.1(9)
C23	- C40	- C61	- C66	= 172.9(6)
C41	- C40	- C61	- C66	= -70.2(7)
C66	- C61	- C62	- C63	= -1.6(10)
C40	- C61	- C62	- C63	= -175.5(6)
C61	- C62	- C63	- C64	= -1.9(11)
C62	- C63	- C64	- C65	= 3.4(12)
C63	- C64	- C65	- C66	= -1.2(12)
C62	- C61	- C66	- C65	= 3.7(11)
C40	- C61	- C66	- C65	= 177.7(7)
C64	- C65	- C66	- C61	= -2.3(12)
C106	- C101	- C102	- C103	= -0.4(13)
C101	- C102	- C103	- C104	= 0.2(13)
C102	- C103	- C104	- C105	= -0.7(13)
C103	- C104	- C105	- C106	= 1.6(13)
C102	- C101	- C106	- C105	= 1.2(12)
C104	- C105	- C106	- C101	= -1.8(12)