Reactions of a Persistent Phosphinyl Radical/diphosphine with Heteroallenes

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Supporting Information

General Synthetic Procedures

All reactions were performed in dry, O_2-free conditions under an atmosphere of N_2 within an mBraun Labmaster SP inert atmosphere drybox or sealed reaction vessels using standard Schlenk techniques. Synthesis of ligand **1** was done via our literature procedure (*Inorg. Chem.,* 2012, **51**, 11837-11850). All reagents were purchased from Sigma-Aldrich and used as received, unless otherwise noted. Alumina and molecular sieves were pre-dried in a 150°C oven before bring dried at 300°C in vacuo. Solvents were purified using an Innovative Technology solvent purification system or purchased as 'anhydrous' from Sigma-Aldrich. Solvents were then dried using KH and subsequently filtered through dry alumina and stored over previously dried 3Å molecular sieves. Glassware was dried at 150°C overnight prior to experimentation. NMR spectra were recorded on a Bruker Avance 300MHz spectrometer. Trace amounts of non-deuterated solvent were used as internal references for ^{1}H NMR spectra and were referenced relative to tetramethylsilane. The deuterated solvent was used as an internal reference

for $^{13}C\{^1H\}$ NMR spectra and referenced relative to tetramethylsilane. ^{31}P NMR spectra were referenced to external phosphoric acid. Coupling constants are reported as absolute values. Melting points were recorded on an Electrothermal MEL-Temp 3.0 using glass capillaries sealed under inert conditions. Elemental analysis was performed by the Centre for Environmental Analysis and Remediation (CEAR) facility at Saint Mary's University using a Perkin Elmer 2400 II series Elemental Analyser.

Preparation of $Dipp_2C_2H_4N_2P$-S-C(=S)-$PN_2H_4C_2Dipp_2$ **2**

In a 20 mL scintillation vial, 200 mg (0.244 mmol) of diphosphine **1** was dissolved in 5 mL of toluene to give an orange colored solution. With rapid stirring, 15.0 µL (0.244 mmol) of CS_2 was added using a micro-pipette. The orange colored solution transitions to bright turquoise color over several seconds. After stirring for 30 min, the solution was filtered through a pad of diatomaceous earth and crystallized *via* slow evaporation of the solvent at ambient temperatures yielded X-ray quality, turquoise colored crystals. Removal of the solvent afforded 205 mg of analytically pure solid. (94 % yield). $^{31}P\{^1H\}$ (121.5 MHz, C_6D_6) δ: 133.10 (d, $^3J_{P\text{-}P}$ = 8 Hz) , 92.36 (d, $^3J_{P\text{-}P}$ = 8 Hz). ^1H (300 MHz, C_6D_6) δ: 7.20-7.16 (m, 6H, Ar-*H*), 7.14-7.03 (m, 6H, Ar-*H*), 4.19-4.04 (m, 4H, overlapping sept(*CH*)/m{C*H*$_2$}) 3.82 (sept, 2H, C*H*, $^3J_{H\text{-}H}$ = 7 Hz), 3.71 (m, 2H, C*H*$_2$, $^3J_{H\text{-}H}$ = 7 Hz), 3.60 (sept, 4H, C*H*, $^3J_{H\text{-}H}$ = 7 Hz), 3.23 (sept, 4H, C*H*, $^3J_{H\text{-}H}$ = 7 Hz), 1.45-1.41 (overlapping doublets, 12H, C*H*$_3$), 1.30-1.26 (overlapping doublets, 27H, C*H*$_3$), 1.15 (d, 6H, C*H*$_3$, $^3J_{H\text{-}H}$ = 7 Hz) 0.94-0.89 (m, 3H, C*H*$_3$). $^{13}C\{^1H\}$ (75.4 MHz, C_6D_6) δ: 149.55, 149.36, 147.59, 147.50, 138.36 (dd, P-*C*(S)-S-P, $^1J_{P\text{-}C}$ = 134.7 Hz, $^2J_{P'\text{-}C}$ = 11.5 Hz), 127.00, 124.54, 124.17, 55.51, 55.40, 34.41, 29.45, 29.31, 29.23, 28.99, 28.80, 26.10, 26.00, 25.91, 25.57, 25.37, 25.31, 24.41, 24.25, 22.69, 14.24. M.P.: 169-172 °C. Anal calc for $C_{53}H_{76}N_4PS_2\cdot 1/2C_7H_8$: C, 72.09; H, 8.57; N, 5.95. Found: C, 71.70; H, 7.98; N, 6.20.

Preparation of $Dipp_2C_2H_4N_2P$-O-C(=N-Ph)-$PN_2H_4C_2Dipp_2$ **3**

In a 20 mL scintillation vial, 100mg (0.122 mmol) of diphosphine **1** was dissolved in 5 mL of toluene to give an orange colored solution. With rapid stirring, 13.3 µL (0.122 mmol) of phenyl isocyanate was added using a micro-pipette. The orange colored solution transitions to pale yellow color overnight. Removal of solvent yielded a colorless powder which was dissolved in ca. 5 mL of pentane and filtered through a pad of diatomaceous earth. Colourless, X-ray quality crystals of 17 were grown from a pentane solution at -35 °C, yielding 92 mg of **3** (80 % yield). $^{31}P\{^1H\}$ (121.5 MHz, C_6D_6) δ: 122.36, 84.74. ^1H (300 MHz, C_6D_6) δ: 7.23-6.99 (br m, 16H, Ar-*H*), 6.61 (br s, 2H, Ar-*H*), 5.56 (br s, 2H, Ar-*H*), 4.37-3.95 (br m, 4H, C*H*/C*H*$_2$), 3.87-3.64 (br m, 2H, C*H*/C*H*$_2$), 3.49 (br m, 4H, C*H*/C*H*$_2$), 3.33 (br m, 2H, C*H*/C*H*$_2$), 3.13 (br m, 4H, C*H*/C*H*$_2$), 1.72-0.57 (br m, 48H, C*H*$_3$). $^{13}C\{^1H\}$ (75.4 MHz, C_6D_6) δ: 149.91, 148.86, 147.41, 139.66, 129.29, 126.74, 124.66, 123.05, 121.91, 55.55, 55.32, 28.88, 28.14, 25.92, 24.85, 24.66, 23.76. M.P.: 112-114 °C. Anal calc for $C_{59}H_{81}N_5PO\cdot 1/2C_7H_8$: C, 76.26; H, 8.70; N, 7.11. Found: C, 76.30; H, 8.57; N, 6.86.

Preparation of $Dipp_2C_2H_4N_2P$-S-C(=N-Ph)-$PN_2H_4C_2Dipp_2$ **4**

In a 20 mL scintillation vial, 100mg (0.122 mmol) of diphosphine **1** was dissolved in 5 mL of toluene to give an orange colored solution. With rapid stirring, 14.5 µL (0.244 mmol) of phenyl isothiocyanate (Ph-NCS) was added using a micro-pipette. The orange solution transitions to a pale yellow over 5 days. Removal of solvent afforded a yellow powder which was subsequently dissolved in ca. 5 mL of pentanes and filtered through a pad of diatomaceous earth. X-ray quality crystals of 18 were grown from a pentane solution at -35 °C containing a trace amount of benzene, yielding 98 mg of material (84 % yield). $^{31}P\{^1H\}$ (121.5 MHz, C_6D_6) δ: 128.07 (br s), 83.81 (br s). ^1H (300 MHz, C_6D_6) δ: 7.26-7.06 (br m, 12H, Ar-H), 6.74-6.69 (br m, 2H, Ar-*H*), 6.62-6.56 (br m, 3H, Ar-*H*), 5.54 (br s, 2H), 4.58 (br s, 1H), 4.30 (br s, 2H), 3.91-3.47 (br m, 11H, C*H*/CH_2), 3.14 (br m, 5H, C*H*/CH_2), 1.76-0.60 (br m, 48H, CH_3). $^{13}C\{^1H\}$ (75.4 MHz, C_6D_6) δ: 149.87, 149.08, 148.58, 147.18, 139.21, 139.03, 129.42, 126.97, 125.70, 124.93, 124.64, 124.18, 123.45, 121.05, 55.25, 54.78, 29.07, 28.77, 25.95, 25.03, 24.13, 22.69, 14.45. M.P.: 193 °C. Anal calc for $C_{59}H_{81}N_5PS$: C, 74.26; H, 8.56; N, 7.34. Found: C, 73.82; H, 8.89; N, 7.2

General X-ray Crystallography Procedures

Crystals of compounds **2**-**4** were mounted from Paratone-N oil on an appropriately sized MiTeGen MicroMount. The data were collected on a Bruker APEX II charge-coupled-device (CCD) diffractometer, with an Oxford 700 Cryocool sample cooling device. The instrument was equipped with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å; 30 mA, 50 mV), with MonoCap X-ray source optics. For data collection, four ω-scan frame series were collected with 0.5° wide scans, 416 frames per series at varying ϕ angles (ϕ = 0°, 90°, 180°, 270°). Data collection, unit cell refinement, data processing and multi-scan absorption correction were applied using the APEX II software package.[1] The structures were solved using direct methods[2] and all non-hydrogen atoms were refined anisotropically using the shelXle[3] graphical user interface and the SHELX suite of programs.[2] Unless otherwise noted, all hydrogen atom positions were idealized and rode on the atom to which they were attached. The final refinement included anisotropic temperature factors on all non- hydrogen atoms. Details of crystal data, data collection, and structure refinement are listed in Table S1. All figures were made using ORTEP-3 for Windows.[4] CCDC 1480970-1480972 contain the supplementary crystallographic data for compounds **2**-**4**. These data can be obtained free of charge from the Cambridge Crystallographic Database Centre via https://summary.ccdc.cam.ac.uk/structure-summary-form.

1. APEX2 Ver. 2008.5, Bruker AXS, Inc., Madison, Wisconsin, USA, 2008.
2. G. M. Sheldrick, *Acta Cryst.,* 2008, A64, 112.
3. C. B. Hübschle, G. M. Sheldrick and B. Dittrich, *J. Appl. Cryst.,* 2011, 44, 1281-1284.
4. L. J. Farrugia, *J. Appl. Cryst.,* 1997, 30, 565.

Table S1. Crystallographic Data for Compounds 2-4

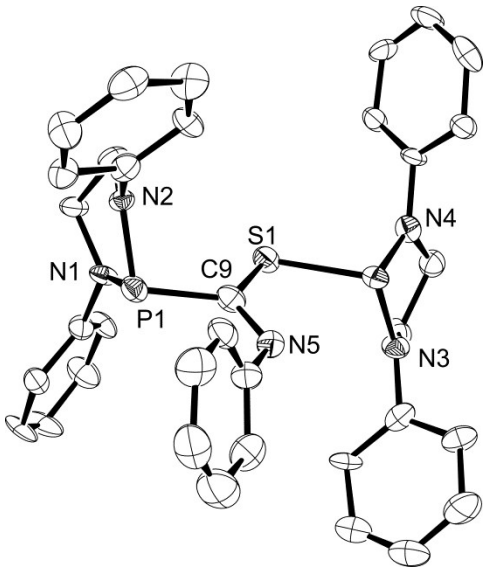
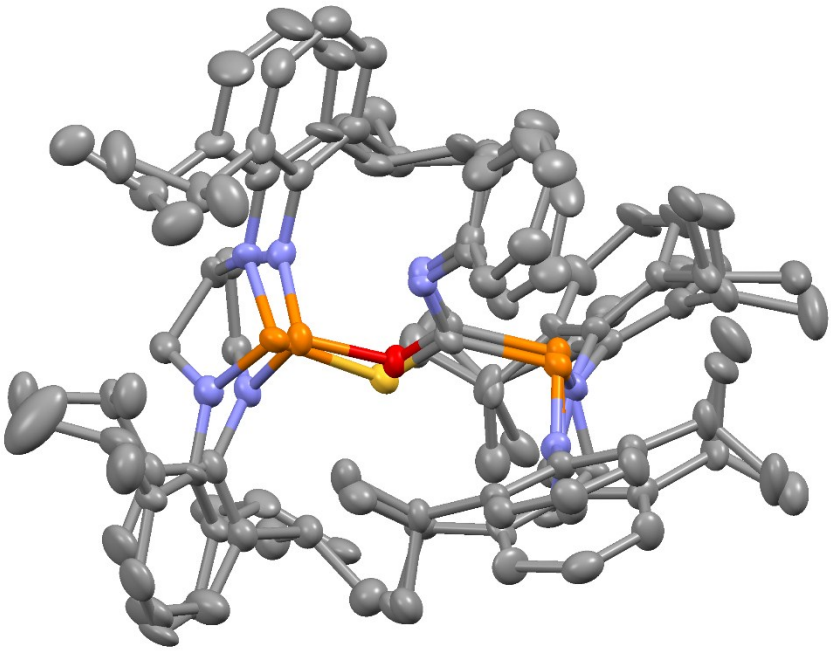


Figure S1. Single crystal structure of 4. Thermal ellipsoids are displayed at 50% probability; isopropyl groups and hydrogen atoms are removed for clarity.

Figure S2. Overlay of structures from compounds **3** (sulfur = yellow) and **4** (oxygen = red).



Crystallography tables for compound 2

Table 1. Crystal data and structure refinement for 2.

Identification code	NG111_0m	
Empirical formula	C53 H76 N4 P2 S2	
Formula weight	895.23	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 16.506(3) Å	α= 90°.
	b = 14.607(2) Å	β= 93.218(2)°.
	c = 21.516(3) Å	γ = 90°.
Volume	5179.4(14) $Å^3$	
Z	4	
Density (calculated)	1.148 Mg/m^3	
Absorption coefficient	0.202 mm^{-1}	
F(000)	1936	
Crystal size	0.124 x 0.111 x 0.108 mm^3	
Theta range for data collection	2.059 to 25.000°.	
Index ranges	-19<=h<=19, -15<=k<=17, -24<=l<=25	
Reflections collected	33942	
Independent reflections	9113 [R(int) = 0.1375]	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.7121	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9113 / 1 / 566	
Goodness-of-fit on F^2	1.012	
Final R indices [I>2sigma(I)]	R1 = 0.0660, wR2 = 0.1196	
R indices (all data)	R1 = 0.1491, wR2 = 0.1538	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.412 and -0.306 $e.Å^{-3}$	

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

	x	y	z	U(eq)
S(1)	1891(1)	-285(1)	2628(1)	32(1)
S(2)	3443(1)	646(1)	3023(1)	48(1)
P(1)	2762(1)	-1410(1)	2970(1)	24(1)
P(2)	2030(1)	1603(1)	2201(1)	25(1)
N(1)	2524(2)	-1590(2)	3705(1)	21(1)
N(2)	2266(2)	-2352(2)	2741(1)	23(1)
N(3)	2547(2)	2561(2)	2404(2)	25(1)
N(4)	2511(2)	1524(2)	1520(1)	25(1)
C(1)	2555(2)	641(3)	2657(2)	28(1)
C(2)	2077(3)	-2432(3)	3816(2)	34(1)
C(3)	1740(3)	-2755(3)	3192(2)	32(1)
C(4)	3257(2)	2728(3)	2046(2)	37(1)
C(5)	3091(3)	2262(3)	1423(2)	39(1)
C(6)	2788(2)	-999(3)	4216(2)	20(1)
C(7)	3597(2)	-1043(3)	4450(2)	26(1)
C(8)	3838(2)	-427(3)	4920(2)	32(1)
C(9)	3313(2)	194(3)	5148(2)	30(1)
C(10)	2518(2)	212(3)	4922(2)	26(1)
C(11)	2237(2)	-383(3)	4453(2)	23(1)
C(12)	4190(2)	-1729(4)	4221(2)	41(1)
C(13)	4595(4)	-2281(4)	4762(2)	87(2)
C(14)	4830(3)	-1273(4)	3838(2)	66(2)
C(15)	1349(2)	-367(3)	4234(2)	29(1)
C(16)	835(2)	-794(3)	4735(2)	39(1)
C(17)	1035(3)	592(3)	4063(2)	45(1)
C(18)	2337(2)	-2700(3)	2120(2)	23(1)
C(19)	1733(2)	-2511(3)	1654(2)	26(1)
C(20)	1874(3)	-2784(3)	1053(2)	34(1)
C(21)	2582(3)	-3230(3)	912(2)	41(1)
C(22)	3148(3)	-3438(3)	1387(2)	37(1)
C(23)	3042(2)	-3191(3)	1996(2)	26(1)

C(24)	3666(2)	-3486(3)	2505(2)	33(1)
C(25)	4498(3)	-3082(4)	2418(3)	72(2)
C(26)	3710(3)	-4528(4)	2547(3)	68(2)
C(27)	934(2)	-2056(3)	1785(2)	31(1)
C(28)	248(2)	-2767(3)	1760(2)	47(1)
C(29)	721(3)	-1267(3)	1341(2)	43(1)
C(30)	2229(2)	3277(3)	2774(2)	22(1)
C(31)	2548(2)	3414(3)	3391(2)	27(1)
C(32)	2218(3)	4104(3)	3741(2)	33(1)
C(33)	1599(3)	4653(3)	3501(2)	34(1)
C(34)	1309(3)	4536(3)	2894(2)	32(1)
C(35)	1616(2)	3862(3)	2523(2)	25(1)
C(36)	3245(2)	2851(3)	3669(2)	34(1)
C(37)	3047(3)	2414(4)	4286(2)	66(2)
C(38)	4013(3)	3430(4)	3763(2)	56(2)
C(39)	1289(2)	3791(3)	1848(2)	28(1)
C(40)	389(2)	3557(3)	1810(2)	40(1)
C(41)	1450(3)	4666(3)	1491(2)	47(1)
C(42)	2318(2)	872(3)	1036(2)	25(1)
C(43)	1574(2)	926(3)	690(2)	29(1)
C(44)	1398(3)	266(3)	228(2)	36(1)
C(45)	1941(3)	-418(3)	117(2)	40(1)
C(46)	2674(3)	-454(3)	449(2)	37(1)
C(47)	2882(3)	179(3)	912(2)	31(1)
C(48)	975(2)	1682(3)	768(2)	30(1)
C(49)	133(3)	1335(4)	881(3)	66(2)
C(50)	955(4)	2324(4)	214(2)	78(2)
C(51)	3705(2)	114(3)	1253(2)	36(1)
C(52)	4381(3)	353(4)	821(2)	52(2)
C(53)	3856(3)	-837(3)	1539(2)	49(1)

Table 3. Bond lengths [Å] and angles [°] for 2.

S(1)-C(1)	1.739(4)
S(1)-P(1)	2.2774(16)
S(2)-C(1)	1.625(4)
P(1)-N(2)	1.663(3)
P(1)-N(1)	1.670(3)
P(2)-N(3)	1.683(3)
P(2)-N(4)	1.710(3)
P(2)-C(1)	1.895(4)
N(1)-C(6)	1.446(5)
N(1)-C(2)	1.461(5)
N(2)-C(18)	1.440(5)
N(2)-C(3)	1.461(5)
N(3)-C(30)	1.432(5)
N(3)-C(4)	1.459(5)
N(4)-C(42)	1.433(5)
N(4)-C(5)	1.463(5)
C(2)-C(3)	1.501(5)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.514(6)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(11)	1.397(5)
C(6)-C(7)	1.402(5)
C(7)-C(8)	1.394(6)
C(7)-C(12)	1.503(6)
C(8)-C(9)	1.364(6)
C(8)-H(8)	0.9500
C(9)-C(10)	1.375(5)
C(9)-H(9)	0.9500

C(10)-C(11)	1.392(5)
C(10)-H(10)	0.9500
C(11)-C(15)	1.514(5)
C(12)-C(14)	1.528(6)
C(12)-C(13)	1.538(6)
C(12)-H(12)	1.0000
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-C(17)	1.532(6)
C(15)-C(16)	1.542(5)
C(15)-H(15)	1.0000
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(19)	1.400(5)
C(18)-C(23)	1.405(5)
C(19)-C(20)	1.385(5)
C(19)-C(27)	1.518(5)
C(20)-C(21)	1.386(6)
C(20)-H(20)	0.9500
C(21)-C(22)	1.380(6)
C(21)-H(21)	0.9500
C(22)-C(23)	1.378(5)
C(22)-H(22)	0.9500
C(23)-C(24)	1.524(5)
C(24)-C(25)	1.516(6)
C(24)-C(26)	1.526(6)
C(24)-H(24)	1.0000
C(25)-H(25A)	0.9800

C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-C(29)	1.524(6)
C(27)-C(28)	1.536(6)
C(27)-H(27)	1.0000
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(35)	1.409(5)
C(30)-C(31)	1.414(5)
C(31)-C(32)	1.388(6)
C(31)-C(36)	1.510(5)
C(32)-C(33)	1.376(6)
C(32)-H(32)	0.9500
C(33)-C(34)	1.376(6)
C(33)-H(33)	0.9500
C(34)-C(35)	1.381(5)
C(34)-H(34)	0.9500
C(35)-C(39)	1.524(5)
C(36)-C(37)	1.523(6)
C(36)-C(38)	1.528(6)
C(36)-H(36)	1.0000
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-C(40)	1.521(5)
C(39)-C(41)	1.523(6)

C(39)-H(39)	1.0000
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-C(43)	1.403(5)
C(42)-C(47)	1.411(5)
C(43)-C(44)	1.402(6)
C(43)-C(48)	1.499(6)
C(44)-C(45)	1.372(6)
C(44)-H(44)	0.9500
C(45)-C(46)	1.371(6)
C(45)-H(45)	0.9500
C(46)-C(47)	1.389(6)
C(46)-H(46)	0.9500
C(47)-C(51)	1.510(6)
C(48)-C(49)	1.511(6)
C(48)-C(50)	1.515(6)
C(48)-H(48)	1.0000
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
C(51)-C(52)	1.533(5)
C(51)-C(53)	1.534(6)
C(51)-H(51)	1.0000
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800

C(1)-S(1)-P(1)	99.48(15)
N(2)-P(1)-N(1)	90.71(16)
N(2)-P(1)-S(1)	102.12(12)
N(1)-P(1)-S(1)	104.05(12)
N(3)-P(2)-N(4)	91.47(16)
N(3)-P(2)-C(1)	105.86(17)
N(4)-P(2)-C(1)	99.93(17)
C(6)-N(1)-C(2)	120.8(3)
C(6)-N(1)-P(1)	123.3(3)
C(2)-N(1)-P(1)	115.8(3)
C(18)-N(2)-C(3)	123.8(3)
C(18)-N(2)-P(1)	120.2(3)
C(3)-N(2)-P(1)	115.9(3)
C(30)-N(3)-C(4)	120.1(3)
C(30)-N(3)-P(2)	123.8(2)
C(4)-N(3)-P(2)	114.3(3)
C(42)-N(4)-C(5)	120.4(3)
C(42)-N(4)-P(2)	124.9(3)
C(5)-N(4)-P(2)	114.2(3)
S(2)-C(1)-S(1)	124.8(3)
S(2)-C(1)-P(2)	128.3(2)
S(1)-C(1)-P(2)	106.9(2)
N(1)-C(2)-C(3)	106.4(3)
N(1)-C(2)-H(2A)	110.4
C(3)-C(2)-H(2A)	110.4
N(1)-C(2)-H(2B)	110.4
C(3)-C(2)-H(2B)	110.4
H(2A)-C(2)-H(2B)	108.6
N(2)-C(3)-C(2)	105.3(3)
N(2)-C(3)-H(3A)	110.7
C(2)-C(3)-H(3A)	110.7
N(2)-C(3)-H(3B)	110.7
C(2)-C(3)-H(3B)	110.7
H(3A)-C(3)-H(3B)	108.8
N(3)-C(4)-C(5)	106.4(3)

N(3)-C(4)-H(4A)	110.5
C(5)-C(4)-H(4A)	110.5
N(3)-C(4)-H(4B)	110.5
C(5)-C(4)-H(4B)	110.5
H(4A)-C(4)-H(4B)	108.6
N(4)-C(5)-C(4)	107.0(3)
N(4)-C(5)-H(5A)	110.3
C(4)-C(5)-H(5A)	110.3
N(4)-C(5)-H(5B)	110.3
C(4)-C(5)-H(5B)	110.3
H(5A)-C(5)-H(5B)	108.6
C(11)-C(6)-C(7)	121.7(4)
C(11)-C(6)-N(1)	119.1(3)
C(7)-C(6)-N(1)	119.1(3)
C(8)-C(7)-C(6)	117.2(4)
C(8)-C(7)-C(12)	120.3(4)
C(6)-C(7)-C(12)	122.5(4)
C(9)-C(8)-C(7)	121.9(4)
C(9)-C(8)-H(8)	119.0
C(7)-C(8)-H(8)	119.0
C(8)-C(9)-C(10)	119.9(4)
C(8)-C(9)-H(9)	120.0
C(10)-C(9)-H(9)	120.0
C(9)-C(10)-C(11)	121.1(4)
C(9)-C(10)-H(10)	119.4
C(11)-C(10)-H(10)	119.4
C(10)-C(11)-C(6)	118.0(4)
C(10)-C(11)-C(15)	119.6(4)
C(6)-C(11)-C(15)	122.4(4)
C(7)-C(12)-C(14)	111.6(4)
C(7)-C(12)-C(13)	111.3(4)
C(14)-C(12)-C(13)	110.7(4)
C(7)-C(12)-H(12)	107.7
C(14)-C(12)-H(12)	107.7
C(13)-C(12)-H(12)	107.7
C(12)-C(13)-H(13A)	109.5

C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(11)-C(15)-C(17)	113.4(4)
C(11)-C(15)-C(16)	109.7(3)
C(17)-C(15)-C(16)	110.2(3)
C(11)-C(15)-H(15)	107.8
C(17)-C(15)-H(15)	107.8
C(16)-C(15)-H(15)	107.8
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(19)-C(18)-C(23)	121.9(4)
C(19)-C(18)-N(2)	120.2(3)
C(23)-C(18)-N(2)	117.9(4)
C(20)-C(19)-C(18)	117.5(4)
C(20)-C(19)-C(27)	119.5(4)
C(18)-C(19)-C(27)	123.0(4)
C(19)-C(20)-C(21)	121.8(4)

C(19)-C(20)-H(20)	119.1
C(21)-C(20)-H(20)	119.1
C(22)-C(21)-C(20)	119.1(4)
C(22)-C(21)-H(21)	120.5
C(20)-C(21)-H(21)	120.5
C(23)-C(22)-C(21)	121.9(4)
C(23)-C(22)-H(22)	119.1
C(21)-C(22)-H(22)	119.1
C(22)-C(23)-C(18)	117.7(4)
C(22)-C(23)-C(24)	119.5(4)
C(18)-C(23)-C(24)	122.8(4)
C(25)-C(24)-C(23)	112.5(4)
C(25)-C(24)-C(26)	110.8(4)
C(23)-C(24)-C(26)	110.7(4)
C(25)-C(24)-H(24)	107.5
C(23)-C(24)-H(24)	107.5
C(26)-C(24)-H(24)	107.5
C(24)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(19)-C(27)-C(29)	112.7(4)
C(19)-C(27)-C(28)	110.2(4)
C(29)-C(27)-C(28)	110.2(4)
C(19)-C(27)-H(27)	107.8
C(29)-C(27)-H(27)	107.8
C(28)-C(27)-H(27)	107.8
C(27)-C(28)-H(28A)	109.5

C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(35)-C(30)-C(31)	119.7(4)
C(35)-C(30)-N(3)	120.4(4)
C(31)-C(30)-N(3)	119.8(4)
C(32)-C(31)-C(30)	118.4(4)
C(32)-C(31)-C(36)	119.6(4)
C(30)-C(31)-C(36)	122.0(4)
C(33)-C(32)-C(31)	121.7(4)
C(33)-C(32)-H(32)	119.1
C(31)-C(32)-H(32)	119.1
C(32)-C(33)-C(34)	119.6(4)
C(32)-C(33)-H(33)	120.2
C(34)-C(33)-H(33)	120.2
C(33)-C(34)-C(35)	121.3(4)
C(33)-C(34)-H(34)	119.4
C(35)-C(34)-H(34)	119.4
C(34)-C(35)-C(30)	119.2(4)
C(34)-C(35)-C(39)	118.6(4)
C(30)-C(35)-C(39)	122.2(4)
C(31)-C(36)-C(37)	112.2(4)
C(31)-C(36)-C(38)	111.0(4)
C(37)-C(36)-C(38)	109.5(4)
C(31)-C(36)-H(36)	108.0
C(37)-C(36)-H(36)	108.0
C(38)-C(36)-H(36)	108.0
C(36)-C(37)-H(37A)	109.5

C(36)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(36)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(36)-C(38)-H(38A)	109.5
C(36)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(36)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(40)-C(39)-C(41)	111.0(4)
C(40)-C(39)-C(35)	111.1(3)
C(41)-C(39)-C(35)	111.2(4)
C(40)-C(39)-H(39)	107.8
C(41)-C(39)-H(39)	107.8
C(35)-C(39)-H(39)	107.8
C(39)-C(40)-H(40A)	109.5
C(39)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(39)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(39)-C(41)-H(41A)	109.5
C(39)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(39)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(43)-C(42)-C(47)	120.4(4)
C(43)-C(42)-N(4)	120.1(4)
C(47)-C(42)-N(4)	119.5(4)
C(44)-C(43)-C(42)	118.6(4)
C(44)-C(43)-C(48)	118.3(4)
C(42)-C(43)-C(48)	123.0(4)
C(45)-C(44)-C(43)	120.8(4)

C(45)-C(44)-H(44)	119.6
C(43)-C(44)-H(44)	119.6
C(46)-C(45)-C(44)	120.2(4)
C(46)-C(45)-H(45)	119.9
C(44)-C(45)-H(45)	119.9
C(45)-C(46)-C(47)	121.5(4)
C(45)-C(46)-H(46)	119.2
C(47)-C(46)-H(46)	119.2
C(46)-C(47)-C(42)	118.4(4)
C(46)-C(47)-C(51)	119.1(4)
C(42)-C(47)-C(51)	122.5(4)
C(43)-C(48)-C(49)	113.0(4)
C(43)-C(48)-C(50)	110.6(4)
C(49)-C(48)-C(50)	110.7(4)
C(43)-C(48)-H(48)	107.4
C(49)-C(48)-H(48)	107.4
C(50)-C(48)-H(48)	107.4
C(48)-C(49)-H(49A)	109.5
C(48)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(48)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(48)-C(50)-H(50A)	109.5
C(48)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(48)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(47)-C(51)-C(52)	110.9(4)
C(47)-C(51)-C(53)	111.9(4)
C(52)-C(51)-C(53)	110.0(4)
C(47)-C(51)-H(51)	108.0
C(52)-C(51)-H(51)	108.0
C(53)-C(51)-H(51)	108.0
C(51)-C(52)-H(52A)	109.5

C(51)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(51)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(51)-C(53)-H(53A)	109.5
C(51)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(51)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	37(1)	23(1)	34(1)	4(1)	-1(1)	-5(1)
S(2)	46(1)	27(1)	68(1)	0(1)	-24(1)	0(1)
P(1)	26(1)	22(1)	22(1)	-2(1)	2(1)	-3(1)
P(2)	25(1)	22(1)	29(1)	2(1)	-2(1)	-2(1)
N(1)	25(2)	18(2)	19(2)	-1(2)	0(2)	-3(2)
N(2)	27(2)	19(2)	22(2)	-4(2)	3(2)	-8(2)
N(3)	21(2)	17(2)	36(2)	0(2)	4(2)	0(2)
N(4)	23(2)	27(2)	26(2)	1(2)	3(2)	-5(2)
C(1)	34(3)	21(3)	28(2)	-1(2)	-4(2)	-3(2)
C(2)	51(3)	24(3)	27(3)	-4(2)	7(2)	-10(2)
C(3)	41(3)	27(3)	27(3)	-2(2)	4(2)	-9(2)
C(4)	23(2)	33(3)	56(3)	-9(3)	14(2)	-7(2)
C(5)	42(3)	34(3)	42(3)	1(2)	11(2)	-14(2)
C(6)	26(2)	18(2)	16(2)	1(2)	0(2)	-3(2)
C(7)	23(2)	28(3)	25(2)	4(2)	3(2)	1(2)
C(8)	20(2)	46(3)	28(3)	2(2)	-4(2)	-7(2)
C(9)	31(3)	32(3)	26(3)	-3(2)	0(2)	-6(2)
C(10)	31(2)	23(3)	23(2)	-2(2)	2(2)	0(2)
C(11)	28(2)	22(3)	19(2)	0(2)	2(2)	-3(2)
C(12)	27(3)	57(4)	38(3)	-9(3)	-7(2)	12(2)
C(13)	97(5)	91(6)	70(4)	3(4)	-13(4)	60(4)
C(14)	29(3)	101(5)	69(4)	-21(4)	13(3)	3(3)
C(15)	27(2)	30(3)	29(3)	-6(2)	-3(2)	7(2)
C(16)	24(2)	54(4)	41(3)	-13(3)	6(2)	-1(2)
C(17)	42(3)	42(3)	52(3)	-9(3)	-7(2)	14(3)
C(18)	30(2)	16(3)	25(2)	-3(2)	3(2)	-6(2)
C(19)	31(2)	19(3)	29(3)	-3(2)	0(2)	-2(2)
C(20)	43(3)	34(3)	25(3)	-3(2)	-5(2)	-2(2)
C(21)	54(3)	43(3)	27(3)	-12(2)	6(2)	4(3)
C(22)	40(3)	29(3)	43(3)	-9(2)	7(2)	4(2)
C(23)	33(3)	20(3)	24(2)	-4(2)	2(2)	-2(2)

C(24)	32(3)	28(3)	38(3)	-9(2)	1(2)	5(2)
C(25)	36(3)	78(5)	99(5)	22(4)	-14(3)	-9(3)
C(26)	76(4)	38(4)	86(4)	13(3)	-20(3)	-6(3)
C(27)	32(3)	32(3)	27(3)	-2(2)	-5(2)	1(2)
C(28)	37(3)	46(4)	56(3)	-15(3)	-1(2)	-13(3)
C(29)	45(3)	45(4)	40(3)	0(3)	1(2)	8(3)
C(30)	20(2)	18(3)	30(3)	1(2)	6(2)	-7(2)
C(31)	22(2)	26(3)	34(3)	5(2)	-2(2)	-5(2)
C(32)	38(3)	33(3)	27(3)	2(2)	-3(2)	2(2)
C(33)	39(3)	26(3)	37(3)	-7(2)	6(2)	0(2)
C(34)	35(3)	26(3)	34(3)	2(2)	3(2)	5(2)
C(35)	25(2)	22(3)	28(2)	0(2)	3(2)	-4(2)
C(36)	30(3)	30(3)	42(3)	5(2)	-10(2)	-3(2)
C(37)	51(3)	74(5)	72(4)	38(4)	-2(3)	2(3)
C(38)	30(3)	59(4)	78(4)	19(3)	-9(3)	-5(3)
C(39)	30(2)	28(3)	26(2)	5(2)	3(2)	6(2)
C(40)	29(3)	56(4)	33(3)	4(2)	-5(2)	-2(2)
C(41)	65(3)	39(3)	37(3)	8(3)	5(3)	-4(3)
C(42)	29(2)	23(3)	22(2)	2(2)	4(2)	0(2)
C(43)	31(3)	30(3)	25(3)	4(2)	5(2)	-2(2)
C(44)	41(3)	35(3)	30(3)	1(2)	-1(2)	2(2)
C(45)	57(3)	31(3)	33(3)	-1(2)	6(3)	0(3)
C(46)	48(3)	30(3)	36(3)	0(2)	16(2)	10(2)
C(47)	34(3)	27(3)	32(3)	5(2)	12(2)	5(2)
C(48)	29(2)	31(3)	29(3)	-5(2)	-4(2)	2(2)
C(49)	39(3)	52(4)	106(5)	-35(4)	11(3)	-7(3)
C(50)	100(5)	68(5)	70(4)	25(4)	33(4)	49(4)
C(51)	31(3)	34(3)	42(3)	3(2)	11(2)	10(2)
C(52)	41(3)	52(4)	64(4)	14(3)	12(3)	5(3)
C(53)	47(3)	52(4)	50(3)	20(3)	15(3)	12(3)

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

	x	y	z	U(eq)
H(2A)	1633	-2313	4096	41
H(2B)	2443	-2901	4011	41
H(3A)	1751	-3431	3168	38
H(3B)	1173	-2543	3114	38
H(4A)	3749	2469	2263	44
H(4B)	3339	3393	1988	44
H(5A)	2860	2704	1113	47
H(5B)	3599	2010	1270	47
H(8)	4384	-440	5086	38
H(9)	3498	613	5462	36
H(10)	2154	639	5088	31
H(12)	3880	-2169	3942	49
H(13A)	4883	-1863	5054	130
H(13B)	4981	-2717	4599	130
H(13C)	4179	-2614	4978	130
H(14A)	4563	-965	3478	99
H(14B)	5205	-1738	3696	99
H(14C)	5132	-822	4097	99
H(15)	1283	-758	3852	35
H(16A)	1010	-1427	4814	59
H(16B)	261	-789	4590	59
H(16C)	906	-439	5121	59
H(17A)	1052	977	4437	68
H(17B)	474	550	3889	68
H(17C)	1376	864	3754	68
H(20)	1474	-2662	729	41
H(21)	2675	-3391	494	49
H(22)	3625	-3761	1292	44
H(24)	3479	-3254	2910	40
H(25A)	4715	-3331	2039	107

H(25B)	4863	-3239	2777	107
H(25C)	4454	-2415	2383	107
H(26A)	3167	-4774	2605	101
H(26B)	4075	-4703	2902	101
H(26C)	3916	-4774	2163	101
H(27)	985	-1802	2217	37
H(28A)	202	-3048	1346	70
H(28B)	-265	-2466	1844	70
H(28C)	368	-3241	2074	70
H(29A)	1174	-832	1347	65
H(29B)	233	-957	1472	65
H(29C)	621	-1507	918	65
H(32)	2424	4200	4157	40
H(33)	1372	5110	3753	41
H(34)	891	4926	2727	38
H(36)	3357	2348	3370	41
H(37A)	2954	2895	4591	99
H(37B)	3502	2029	4438	99
H(37C)	2558	2038	4224	99
H(38A)	4141	3709	3366	84
H(38B)	4466	3040	3914	84
H(38C)	3925	3912	4069	84
H(39)	1583	3280	1648	33
H(40A)	86	4045	2005	60
H(40B)	304	2978	2027	60
H(40C)	198	3496	1372	60
H(41A)	1162	5177	1675	71
H(41B)	1257	4591	1055	71
H(41C)	2034	4793	1513	71
H(44)	897	293	-10	43
H(45)	1809	-867	-191	48
H(46)	3049	-924	360	45
H(48)	1166	2043	1143	36
H(49A)	-77	987	517	98
H(49B)	-226	1856	950	98
H(49C)	156	938	1249	98

H(50A)	1496	2584	172	117
H(50B)	567	2818	277	117
H(50C)	788	1984	-164	117
H(51)	3722	572	1600	43
H(52A)	4407	-116	498	78
H(52B)	4902	380	1063	78
H(52C)	4267	950	626	78
H(53A)	3411	-993	1803	74
H(53B)	4369	-833	1792	74
H(53C)	3884	-1291	1206	74

Crystallography tables for compound 3

Table 1. Crystal data and structure refinement for 3.

Identification code	NG122_0m	
Empirical formula	C59 H81 N5 O P2	
Formula weight	938.22	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 29.594(7) Å	α= 90°.
	b = 19.280(5) Å	β= 112.239(3)°.
	c = 22.869(6) Å	γ = 90°.
Volume	12078(5) $Å^3$	
Z	8	
Density (calculated)	1.032 Mg/m^3	
Absorption coefficient	0.111 mm^{-1}	
F(000)	4064	
Crystal size	0.237 x 0.154 x 0.094 mm^3	
Theta range for data collection	1.936 to 24.997°.	
Index ranges	-35<=h<=35, -22<=k<=22, -25<=l<=27	
Reflections collected	39221	
Independent reflections	10618 [R(int) = 0.0809]	
Completeness to theta = 24.997°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6802	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10618 / 0 / 620	
Goodness-of-fit on F^2	0.921	
Final R indices [I>2sigma(I)]	R1 = 0.0560, wR2 = 0.1218	
R indices (all data)	R1 = 0.1020, wR2 = 0.1368	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.226 and -0.297 $e.Å^{-3}$	

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

	x	y	z	U(eq)
P(1)	1432(1)	10240(1)	1114(1)	27(1)
P(2)	2858(1)	9516(1)	1212(1)	27(1)
O(1)	1846(1)	9710(1)	941(1)	27(1)
N(1)	2315(1)	10647(1)	1328(1)	31(1)
N(2)	1228(1)	10752(1)	462(1)	27(1)
N(3)	933(1)	9742(1)	816(1)	25(1)
N(4)	2656(1)	8890(1)	657(1)	28(1)
N(5)	2908(1)	8933(1)	1793(1)	28(1)
C(1)	2298(1)	10007(1)	1170(1)	27(1)
C(2)	2761(1)	10998(1)	1637(1)	33(1)
C(3)	3031(1)	10871(1)	2268(1)	38(1)
C(4)	3452(1)	11249(2)	2584(1)	45(1)
C(5)	3606(1)	11753(2)	2278(2)	49(1)
C(6)	3335(1)	11882(2)	1650(2)	51(1)
C(7)	2909(1)	11520(2)	1334(1)	43(1)
C(8)	740(1)	10570(1)	3(1)	30(1)
C(9)	675(1)	9815(1)	132(1)	28(1)
C(10)	2475(1)	8273(1)	888(1)	31(1)
C(11)	2797(1)	8220(1)	1583(1)	30(1)
C(12)	1439(1)	11401(1)	391(1)	29(1)
C(13)	1442(1)	11967(1)	778(1)	34(1)
C(14)	1640(1)	12590(2)	679(2)	43(1)
C(15)	1831(1)	12656(2)	218(2)	43(1)
C(16)	1831(1)	12090(1)	-157(1)	36(1)
C(17)	1638(1)	11461(1)	-74(1)	30(1)
C(18)	1652(1)	10852(1)	-492(1)	33(1)
C(19)	1332(1)	10989(2)	-1186(1)	45(1)
C(20)	2181(1)	10691(2)	-421(1)	42(1)
C(21)	1237(1)	11931(2)	1291(1)	39(1)
C(22)	784(1)	12387(2)	1133(2)	64(1)
C(23)	1623(1)	12107(2)	1937(2)	60(1)

C(24)	759(1)	9320(1)	1205(1)	31(1)
C(25)	776(1)	8595(2)	1162(1)	37(1)
C(26)	613(1)	8202(2)	1552(2)	58(1)
C(27)	458(1)	8507(2)	1984(2)	67(1)
C(28)	440(1)	9213(2)	2019(2)	53(1)
C(29)	579(1)	9638(2)	1627(1)	35(1)
C(30)	522(1)	10419(1)	1661(1)	34(1)
C(31)	871(1)	10714(2)	2289(1)	47(1)
C(32)	-5(1)	10612(2)	1555(1)	47(1)
C(33)	956(1)	8234(1)	704(1)	36(1)
C(34)	1295(1)	7625(2)	1012(2)	50(1)
C(35)	517(1)	7979(2)	126(2)	50(1)
C(36)	2670(1)	8893(1)	37(1)	31(1)
C(37)	2249(1)	8707(1)	-488(1)	33(1)
C(38)	2279(1)	8644(1)	-1080(1)	41(1)
C(39)	2709(1)	8798(2)	-1165(2)	48(1)
C(40)	3112(1)	9011(2)	-657(2)	44(1)
C(41)	3111(1)	9054(1)	-46(1)	36(1)
C(42)	3577(1)	9288(2)	476(1)	40(1)
C(43)	4030(1)	8900(2)	478(2)	66(1)
C(44)	3640(1)	10074(2)	449(2)	58(1)
C(45)	1751(1)	8583(1)	-452(1)	35(1)
C(46)	1346(1)	8981(2)	-968(1)	50(1)
C(47)	1612(1)	7819(2)	-507(1)	43(1)
C(48)	3168(1)	9076(1)	2450(1)	28(1)
C(49)	3679(1)	9151(1)	2691(1)	34(1)
C(50)	3914(1)	9314(2)	3327(1)	39(1)
C(51)	3662(1)	9391(2)	3715(1)	38(1)
C(52)	3160(1)	9299(1)	3480(1)	32(1)
C(53)	2904(1)	9139(1)	2846(1)	28(1)
C(54)	2354(1)	9032(1)	2599(1)	32(1)
C(55)	2091(1)	9644(2)	2757(1)	40(1)
C(56)	2225(1)	8361(2)	2855(1)	43(1)
C(57)	3975(1)	9051(2)	2281(1)	41(1)
C(58)	4240(1)	9715(2)	2235(2)	63(1)
C(59)	4330(1)	8443(2)	2509(2)	67(1)

Table 3. Bond lengths [Å] and angles [°] for 3.

P(1)-N(3)	1.675(2)
P(1)-N(2)	1.697(2)
P(1)-O(1)	1.7510(17)
P(2)-N(4)	1.688(2)
P(2)-N(5)	1.702(2)
P(2)-C(1)	1.881(3)
O(1)-C(1)	1.363(3)
N(1)-C(1)	1.281(3)
N(1)-C(2)	1.412(3)
N(2)-C(12)	1.435(3)
N(2)-C(8)	1.470(3)
N(3)-C(24)	1.439(3)
N(3)-C(9)	1.463(3)
N(4)-C(36)	1.434(3)
N(4)-C(10)	1.481(3)
N(5)-C(48)	1.433(3)
N(5)-C(11)	1.451(3)
C(2)-C(3)	1.382(4)
C(2)-C(7)	1.384(4)
C(3)-C(4)	1.385(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.373(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.376(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.382(4)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-C(9)	1.513(3)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.517(3)

C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.403(4)
C(12)-C(17)	1.403(4)
C(13)-C(14)	1.393(4)
C(13)-C(21)	1.511(4)
C(14)-C(15)	1.378(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.387(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.383(4)
C(16)-H(16)	0.9500
C(17)-C(18)	1.524(4)
C(18)-C(19)	1.532(4)
C(18)-C(20)	1.544(4)
C(18)-H(18)	1.0000
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(23)	1.525(4)
C(21)-C(22)	1.529(4)
C(21)-H(21)	1.0000
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-C(25)	1.403(4)
C(24)-C(29)	1.406(4)
C(25)-C(26)	1.388(4)

C(25)-C(33)	1.513(4)
C(26)-C(27)	1.370(4)
C(26)-H(26)	0.9500
C(27)-C(28)	1.366(4)
C(27)-H(27)	0.9500
C(28)-C(29)	1.386(4)
C(28)-H(28)	0.9500
C(29)-C(30)	1.521(4)
C(30)-C(31)	1.526(4)
C(30)-C(32)	1.531(3)
C(30)-H(30)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.532(4)
C(33)-C(35)	1.542(4)
C(33)-H(33)	1.0000
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-C(37)	1.409(4)
C(36)-C(41)	1.424(4)
C(37)-C(38)	1.395(4)
C(37)-C(45)	1.526(4)
C(38)-C(39)	1.389(4)
C(38)-H(38)	0.9500
C(39)-C(40)	1.375(4)
C(39)-H(39)	0.9500
C(40)-C(41)	1.399(4)
C(40)-H(40)	0.9500

C(41)-C(42)	1.511(4)
C(42)-C(44)	1.531(4)
C(42)-C(43)	1.534(4)
C(42)-H(42)	1.0000
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-C(47)	1.521(4)
C(45)-C(46)	1.534(4)
C(45)-H(45)	1.0000
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-C(53)	1.407(3)
C(48)-C(49)	1.407(3)
C(49)-C(50)	1.390(4)
C(49)-C(57)	1.519(4)
C(50)-C(51)	1.365(4)
C(50)-H(50)	0.9500
C(51)-C(52)	1.387(4)
C(51)-H(51)	0.9500
C(52)-C(53)	1.392(4)
C(52)-H(52)	0.9500
C(53)-C(54)	1.524(3)
C(54)-C(56)	1.527(4)
C(54)-C(55)	1.530(4)
C(54)-H(54)	1.0000
C(55)-H(55A)	0.9800
C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800

C(56)-H(56A)	0.9800
C(56)-H(56B)	0.9800
C(56)-H(56C)	0.9800
C(57)-C(58)	1.526(4)
C(57)-C(59)	1.527(4)
C(57)-H(57)	1.0000
C(58)-H(58A)	0.9800
C(58)-H(58B)	0.9800
C(58)-H(58C)	0.9800
C(59)-H(59A)	0.9800
C(59)-H(59B)	0.9800
C(59)-H(59C)	0.9800

N(3)-P(1)-N(2)	90.55(10)
N(3)-P(1)-O(1)	99.12(9)
N(2)-P(1)-O(1)	100.89(9)
N(4)-P(2)-N(5)	90.89(11)
N(4)-P(2)-C(1)	105.44(11)
N(5)-P(2)-C(1)	100.76(11)
C(1)-O(1)-P(1)	109.61(15)
C(1)-N(1)-C(2)	122.2(2)
C(12)-N(2)-C(8)	118.65(19)
C(12)-N(2)-P(1)	125.51(17)
C(8)-N(2)-P(1)	114.54(16)
C(24)-N(3)-C(9)	123.4(2)
C(24)-N(3)-P(1)	122.68(17)
C(9)-N(3)-P(1)	113.79(16)
C(36)-N(4)-C(10)	120.3(2)
C(36)-N(4)-P(2)	127.26(18)
C(10)-N(4)-P(2)	112.32(16)
C(48)-N(5)-C(11)	119.48(19)
C(48)-N(5)-P(2)	123.00(17)
C(11)-N(5)-P(2)	115.20(17)
N(1)-C(1)-O(1)	116.2(2)
N(1)-C(1)-P(2)	122.01(19)
O(1)-C(1)-P(2)	121.68(19)

C(3)-C(2)-C(7)	119.0(3)
C(3)-C(2)-N(1)	120.1(3)
C(7)-C(2)-N(1)	120.6(3)
C(2)-C(3)-C(4)	120.1(3)
C(2)-C(3)-H(3)	120.0
C(4)-C(3)-H(3)	120.0
C(5)-C(4)-C(3)	120.9(3)
C(5)-C(4)-H(4)	119.5
C(3)-C(4)-H(4)	119.5
C(4)-C(5)-C(6)	119.0(3)
C(4)-C(5)-H(5)	120.5
C(6)-C(5)-H(5)	120.5
C(5)-C(6)-C(7)	120.8(3)
C(5)-C(6)-H(6)	119.6
C(7)-C(6)-H(6)	119.6
C(6)-C(7)-C(2)	120.2(3)
C(6)-C(7)-H(7)	119.9
C(2)-C(7)-H(7)	119.9
N(2)-C(8)-C(9)	104.7(2)
N(2)-C(8)-H(8A)	110.8
C(9)-C(8)-H(8A)	110.8
N(2)-C(8)-H(8B)	110.8
C(9)-C(8)-H(8B)	110.8
H(8A)-C(8)-H(8B)	108.9
N(3)-C(9)-C(8)	104.29(19)
N(3)-C(9)-H(9A)	110.9
C(8)-C(9)-H(9A)	110.9
N(3)-C(9)-H(9B)	110.9
C(8)-C(9)-H(9B)	110.9
H(9A)-C(9)-H(9B)	108.9
N(4)-C(10)-C(11)	105.0(2)
N(4)-C(10)-H(10A)	110.8
C(11)-C(10)-H(10A)	110.8
N(4)-C(10)-H(10B)	110.8
C(11)-C(10)-H(10B)	110.8
H(10A)-C(10)-H(10B)	108.8

N(5)-C(11)-C(10)	104.9(2)
N(5)-C(11)-H(11A)	110.8
C(10)-C(11)-H(11A)	110.8
N(5)-C(11)-H(11B)	110.8
C(10)-C(11)-H(11B)	110.8
H(11A)-C(11)-H(11B)	108.8
C(13)-C(12)-C(17)	120.7(2)
C(13)-C(12)-N(2)	120.4(2)
C(17)-C(12)-N(2)	118.9(2)
C(14)-C(13)-C(12)	118.1(3)
C(14)-C(13)-C(21)	118.9(3)
C(12)-C(13)-C(21)	123.1(3)
C(15)-C(14)-C(13)	121.6(3)
C(15)-C(14)-H(14)	119.2
C(13)-C(14)-H(14)	119.2
C(14)-C(15)-C(16)	119.8(3)
C(14)-C(15)-H(15)	120.1
C(16)-C(15)-H(15)	120.1
C(17)-C(16)-C(15)	120.5(3)
C(17)-C(16)-H(16)	119.7
C(15)-C(16)-H(16)	119.7
C(16)-C(17)-C(12)	119.3(3)
C(16)-C(17)-C(18)	118.7(2)
C(12)-C(17)-C(18)	122.0(2)
C(17)-C(18)-C(19)	111.4(2)
C(17)-C(18)-C(20)	110.9(2)
C(19)-C(18)-C(20)	110.3(2)
C(17)-C(18)-H(18)	108.1
C(19)-C(18)-H(18)	108.1
C(20)-C(18)-H(18)	108.1
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(13)-C(21)-C(23)	111.6(2)
C(13)-C(21)-C(22)	111.4(3)
C(23)-C(21)-C(22)	111.7(3)
C(13)-C(21)-H(21)	107.3
C(23)-C(21)-H(21)	107.3
C(22)-C(21)-H(21)	107.3
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(21)-C(23)-H(23A)	109.5
C(21)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(21)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(25)-C(24)-C(29)	121.0(3)
C(25)-C(24)-N(3)	119.2(2)
C(29)-C(24)-N(3)	119.7(2)
C(26)-C(25)-C(24)	117.9(3)
C(26)-C(25)-C(33)	119.5(3)
C(24)-C(25)-C(33)	122.6(3)
C(27)-C(26)-C(25)	121.4(3)
C(27)-C(26)-H(26)	119.3
C(25)-C(26)-H(26)	119.3
C(28)-C(27)-C(26)	120.1(3)
C(28)-C(27)-H(27)	120.0
C(26)-C(27)-H(27)	120.0

C(27)-C(28)-C(29)	121.5(3)
C(27)-C(28)-H(28)	119.2
C(29)-C(28)-H(28)	119.2
C(28)-C(29)-C(24)	117.9(3)
C(28)-C(29)-C(30)	119.1(3)
C(24)-C(29)-C(30)	123.0(2)
C(29)-C(30)-C(31)	111.6(2)
C(29)-C(30)-C(32)	111.0(2)
C(31)-C(30)-C(32)	110.2(2)
C(29)-C(30)-H(30)	107.9
C(31)-C(30)-H(30)	107.9
C(32)-C(30)-H(30)	107.9
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(25)-C(33)-C(34)	112.1(2)
C(25)-C(33)-C(35)	109.7(2)
C(34)-C(33)-C(35)	110.0(2)
C(25)-C(33)-H(33)	108.3
C(34)-C(33)-H(33)	108.3
C(35)-C(33)-H(33)	108.3
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5

C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(37)-C(36)-C(41)	120.0(2)
C(37)-C(36)-N(4)	119.6(2)
C(41)-C(36)-N(4)	120.3(2)
C(38)-C(37)-C(36)	119.3(3)
C(38)-C(37)-C(45)	117.1(3)
C(36)-C(37)-C(45)	123.6(2)
C(39)-C(38)-C(37)	121.0(3)
C(39)-C(38)-H(38)	119.5
C(37)-C(38)-H(38)	119.5
C(40)-C(39)-C(38)	119.5(3)
C(40)-C(39)-H(39)	120.3
C(38)-C(39)-H(39)	120.3
C(39)-C(40)-C(41)	122.2(3)
C(39)-C(40)-H(40)	118.9
C(41)-C(40)-H(40)	118.9
C(40)-C(41)-C(36)	117.9(3)
C(40)-C(41)-C(42)	117.5(3)
C(36)-C(41)-C(42)	124.6(2)
C(41)-C(42)-C(44)	110.6(2)
C(41)-C(42)-C(43)	113.0(3)
C(44)-C(42)-C(43)	111.2(3)
C(41)-C(42)-H(42)	107.2
C(44)-C(42)-H(42)	107.2
C(43)-C(42)-H(42)	107.2
C(42)-C(43)-H(43A)	109.5
C(42)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(42)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5

C(42)-C(44)-H(44A)	109.5
C(42)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(42)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(47)-C(45)-C(37)	112.7(2)
C(47)-C(45)-C(46)	108.2(2)
C(37)-C(45)-C(46)	111.7(2)
C(47)-C(45)-H(45)	108.0
C(37)-C(45)-H(45)	108.0
C(46)-C(45)-H(45)	108.0
C(45)-C(46)-H(46A)	109.5
C(45)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(45)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
C(45)-C(47)-H(47A)	109.5
C(45)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(45)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(53)-C(48)-C(49)	121.0(2)
C(53)-C(48)-N(5)	118.8(2)
C(49)-C(48)-N(5)	120.2(2)
C(50)-C(49)-C(48)	118.1(2)
C(50)-C(49)-C(57)	119.9(2)
C(48)-C(49)-C(57)	122.0(2)
C(51)-C(50)-C(49)	121.6(3)
C(51)-C(50)-H(50)	119.2
C(49)-C(50)-H(50)	119.2
C(50)-C(51)-C(52)	120.2(3)
C(50)-C(51)-H(51)	119.9
C(52)-C(51)-H(51)	119.9

C(51)-C(52)-C(53)	120.8(3)
C(51)-C(52)-H(52)	119.6
C(53)-C(52)-H(52)	119.6
C(52)-C(53)-C(48)	118.3(2)
C(52)-C(53)-C(54)	120.0(2)
C(48)-C(53)-C(54)	121.7(2)
C(53)-C(54)-C(56)	111.0(2)
C(53)-C(54)-C(55)	112.1(2)
C(56)-C(54)-C(55)	109.9(2)
C(53)-C(54)-H(54)	107.9
C(56)-C(54)-H(54)	107.9
C(55)-C(54)-H(54)	107.9
C(54)-C(55)-H(55A)	109.5
C(54)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
C(54)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
C(54)-C(56)-H(56A)	109.5
C(54)-C(56)-H(56B)	109.5
H(56A)-C(56)-H(56B)	109.5
C(54)-C(56)-H(56C)	109.5
H(56A)-C(56)-H(56C)	109.5
H(56B)-C(56)-H(56C)	109.5
C(49)-C(57)-C(58)	111.5(3)
C(49)-C(57)-C(59)	111.6(2)
C(58)-C(57)-C(59)	111.3(3)
C(49)-C(57)-H(57)	107.4
C(58)-C(57)-H(57)	107.4
C(59)-C(57)-H(57)	107.4
C(57)-C(58)-H(58A)	109.5
C(57)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
C(57)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5

C(57)-C(59)-H(59A)	109.5
C(57)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	109.5
C(57)-C(59)-H(59C)	109.5
H(59A)-C(59)-H(59C)	109.5
H(59B)-C(59)-H(59C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	23(1)	34(1)	23(1)	-4(1)	10(1)	2(1)
P(2)	24(1)	34(1)	24(1)	3(1)	12(1)	5(1)
O(1)	23(1)	32(1)	26(1)	-2(1)	10(1)	4(1)
N(1)	27(1)	34(1)	32(1)	-2(1)	10(1)	1(1)
N(2)	25(1)	28(1)	25(1)	-2(1)	6(1)	2(1)
N(3)	22(1)	34(1)	21(1)	-3(1)	9(1)	-3(1)
N(4)	31(1)	33(1)	26(1)	4(1)	16(1)	4(1)
N(5)	32(1)	32(1)	20(1)	3(1)	11(1)	6(1)
C(1)	25(1)	36(2)	21(2)	2(1)	10(1)	2(1)
C(2)	29(2)	32(2)	38(2)	-4(1)	14(1)	4(1)
C(3)	38(2)	38(2)	36(2)	1(1)	14(2)	-5(1)
C(4)	46(2)	49(2)	29(2)	1(2)	4(2)	-6(2)
C(5)	43(2)	48(2)	47(2)	-1(2)	4(2)	-11(2)
C(6)	45(2)	53(2)	51(2)	11(2)	14(2)	-15(2)
C(7)	39(2)	48(2)	35(2)	10(2)	7(2)	-3(2)
C(8)	27(1)	34(2)	27(2)	-1(1)	9(1)	0(1)
C(9)	26(1)	30(2)	25(2)	-2(1)	7(1)	0(1)
C(10)	33(2)	35(2)	30(2)	3(1)	17(1)	6(1)
C(11)	36(2)	32(2)	27(2)	3(1)	15(1)	6(1)
C(12)	22(1)	27(2)	31(2)	-1(1)	4(1)	1(1)
C(13)	25(1)	34(2)	40(2)	-9(1)	10(1)	-2(1)
C(14)	34(2)	37(2)	53(2)	-10(2)	12(2)	-1(1)
C(15)	35(2)	36(2)	50(2)	6(2)	8(2)	-7(1)
C(16)	34(2)	39(2)	34(2)	6(1)	12(1)	0(1)
C(17)	30(2)	30(2)	27(2)	5(1)	7(1)	1(1)
C(18)	40(2)	36(2)	27(2)	2(1)	15(1)	0(1)
C(19)	52(2)	50(2)	33(2)	-2(2)	15(2)	-4(2)
C(20)	46(2)	48(2)	37(2)	1(1)	20(2)	4(2)
C(21)	37(2)	36(2)	50(2)	-18(1)	22(2)	-4(1)
C(22)	49(2)	68(2)	84(3)	-23(2)	34(2)	-1(2)
C(23)	53(2)	82(3)	46(2)	-22(2)	21(2)	-15(2)

C(24)	26(1)	41(2)	28(2)	0(1)	13(1)	-2(1)
C(25)	39(2)	41(2)	39(2)	3(1)	22(2)	3(1)
C(26)	83(2)	46(2)	68(3)	4(2)	53(2)	-1(2)
C(27)	99(3)	59(2)	74(3)	12(2)	68(3)	-2(2)
C(28)	63(2)	64(2)	54(2)	2(2)	45(2)	1(2)
C(29)	33(2)	49(2)	29(2)	-1(1)	17(1)	2(1)
C(30)	30(2)	49(2)	29(2)	-6(1)	16(1)	4(1)
C(31)	37(2)	62(2)	38(2)	-7(2)	10(2)	7(2)
C(32)	33(2)	72(2)	35(2)	-9(2)	11(2)	11(2)
C(33)	40(2)	35(2)	39(2)	1(1)	24(2)	5(1)
C(34)	54(2)	45(2)	54(2)	5(2)	24(2)	9(2)
C(35)	47(2)	51(2)	54(2)	-9(2)	23(2)	-2(2)
C(36)	44(2)	30(2)	23(2)	4(1)	18(1)	14(1)
C(37)	45(2)	31(2)	28(2)	2(1)	18(2)	13(1)
C(38)	59(2)	34(2)	32(2)	-1(1)	18(2)	5(2)
C(39)	81(3)	41(2)	38(2)	3(2)	40(2)	7(2)
C(40)	59(2)	43(2)	44(2)	1(2)	35(2)	1(2)
C(41)	47(2)	34(2)	37(2)	7(1)	29(2)	11(1)
C(42)	40(2)	47(2)	45(2)	3(2)	30(2)	3(2)
C(43)	42(2)	83(3)	84(3)	-19(2)	38(2)	1(2)
C(44)	79(2)	54(2)	48(2)	2(2)	34(2)	-15(2)
C(45)	36(2)	42(2)	27(2)	-4(1)	11(1)	17(1)
C(46)	51(2)	55(2)	34(2)	-6(2)	4(2)	20(2)
C(47)	42(2)	52(2)	37(2)	-5(2)	18(2)	2(2)
C(48)	29(2)	32(2)	24(2)	5(1)	12(1)	3(1)
C(49)	30(2)	42(2)	31(2)	8(1)	13(1)	4(1)
C(50)	24(2)	58(2)	34(2)	4(2)	8(1)	-1(1)
C(51)	36(2)	47(2)	27(2)	2(1)	8(1)	-3(1)
C(52)	37(2)	36(2)	27(2)	1(1)	16(1)	1(1)
C(53)	32(2)	29(2)	25(2)	4(1)	14(1)	4(1)
C(54)	26(1)	43(2)	29(2)	3(1)	13(1)	5(1)
C(55)	35(2)	55(2)	34(2)	7(2)	18(1)	10(1)
C(56)	35(2)	50(2)	48(2)	5(2)	21(2)	-1(1)
C(57)	27(2)	64(2)	36(2)	7(2)	16(1)	9(2)
C(58)	54(2)	89(3)	59(2)	4(2)	37(2)	-11(2)
C(59)	47(2)	103(3)	61(3)	20(2)	33(2)	31(2)

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

	x	y	z	U(eq)
H(3)	2929	10523	2486	45
H(4)	3635	11159	3018	53
H(5)	3896	12008	2496	59
H(6)	3442	12223	1432	61
H(7)	2717	11630	906	51
H(8A)	722	10634	-435	36
H(8B)	486	10860	67	36
H(9A)	325	9699	6	33
H(9B)	819	9509	-99	33
H(10A)	2505	7851	658	37
H(10B)	2129	8333	831	37
H(11A)	2623	7984	1821	36
H(11B)	3100	7961	1643	36
H(14)	1644	12979	936	51
H(15)	1963	13087	158	52
H(16)	1964	12135	-474	43
H(18)	1519	10436	-350	40
H(19A)	995	11071	-1227	68
H(19B)	1343	10586	-1441	68
H(19C)	1454	11398	-1334	68
H(20A)	2312	11083	-578	63
H(20B)	2184	10274	-665	63
H(20C)	2382	10612	26	63
H(21)	1133	11441	1311	47
H(22A)	879	12876	1161	97
H(22B)	627	12293	1433	97
H(22C)	554	12284	703	97
H(23A)	1900	11788	2033	90
H(23B)	1482	12062	2260	90
H(23C)	1736	12584	1933	90

H(26)	609	7711	1518	70
H(27)	363	8227	2260	80
H(28)	329	9418	2318	64
H(30)	603	10636	1316	41
H(31A)	818	10479	2638	70
H(31B)	811	11212	2306	70
H(31C)	1209	10640	2327	70
H(32A)	-85	10438	1907	70
H(32B)	-227	10405	1159	70
H(32C)	-41	11118	1530	70
H(33)	1143	8578	555	43
H(34A)	1563	7786	1392	75
H(34B)	1428	7434	713	75
H(34C)	1111	7264	1127	75
H(35A)	317	7666	267	74
H(35B)	635	7731	-162	74
H(35C)	320	8377	-93	74
H(38)	2002	8494	-1430	49
H(39)	2724	8755	-1571	58
H(40)	3399	9134	-723	53
H(42)	3543	9183	886	48
H(43A)	3980	8399	498	99
H(43B)	4315	9042	847	99
H(43C)	4084	9010	91	99
H(44A)	3651	10200	39	86
H(44B)	3946	10215	788	86
H(44C)	3365	10309	502	86
H(45)	1765	8753	-33	42
H(46A)	1440	9470	-960	75
H(46B)	1042	8947	-892	75
H(46C)	1296	8781	-1382	75
H(47A)	1602	7638	-912	64
H(47B)	1289	7768	-484	64
H(47C)	1854	7560	-161	64
H(50)	4259	9373	3496	47
H(51)	3831	9509	4146	45

H(52)	2989	9346	3755	39
H(54)	2233	8992	2128	38
H(55A)	2211	9704	3216	60
H(55B)	1739	9554	2592	60
H(55C)	2155	10068	2564	60
H(56A)	2381	7968	2733	64
H(56B)	1870	8297	2681	64
H(56C)	2343	8386	3317	64
H(57)	3741	8936	1845	49
H(58A)	4481	9835	2654	94
H(58B)	4003	10093	2080	94
H(58C)	4407	9644	1942	94
H(59A)	4506	8382	2225	100
H(59B)	4147	8019	2510	100
H(59C)	4564	8537	2938	100

Crystallography tables for compound 4

Table 1. Crystal data and structure refinement for 4.

Identification code	NG128_0m	
Empirical formula	C59 H81 N5 P2 S	
Formula weight	954.28	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.751(6) Å	α= 86.729(7)°.
	b = 13.140(6) Å	β= 85.693(8)°.
	c = 17.906(9) Å	γ = 65.164(7)°.
Volume	2714(2) $Å^3$	
Z	2	
Density (calculated)	1.168 Mg/m^3	
Absorption coefficient	0.161 mm^{-1}	
F(000)	1032	
Crystal size	.118 x .113 x .087 mm^3	
Theta range for data collection	1.874 to 24.997°.	
Index ranges	-13<=h<=15, -14<=k<=15, -21<=l<=21	
Reflections collected	18107	
Independent reflections	9374 [R(int) = 0.2306]	
Completeness to theta = 24.997°	98.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.5617	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9374 / 0 / 620	
Goodness-of-fit on F^2	0.947	
Final R indices [I>2sigma(I)]	R1 = 0.1097, wR2 = 0.1989	
R indices (all data)	R1 = 0.3317, wR2 = 0.3029	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.389 and -0.454 $e.Å^{-3}$	

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

	x	y	z	U(eq)
S(1)	7200(2)	847(2)	2485(2)	29(1)
P(1)	4827(2)	2546(2)	3223(2)	27(1)
P(2)	7420(2)	39(2)	1394(2)	27(1)
N(1)	5854(6)	2660(6)	3741(5)	25(2)
N(2)	4727(6)	1554(6)	3853(4)	21(2)
N(3)	8028(7)	708(6)	804(5)	27(2)
N(4)	8745(7)	-1011(7)	1514(5)	29(2)
N(5)	5357(7)	1958(7)	1732(5)	31(2)
C(1)	5975(9)	2055(8)	4467(5)	27(3)
C(2)	5677(8)	1072(8)	4333(6)	30(3)
C(3)	9249(8)	388(8)	948(6)	28(3)
C(4)	9719(9)	-876(8)	1131(6)	32(3)
C(9)	5744(8)	1744(8)	2403(6)	29(3)
C(11)	4161(10)	2586(9)	1637(6)	36(3)
C(12)	3823(10)	3509(10)	1143(6)	43(3)
C(13)	2643(12)	4176(11)	1077(8)	61(4)
C(14)	1830(11)	3877(11)	1455(7)	52(4)
C(15)	2175(10)	2934(10)	1910(7)	46(3)
C(16)	3340(9)	2292(8)	2003(6)	33(3)
C(23)	6176(8)	3583(8)	3676(6)	27(3)
C(24)	5322(9)	4725(8)	3644(6)	30(3)
C(25)	5716(10)	5560(8)	3544(6)	41(3)
C(26)	6859(10)	5349(9)	3520(7)	50(4)
C(27)	7682(9)	4231(9)	3573(7)	45(3)
C(28)	7361(9)	3348(8)	3649(6)	30(3)
C(29)	4042(8)	5028(8)	3712(6)	31(3)
C(30)	3515(9)	5446(8)	2942(6)	43(3)
C(31)	3438(9)	5918(8)	4292(6)	46(3)
C(32)	8317(9)	2166(9)	3716(6)	36(3)
C(33)	9272(9)	1928(9)	3077(6)	45(3)
C(34)	8846(9)	1978(8)	4469(6)	41(3)

C(35)	3847(8)	1162(8)	3869(6)	28(3)
C(36)	4129(8)	60(8)	3614(6)	28(3)
C(37)	3312(8)	-354(9)	3703(6)	37(3)
C(38)	2234(10)	261(10)	4031(6)	42(3)
C(39)	1958(9)	1333(9)	4270(6)	36(3)
C(40)	2733(8)	1808(8)	4193(6)	29(3)
C(41)	5286(8)	-612(8)	3231(6)	30(3)
C(42)	5198(9)	-1047(9)	2497(6)	43(3)
C(43)	6027(9)	-1585(8)	3726(6)	42(3)
C(44)	2398(9)	2998(8)	4448(6)	34(3)
C(45)	1779(9)	3835(8)	3818(6)	44(3)
C(46)	1594(9)	3311(9)	5143(6)	44(3)
C(47)	7422(9)	1607(9)	272(6)	35(3)
C(48)	7181(9)	2723(9)	452(6)	37(3)
C(49)	6625(10)	3539(10)	-90(7)	56(4)
C(50)	6290(12)	3295(11)	-733(8)	71(5)
C(51)	6546(10)	2203(11)	-885(7)	54(4)
C(52)	7134(8)	1338(9)	-396(6)	33(3)
C(53)	7519(9)	3028(9)	1153(6)	36(3)
C(54)	6566(9)	4028(8)	1538(6)	44(3)
C(55)	8594(10)	3275(9)	1012(6)	50(4)
C(56)	7384(10)	125(9)	-571(6)	42(3)
C(57)	7868(9)	-171(10)	-1381(6)	48(3)
C(58)	6285(10)	-62(11)	-426(7)	61(4)
C(59)	8934(8)	-2022(8)	1954(6)	25(3)
C(60)	9476(8)	-2219(8)	2614(6)	28(3)
C(61)	9688(9)	-3229(9)	3010(6)	41(3)
C(62)	9330(10)	-3983(9)	2759(7)	44(3)
C(63)	8776(9)	-3779(9)	2105(7)	46(3)
C(64)	8591(9)	-2804(8)	1664(6)	29(3)
C(65)	9819(8)	-1369(8)	2935(6)	32(3)
C(66)	9293(10)	-1058(8)	3744(6)	45(3)
C(67)	11135(9)	-1758(9)	2930(6)	48(3)
C(68)	8090(11)	-2686(9)	924(7)	49(4)
C(69)	9004(13)	-3234(15)	328(8)	109(7)
C(70)	7107(10)	-3052(10)	886(7)	66(4)

Table 3. Bond lengths [Å] and angles [°] for 4.

S(1)-C(9)	1.744(9)
S(1)-P(2)	2.220(4)
P(1)-N(2)	1.713(8)
P(1)-N(1)	1.721(8)
P(1)-C(9)	1.876(10)
P(2)-N(3)	1.683(9)
P(2)-N(4)	1.693(8)
N(1)-C(23)	1.431(12)
N(1)-C(1)	1.468(12)
N(2)-C(35)	1.416(12)
N(2)-C(2)	1.435(11)
N(3)-C(47)	1.455(12)
N(3)-C(3)	1.471(11)
N(4)-C(59)	1.443(12)
N(4)-C(4)	1.445(12)
N(5)-C(9)	1.303(11)
N(5)-C(11)	1.415(12)
C(1)-C(2)	1.527(13)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.534(13)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(11)-C(16)	1.372(15)
C(11)-C(12)	1.392(15)
C(12)-C(13)	1.397(15)
C(12)-H(12)	0.9500
C(13)-C(14)	1.376(17)
C(13)-H(13)	0.9500
C(14)-C(15)	1.369(16)

C(14)-H(14)	0.9500
C(15)-C(16)	1.384(13)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(23)-C(28)	1.407(13)
C(23)-C(24)	1.437(12)
C(24)-C(25)	1.383(14)
C(24)-C(29)	1.506(13)
C(25)-C(26)	1.363(14)
C(25)-H(25A)	0.9500
C(26)-C(27)	1.405(13)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.380(14)
C(27)-H(27A)	0.9500
C(28)-C(32)	1.524(12)
C(29)-C(31)	1.517(12)
C(29)-C(30)	1.547(13)
C(29)-H(29A)	1.0000
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-C(34)	1.514(13)
C(32)-C(33)	1.551(14)
C(32)-H(32)	1.0000
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-C(40)	1.412(12)
C(35)-C(36)	1.430(13)
C(36)-C(37)	1.361(14)

C(36)-C(41)	1.499(13)
C(37)-C(38)	1.374(13)
C(37)-H(37A)	0.9500
C(38)-C(39)	1.385(13)
C(38)-H(38A)	0.9500
C(39)-C(40)	1.368(13)
C(39)-H(39A)	0.9500
C(40)-C(44)	1.526(13)
C(41)-C(42)	1.493(12)
C(41)-C(43)	1.515(13)
C(41)-H(41A)	1.0000
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-C(46)	1.510(14)
C(44)-C(45)	1.539(13)
C(44)-H(44A)	1.0000
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
C(47)-C(52)	1.385(13)
C(47)-C(48)	1.418(14)
C(48)-C(49)	1.393(14)
C(48)-C(53)	1.485(13)
C(49)-C(50)	1.357(15)
C(49)-H(49A)	0.9500
C(50)-C(51)	1.370(16)
C(50)-H(50A)	0.9500
C(51)-C(52)	1.375(14)
C(51)-H(51A)	0.9500

C(52)-C(56)	1.534(14)
C(53)-C(54)	1.521(13)
C(53)-C(55)	1.535(14)
C(53)-H(53A)	1.0000
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(55)-H(55A)	0.9800
C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800
C(56)-C(58)	1.522(15)
C(56)-C(57)	1.538(14)
C(56)-H(56A)	1.0000
C(57)-H(57A)	0.9800
C(57)-H(57B)	0.9800
C(57)-H(57C)	0.9800
C(58)-H(58A)	0.9800
C(58)-H(58B)	0.9800
C(58)-H(58C)	0.9800
C(59)-C(60)	1.371(12)
C(59)-C(64)	1.410(13)
C(60)-C(61)	1.400(14)
C(60)-C(65)	1.512(13)
C(61)-C(62)	1.362(14)
C(61)-H(61A)	0.9500
C(62)-C(63)	1.368(13)
C(62)-H(62A)	0.9500
C(63)-C(64)	1.407(14)
C(63)-H(63A)	0.9500
C(64)-C(68)	1.487(13)
C(65)-C(67)	1.535(13)
C(65)-C(66)	1.551(13)
C(65)-H(65A)	1.0000
C(66)-H(66A)	0.9800
C(66)-H(66B)	0.9800
C(66)-H(66C)	0.9800

C(67)-H(67A)	0.9800
C(67)-H(67B)	0.9800
C(67)-H(67C)	0.9800
C(68)-C(69)	1.488(16)
C(68)-C(70)	1.526(15)
C(68)-H(68A)	1.0000
C(69)-H(69A)	0.9800
C(69)-H(69B)	0.9800
C(69)-H(69C)	0.9800
C(70)-H(70A)	0.9800
C(70)-H(70B)	0.9800
C(70)-H(70C)	0.9800

C(9)-S(1)-P(2)	95.5(4)
N(2)-P(1)-N(1)	90.0(4)
N(2)-P(1)-C(9)	105.5(4)
N(1)-P(1)-C(9)	101.2(4)
N(3)-P(2)-N(4)	89.7(4)
N(3)-P(2)-S(1)	104.5(3)
N(4)-P(2)-S(1)	97.6(3)
C(23)-N(1)-C(1)	117.8(8)
C(23)-N(1)-P(1)	124.2(7)
C(1)-N(1)-P(1)	112.5(6)
C(35)-N(2)-C(2)	121.6(8)
C(35)-N(2)-P(1)	124.1(6)
C(2)-N(2)-P(1)	114.0(7)
C(47)-N(3)-C(3)	121.6(9)
C(47)-N(3)-P(2)	125.8(7)
C(3)-N(3)-P(2)	112.1(6)
C(59)-N(4)-C(4)	119.7(8)
C(59)-N(4)-P(2)	123.6(7)
C(4)-N(4)-P(2)	116.7(7)
C(9)-N(5)-C(11)	120.0(8)
N(1)-C(1)-C(2)	104.9(8)
N(1)-C(1)-H(1A)	110.8
C(2)-C(1)-H(1A)	110.8

N(1)-C(1)-H(1B)	110.8
C(2)-C(1)-H(1B)	110.8
H(1A)-C(1)-H(1B)	108.8
N(2)-C(2)-C(1)	103.3(8)
N(2)-C(2)-H(2A)	111.1
C(1)-C(2)-H(2A)	111.1
N(2)-C(2)-H(2B)	111.1
C(1)-C(2)-H(2B)	111.1
H(2A)-C(2)-H(2B)	109.1
N(3)-C(3)-C(4)	103.9(8)
N(3)-C(3)-H(3A)	111.0
C(4)-C(3)-H(3A)	111.0
N(3)-C(3)-H(3B)	111.0
C(4)-C(3)-H(3B)	111.0
H(3A)-C(3)-H(3B)	109.0
N(4)-C(4)-C(3)	103.8(8)
N(4)-C(4)-H(4A)	111.0
C(3)-C(4)-H(4A)	111.0
N(4)-C(4)-H(4B)	111.0
C(3)-C(4)-H(4B)	111.0
H(4A)-C(4)-H(4B)	109.0
N(5)-C(9)-S(1)	117.6(8)
N(5)-C(9)-P(1)	120.6(7)
S(1)-C(9)-P(1)	121.2(6)
C(16)-C(11)-C(12)	119.8(11)
C(16)-C(11)-N(5)	121.9(11)
C(12)-C(11)-N(5)	118.4(11)
C(11)-C(12)-C(13)	119.0(12)
C(11)-C(12)-H(12)	120.5
C(13)-C(12)-H(12)	120.5
C(14)-C(13)-C(12)	120.3(13)
C(14)-C(13)-H(13)	119.8
C(12)-C(13)-H(13)	119.8
C(15)-C(14)-C(13)	120.0(12)
C(15)-C(14)-H(14)	120.0
C(13)-C(14)-H(14)	120.0

C(14)-C(15)-C(16)	120.1(13)
C(14)-C(15)-H(15)	119.9
C(16)-C(15)-H(15)	119.9
C(11)-C(16)-C(15)	120.6(11)
C(11)-C(16)-H(16)	119.7
C(15)-C(16)-H(16)	119.7
C(28)-C(23)-N(1)	118.2(9)
C(28)-C(23)-C(24)	120.2(9)
N(1)-C(23)-C(24)	121.6(9)
C(25)-C(24)-C(23)	117.5(9)
C(25)-C(24)-C(29)	120.0(9)
C(23)-C(24)-C(29)	122.5(9)
C(26)-C(25)-C(24)	123.1(10)
C(26)-C(25)-H(25A)	118.5
C(24)-C(25)-H(25A)	118.5
C(25)-C(26)-C(27)	118.7(10)
C(25)-C(26)-H(26A)	120.7
C(27)-C(26)-H(26A)	120.7
C(28)-C(27)-C(26)	121.8(10)
C(28)-C(27)-H(27A)	119.1
C(26)-C(27)-H(27A)	119.1
C(27)-C(28)-C(23)	118.6(9)
C(27)-C(28)-C(32)	117.9(9)
C(23)-C(28)-C(32)	123.5(9)
C(24)-C(29)-C(31)	110.9(9)
C(24)-C(29)-C(30)	109.9(9)
C(31)-C(29)-C(30)	110.2(8)
C(24)-C(29)-H(29A)	108.6
C(31)-C(29)-H(29A)	108.6
C(30)-C(29)-H(29A)	108.6
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5

C(29)-C(31)-H(31A)	109.5
C(29)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(29)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(34)-C(32)-C(28)	110.5(8)
C(34)-C(32)-C(33)	109.9(8)
C(28)-C(32)-C(33)	111.9(9)
C(34)-C(32)-H(32)	108.1
C(28)-C(32)-H(32)	108.1
C(33)-C(32)-H(32)	108.1
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(32)-C(34)-H(34A)	109.5
C(32)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(32)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(40)-C(35)-N(2)	120.4(9)
C(40)-C(35)-C(36)	120.2(10)
N(2)-C(35)-C(36)	119.1(8)
C(37)-C(36)-C(35)	118.7(9)
C(37)-C(36)-C(41)	120.4(9)
C(35)-C(36)-C(41)	120.9(10)
C(36)-C(37)-C(38)	121.3(11)
C(36)-C(37)-H(37A)	119.3
C(38)-C(37)-H(37A)	119.3
C(37)-C(38)-C(39)	119.9(11)
C(37)-C(38)-H(38A)	120.1
C(39)-C(38)-H(38A)	120.1

C(40)-C(39)-C(38)	122.0(10)
C(40)-C(39)-H(39A)	119.0
C(38)-C(39)-H(39A)	119.0
C(39)-C(40)-C(35)	117.9(9)
C(39)-C(40)-C(44)	120.8(9)
C(35)-C(40)-C(44)	121.3(10)
C(42)-C(41)-C(36)	113.1(8)
C(42)-C(41)-C(43)	109.1(8)
C(36)-C(41)-C(43)	111.3(9)
C(42)-C(41)-H(41A)	107.7
C(36)-C(41)-H(41A)	107.7
C(43)-C(41)-H(41A)	107.7
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(41)-C(43)-H(43A)	109.5
C(41)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(41)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(46)-C(44)-C(40)	114.4(10)
C(46)-C(44)-C(45)	107.2(9)
C(40)-C(44)-C(45)	108.9(8)
C(46)-C(44)-H(44A)	108.7
C(40)-C(44)-H(44A)	108.7
C(45)-C(44)-H(44A)	108.7
C(44)-C(45)-H(45A)	109.5
C(44)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(44)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5

C(44)-C(46)-H(46A)	109.5
C(44)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(44)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
C(52)-C(47)-C(48)	122.7(10)
C(52)-C(47)-N(3)	118.9(10)
C(48)-C(47)-N(3)	118.4(9)
C(49)-C(48)-C(47)	115.4(11)
C(49)-C(48)-C(53)	121.0(10)
C(47)-C(48)-C(53)	123.7(9)
C(50)-C(49)-C(48)	122.7(12)
C(50)-C(49)-H(49A)	118.6
C(48)-C(49)-H(49A)	118.6
C(49)-C(50)-C(51)	119.8(12)
C(49)-C(50)-H(50A)	120.1
C(51)-C(50)-H(50A)	120.1
C(50)-C(51)-C(52)	121.5(12)
C(50)-C(51)-H(51A)	119.3
C(52)-C(51)-H(51A)	119.3
C(51)-C(52)-C(47)	117.8(11)
C(51)-C(52)-C(56)	120.4(10)
C(47)-C(52)-C(56)	121.6(10)
C(48)-C(53)-C(54)	114.0(8)
C(48)-C(53)-C(55)	111.4(9)
C(54)-C(53)-C(55)	108.4(9)
C(48)-C(53)-H(53A)	107.6
C(54)-C(53)-H(53A)	107.6
C(55)-C(53)-H(53A)	107.6
C(53)-C(54)-H(54A)	109.5
C(53)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(53)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5

C(53)-C(55)-H(55A)	109.5
C(53)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
C(53)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
C(58)-C(56)-C(52)	109.8(9)
C(58)-C(56)-C(57)	110.0(9)
C(52)-C(56)-C(57)	112.2(10)
C(58)-C(56)-H(56A)	108.2
C(52)-C(56)-H(56A)	108.2
C(57)-C(56)-H(56A)	108.2
C(56)-C(57)-H(57A)	109.5
C(56)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5
C(56)-C(57)-H(57C)	109.5
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5
C(56)-C(58)-H(58A)	109.5
C(56)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
C(56)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
C(60)-C(59)-C(64)	122.1(10)
C(60)-C(59)-N(4)	120.0(9)
C(64)-C(59)-N(4)	117.8(9)
C(59)-C(60)-C(61)	118.4(9)
C(59)-C(60)-C(65)	122.2(10)
C(61)-C(60)-C(65)	119.3(9)
C(62)-C(61)-C(60)	120.9(10)
C(62)-C(61)-H(61A)	119.6
C(60)-C(61)-H(61A)	119.6
C(61)-C(62)-C(63)	120.6(11)
C(61)-C(62)-H(62A)	119.7
C(63)-C(62)-H(62A)	119.7

C(62)-C(63)-C(64)	121.0(10)
C(62)-C(63)-H(63A)	119.5
C(64)-C(63)-H(63A)	119.5
C(63)-C(64)-C(59)	116.8(9)
C(63)-C(64)-C(68)	118.4(9)
C(59)-C(64)-C(68)	124.8(10)
C(60)-C(65)-C(67)	113.0(8)
C(60)-C(65)-C(66)	112.1(10)
C(67)-C(65)-C(66)	109.0(8)
C(60)-C(65)-H(65A)	107.5
C(67)-C(65)-H(65A)	107.5
C(66)-C(65)-H(65A)	107.5
C(65)-C(66)-H(66A)	109.5
C(65)-C(66)-H(66B)	109.5
H(66A)-C(66)-H(66B)	109.5
C(65)-C(66)-H(66C)	109.5
H(66A)-C(66)-H(66C)	109.5
H(66B)-C(66)-H(66C)	109.5
C(65)-C(67)-H(67A)	109.5
C(65)-C(67)-H(67B)	109.5
H(67A)-C(67)-H(67B)	109.5
C(65)-C(67)-H(67C)	109.5
H(67A)-C(67)-H(67C)	109.5
H(67B)-C(67)-H(67C)	109.5
C(64)-C(68)-C(69)	111.5(11)
C(64)-C(68)-C(70)	116.9(11)
C(69)-C(68)-C(70)	109.8(10)
C(64)-C(68)-H(68A)	105.9
C(69)-C(68)-H(68A)	105.9
C(70)-C(68)-H(68A)	105.9
C(68)-C(69)-H(69A)	109.5
C(68)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	109.5
C(68)-C(69)-H(69C)	109.5
H(69A)-C(69)-H(69C)	109.5
H(69B)-C(69)-H(69C)	109.5

C(68)-C(70)-H(70A)	109.5
C(68)-C(70)-H(70B)	109.5
H(70A)-C(70)-H(70B)	109.5
C(68)-C(70)-H(70C)	109.5
H(70A)-C(70)-H(70C)	109.5
H(70B)-C(70)-H(70C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 4. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	30(2)	23(2)	32(2)	-2(1)	-3(1)	-9(1)
P(1)	30(2)	22(2)	30(2)	-2(1)	-4(1)	-11(1)
P(2)	34(2)	20(2)	28(2)	2(1)	-3(1)	-12(1)
N(1)	31(5)	16(5)	31(6)	6(4)	-9(4)	-13(4)
N(2)	21(5)	21(5)	19(5)	4(4)	-3(4)	-7(4)
N(3)	28(5)	24(5)	31(6)	2(4)	3(4)	-15(4)
N(4)	29(5)	28(5)	32(6)	-3(4)	-1(4)	-12(4)
N(5)	34(6)	27(5)	26(6)	0(4)	-1(4)	-8(4)
C(1)	40(7)	21(6)	26(7)	6(5)	-10(5)	-17(5)
C(2)	41(7)	35(7)	22(6)	7(5)	-10(5)	-24(6)
C(3)	33(6)	20(6)	36(7)	-6(5)	7(5)	-16(5)
C(4)	33(7)	30(7)	30(7)	-1(5)	-3(5)	-9(6)
C(9)	23(6)	24(6)	35(7)	1(5)	-6(5)	-5(5)
C(11)	41(8)	29(7)	30(7)	2(6)	-6(6)	-9(6)
C(12)	43(8)	55(9)	35(8)	0(7)	-11(6)	-23(7)
C(13)	65(10)	48(9)	59(10)	3(7)	-27(8)	-10(8)
C(14)	41(8)	50(9)	50(10)	-10(7)	-23(7)	2(7)
C(15)	46(8)	53(9)	44(8)	0(7)	-15(6)	-25(7)
C(16)	39(7)	24(6)	36(8)	-4(5)	-8(6)	-11(6)
C(23)	31(7)	24(6)	30(7)	-1(5)	3(5)	-17(5)
C(24)	32(7)	24(6)	32(7)	-3(5)	3(5)	-10(5)
C(25)	50(8)	8(6)	65(9)	-2(6)	-1(7)	-12(6)
C(26)	51(8)	20(7)	82(10)	12(6)	-3(7)	-19(6)
C(27)	33(7)	30(7)	71(10)	-4(6)	3(6)	-13(6)
C(28)	30(7)	18(6)	47(8)	-4(5)	-1(6)	-13(5)
C(29)	34(7)	23(6)	35(7)	-5(5)	-7(6)	-8(5)
C(30)	53(8)	21(6)	52(8)	-4(6)	-5(6)	-13(6)
C(31)	62(8)	32(7)	33(8)	-3(6)	-3(6)	-9(6)
C(32)	35(7)	34(7)	35(7)	-17(6)	-7(6)	-8(6)
C(33)	32(7)	45(8)	52(8)	-13(6)	1(6)	-9(6)
C(34)	33(7)	30(7)	63(9)	-1(6)	-8(6)	-15(6)

C(35)	23(6)	32(7)	26(7)	3(5)	-2(5)	-10(5)
C(36)	20(6)	19(6)	40(7)	1(5)	-9(5)	-1(5)
C(37)	18(6)	47(8)	48(8)	1(6)	5(6)	-18(6)
C(38)	47(8)	52(8)	35(8)	7(6)	-5(6)	-30(7)
C(39)	29(6)	38(7)	48(8)	-9(6)	8(6)	-21(6)
C(40)	25(6)	36(7)	31(7)	-2(5)	3(5)	-17(6)
C(41)	40(7)	25(6)	30(7)	5(5)	-2(5)	-20(6)
C(42)	53(8)	35(7)	41(8)	1(6)	-10(6)	-17(6)
C(43)	44(7)	26(7)	51(8)	5(6)	-6(6)	-9(6)
C(44)	40(7)	31(7)	30(7)	-12(6)	-5(6)	-12(6)
C(45)	41(7)	26(7)	49(8)	6(6)	3(6)	-1(6)
C(46)	41(7)	43(8)	46(8)	-15(6)	-1(6)	-14(6)
C(47)	34(7)	44(8)	24(7)	5(6)	-1(5)	-16(6)
C(48)	53(8)	20(6)	37(8)	14(6)	-3(6)	-14(6)
C(49)	79(10)	30(8)	48(9)	10(7)	-9(8)	-14(7)
C(50)	101(12)	36(9)	56(11)	17(7)	-23(9)	-8(8)
C(51)	68(9)	56(9)	36(8)	9(7)	-27(7)	-22(8)
C(52)	25(6)	43(7)	31(7)	12(6)	-11(5)	-15(6)
C(53)	41(7)	29(7)	38(8)	14(6)	-10(6)	-15(6)
C(54)	61(8)	19(6)	50(8)	3(6)	14(6)	-17(6)
C(55)	61(9)	34(7)	47(8)	2(6)	-6(7)	-12(7)
C(56)	61(8)	38(7)	33(8)	-4(6)	-15(6)	-25(6)
C(57)	45(8)	66(9)	47(8)	1(7)	-6(6)	-36(7)
C(58)	73(9)	83(11)	51(9)	0(8)	-9(7)	-56(9)
C(59)	32(6)	13(6)	30(7)	4(5)	3(5)	-10(5)
C(60)	34(6)	19(6)	29(7)	0(5)	-9(5)	-8(5)
C(61)	57(8)	29(7)	22(7)	11(6)	0(6)	-5(6)
C(62)	67(9)	16(6)	44(8)	9(6)	-18(7)	-12(6)
C(63)	53(8)	28(7)	61(10)	-15(7)	-3(7)	-21(6)
C(64)	37(7)	22(6)	29(7)	1(5)	-8(5)	-13(5)
C(65)	36(7)	28(6)	31(7)	6(5)	-20(6)	-9(5)
C(66)	71(9)	25(7)	37(8)	9(6)	-14(7)	-17(6)
C(67)	55(8)	46(8)	54(9)	14(6)	-19(7)	-29(7)
C(68)	78(10)	29(7)	44(9)	4(6)	-12(8)	-25(7)
C(69)	118(14)	200(20)	58(11)	-31(12)	8(10)	-118(15)
C(70)	66(9)	67(10)	66(10)	-21(8)	13(8)	-30(8)

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

	x	y	z	U(eq)
H(1A)	5436	2545	4856	33
H(1B)	6776	1783	4628	33
H(2A)	6341	454	4085	36
H(2B)	5445	782	4809	36
H(3A)	9316	798	1376	34
H(3B)	9670	542	501	34
H(4A)	9972	-1312	667	39
H(4B)	10379	-1119	1457	39
H(12)	4386	3684	855	51
H(13)	2401	4839	769	73
H(14)	1030	4326	1401	63
H(15)	1614	2719	2162	55
H(16)	3574	1643	2324	40
H(25A)	5163	6315	3489	49
H(26A)	7095	5947	3468	60
H(27A)	8480	4078	3557	54
H(29A)	3924	4341	3874	37
H(30A)	3913	4865	2573	64
H(30B)	3610	6130	2782	64
H(30C)	2690	5608	2986	64
H(31A)	2620	6057	4356	69
H(31B)	3502	6614	4123	69
H(31C)	3803	5659	4770	69
H(32)	7963	1621	3682	44
H(33A)	8915	2122	2593	68
H(33B)	9803	1131	3093	68
H(33C)	9702	2382	3141	68
H(34A)	9513	1247	4481	61
H(34B)	8269	1994	4867	61
H(34C)	9099	2571	4545	61

H(37A)	3490	-1084	3535	44
H(38A)	1679	-47	4095	50
H(39A)	1209	1751	4494	44
H(41A)	5693	-108	3132	35
H(42A)	4781	-416	2158	65
H(42B)	4778	-1525	2575	65
H(42C)	5976	-1486	2277	65
H(43A)	6780	-2000	3465	63
H(43B)	5640	-2086	3841	63
H(43C)	6140	-1299	4193	63
H(44A)	3119	3083	4545	41
H(45A)	2304	3701	3370	65
H(45B)	1548	4602	3981	65
H(45C)	1090	3734	3702	65
H(46A)	1908	2731	5535	66
H(46B)	830	3375	5025	66
H(46C)	1523	4031	5318	66
H(49A)	6474	4296	-7	67
H(50A)	5878	3881	-1078	86
H(51A)	6313	2040	-1338	65
H(53A)	7723	2368	1510	44
H(54A)	5849	3919	1586	66
H(54B)	6440	4714	1239	66
H(54C)	6795	4096	2036	66
H(55A)	9240	2610	810	75
H(55B)	8800	3464	1485	75
H(55C)	8426	3906	653	75
H(56A)	7973	-388	-225	50
H(57A)	8577	-52	-1468	57
H(57B)	7293	310	-1729	57
H(57C)	8043	-958	-1462	57
H(58A)	6013	76	101	91
H(58B)	6449	-838	-538	91
H(58C)	5687	453	-748	91
H(61A)	10087	-3391	3459	50
H(62A)	9466	-4657	3041	52

H(63A)	8511	-4304	1947	55
H(65A)	9503	-670	2614	39
H(66A)	8451	-800	3751	67
H(66B)	9476	-457	3913	67
H(66C)	9620	-1718	4078	67
H(67A)	11480	-2007	2429	73
H(67B)	11458	-2380	3294	73
H(67C)	11307	-1133	3065	73
H(68A)	7754	-1866	792	59
H(69A)	8674	-3015	-164	131
H(69B)	9307	-4051	398	131
H(69C)	9633	-2997	355	131
H(70A)	6537	-2734	1303	98
H(70B)	7418	-3872	919	98
H(70C)	6735	-2783	410	98

Table 6. Torsion angles [°] for 4.

N(2)-P(1)-N(1)-C(23)	-162.3(8)
C(9)-P(1)-N(1)-C(23)	91.9(8)
N(2)-P(1)-N(1)-C(1)	-9.3(6)
C(9)-P(1)-N(1)-C(1)	-115.1(7)
N(1)-P(1)-N(2)-C(35)	168.4(7)
C(9)-P(1)-N(2)-C(35)	-90.0(8)
N(1)-P(1)-N(2)-C(2)	-16.7(7)
C(9)-P(1)-N(2)-C(2)	84.9(7)
N(4)-P(2)-N(3)-C(47)	162.6(8)
S(1)-P(2)-N(3)-C(47)	-99.6(8)
N(4)-P(2)-N(3)-C(3)	-24.9(6)
S(1)-P(2)-N(3)-C(3)	72.9(6)
N(3)-P(2)-N(4)-C(59)	-175.8(8)
S(1)-P(2)-N(4)-C(59)	79.6(7)
N(3)-P(2)-N(4)-C(4)	2.3(7)
S(1)-P(2)-N(4)-C(4)	-102.2(6)
C(23)-N(1)-C(1)-C(2)	-174.9(8)
P(1)-N(1)-C(1)-C(2)	30.2(9)
C(35)-N(2)-C(2)-C(1)	-149.3(8)
P(1)-N(2)-C(2)-C(1)	35.7(9)
N(1)-C(1)-C(2)-N(2)	-39.4(10)
C(47)-N(3)-C(3)-C(4)	-148.2(9)
P(2)-N(3)-C(3)-C(4)	39.0(9)
C(59)-N(4)-C(4)-C(3)	-162.8(8)
P(2)-N(4)-C(4)-C(3)	18.9(9)
N(3)-C(3)-C(4)-N(4)	-33.9(9)
C(11)-N(5)-C(9)-S(1)	173.5(8)
C(11)-N(5)-C(9)-P(1)	-15.7(14)
P(2)-S(1)-C(9)-N(5)	-21.3(9)
P(2)-S(1)-C(9)-P(1)	168.0(6)
N(2)-P(1)-C(9)-N(5)	123.4(9)
N(1)-P(1)-C(9)-N(5)	-143.4(9)
N(2)-P(1)-C(9)-S(1)	-66.1(7)
N(1)-P(1)-C(9)-S(1)	27.0(8)

C(9)-N(5)-C(11)-C(16)	-53.1(15)
C(9)-N(5)-C(11)-C(12)	128.4(11)
C(16)-C(11)-C(12)-C(13)	5.2(16)
N(5)-C(11)-C(12)-C(13)	-176.2(9)
C(11)-C(12)-C(13)-C(14)	-4.5(17)
C(12)-C(13)-C(14)-C(15)	1.2(18)
C(13)-C(14)-C(15)-C(16)	1.4(17)
C(12)-C(11)-C(16)-C(15)	-2.7(16)
N(5)-C(11)-C(16)-C(15)	178.8(9)
C(14)-C(15)-C(16)-C(11)	-0.7(16)
C(1)-N(1)-C(23)-C(28)	73.0(12)
P(1)-N(1)-C(23)-C(28)	-135.3(8)
C(1)-N(1)-C(23)-C(24)	-106.5(10)
P(1)-N(1)-C(23)-C(24)	45.2(13)
C(28)-C(23)-C(24)-C(25)	3.6(15)
N(1)-C(23)-C(24)-C(25)	-176.9(10)
C(28)-C(23)-C(24)-C(29)	-176.7(10)
N(1)-C(23)-C(24)-C(29)	2.9(14)
C(23)-C(24)-C(25)-C(26)	-4.0(17)
C(29)-C(24)-C(25)-C(26)	176.3(10)
C(24)-C(25)-C(26)-C(27)	2.3(18)
C(25)-C(26)-C(27)-C(28)	0.0(18)
C(26)-C(27)-C(28)-C(23)	-0.2(17)
C(26)-C(27)-C(28)-C(32)	-179.0(10)
N(1)-C(23)-C(28)-C(27)	178.9(10)
C(24)-C(23)-C(28)-C(27)	-1.6(15)
N(1)-C(23)-C(28)-C(32)	-2.4(15)
C(24)-C(23)-C(28)-C(32)	177.1(9)
C(25)-C(24)-C(29)-C(31)	-50.5(14)
C(23)-C(24)-C(29)-C(31)	129.7(10)
C(25)-C(24)-C(29)-C(30)	71.6(12)
C(23)-C(24)-C(29)-C(30)	-108.1(11)
C(27)-C(28)-C(32)-C(34)	71.1(13)
C(23)-C(28)-C(32)-C(34)	-107.6(12)
C(27)-C(28)-C(32)-C(33)	-51.8(13)
C(23)-C(28)-C(32)-C(33)	129.5(11)

C(2)-N(2)-C(35)-C(40)	106.8(11)
P(1)-N(2)-C(35)-C(40)	-78.6(11)
C(2)-N(2)-C(35)-C(36)	-67.7(12)
P(1)-N(2)-C(35)-C(36)	106.9(9)
C(40)-C(35)-C(36)-C(37)	-1.2(15)
N(2)-C(35)-C(36)-C(37)	173.3(9)
C(40)-C(35)-C(36)-C(41)	176.6(9)
N(2)-C(35)-C(36)-C(41)	-8.9(14)
C(35)-C(36)-C(37)-C(38)	-0.1(16)
C(41)-C(36)-C(37)-C(38)	-178.0(9)
C(36)-C(37)-C(38)-C(39)	0.9(17)
C(37)-C(38)-C(39)-C(40)	-0.3(17)
C(38)-C(39)-C(40)-C(35)	-1.0(16)
C(38)-C(39)-C(40)-C(44)	178.9(10)
N(2)-C(35)-C(40)-C(39)	-172.7(10)
C(36)-C(35)-C(40)-C(39)	1.7(15)
N(2)-C(35)-C(40)-C(44)	7.4(15)
C(36)-C(35)-C(40)-C(44)	-178.2(9)
C(37)-C(36)-C(41)-C(42)	50.0(13)
C(35)-C(36)-C(41)-C(42)	-127.7(10)
C(37)-C(36)-C(41)-C(43)	-73.2(12)
C(35)-C(36)-C(41)-C(43)	109.0(11)
C(39)-C(40)-C(44)-C(46)	35.3(14)
C(35)-C(40)-C(44)-C(46)	-144.7(10)
C(39)-C(40)-C(44)-C(45)	-84.5(13)
C(35)-C(40)-C(44)-C(45)	95.4(11)
C(3)-N(3)-C(47)-C(52)	109.4(11)
P(2)-N(3)-C(47)-C(52)	-78.8(12)
C(3)-N(3)-C(47)-C(48)	-68.8(13)
P(2)-N(3)-C(47)-C(48)	103.0(11)
C(52)-C(47)-C(48)-C(49)	0.4(17)
N(3)-C(47)-C(48)-C(49)	178.5(10)
C(52)-C(47)-C(48)-C(53)	-177.8(10)
N(3)-C(47)-C(48)-C(53)	0.4(16)
C(47)-C(48)-C(49)-C(50)	2.7(19)
C(53)-C(48)-C(49)-C(50)	-179.2(12)

C(48)-C(49)-C(50)-C(51)	-3(2)
C(49)-C(50)-C(51)-C(52)	0(2)
C(50)-C(51)-C(52)-C(47)	2.4(19)
C(50)-C(51)-C(52)-C(56)	178.5(13)
C(48)-C(47)-C(52)-C(51)	-2.8(17)
N(3)-C(47)-C(52)-C(51)	179.1(10)
C(48)-C(47)-C(52)-C(56)	-178.8(11)
N(3)-C(47)-C(52)-C(56)	3.1(15)
C(49)-C(48)-C(53)-C(54)	47.2(15)
C(47)-C(48)-C(53)-C(54)	-134.7(11)
C(49)-C(48)-C(53)-C(55)	-75.7(13)
C(47)-C(48)-C(53)-C(55)	102.3(13)
C(51)-C(52)-C(56)-C(58)	-75.8(14)
C(47)-C(52)-C(56)-C(58)	100.1(12)
C(51)-C(52)-C(56)-C(57)	46.9(15)
C(47)-C(52)-C(56)-C(57)	-137.3(10)
C(4)-N(4)-C(59)-C(60)	70.2(12)
P(2)-N(4)-C(59)-C(60)	-111.7(9)
C(4)-N(4)-C(59)-C(64)	-107.0(10)
P(2)-N(4)-C(59)-C(64)	71.1(11)
C(64)-C(59)-C(60)-C(61)	-0.3(15)
N(4)-C(59)-C(60)-C(61)	-177.4(9)
C(64)-C(59)-C(60)-C(65)	-178.5(9)
N(4)-C(59)-C(60)-C(65)	4.4(15)
C(59)-C(60)-C(61)-C(62)	-2.2(16)
C(65)-C(60)-C(61)-C(62)	176.1(10)
C(60)-C(61)-C(62)-C(63)	1.4(17)
C(61)-C(62)-C(63)-C(64)	1.9(17)
C(62)-C(63)-C(64)-C(59)	-4.1(16)
C(62)-C(63)-C(64)-C(68)	174.0(10)
C(60)-C(59)-C(64)-C(63)	3.3(15)
N(4)-C(59)-C(64)-C(63)	-179.6(9)
C(60)-C(59)-C(64)-C(68)	-174.6(10)
N(4)-C(59)-C(64)-C(68)	2.5(15)
C(59)-C(60)-C(65)-C(67)	-112.6(11)
C(61)-C(60)-C(65)-C(67)	69.2(13)

C(59)-C(60)-C(65)-C(66)	123.9(11)
C(61)-C(60)-C(65)-C(66)	-54.3(12)
C(63)-C(64)-C(68)-C(69)	-86.1(14)
C(59)-C(64)-C(68)-C(69)	91.7(14)
C(63)-C(64)-C(68)-C(70)	41.4(14)
C(59)-C(64)-C(68)-C(70)	-140.7(11)

Symmetry transformations used to generate equivalent atoms: