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Tetracarbonyl[*N*-(diphenylphosphanyl-κ*P*)-*N*,*N*′-diisopropyl-*P*-phenylphosphorus diamide-κ*P*]-molybdenum(0) with an unknown solvent

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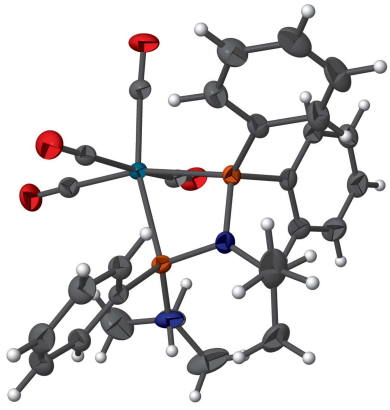
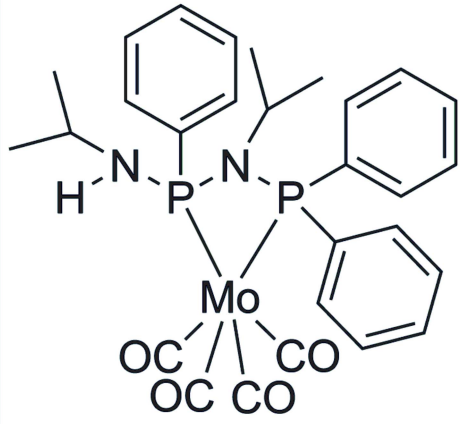
The title complex, $[Mo(C_{24}H_{30}N_2P_2)(CO)_4]$, contains a molybdenum centre bearing a *P*,*P*′-*cis*-chelating $Ph_2PN(^iPr)P(Ph)NH(^iPr)$ and four carbonyl ligands in a distorted octahedral coordination geometry. This results in a nearly planar four-membered metallacycle. In the crystal, molecules are linked by N—H···O and C—H···O hydrogen bonds to form layers parallel to the *ac* plane. For the final refinement, the contributions of disordered solvent molecules were removed from the diffraction data with SQUEEZE in *PLATON* [Spek (2015). *Acta Cryst.* C**71**, 9–18]. The given chemical formula and other crystal data do not take into account the unknown solvent molecule(*s*).

3D view



Chemical scheme



Structure description

The title complex (Fig. 1) contains a molybdenum centre coordinated to a *P*,*P*′-cis-chelating $Ph_2PN(^iPr)P(Ph)NH(^iPr)$ ligand and four carbonyl ligands in a distorted octahedral geometry, forming a nearly planar four-membered Mo—P—N—P metallacycle (r.m.s. deviation for Mo1, P1, N1, P2 = 0.053 Å). The P—Mo—P bite angle amounts to 64.948 (13)° and complies with those in comparable $[Mo(CO)_4\{Ph_2PN(R)PPh_2\}]$ ($R \neq$ H) complexes [range from 64.38 (8) to 66.14 (3)°; Al-Masri *et al.*, 2013; Biricik *et al.*, 2003; Gaw *et al.*, 2000, 2002; Majoumo *et al.*, 2004; Majoumo-Mbe *et al.*, 2015; Payne *et al.*, 1965] and is slightly smaller than that found in the analogous chromium complex [P—Cr—P = 67.90 (2), 67.95 (12)°] published by Aluri *et al.* (2010) and Dulai *et al.* (2011). As a result of the ring strain, the P—N—P bond angle [103.10 (6)°] is clearly smaller than that observed in the uncoordinated $Ph_2PN(^iPr)P(Ph)NH(^iPr)$ molecule [121.53 (11)°; Peitz *et al.*, 2010] but conforms with comparable $[Mo(CO)_4\{Ph_2PN(R)PPh_2\}]$ ($R \neq$ H) complexes

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1^{i}	0.95	2.53	3.338 (2)	143
N2—H2···O1^{ii}	0.83 (1)	2.54 (1)	3.3419 (18)	163 (1)

Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x+\frac{1}{2}, y, -z+\frac{1}{2}$.

(Al-Masri *et al.*, 2013; Biricik *et al.*, 2003; Gaw *et al.*, 2000, 2002; Majoumo *et al.*, 2004; Majoumo-Mbe *et al.*, 2015; Payne *et al.*, 1965). The P—N bond lengths [range from 1.6462 (13) to 1.7185 (13) Å] are noticeably shortened compared to the calculated sum of the covalent radii by Pyykkö [single: Σ*r*cov(P—N) = 1.82 Å; Pyykkö, 2015] and show some multiple-bond character [double: Σ*r*cov(P=N) = 1.62 Å; Pyykkö, 2015]. Consistent with this geometry, the central N1 atom is nearly trigonal planar [Σ(∠N1) = 359°]. The Mo—P distances are slightly different [Mo1—P1 = 2.4731 (5), Mo1—P2 = 2.5056 (6) Å], which might be an effect of the asymmetric *P*,*P*′-cis-ligating $Ph_2PN(^iPr)P(Ph)NH(^iPr)$ ligand.

In the crystal, N—H···O and C—H···O hydrogen bonds (Table 1) link the molecules into layers parallel to the *ac* plane.

Synthesis and crystallization

$Mo(CO)_4(pip)_2$ (pip = piperidine; 0.99 g, 2.617 mmol) and $Ph_2PN(^iPr)P(Ph)NH(^iPr)$ (1.305 g, 3.193 mmol), were dissolved in CH_2Cl_2 (30 ml) at r.t. After 2 h of refluxing, 20 ml CH_2Cl_2 was removed *in vacuo*. Ethanol (15 ml) was added and the solution was cooled. The white solid was washed with *n*-hexane at −78°C and dried under vacuum. Yield 1.45 g (90%). Crystals were obtained from a saturated CH_2Cl_2/EtOH solution at −78°C.

^{1}H NMR (300 MHz, C_6D_6, 298 K): δ (p.p.m.) 7.95–7.88 (*m*, 2H, Ar*H*), 7.69–7.53 (*m*, 4H, Ar*H*), 7.14–6.98 (*m*, 9H, Ar*H*), 4.17 (*m*, 1H, C*H*CH$_3$), 3.31 (*m*, 1H, C*H*CH$_3$), 2.19 (*t*, 1H, N*H*), 1.22 (*d*, $^3J_{H,H}$ = 6.5 Hz, 3H, CHC*H*$_3$), 1.15 (*d*, $^3J_{H,H}$ = 6.4 Hz, 3H, CHC*H*$_3$), 0.89 (*d*, *J* = 6.7 Hz, 3H, CHC*H*$_3$), 0.38 (*d*, $^3J_{H,H}$ = 6.7 Hz, 3H, CHC*H*$_3$). ^{13}C NMR (100 MHz, C_6D_6, 298 K): δ (p.p.m.) 219.7 (*m*, *C*O), 212.4 (*m*, *C*O), 141.7, 141.0, 138.7, 138.2, 136.2, 138.8, 133.8, 131.3, 130.8, 130.0, 128.9, 128.7, 128.5 (Ar*C*), 55.7 (*t*, $^2J_{PC}$ = 6.0 Hz, *C*HCH$_3$), 49.3 (*d*, $^2J_{PC}$ = 18.0 Hz, *C*HCH$_3$), 26.3 (*d*, $^3J_{PC}$ = 4.5 Hz, CH*C*H$_3$), 25.6 (*d*, $^3J_{PC}$ = 4.5 Hz, CH*C*H$_3$), 24.3 (*br s*, CH*C*H$_3$) 24.2 (*br s*, CH*C*H$_3$). ^{31}P NMR (121 MHz, CD_2Cl_2, 298 K): δ = 96.7 (*d*, $^2J_{PP}$ = 8.7 Hz), 80.2 (*d*, $^2J_{PP}$ = 8.7 Hz). Elemental analysis calcd. (%) for $C_{28}H_{30}MoN_2O_4P_2$ (616.44): C 54.56, H 4.91, N 4.54. Found: C 55.42, H 4.96, N 4.65. IR (CH_2Cl_2, cm^{-1}): ν (CO) 1870, 1896, 1918, 2005. M.p. 180°C (dec.).

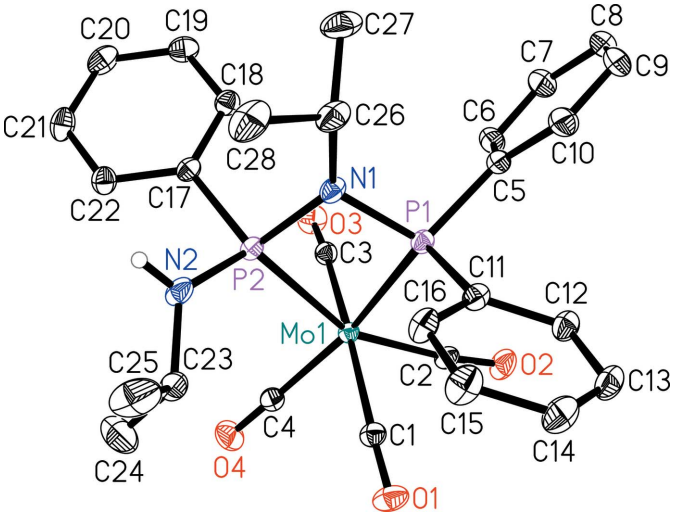


Figure 1
The molecular structure of the title compound with atom labelling and displacement ellipsoids drawn at 30% probability level. C-bound hydrogen atoms are omitted for clarity.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Mo(C_{24}H_{30}N_2P_2)(CO)_4]$
M_r	616.42
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	150
a, *b*, *c* (Å)	15.634 (3), 17.716 (4), 21.661 (4)
V (Å^3)	5999 (2)
Z	8
Radiation type	Mo *Kα*
μ (mm^{-1})	0.58
Crystal size (mm)	0.46 × 0.38 × 0.36
Data collection	
Diffractometer	Stoe IPDS II
Absorption correction	Numerical (*X-SHAPE* and *X-RED32*; Stoe & Cie, 2005)
T_{min}, T_{max}	0.75, 0.89
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	95647, 6886, 5657
R_{int}	0.041
(sin θ/λ)$_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.022, 0.050, 0.92
No. of reflections	6886
No. of parameters	342
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.31

Computer programs: *X-AREA* (Stoe & Cie, 2005), *XP* in *SHELXTL* and *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015)and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Six outliers (4 0 10, 6 3 4, 1 2 11, 5 7 4, 1 2 8, 2 3 8) were omitted in the last cycles of refinement. For the final refinement, the contributions of disordered solvent molecules were removed from the diffraction data with SQUEEZE in *PLATON* (Spek, 2015). SQUEEZE estimated the electron counts in each of the four voids of 111 and 112 Å^3, respectively to be 34.

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full crystallographic data

IUCrData (2018). **3**, x180846 [https://doi.org/10.1107/S2414314618008465]

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Tetracarbonyl[*N*-(diphenylphosphanyl-κ*P*)-*N*,*N*′-diisopropyl-*P*-phenylphosphorus diamide-κ*P*]molybdenum(0)

Crystal data

$[Mo(C_{24}H_{30}N_2P_2)(CO)_4]$
M_r = 616.42
Orthorhombic, *Pbca*
a = 15.634 (3) Å
b = 17.716 (4) Å
c = 21.661 (4) Å
V = 5999 (2) Å^3
Z = 8
F(000) = 2528
D_x = 1.365 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 11600 reflections
θ = 1.8–29.7°
μ = 0.58 mm^{-1}
T = 150 K
Prism, colourless
0.46 × 0.38 × 0.36 mm

Data collection

Stoe IPDS II diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: numerical (X-SHAPE and X-RED32; Stoe & Cie, 2005)
T_{min} = 0.75, T_{max} = 0.89
95647 measured reflections
6886 independent reflections
5657 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 27.5°, θ_{min} = 1.9°
h = −20→20
k = −22→23
l = −28→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.050
S = 0.92
6886 reflections
342 parameters
1 restraint
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0338P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The N-bound H atom was located in a difference Fourier map and refined with the N–H distance constrained to be 0.87 Å. All other H atoms were placed geometrically and refined using a riding atom approximation, with C–H = 0.95–1.00 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C) for methyl H atoms. A rotating model was used for the methyl groups.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.34111 (9)	0.15827 (8)	0.28181 (6)	0.0269 (3)
C2	0.28472 (9)	0.07619 (8)	0.38433 (7)	0.0271 (3)
C3	0.44531 (9)	0.01870 (8)	0.40890 (7)	0.0262 (3)
C4	0.40591 (9)	0.01114 (9)	0.28804 (7)	0.0288 (3)
C5	0.40138 (9)	0.22378 (9)	0.48935 (7)	0.0287 (3)
C6	0.39750 (10)	0.15799 (10)	0.52376 (7)	0.0343 (3)
H6	0.4040	0.1106	0.5037	0.041*
C7	0.38431 (11)	0.16021 (11)	0.58705 (8)	0.0416 (4)
H7	0.3828	0.1147	0.6102	0.050*
C8	0.37339 (12)	0.22824 (12)	0.61608 (8)	0.0450 (4)
H8	0.3645	0.2299	0.6594	0.054*
C9	0.37530 (12)	0.29434 (12)	0.58244 (9)	0.0487 (5)
H9	0.3665	0.3413	0.6026	0.058*
C10	0.38998 (11)	0.29266 (10)	0.51939 (8)	0.0399 (4)
H10	0.3923	0.3384	0.4966	0.048*
C11	0.37638 (9)	0.29940 (8)	0.37296 (7)	0.0271 (3)
C12	0.29425 (10)	0.32308 (9)	0.38861 (7)	0.0314 (3)
H12	0.2642	0.2987	0.4211	0.038*
C13	0.25641 (11)	0.38204 (9)	0.35696 (8)	0.0372 (4)
H13	0.2006	0.3983	0.3681	0.045*
C14	0.29902 (12)	0.41738 (9)	0.30934 (9)	0.0417 (4)
H14	0.2726	0.4578	0.2878	0.050*
C15	0.38000 (12)	0.39387 (10)	0.29309 (9)	0.0432 (4)
H15	0.4095	0.4182	0.2603	0.052*
C16	0.41847 (10)	0.33487 (9)	0.32456 (8)	0.0354 (4)
H16	0.4741	0.3186	0.3129	0.042*
C17	0.63680 (9)	0.09612 (8)	0.37610 (6)	0.0241 (3)
C18	0.64070 (10)	0.08548 (8)	0.43972 (7)	0.0290 (3)
H18	0.5987	0.1080	0.4655	0.035*
C19	0.70499 (11)	0.04247 (9)	0.46573 (8)	0.0361 (3)
H19	0.7077	0.0364	0.5093	0.043*
C20	0.76512 (11)	0.00839 (9)	0.42858 (8)	0.0394 (4)
H20	0.8094	−0.0210	0.4466	0.047*
C21	0.76123 (11)	0.01667 (10)	0.36556 (8)	0.0394 (4)
H21	0.8025	−0.0074	0.3401	0.047*
C22	0.69701 (10)	0.06027 (9)	0.33895 (7)	0.0310 (3)
H22	0.6943	0.0656	0.2954	0.037*
C23	0.54833 (10)	0.19268 (10)	0.21953 (7)	0.0363 (4)
H23	0.4871	0.2051	0.2283	0.044*
C24	0.55048 (17)	0.12180 (16)	0.18082 (10)	0.0691 (7)

H24A	0.6100	0.1082	0.1720	0.104*
H24B	0.5201	0.1307	0.1419	0.104*
H24C	0.5228	0.0806	0.2034	0.104*
C25	0.58778 (15)	0.25923 (16)	0.18724 (11)	0.0718 (8)
H25A	0.5816	0.3043	0.2130	0.108*
H25B	0.5589	0.2674	0.1477	0.108*
H25C	0.6486	0.2494	0.1800	0.108*
C26	0.58322 (10)	0.28343 (9)	0.41876 (9)	0.0395 (4)
H26	0.5443	0.3277	0.4244	0.047*
C27	0.62182 (13)	0.26694 (12)	0.48171 (10)	0.0537 (5)
H27A	0.5774	0.2472	0.5093	0.081*
H27B	0.6454	0.3135	0.4991	0.081*
H27C	0.6675	0.2295	0.4774	0.081*
C28	0.65060 (13)	0.30750 (11)	0.37253 (11)	0.0554 (5)
H28A	0.6886	0.2648	0.3637	0.083*
H28B	0.6841	0.3493	0.3897	0.083*
H28C	0.6227	0.3239	0.3343	0.083*
N1	0.52898 (7)	0.22025 (7)	0.39514 (6)	0.0271 (3)
N2	0.59168 (8)	0.18048 (8)	0.27863 (6)	0.0332 (3)
O1	0.30266 (7)	0.18956 (7)	0.24502 (5)	0.0397 (3)
O2	0.22161 (7)	0.06770 (8)	0.41024 (6)	0.0427 (3)
O3	0.46686 (8)	−0.03061 (7)	0.43865 (5)	0.0418 (3)
O4	0.41082 (8)	−0.03731 (7)	0.25315 (6)	0.0459 (3)
P1	0.42203 (2)	0.21436 (2)	0.40705 (2)	0.02325 (7)
P2	0.54809 (2)	0.14920 (2)	0.34291 (2)	0.02225 (7)
Mo1	0.39963 (2)	0.09633 (2)	0.34827 (2)	0.01978 (4)
H2	0.6430 (9)	0.1912 (10)	0.2777 (8)	0.035 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0232 (7)	0.0302 (8)	0.0274 (7)	−0.0046 (6)	−0.0005 (6)	0.0038 (6)
C2	0.0247 (7)	0.0285 (7)	0.0282 (7)	0.0004 (6)	−0.0026 (6)	0.0055 (6)
C3	0.0255 (7)	0.0273 (7)	0.0257 (7)	−0.0001 (6)	0.0015 (6)	0.0007 (6)
C4	0.0266 (7)	0.0304 (7)	0.0294 (7)	−0.0012 (6)	−0.0011 (6)	−0.0013 (6)
C5	0.0259 (7)	0.0305 (8)	0.0295 (7)	0.0043 (6)	−0.0041 (6)	−0.0062 (6)
C6	0.0389 (8)	0.0350 (8)	0.0291 (7)	0.0049 (7)	−0.0004 (7)	−0.0050 (6)
C7	0.0453 (10)	0.0508 (11)	0.0286 (8)	0.0027 (8)	0.0016 (7)	−0.0017 (7)
C8	0.0393 (9)	0.0657 (13)	0.0301 (8)	0.0075 (9)	−0.0017 (7)	−0.0139 (8)
C9	0.0477 (10)	0.0526 (12)	0.0458 (10)	0.0118 (9)	−0.0071 (8)	−0.0274 (9)
C10	0.0431 (9)	0.0341 (9)	0.0425 (9)	0.0051 (7)	−0.0070 (7)	−0.0109 (7)
C11	0.0258 (7)	0.0204 (7)	0.0349 (7)	0.0008 (5)	−0.0041 (6)	−0.0011 (6)
C12	0.0273 (7)	0.0270 (7)	0.0399 (8)	0.0027 (6)	−0.0009 (6)	−0.0010 (6)
C13	0.0295 (8)	0.0307 (8)	0.0515 (10)	0.0083 (6)	−0.0031 (7)	−0.0012 (7)
C14	0.0414 (9)	0.0284 (8)	0.0552 (10)	0.0087 (7)	−0.0069 (8)	0.0095 (7)
C15	0.0405 (9)	0.0364 (9)	0.0528 (10)	0.0021 (7)	0.0022 (8)	0.0156 (8)
C16	0.0277 (8)	0.0313 (8)	0.0471 (9)	0.0032 (6)	0.0017 (7)	0.0065 (7)
C17	0.0213 (6)	0.0214 (6)	0.0297 (7)	−0.0012 (6)	−0.0017 (5)	0.0022 (6)

C18	0.0285 (7)	0.0285 (8)	0.0302 (7)	0.0021 (6)	−0.0009 (6)	0.0021 (6)
C19	0.0391 (9)	0.0347 (8)	0.0345 (8)	0.0026 (7)	−0.0082 (7)	0.0071 (7)
C20	0.0328 (8)	0.0316 (8)	0.0540 (10)	0.0085 (7)	−0.0092 (7)	0.0082 (8)
C21	0.0334 (8)	0.0338 (8)	0.0510 (10)	0.0109 (7)	0.0071 (7)	0.0024 (7)
C22	0.0312 (8)	0.0291 (8)	0.0325 (8)	0.0028 (6)	0.0032 (6)	0.0015 (6)
C23	0.0271 (8)	0.0521 (10)	0.0297 (8)	0.0028 (7)	0.0024 (6)	0.0148 (7)
C24	0.0814 (17)	0.0884 (18)	0.0377 (11)	0.0139 (14)	0.0051 (11)	−0.0063 (11)
C25	0.0556 (13)	0.0973 (19)	0.0625 (14)	−0.0232 (12)	−0.0123 (10)	0.0524 (14)
C26	0.0307 (8)	0.0263 (8)	0.0616 (11)	−0.0042 (6)	−0.0097 (7)	−0.0082 (8)
C27	0.0471 (11)	0.0448 (11)	0.0692 (13)	−0.0016 (9)	−0.0272 (10)	−0.0155 (10)
C28	0.0385 (10)	0.0386 (10)	0.0891 (16)	−0.0155 (8)	−0.0037 (10)	−0.0024 (10)
N1	0.0214 (6)	0.0224 (6)	0.0375 (7)	−0.0001 (5)	−0.0035 (5)	−0.0027 (5)
N2	0.0200 (6)	0.0465 (8)	0.0330 (7)	−0.0036 (6)	0.0010 (5)	0.0143 (6)
O1	0.0351 (6)	0.0473 (7)	0.0368 (6)	−0.0053 (5)	−0.0095 (5)	0.0157 (5)
O2	0.0257 (6)	0.0557 (8)	0.0465 (7)	−0.0005 (5)	0.0076 (5)	0.0122 (6)
O3	0.0477 (7)	0.0373 (6)	0.0404 (6)	0.0068 (5)	−0.0008 (5)	0.0144 (5)
O4	0.0517 (8)	0.0420 (7)	0.0440 (7)	−0.0003 (6)	0.0014 (6)	−0.0174 (6)
P1	0.02145 (16)	0.02076 (17)	0.02755 (17)	0.00172 (13)	−0.00178 (13)	−0.00073 (14)
P2	0.01931 (16)	0.02283 (16)	0.02462 (16)	−0.00003 (13)	−0.00046 (13)	0.00359 (14)
Mo1	0.01891 (6)	0.02026 (6)	0.02017 (6)	−0.00123 (4)	−0.00037 (4)	0.00138 (4)

Geometric parameters (Å, º)

C1—O1	1.1417 (17)	C15—C16	1.385 (2)
C1—Mo1	2.0282 (15)	C17—C22	1.392 (2)
C2—O2	1.1450 (18)	C17—C18	1.392 (2)
C2—Mo1	1.9912 (15)	C17—P2	1.8234 (14)
C3—O3	1.1366 (18)	C18—C19	1.381 (2)
C3—Mo1	2.0313 (15)	C19—C20	1.377 (2)
C4—O4	1.1463 (19)	C20—C21	1.374 (3)
C4—Mo1	1.9973 (15)	C21—C22	1.392 (2)
C5—C6	1.385 (2)	C23—N2	1.4646 (19)
C5—C10	1.394 (2)	C23—C25	1.503 (3)
C5—P1	1.8194 (15)	C23—C24	1.510 (3)
C6—C7	1.387 (2)	C26—N1	1.4946 (19)
C7—C8	1.370 (3)	C26—C28	1.515 (3)
C8—C9	1.380 (3)	C26—C27	1.520 (3)
C9—C10	1.385 (3)	N1—P1	1.6949 (13)
C11—C16	1.388 (2)	N1—P2	1.7185 (13)
C11—C12	1.393 (2)	N2—P2	1.6462 (13)
C11—P1	1.8232 (15)	P1—Mo1	2.4731 (5)
C12—C13	1.382 (2)	P1—P2	2.6733 (6)
C13—C14	1.378 (3)	P2—Mo1	2.5056 (6)
C14—C15	1.378 (3)		
O1—C1—Mo1	174.59 (12)	C23—N2—P2	126.68 (11)
O2—C2—Mo1	173.34 (13)	N1—P1—C5	108.58 (6)
O3—C3—Mo1	172.36 (13)	N1—P1—C11	105.88 (7)

O4—C4—Mo1	178.85 (14)	C5—P1—C11	104.57 (7)
C6—C5—C10	118.67 (14)	N1—P1—Mo1	96.51 (4)
C6—C5—P1	117.26 (11)	C5—P1—Mo1	123.84 (5)
C10—C5—P1	124.07 (13)	C11—P1—Mo1	115.77 (5)
C5—C6—C7	120.99 (16)	N1—P1—P2	38.76 (4)
C8—C7—C6	119.81 (18)	C5—P1—P2	132.82 (5)
C7—C8—C9	120.10 (16)	C11—P1—P2	115.78 (5)
C8—C9—C10	120.40 (17)	Mo1—P1—P2	58.112 (14)
C9—C10—C5	120.01 (17)	N2—P2—N1	112.48 (7)
C16—C11—C12	118.98 (14)	N2—P2—C17	101.08 (7)
C16—C11—P1	119.63 (11)	N1—P2—C17	104.50 (6)
C12—C11—P1	120.75 (12)	N2—P2—Mo1	123.27 (5)
C13—C12—C11	120.10 (15)	N1—P2—Mo1	94.72 (4)
C14—C13—C12	120.49 (15)	C17—P2—Mo1	119.57 (5)
C13—C14—C15	119.85 (15)	N2—P2—P1	126.83 (5)
C14—C15—C16	120.07 (16)	N1—P2—P1	38.13 (4)
C15—C16—C11	120.49 (15)	C17—P2—P1	125.34 (5)
C22—C17—C18	118.74 (13)	Mo1—P2—P1	56.940 (15)
C22—C17—P2	121.45 (11)	C2—Mo1—C4	99.51 (6)
C18—C17—P2	119.57 (11)	C2—Mo1—C1	88.19 (6)
C19—C18—C17	120.68 (15)	C4—Mo1—C1	88.13 (6)
C20—C19—C18	120.02 (15)	C2—Mo1—C3	86.69 (6)
C21—C20—C19	120.23 (15)	C4—Mo1—C3	83.89 (6)
C20—C21—C22	120.17 (15)	C1—Mo1—C3	169.67 (6)
C21—C22—C17	120.11 (14)	C2—Mo1—P1	94.44 (5)
N2—C23—C25	109.43 (15)	C4—Mo1—P1	165.51 (4)
N2—C23—C24	110.63 (15)	C1—Mo1—P1	88.39 (4)
C25—C23—C24	112.62 (18)	C3—Mo1—P1	100.94 (4)
N1—C26—C28	112.27 (15)	C2—Mo1—P2	157.06 (4)
N1—C26—C27	112.87 (15)	C4—Mo1—P2	101.93 (4)
C28—C26—C27	111.79 (16)	C1—Mo1—P2	100.52 (4)
C26—N1—P1	123.61 (10)	C3—Mo1—P2	87.56 (4)
C26—N1—P2	132.47 (11)	P1—Mo1—P2	64.948 (13)
P1—N1—P2	103.10 (6)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O1^{i}	0.95	2.53	3.338 (2)	143
N2—H2···O1^{ii}	0.83 (1)	2.54 (1)	3.3419 (18)	163 (1)

Symmetry codes: (i) x, $-y+1/2$, $z+1/2$; (ii) $x+1/2$, y, $-z+1/2$.