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(*RS*)-Efonidipine acetone hemisolvate

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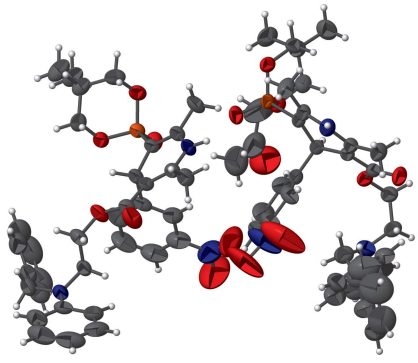
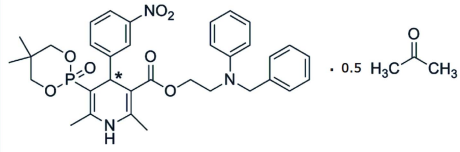
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{34}H_{38}N_3O_7P\cdot0.5C_3H_6O$ {systematic name: (*RS*)-2-[phenyl(phenylmethyl)amino]ethyl 5-(5,5-dimethyl-2-oxo-1,3-dioxa-2λ^5-phosphacyclohex-2-yl)-2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3-carboxylate acetone hemisolvate}, contains one *R*-efonidipine molecule, one *S*-efonidipine molecule and half of a solvate acetone molecule. In both efonidipine molecules, the six-membered rings of the dioxaphosphinanyl moieties display a chair conformation and the dihydropyridine rings display a flattened boat conformation. In the crystal, N—H···O, C—H···O hydrogen bonds and weak C—H···π interactions link the molecules into a three-dimensional supramolecular structure. A solvent-accessible void of 199 Å^3 is found in the structure; the contribution of the heavily disordered solvate molecule was suppressed by use of the SQUEEZE routine in *PLATON* [Spek (2015). *Acta Cryst.* C**71**, 9–18].

3D view



Chemical scheme



Structure description

(*RS*)-Efonidipine is an efficient and long-acting Ca^{2+} channel blocker with renal protection, and has been used clinically in Japan and Korea (Yamashita *et al.*, 1991; Saito *et al.*, 1992). (*S*)-efonidipine has been synthesized by asymmetric synthesis and its crystal structure reported in the space group $P2_12_12_1$ (Guo *et al.*, 2008; Sakoda *et al.*, 1992). Here we report the crystal structure of (*RS*)-efonidipine acetone hemisolvate. For the structure of an efonidipine analogue, 1,2,3,4,5,6,7,8-octahydro-3,3,6,6-tetramethyl-9-(2-nitrophenyl)xanthene-1,8-dione, see: Jeyakanthan *et al.* (1999).

As shown in Fig. 1, the asymmetric unit of the title compound contains a (*R*)-efonidipine molecule, a (*S*)-efonidipine molecule and half of an acetone molecule. In both efonidipine molecules, the six-membered rings of the dioxaphosphinanyl moieties display

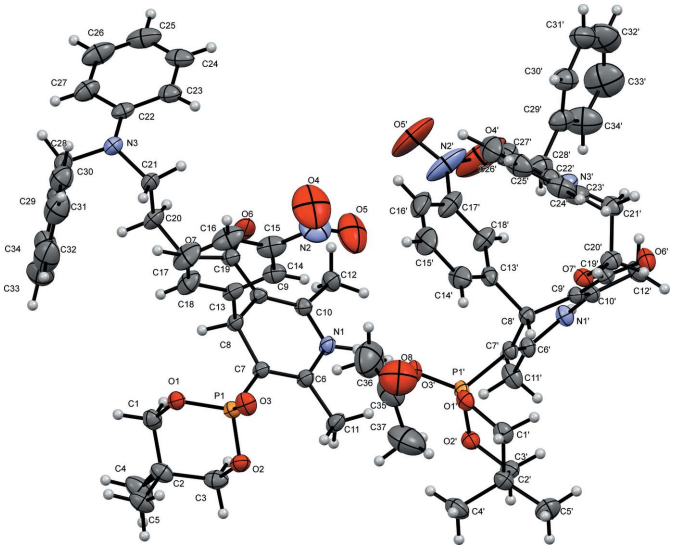


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

a chair conformation and the dihydropyridine rings display a flattened boat conformation.

In the crystal, classical N—H···O hydrogen bonds and weak C—H···O and C—H···π interactions (Table 1) link the molecules into a three-dimensional network.

Synthesis and crystallization

(*RS*)-Efonidipine was prepared using a Hantzsch pyridine reaction, starting with two intermediates I {2-butenoic acid, 3-amino-2-[phenyl(phenylmethyl)amino] ethyl ester} and II {3-buten-2-one, 3-(5,5-dimethyl-2-oxido-1,3,2-dioxaphosphorinan-2-yl)-4-(3-nitrophenyl)}. The intermediates I (7.0 g, 22.55 mmol) and II (7.6 g, 22.40 mmol) were dissolved in 150 ml of 2-propanol at 83° C with reflux, stirred for 3 h, then cooled down to room temperature and stirred for 8 h, vacuum filtration, recrystallized in 100 ml of ethanol, vacuum drying, yield 11.05 g (78.09%). Slow evaporation of a solution in acetone while left to stand for 4 days gave light-yellow rhombus-shaped columnar crystals.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The solvent-accessible void of 199 Å^3 is found in the structure, the presumed contribution of a heavily disordered solvate molecule was suppressed by the SQUEEZE routine in *PLATON* (Spek, 2015).

Acknowledgements

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

*Cg*4 and *Cg*9 are the centroids of the C22′–C27′ and C22–C27 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3′	0.86	2.04	2.847 (2)	155
N1′—H1′···O3^{i}	0.86	2.20	2.917 (2)	141
C1—H1*A*···O6^{ii}	0.97	2.54	3.456 (4)	157
C1′—H1′*B*···O6′^{iii}	0.97	2.42	3.346 (4)	160
C15′—H15′···O5	0.93	2.55	3.470 (7)	173
C37—H37*C*···*Cg*4^{iv}	0.96	2.88	3.667 (9)	139
C3′—H3′*B*···*Cg*9^{v}	0.97	2.66	3.599 (3)	163

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{34}H_{38}N_3O_7P{\cdot}0.5C_3H_6O$
M_r	660.68
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	13.9972 (6), 17.2985 (4), 18.4787 (6)
α, β, γ (°)	63.725 (3), 68.593 (3), 67.115 (4)
V (Å^3)	3594.1 (3)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.10
Crystal size (mm)	0.32 × 0.25 × 0.2
Data collection	
Diffractometer	Agilent Xcalibur, Eos, Gemini
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.575, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	56083, 12829, 10943
R_{int}	0.050
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.597
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.062, 0.196, 1.05
No. of reflections	12829
No. of parameters	857
No. of restraints	38
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.93, −0.49

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

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full crystallographic data

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***RS*-2-(Phenyl(phenylmethyl)amino)ethyl 5-(5,5-dimethyl-2-oxo-1,3-dioxa-2λ^5-phosphacyclohex-2-yl)-2,6-dimethyl-4-(3-nitrophenyl)-1,4-dihydropyridine-3-carboxylate acetone hemisolvate**

Crystal data

$C_{34}H_{38}N_3O_7P{\cdot}0.5C_3H_6O$
M_r = 660.68
Triclinic, $P\overline{1}$
a = 13.9972 (6) Å
b = 17.2985 (4) Å
c = 18.4787 (6) Å
α = 63.725 (3)°
β = 68.593 (3)°
γ = 67.115 (4)°
V = 3594.1 (3) Å^3
Z = 4
$F(000)$ = 1400
D_x = 1.221 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 17758 reflections
θ = 3.6–70.8°
μ = 1.10 mm^{-1}
T = 293 K
Block, yellow
0.32 × 0.25 × 0.2 mm

Data collection

Agilent Xcalibur, Eos, Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.2312 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis Pro; Agilent, 2014)
T_{min} = 0.575, T_{max} = 1.000
56083 measured reflections
12829 independent reflections
10943 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 67.1°, θ_{min} = 3.5°
h = −16→16
k = −20→20
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.196
S = 1.05
12829 reflections
857 parameters
38 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1265P)^2 + 0.9921P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.93 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3215 (2)	0.82686 (17)	−0.00144 (16)	0.0549 (6)
H1A	0.3687	0.8624	−0.0143	0.066*
H1B	0.2636	0.8653	−0.0291	0.066*
C2	0.3824 (2)	0.75075 (19)	−0.03425 (16)	0.0561 (6)
C3	0.4714 (2)	0.6915 (2)	0.01101 (18)	0.0622 (7)
H3A	0.5128	0.6427	−0.0099	0.075*
H3B	0.5185	0.7262	0.0001	0.075*
C4	0.4328 (3)	0.7904 (3)	−0.12659 (19)	0.0829 (10)
H4A	0.3783	0.8343	−0.1550	0.124*
H4B	0.4674	0.7436	−0.1496	0.124*
H4C	0.4843	0.8183	−0.1331	0.124*
C5	0.3101 (3)	0.6968 (2)	−0.02151 (19)	0.0685 (8)
H5A	0.2870	0.6657	0.0367	0.103*
H5B	0.3486	0.6543	−0.0494	0.103*
H5C	0.2491	0.7365	−0.0439	0.103*
C6	0.52984 (16)	0.74078 (14)	0.16638 (14)	0.0419 (5)
C7	0.43285 (16)	0.78168 (14)	0.14929 (13)	0.0388 (4)
C8	0.37752 (16)	0.87938 (14)	0.14128 (14)	0.0403 (4)
H8	0.3490	0.9090	0.0915	0.048*
C9	0.45699 (16)	0.92695 (14)	0.12951 (13)	0.0390 (4)
C10	0.55301 (16)	0.88028 (15)	0.14821 (14)	0.0416 (5)
C11	0.5922 (2)	0.64459 (16)	0.1784 (2)	0.0588 (6)
H11D	0.6456	0.6412	0.1286	0.088*
H11E	0.5448	0.6102	0.1908	0.088*
H11F	0.6259	0.6210	0.2236	0.088*
C12	0.63500 (19)	0.91921 (18)	0.14379 (18)	0.0552 (6)
H12D	0.6908	0.8719	0.1686	0.083*
H12E	0.6020	0.9605	0.1732	0.083*
H12F	0.6646	0.9501	0.0868	0.083*
C13	0.28356 (17)	0.88676 (15)	0.21580 (17)	0.0484 (5)
C14	0.3000 (2)	0.85466 (18)	0.29409 (18)	0.0589 (6)
H14	0.3689	0.8295	0.3024	0.071*
C15	0.2133 (3)	0.8601 (2)	0.3605 (2)	0.0747 (9)
C16	0.1102 (3)	0.8963 (3)	0.3506 (3)	0.0912 (12)
H16	0.0529	0.8989	0.3961	0.109*
C17	0.0936 (2)	0.9283 (3)	0.2728 (3)	0.0955 (13)
H17	0.0243	0.9528	0.2653	0.115*
C18	0.1793 (2)	0.9248 (2)	0.2045 (2)	0.0738 (8)
H18	0.1674	0.9476	0.1517	0.089*

C19	0.42528 (17)	1.02457 (15)	0.09720 (14)	0.0439 (5)
C20	0.2875 (2)	1.15274 (16)	0.04375 (17)	0.0561 (6)
H20C	0.2614	1.1723	−0.0052	0.067*
H20D	0.3405	1.1833	0.0298	0.067*
C21	0.1962 (2)	1.17484 (15)	0.11350 (15)	0.0497 (5)
H21C	0.1508	1.1356	0.1338	0.060*
H21D	0.2246	1.1636	0.1589	0.060*
C22	0.1755 (2)	1.33439 (16)	0.07568 (16)	0.0532 (6)
C23	0.2416 (2)	1.3172 (2)	0.12598 (19)	0.0635 (7)
H23	0.2583	1.2607	0.1660	0.076*
C24	0.2818 (3)	1.3827 (3)	0.1168 (2)	0.0782 (9)
H24	0.3261	1.3695	0.1503	0.094*
C25	0.2580 (3)	1.4672 (3)	0.0592 (3)	0.0962 (13)
H25	0.2854	1.5112	0.0536	0.115*
C26	0.1941 (4)	1.4852 (2)	0.0108 (3)	0.0980 (14)
H26	0.1772	1.5426	−0.0279	0.118*
C27	0.1522 (3)	1.42034 (19)	0.0170 (2)	0.0724 (8)
H27	0.1091	1.4345	−0.0178	0.087*
C28	0.0648 (2)	1.29038 (18)	0.03193 (19)	0.0622 (7)
H28C	0.1081	1.2997	−0.0243	0.075*
H28D	0.0101	1.3459	0.0324	0.075*
C29	0.0127 (2)	1.21837 (19)	0.0569 (2)	0.0649 (7)
C30	−0.0632 (3)	1.1985 (2)	0.1317 (2)	0.0812 (9)
H30	−0.0840	1.2320	0.1654	0.097*
C31	−0.1071 (3)	1.1306 (3)	0.1558 (4)	0.1045 (14)
H31	−0.1567	1.1173	0.2062	0.125*
C32	−0.0786 (4)	1.0820 (3)	0.1062 (4)	0.1177 (18)
H32	−0.1081	1.0353	0.1228	0.141*
C33	−0.0063 (5)	1.1024 (3)	0.0319 (4)	0.1131 (15)
H33	0.0119	1.0701	−0.0024	0.136*
C34	0.0401 (3)	1.1700 (3)	0.0069 (3)	0.0864 (10)
H34	0.0897	1.1827	−0.0436	0.104*
N1	0.58447 (14)	0.78856 (12)	0.17179 (13)	0.0457 (4)
H1	0.6410	0.7596	0.1909	0.055*
N2	0.2307 (4)	0.8258 (3)	0.4430 (2)	0.1114 (12)
N3	0.13209 (16)	1.26804 (13)	0.08721 (13)	0.0507 (5)
O1	0.27786 (11)	0.79476 (10)	0.08821 (10)	0.0451 (4)
O2	0.42944 (13)	0.65511 (11)	0.09956 (11)	0.0510 (4)
O3	0.29406 (14)	0.67610 (13)	0.22736 (11)	0.0563 (4)
O4	0.1529 (4)	0.8275 (4)	0.5002 (2)	0.191 (2)
O5	0.3205 (4)	0.7993 (4)	0.4505 (2)	0.1607 (18)
O6	0.47088 (17)	1.07441 (12)	0.09126 (15)	0.0716 (6)
O7	0.33406 (13)	1.05736 (11)	0.07105 (12)	0.0565 (4)
P1	0.35504 (4)	0.72254 (4)	0.14661 (3)	0.03924 (16)
C1′	0.8422 (2)	0.46689 (17)	0.34018 (16)	0.0540 (6)
H1′A	0.7874	0.4359	0.3740	0.065*
H1′B	0.8822	0.4609	0.3765	0.065*
C2′	0.9168 (2)	0.42312 (18)	0.27692 (17)	0.0558 (6)

C3′	0.99985 (19)	0.47459 (17)	0.22293 (17)	0.0539 (6)
H3′A	1.0406	0.4715	0.2573	0.065*
H3′B	1.0488	0.4472	0.1824	0.065*
C4′	0.8536 (3)	0.4228 (3)	0.2244 (2)	0.0767 (9)
H4′A	0.8224	0.4834	0.1925	0.115*
H4′B	0.7983	0.3939	0.2602	0.115*
H4′C	0.9007	0.3910	0.1876	0.115*
C5′	0.9748 (3)	0.3270 (2)	0.3238 (2)	0.0829 (9)
H5′A	1.0245	0.2991	0.2847	0.124*
H5′B	0.9236	0.2934	0.3588	0.124*
H5′C	1.0124	0.3285	0.3572	0.124*
C6′	1.02119 (17)	0.66646 (15)	0.25335 (13)	0.0426 (5)
C7′	0.92907 (16)	0.64304 (14)	0.29022 (13)	0.0391 (4)
C8′	0.86958 (16)	0.64201 (15)	0.37817 (13)	0.0398 (4)
H8′	0.8416	0.5894	0.4074	0.048*
C9′	0.94629 (16)	0.63279 (14)	0.42430 (13)	0.0388 (4)
C10′	1.03893 (17)	0.65626 (14)	0.38304 (14)	0.0421 (5)
C11′	1.0839 (2)	0.6770 (2)	0.16599 (15)	0.0603 (7)
H11A	1.0999	0.7339	0.1399	0.091*
H11B	1.0430	0.6742	0.1358	0.091*
H11C	1.1492	0.6298	0.1662	0.091*
C12′	1.1179 (2)	0.6566 (2)	0.42041 (17)	0.0562 (6)
H12A	1.1498	0.5963	0.4524	0.084*
H12B	1.0819	0.6916	0.4558	0.084*
H12C	1.1724	0.6821	0.3769	0.084*
C13′	0.77520 (17)	0.72550 (17)	0.37620 (14)	0.0480 (5)
C14′	0.6721 (2)	0.7201 (3)	0.3965 (2)	0.0778 (9)
H14′	0.6596	0.6654	0.4113	0.093*
C15′	0.5864 (3)	0.7974 (4)	0.3946 (3)	0.1037 (14)
H15′	0.5173	0.7931	0.4086	0.124*
C16′	0.6016 (3)	0.8775 (3)	0.3731 (2)	0.0926 (12)
H16′	0.5444	0.9285	0.3720	0.111*
C17′	0.7049 (3)	0.8812 (2)	0.3529 (2)	0.0846 (11)
C18′	0.7913 (2)	0.80735 (18)	0.35421 (17)	0.0635 (7)
H18′	0.8599	0.8126	0.3404	0.076*
C19′	0.91776 (17)	0.59837 (15)	0.51501 (14)	0.0429 (5)
C20′	0.7868 (2)	0.54706 (17)	0.63447 (15)	0.0538 (6)
H20A	0.8463	0.5009	0.6565	0.065*
H20B	0.7305	0.5195	0.6496	0.065*
C21′	0.7468 (2)	0.61830 (19)	0.67325 (16)	0.0573 (6)
H21A	0.7344	0.5893	0.7331	0.069*
H21B	0.8022	0.6477	0.6554	0.069*
C22′	0.5513 (2)	0.67157 (18)	0.69936 (17)	0.0568 (6)
C23′	0.5416 (3)	0.5900 (2)	0.76480 (19)	0.0659 (7)
H23′	0.6028	0.5442	0.7766	0.079*
C24′	0.4427 (3)	0.5771 (3)	0.8117 (2)	0.0783 (9)
H24′	0.4387	0.5230	0.8551	0.094*
C25′	0.3514 (3)	0.6416 (3)	0.7959 (3)	0.0891 (11)

H25′	0.2853	0.6324	0.8281	0.107*
C26′	0.3586 (3)	0.7200 (3)	0.7320 (3)	0.0966 (12)
H26′	0.2961	0.7638	0.7199	0.116*
C27′	0.4559 (3)	0.7371 (2)	0.6842 (2)	0.0791 (9)
H27′	0.4577	0.7922	0.6420	0.095*
C28′	0.6654 (3)	0.7689 (2)	0.58599 (19)	0.0720 (8)
H28A	0.5997	0.8024	0.5673	0.086*
H28B	0.7205	0.7549	0.5397	0.086*
C29′	0.6958 (3)	0.8272 (2)	0.61009 (19)	0.0719 (8)
C30′	0.6320 (3)	0.8580 (2)	0.6734 (2)	0.0838 (9)
H30′	0.5684	0.8421	0.7020	0.101*
C31′	0.6573 (5)	0.9111 (3)	0.6965 (3)	0.1077 (12)
H31′	0.6095	0.9354	0.7365	0.129*
C32′	0.7567 (7)	0.9278 (4)	0.6586 (5)	0.141 (2)
H32′	0.7756	0.9631	0.6744	0.169*
C33′	0.8295 (6)	0.8930 (5)	0.5972 (6)	0.165 (3)
H33′	0.8966	0.9033	0.5730	0.198*
C34′	0.7969 (5)	0.8425 (4)	0.5743 (4)	0.131 (2)
H34′	0.8435	0.8181	0.5341	0.158*
N1′	1.06906 (15)	0.68152 (14)	0.29796 (12)	0.0470 (4)
H1′	1.1194	0.7076	0.2714	0.056*
N2′	0.7245 (4)	0.9673 (2)	0.3311 (4)	0.155 (2)
N3′	0.65064 (18)	0.68538 (15)	0.65318 (15)	0.0624 (6)
O1′	0.79168 (12)	0.56194 (12)	0.30105 (10)	0.0475 (4)
O2′	0.94974 (12)	0.56802 (11)	0.18010 (9)	0.0470 (4)
O3′	0.80143 (13)	0.70705 (12)	0.18227 (11)	0.0552 (4)
O4′	0.8163 (4)	0.9680 (2)	0.3326 (5)	0.220 (3)
O5′	0.6487 (4)	1.0330 (2)	0.3217 (4)	0.220 (3)
O6′	0.97116 (14)	0.58385 (14)	0.56099 (11)	0.0610 (5)
O7′	0.82021 (12)	0.58317 (11)	0.54522 (9)	0.0473 (4)
P1′	0.86414 (4)	0.62486 (4)	0.23432 (3)	0.03975 (16)
C35	0.4273 (4)	0.5150 (4)	0.4367 (3)	0.1148 (15)
C36	0.4288 (6)	0.6091 (5)	0.3903 (4)	0.159 (3)
H36A	0.3998	0.6319	0.3427	0.238*
H36B	0.5008	0.6130	0.3725	0.238*
H36C	0.3866	0.6439	0.4254	0.238*
C37	0.5091 (6)	0.4464 (6)	0.4009 (5)	0.170 (3)
H37A	0.5767	0.4597	0.3799	0.255*
H37B	0.4878	0.4476	0.3565	0.255*
H37C	0.5152	0.3881	0.4432	0.255*
O8	0.3668 (4)	0.4943 (4)	0.5027 (3)	0.1588 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0630 (15)	0.0539 (13)	0.0562 (13)	−0.0234 (11)	−0.0201 (11)	−0.0152 (11)
C2	0.0627 (15)	0.0672 (16)	0.0503 (13)	−0.0345 (13)	−0.0055 (11)	−0.0223 (11)
C3	0.0511 (14)	0.0705 (17)	0.0733 (17)	−0.0211 (12)	0.0015 (12)	−0.0411 (14)

C4	0.104 (3)	0.109 (3)	0.0541 (16)	−0.063 (2)	−0.0018 (16)	−0.0286 (17)
C5	0.0800 (19)	0.083 (2)	0.0680 (16)	−0.0431 (16)	−0.0114 (14)	−0.0344 (15)
C6	0.0329 (10)	0.0398 (11)	0.0554 (12)	−0.0100 (8)	−0.0112 (9)	−0.0180 (9)
C7	0.0313 (9)	0.0370 (10)	0.0514 (11)	−0.0090 (8)	−0.0089 (8)	−0.0191 (9)
C8	0.0309 (10)	0.0370 (10)	0.0573 (12)	−0.0091 (8)	−0.0132 (9)	−0.0181 (9)
C9	0.0343 (10)	0.0383 (10)	0.0487 (11)	−0.0113 (8)	−0.0073 (8)	−0.0197 (9)
C10	0.0342 (10)	0.0462 (11)	0.0496 (11)	−0.0134 (9)	−0.0082 (8)	−0.0203 (9)
C11	0.0443 (12)	0.0414 (12)	0.0928 (19)	−0.0020 (10)	−0.0267 (13)	−0.0250 (12)
C12	0.0438 (12)	0.0564 (14)	0.0769 (16)	−0.0176 (10)	−0.0204 (11)	−0.0247 (12)
C13	0.0317 (10)	0.0375 (11)	0.0757 (16)	−0.0102 (8)	−0.0043 (10)	−0.0254 (11)
C14	0.0493 (13)	0.0588 (15)	0.0698 (16)	−0.0193 (11)	−0.0009 (12)	−0.0299 (13)
C15	0.0636 (17)	0.0707 (18)	0.084 (2)	−0.0324 (15)	0.0159 (15)	−0.0361 (16)
C16	0.0591 (19)	0.081 (2)	0.107 (3)	−0.0245 (16)	0.0261 (19)	−0.042 (2)
C17	0.0334 (14)	0.093 (2)	0.133 (4)	−0.0069 (14)	0.0035 (17)	−0.044 (2)
C18	0.0377 (13)	0.0678 (17)	0.106 (2)	−0.0066 (12)	−0.0120 (14)	−0.0319 (16)
C19	0.0369 (10)	0.0437 (11)	0.0543 (12)	−0.0118 (9)	−0.0075 (9)	−0.0216 (9)
C20	0.0500 (13)	0.0357 (11)	0.0696 (15)	−0.0048 (10)	−0.0134 (11)	−0.0139 (11)
C21	0.0514 (13)	0.0380 (11)	0.0559 (13)	−0.0053 (9)	−0.0196 (10)	−0.0136 (10)
C22	0.0510 (13)	0.0438 (12)	0.0557 (13)	−0.0078 (10)	0.0024 (10)	−0.0258 (10)
C23	0.0585 (15)	0.0633 (16)	0.0720 (17)	−0.0100 (12)	−0.0068 (13)	−0.0388 (14)
C24	0.0650 (18)	0.088 (2)	0.101 (2)	−0.0252 (16)	0.0062 (16)	−0.066 (2)
C25	0.077 (2)	0.081 (2)	0.137 (4)	−0.036 (2)	0.022 (2)	−0.068 (3)
C26	0.096 (3)	0.0512 (18)	0.111 (3)	−0.0243 (17)	0.014 (2)	−0.0243 (18)
C27	0.0732 (18)	0.0478 (15)	0.0741 (18)	−0.0127 (13)	−0.0049 (15)	−0.0155 (13)
C28	0.0581 (15)	0.0513 (14)	0.0683 (16)	−0.0025 (11)	−0.0268 (13)	−0.0144 (12)
C29	0.0552 (15)	0.0574 (15)	0.0807 (18)	−0.0055 (12)	−0.0309 (14)	−0.0196 (13)
C30	0.0619 (18)	0.078 (2)	0.096 (2)	−0.0171 (15)	−0.0173 (17)	−0.0268 (18)
C31	0.075 (2)	0.090 (3)	0.137 (4)	−0.028 (2)	−0.028 (2)	−0.022 (3)
C32	0.106 (3)	0.088 (3)	0.171 (5)	−0.042 (3)	−0.063 (4)	−0.018 (3)
C33	0.137 (4)	0.095 (3)	0.148 (4)	−0.036 (3)	−0.065 (4)	−0.047 (3)
C34	0.089 (2)	0.088 (2)	0.096 (2)	−0.0158 (19)	−0.044 (2)	−0.034 (2)
N1	0.0335 (9)	0.0401 (9)	0.0677 (12)	−0.0061 (7)	−0.0212 (8)	−0.0185 (8)
N2	0.107 (3)	0.144 (3)	0.0703 (19)	−0.047 (3)	0.015 (2)	−0.044 (2)
N3	0.0519 (11)	0.0393 (10)	0.0573 (11)	−0.0037 (8)	−0.0174 (9)	−0.0176 (8)
O1	0.0352 (7)	0.0488 (8)	0.0576 (9)	−0.0124 (6)	−0.0120 (6)	−0.0223 (7)
O2	0.0495 (9)	0.0445 (8)	0.0648 (10)	−0.0110 (7)	−0.0132 (7)	−0.0257 (7)
O3	0.0500 (9)	0.0670 (11)	0.0539 (9)	−0.0333 (8)	−0.0060 (7)	−0.0130 (8)
O4	0.138 (3)	0.303 (7)	0.083 (2)	−0.083 (4)	0.042 (2)	−0.061 (3)
O5	0.120 (3)	0.259 (6)	0.082 (2)	−0.038 (3)	−0.013 (2)	−0.061 (3)
O6	0.0704 (12)	0.0439 (9)	0.1145 (17)	−0.0208 (9)	−0.0415 (12)	−0.0195 (10)
O7	0.0435 (9)	0.0363 (8)	0.0875 (12)	−0.0047 (7)	−0.0227 (8)	−0.0193 (8)
P1	0.0322 (3)	0.0397 (3)	0.0505 (3)	−0.0139 (2)	−0.0076 (2)	−0.0179 (2)
C1′	0.0544 (13)	0.0594 (14)	0.0512 (12)	−0.0257 (11)	−0.0112 (10)	−0.0141 (11)
C2′	0.0585 (14)	0.0567 (14)	0.0624 (14)	−0.0167 (11)	−0.0186 (12)	−0.0252 (12)
C3′	0.0414 (12)	0.0565 (14)	0.0659 (14)	−0.0059 (10)	−0.0111 (11)	−0.0307 (12)
C4′	0.084 (2)	0.091 (2)	0.086 (2)	−0.0327 (18)	−0.0256 (17)	−0.0454 (18)
C5′	0.096 (2)	0.0528 (16)	0.094 (2)	−0.0149 (16)	−0.0293 (19)	−0.0203 (16)
C6′	0.0345 (10)	0.0520 (12)	0.0431 (11)	−0.0159 (9)	−0.0097 (8)	−0.0141 (9)

C7′	0.0324 (10)	0.0470 (11)	0.0402 (10)	−0.0121 (8)	−0.0096 (8)	−0.0152 (9)
C8′	0.0327 (10)	0.0472 (11)	0.0422 (10)	−0.0128 (8)	−0.0073 (8)	−0.0173 (9)
C9′	0.0350 (10)	0.0399 (10)	0.0446 (11)	−0.0089 (8)	−0.0099 (8)	−0.0180 (9)
C10′	0.0395 (11)	0.0426 (11)	0.0494 (11)	−0.0104 (9)	−0.0139 (9)	−0.0184 (9)
C11′	0.0473 (13)	0.094 (2)	0.0459 (12)	−0.0374 (13)	−0.0017 (10)	−0.0213 (13)
C12′	0.0515 (13)	0.0721 (16)	0.0608 (14)	−0.0275 (12)	−0.0158 (11)	−0.0256 (12)
C13′	0.0344 (11)	0.0644 (14)	0.0442 (11)	−0.0056 (10)	−0.0094 (9)	−0.0246 (10)
C14′	0.0379 (13)	0.105 (2)	0.109 (2)	−0.0099 (14)	−0.0120 (14)	−0.065 (2)
C15′	0.0346 (15)	0.148 (4)	0.135 (3)	0.0077 (19)	−0.0234 (18)	−0.081 (3)
C16′	0.068 (2)	0.091 (3)	0.092 (2)	0.0254 (19)	−0.0327 (18)	−0.039 (2)
C17′	0.0681 (19)	0.0615 (18)	0.0729 (19)	0.0089 (15)	−0.0067 (15)	−0.0106 (14)
C18′	0.0492 (14)	0.0506 (14)	0.0626 (15)	−0.0065 (11)	−0.0043 (11)	−0.0089 (12)
C19′	0.0399 (11)	0.0444 (11)	0.0463 (11)	−0.0051 (9)	−0.0124 (9)	−0.0210 (9)
C20′	0.0548 (13)	0.0544 (13)	0.0440 (12)	−0.0142 (11)	−0.0024 (10)	−0.0181 (10)
C21′	0.0541 (14)	0.0695 (16)	0.0499 (13)	−0.0174 (12)	−0.0035 (11)	−0.0288 (12)
C22′	0.0545 (14)	0.0593 (15)	0.0656 (15)	−0.0126 (11)	−0.0091 (12)	−0.0359 (12)
C23′	0.0674 (17)	0.0644 (16)	0.0679 (16)	−0.0181 (13)	−0.0048 (13)	−0.0334 (14)
C24′	0.086 (2)	0.090 (2)	0.0777 (19)	−0.0440 (19)	0.0031 (17)	−0.0461 (17)
C25′	0.070 (2)	0.122 (3)	0.104 (3)	−0.043 (2)	−0.0038 (19)	−0.063 (3)
C26′	0.0522 (18)	0.128 (3)	0.120 (3)	−0.0054 (19)	−0.0224 (19)	−0.067 (3)
C27′	0.0674 (19)	0.074 (2)	0.097 (2)	−0.0054 (15)	−0.0255 (17)	−0.0380 (18)
C28′	0.084 (2)	0.0671 (17)	0.0580 (15)	−0.0199 (15)	−0.0076 (14)	−0.0237 (13)
C29′	0.087 (2)	0.0541 (15)	0.0602 (15)	−0.0224 (14)	−0.0065 (14)	−0.0136 (12)
C30′	0.100 (2)	0.078 (2)	0.0734 (19)	−0.0219 (17)	−0.0138 (17)	−0.0337 (16)
C31′	0.158 (3)	0.077 (2)	0.100 (3)	−0.023 (2)	−0.044 (2)	−0.038 (2)
C32′	0.198 (5)	0.101 (3)	0.156 (5)	−0.075 (4)	−0.056 (4)	−0.032 (3)
C33′	0.154 (6)	0.152 (6)	0.204 (8)	−0.093 (5)	−0.009 (5)	−0.057 (5)
C34′	0.138 (4)	0.130 (4)	0.138 (4)	−0.078 (4)	0.020 (3)	−0.062 (3)
N1′	0.0391 (9)	0.0586 (11)	0.0494 (10)	−0.0247 (8)	−0.0082 (8)	−0.0158 (9)
N2′	0.126 (3)	0.0446 (17)	0.191 (4)	0.003 (2)	0.012 (3)	−0.013 (2)
N3′	0.0561 (12)	0.0555 (12)	0.0674 (13)	−0.0110 (10)	−0.0066 (10)	−0.0245 (10)
O1′	0.0333 (7)	0.0649 (10)	0.0509 (8)	−0.0184 (7)	−0.0062 (6)	−0.0244 (7)
O2′	0.0406 (8)	0.0581 (9)	0.0443 (8)	−0.0130 (7)	−0.0070 (6)	−0.0222 (7)
O3′	0.0419 (8)	0.0616 (10)	0.0622 (10)	−0.0066 (7)	−0.0248 (7)	−0.0180 (8)
O4′	0.124 (3)	0.069 (2)	0.338 (7)	−0.034 (2)	0.047 (4)	−0.035 (3)
O5′	0.177 (4)	0.066 (2)	0.295 (7)	0.037 (2)	−0.043 (4)	−0.029 (3)
O6′	0.0511 (9)	0.0853 (13)	0.0502 (9)	−0.0164 (9)	−0.0183 (8)	−0.0235 (9)
O7′	0.0429 (8)	0.0573 (9)	0.0428 (8)	−0.0166 (7)	−0.0041 (6)	−0.0208 (7)
P1′	0.0282 (3)	0.0511 (3)	0.0426 (3)	−0.0096 (2)	−0.0105 (2)	−0.0178 (2)
C35	0.110 (3)	0.153 (5)	0.100 (3)	−0.045 (3)	−0.028 (3)	−0.049 (3)
C36	0.170 (6)	0.160 (6)	0.111 (4)	−0.024 (5)	−0.046 (4)	−0.025 (4)
C37	0.193 (7)	0.210 (8)	0.152 (5)	−0.064 (6)	−0.019 (5)	−0.112 (6)
O8	0.149 (3)	0.180 (4)	0.131 (3)	−0.069 (3)	0.011 (3)	−0.054 (3)

Geometric parameters (Å, º)

C1—H1A	0.9700	C2′—C4′	1.536 (4)
C1—H1B	0.9700	C2′—C5′	1.537 (4)

C1—C2	1.511 (4)	C3′—H3′A	0.9700
C1—O1	1.462 (3)	C3′—H3′B	0.9700
C2—C3	1.520 (4)	C3′—O2′	1.457 (3)
C2—C4	1.530 (4)	C4′—H4′A	0.9600
C2—C5	1.522 (4)	C4′—H4′B	0.9600
C3—H3A	0.9700	C4′—H4′C	0.9600
C3—H3B	0.9700	C5′—H5′A	0.9600
C3—O2	1.446 (3)	C5′—H5′B	0.9600
C4—H4A	0.9600	C5′—H5′C	0.9600
C4—H4B	0.9600	C6′—C7′	1.346 (3)
C4—H4C	0.9600	C6′—C11′	1.496 (3)
C5—H5A	0.9600	C6′—N1′	1.388 (3)
C5—H5B	0.9600	C7′—C8′	1.527 (3)
C5—H5C	0.9600	C7′—P1′	1.785 (2)
C6—C7	1.346 (3)	C8′—H8′	0.9800
C6—C11	1.505 (3)	C8′—C9′	1.523 (3)
C6—N1	1.378 (3)	C8′—C13′	1.529 (3)
C7—C8	1.524 (3)	C9′—C10′	1.357 (3)
C7—P1	1.785 (2)	C9′—C19′	1.462 (3)
C8—H8	0.9800	C10′—C12′	1.505 (3)
C8—C9	1.529 (3)	C10′—N1′	1.375 (3)
C8—C13	1.531 (3)	C11′—H11A	0.9600
C9—C10	1.351 (3)	C11′—H11B	0.9600
C9—C19	1.457 (3)	C11′—H11C	0.9600
C10—C12	1.504 (3)	C12′—H12A	0.9600
C10—N1	1.373 (3)	C12′—H12B	0.9600
C11—H11D	0.9600	C12′—H12C	0.9600
C11—H11E	0.9600	C13′—C14′	1.382 (4)
C11—H11F	0.9600	C13′—C18′	1.376 (4)
C12—H12D	0.9600	C14′—H14′	0.9300
C12—H12E	0.9600	C14′—C15′	1.404 (5)
C12—H12F	0.9600	C15′—H15′	0.9300
C13—C14	1.373 (4)	C15′—C16′	1.342 (7)
C13—C18	1.399 (4)	C16′—H16′	0.9300
C14—H14	0.9300	C16′—C17′	1.375 (6)
C14—C15	1.383 (4)	C17′—C18′	1.374 (4)
C15—C16	1.377 (6)	C17′—N2′	1.470 (6)
C15—N2	1.447 (6)	C18′—H18′	0.9300
C16—H16	0.9300	C19′—O6′	1.213 (3)
C16—C17	1.367 (7)	C19′—O7′	1.356 (3)
C17—H17	0.9300	C20′—H20A	0.9700
C17—C18	1.393 (5)	C20′—H20B	0.9700
C18—H18	0.9300	C20′—C21′	1.516 (4)
C19—O6	1.207 (3)	C20′—O7′	1.443 (3)
C19—O7	1.353 (3)	C21′—H21A	0.9700
C20—H20C	0.9700	C21′—H21B	0.9700
C20—H20D	0.9700	C21′—N3′	1.436 (4)
C20—C21	1.515 (4)	C22′—C23′	1.410 (4)

C20—O7	1.438 (3)	C22′—C27′	1.401 (4)
C21—H21C	0.9700	C22′—N3′	1.390 (4)
C21—H21D	0.9700	C23′—H23′	0.9300
C21—N3	1.463 (3)	C23′—C24′	1.382 (4)
C22—C23	1.406 (4)	C24′—H24′	0.9300
C22—C27	1.395 (4)	C24′—C25′	1.356 (6)
C22—N3	1.401 (3)	C25′—H25′	0.9300
C23—H23	0.9300	C25′—C26′	1.358 (6)
C23—C24	1.373 (4)	C26′—H26′	0.9300
C24—H24	0.9300	C26′—C27′	1.388 (6)
C24—C25	1.373 (6)	C27′—H27′	0.9300
C25—H25	0.9300	C28′—H28A	0.9700
C25—C26	1.348 (7)	C28′—H28B	0.9700
C26—H26	0.9300	C28′—C29′	1.505 (5)
C26—C27	1.402 (6)	C28′—N3′	1.459 (4)
C27—H27	0.9300	C29′—C30′	1.367 (5)
C28—H28C	0.9700	C29′—C34′	1.401 (6)
C28—H28D	0.9700	C30′—H30′	0.9300
C28—C29	1.499 (4)	C30′—C31′	1.366 (6)
C28—N3	1.466 (3)	C31′—H31′	0.9300
C29—C30	1.397 (5)	C31′—C32′	1.390 (9)
C29—C34	1.369 (5)	C32′—H32′	0.9300
C30—H30	0.9300	C32′—C33′	1.404 (10)
C30—C31	1.362 (6)	C33′—H33′	0.9300
C31—H31	0.9300	C33′—C34′	1.389 (9)
C31—C32	1.363 (8)	C34′—H34′	0.9300
C32—H32	0.9300	N1′—H1′	0.8600
C32—C33	1.367 (8)	N2′—O4′	1.301 (8)
C33—H33	0.9300	N2′—O5′	1.212 (5)
C33—C34	1.377 (6)	O1′—P1′	1.5784 (16)
C34—H34	0.9300	O2′—P1′	1.5767 (16)
N1—H1	0.8600	O3′—P1′	1.4670 (17)
N2—O4	1.210 (5)	C35—C36	1.471 (9)
N2—O5	1.198 (5)	C35—C37	1.497 (9)
O1—P1	1.5811 (16)	C35—O8	1.195 (6)
O2—P1	1.5790 (16)	C36—H36A	0.9600
O3—P1	1.4637 (17)	C36—H36B	0.9600
C1′—H1′A	0.9700	C36—H36C	0.9600
C1′—H1′B	0.9700	C37—H37A	0.9600
C1′—C2′	1.519 (4)	C37—H37B	0.9600
C1′—O1′	1.464 (3)	C37—H37C	0.9600
C2′—C3′	1.520 (4)		

H1A—C1—H1B	107.9	C1′—C2′—C5′	108.3 (2)
C2—C1—H1A	109.2	C3′—C2′—C4′	111.2 (2)
C2—C1—H1B	109.2	C3′—C2′—C5′	108.1 (2)
O1—C1—H1A	109.2	C4′—C2′—C5′	110.7 (3)
O1—C1—H1B	109.2	C2′—C3′—H3′A	109.4

O1—C1—C2	112.1 (2)	C2′—C3′—H3′B	109.4
C1—C2—C3	107.7 (2)	H3′A—C3′—H3′B	108.0
C1—C2—C4	108.2 (2)	O2′—C3′—C2′	111.04 (19)
C1—C2—C5	111.5 (2)	O2′—C3′—H3′A	109.4
C3—C2—C4	108.4 (3)	O2′—C3′—H3′B	109.4
C3—C2—C5	110.5 (2)	C2′—C4′—H4′A	109.5
C5—C2—C4	110.5 (2)	C2′—C4′—H4′B	109.5
C2—C3—H3A	109.4	C2′—C4′—H4′C	109.5
C2—C3—H3B	109.4	H4′A—C4′—H4′B	109.5
H3A—C3—H3B	108.0	H4′A—C4′—H4′C	109.5
O2—C3—C2	111.4 (2)	H4′B—C4′—H4′C	109.5
O2—C3—H3A	109.4	C2′—C5′—H5′A	109.5
O2—C3—H3B	109.4	C2′—C5′—H5′B	109.5
C2—C4—H4A	109.5	C2′—C5′—H5′C	109.5
C2—C4—H4B	109.5	H5′A—C5′—H5′B	109.5
C2—C4—H4C	109.5	H5′A—C5′—H5′C	109.5
H4A—C4—H4B	109.5	H5′B—C5′—H5′C	109.5
H4A—C4—H4C	109.5	C7′—C6′—C11′	127.1 (2)
H4B—C4—H4C	109.5	C7′—C6′—N1′	120.0 (2)
C2—C5—H5A	109.5	N1′—C6′—C11′	112.90 (19)
C2—C5—H5B	109.5	C6′—C7′—C8′	121.03 (19)
C2—C5—H5C	109.5	C6′—C7′—P1′	121.26 (16)
H5A—C5—H5B	109.5	C8′—C7′—P1′	117.32 (14)
H5A—C5—H5C	109.5	C7′—C8′—H8′	108.0
H5B—C5—H5C	109.5	C7′—C8′—C13′	110.64 (17)
C7—C6—C11	127.1 (2)	C9′—C8′—C7′	109.97 (16)
C7—C6—N1	120.19 (19)	C9′—C8′—H8′	108.0
N1—C6—C11	112.64 (18)	C9′—C8′—C13′	112.01 (18)
C6—C7—C8	121.41 (19)	C13′—C8′—H8′	108.0
C6—C7—P1	122.43 (16)	C10′—C9′—C8′	121.47 (19)
C8—C7—P1	115.78 (14)	C10′—C9′—C19′	120.07 (19)
C7—C8—H8	107.7	C19′—C9′—C8′	118.46 (18)
C7—C8—C9	110.85 (16)	C9′—C10′—C12′	127.0 (2)
C7—C8—C13	110.87 (18)	C9′—C10′—N1′	119.47 (19)
C9—C8—H8	107.7	N1′—C10′—C12′	113.5 (2)
C9—C8—C13	111.82 (18)	C6′—C11′—H11A	109.5
C13—C8—H8	107.7	C6′—C11′—H11B	109.5
C10—C9—C8	121.29 (19)	C6′—C11′—H11C	109.5
C10—C9—C19	121.26 (19)	H11A—C11′—H11B	109.5
C19—C9—C8	117.45 (18)	H11A—C11′—H11C	109.5
C9—C10—C12	126.2 (2)	H11B—C11′—H11C	109.5
C9—C10—N1	119.97 (19)	C10′—C12′—H12A	109.5
N1—C10—C12	113.85 (19)	C10′—C12′—H12B	109.5
C6—C11—H11D	109.5	C10′—C12′—H12C	109.5
C6—C11—H11E	109.5	H12A—C12′—H12B	109.5
C6—C11—H11F	109.5	H12A—C12′—H12C	109.5
H11D—C11—H11E	109.5	H12B—C12′—H12C	109.5
H11D—C11—H11F	109.5	C14′—C13′—C8′	120.6 (3)

H11E—C11—H11F	109.5	C18′—C13′—C8′	120.6 (2)
C10—C12—H12D	109.5	C18′—C13′—C14′	118.8 (3)
C10—C12—H12E	109.5	C13′—C14′—H14′	120.1
C10—C12—H12F	109.5	C13′—C14′—C15′	119.7 (4)
H12D—C12—H12E	109.5	C15′—C14′—H14′	120.1
H12D—C12—H12F	109.5	C14′—C15′—H15′	119.1
H12E—C12—H12F	109.5	C16′—C15′—C14′	121.8 (3)
C14—C13—C8	120.8 (2)	C16′—C15′—H15′	119.1
C14—C13—C18	119.4 (3)	C15′—C16′—H16′	121.3
C18—C13—C8	119.7 (3)	C15′—C16′—C17′	117.3 (3)
C13—C14—H14	120.3	C17′—C16′—H16′	121.3
C13—C14—C15	119.5 (3)	C16′—C17′—N2′	118.9 (3)
C15—C14—H14	120.3	C18′—C17′—C16′	123.1 (4)
C14—C15—N2	119.5 (3)	C18′—C17′—N2′	118.0 (4)
C16—C15—C14	121.8 (4)	C13′—C18′—H18′	120.4
C16—C15—N2	118.7 (3)	C17′—C18′—C13′	119.3 (3)
C15—C16—H16	120.6	C17′—C18′—H18′	120.4
C17—C16—C15	118.8 (3)	O6′—C19′—C9′	126.9 (2)
C17—C16—H16	120.6	O6′—C19′—O7′	121.3 (2)
C16—C17—H17	119.7	O7′—C19′—C9′	111.78 (18)
C16—C17—C18	120.7 (3)	H20A—C20′—H20B	107.9
C18—C17—H17	119.7	C21′—C20′—H20A	109.2
C13—C18—H18	120.1	C21′—C20′—H20B	109.2
C17—C18—C13	119.8 (4)	O7′—C20′—H20A	109.2
C17—C18—H18	120.1	O7′—C20′—H20B	109.2
O6—C19—C9	127.8 (2)	O7′—C20′—C21′	112.2 (2)
O6—C19—O7	120.7 (2)	C20′—C21′—H21A	108.6
O7—C19—C9	111.49 (18)	C20′—C21′—H21B	108.6
H20C—C20—H20D	108.4	H21A—C21′—H21B	107.6
C21—C20—H20C	110.1	N3′—C21′—C20′	114.7 (2)
C21—C20—H20D	110.1	N3′—C21′—H21A	108.6
O7—C20—H20C	110.1	N3′—C21′—H21B	108.6
O7—C20—H20D	110.1	C27′—C22′—C23′	116.4 (3)
O7—C20—C21	108.2 (2)	N3′—C22′—C23′	121.2 (3)
C20—C21—H21C	109.1	N3′—C22′—C27′	122.4 (3)
C20—C21—H21D	109.1	C22′—C23′—H23′	119.4
H21C—C21—H21D	107.9	C24′—C23′—C22′	121.1 (3)
N3—C21—C20	112.4 (2)	C24′—C23′—H23′	119.4
N3—C21—H21C	109.1	C23′—C24′—H24′	119.3
N3—C21—H21D	109.1	C25′—C24′—C23′	121.4 (4)
C27—C22—C23	117.4 (3)	C25′—C24′—H24′	119.3
C27—C22—N3	122.1 (3)	C24′—C25′—H25′	120.7
N3—C22—C23	120.5 (2)	C24′—C25′—C26′	118.6 (4)
C22—C23—H23	119.6	C26′—C25′—H25′	120.7
C24—C23—C22	120.9 (3)	C25′—C26′—H26′	118.9
C24—C23—H23	119.6	C25′—C26′—C27′	122.2 (4)
C23—C24—H24	119.3	C27′—C26′—H26′	118.9
C25—C24—C23	121.4 (4)	C22′—C27′—H27′	119.9

C25—C24—H24	119.3	C26′—C27′—C22′	120.2 (4)
C24—C25—H25	120.7	C26′—C27′—H27′	119.9
C26—C25—C24	118.6 (4)	H28A—C28′—H28B	107.7
C26—C25—H25	120.7	C29′—C28′—H28A	108.8
C25—C26—H26	118.9	C29′—C28′—H28B	108.8
C25—C26—C27	122.2 (4)	N3′—C28′—H28A	108.8
C27—C26—H26	118.9	N3′—C28′—H28B	108.8
C22—C27—C26	119.6 (4)	N3′—C28′—C29′	113.7 (3)
C22—C27—H27	120.2	C30′—C29′—C28′	121.6 (3)
C26—C27—H27	120.2	C30′—C29′—C34′	117.9 (4)
H28C—C28—H28D	107.9	C34′—C29′—C28′	120.1 (3)
C29—C28—H28C	109.1	C29′—C30′—H30′	118.5
C29—C28—H28D	109.1	C31′—C30′—C29′	122.9 (4)
N3—C28—H28C	109.1	C31′—C30′—H30′	118.5
N3—C28—H28D	109.1	C30′—C31′—H31′	121.0
N3—C28—C29	112.4 (2)	C30′—C31′—C32′	118.0 (5)
C30—C29—C28	120.8 (3)	C32′—C31′—H31′	121.0
C34—C29—C28	120.4 (3)	C31′—C32′—H32′	119.0
C34—C29—C30	118.8 (3)	C31′—C32′—C33′	122.0 (5)
C29—C30—H30	119.7	C33′—C32′—H32′	119.0
C31—C30—C29	120.6 (4)	C32′—C33′—H33′	121.5
C31—C30—H30	119.7	C34′—C33′—C32′	117.0 (6)
C30—C31—H31	119.9	C34′—C33′—H33′	121.5
C30—C31—C32	120.2 (5)	C29′—C34′—H34′	119.1
C32—C31—H31	119.9	C33′—C34′—C29′	121.9 (6)
C31—C32—H32	120.2	C33′—C34′—H34′	119.1
C31—C32—C33	119.6 (4)	C6′—N1′—H1′	118.8
C33—C32—H32	120.2	C10′—N1′—C6′	122.39 (18)
C32—C33—H33	119.4	C10′—N1′—H1′	118.8
C32—C33—C34	121.2 (5)	O4′—N2′—C17′	119.3 (3)
C34—C33—H33	119.4	O5′—N2′—C17′	116.8 (6)
C29—C34—C33	119.6 (4)	O5′—N2′—O4′	123.4 (6)
C29—C34—H34	120.2	C21′—N3′—C28′	115.5 (2)
C33—C34—H34	120.2	C22′—N3′—C21′	120.8 (2)
C6—N1—H1	118.4	C22′—N3′—C28′	123.6 (2)
C10—N1—C6	123.14 (18)	C1′—O1′—P1′	118.92 (14)
C10—N1—H1	118.4	C3′—O2′—P1′	117.97 (14)
O4—N2—C15	117.7 (5)	C19′—O7′—C20′	115.43 (18)
O5—N2—C15	118.3 (3)	O1′—P1′—C7′	106.47 (9)
O5—N2—O4	124.0 (5)	O2′—P1′—C7′	109.21 (9)
C21—N3—C28	115.6 (2)	O2′—P1′—O1′	104.98 (9)
C22—N3—C21	117.7 (2)	O3′—P1′—C7′	114.43 (10)
C22—N3—C28	117.5 (2)	O3′—P1′—O1′	111.05 (9)
C1—O1—P1	118.88 (14)	O3′—P1′—O2′	110.22 (10)
C3—O2—P1	118.32 (16)	C36—C35—C37	117.4 (6)
C19—O7—C20	118.22 (19)	O8—C35—C36	120.7 (6)
O1—P1—C7	105.67 (9)	O8—C35—C37	121.8 (7)
O2—P1—C7	109.22 (9)	C35—C36—H36A	109.5

O2—P1—O1	104.83 (9)	C35—C36—H36B	109.5
O3—P1—C7	115.41 (10)	C35—C36—H36C	109.5
O3—P1—O1	110.54 (9)	H36A—C36—H36B	109.5
O3—P1—O2	110.54 (10)	H36A—C36—H36C	109.5
H1′A—C1′—H1′B	107.9	H36B—C36—H36C	109.5
C2′—C1′—H1′A	109.1	C35—C37—H37A	109.5
C2′—C1′—H1′B	109.1	C35—C37—H37B	109.5
O1′—C1′—H1′A	109.1	C35—C37—H37C	109.5
O1′—C1′—H1′B	109.1	H37A—C37—H37B	109.5
O1′—C1′—C2′	112.3 (2)	H37A—C37—H37C	109.5
C1′—C2′—C3′	108.2 (2)	H37B—C37—H37C	109.5
C1′—C2′—C4′	110.3 (2)		

C1—C2—C3—O2	60.3 (3)	C1′—C2′—C3′—O2′	−59.7 (3)
C1—O1—P1—C7	74.60 (17)	C1′—O1′—P1′—C7′	−74.34 (18)
C1—O1—P1—O2	−40.74 (17)	C1′—O1′—P1′—O2′	41.40 (17)
C1—O1—P1—O3	−159.87 (16)	C1′—O1′—P1′—O3′	160.50 (16)
C2—C1—O1—P1	52.4 (2)	C2′—C1′—O1′—P1′	−51.6 (2)
C2—C3—O2—P1	−56.5 (3)	C2′—C3′—O2′—P1′	57.3 (2)
C3—O2—P1—C7	−69.90 (19)	C3′—O2′—P1′—C7′	69.47 (18)
C3—O2—P1—O1	42.94 (19)	C3′—O2′—P1′—O1′	−44.36 (17)
C3—O2—P1—O3	162.08 (17)	C3′—O2′—P1′—O3′	−164.02 (16)
C4—C2—C3—O2	177.1 (2)	C4′—C2′—C3′—O2′	61.6 (3)
C5—C2—C3—O2	−61.7 (3)	C5′—C2′—C3′—O2′	−176.8 (2)
C6—C7—C8—C9	16.7 (3)	C6′—C7′—C8′—C9′	−22.6 (3)
C6—C7—C8—C13	−108.1 (2)	C6′—C7′—C8′—C13′	101.7 (2)
C6—C7—P1—O1	−155.43 (19)	C6′—C7′—P1′—O1′	156.74 (18)
C6—C7—P1—O2	−43.1 (2)	C6′—C7′—P1′—O2′	43.9 (2)
C6—C7—P1—O3	82.1 (2)	C6′—C7′—P1′—O3′	−80.2 (2)
C7—C6—N1—C10	−10.3 (3)	C7′—C6′—N1′—C10′	13.6 (3)
C7—C8—C9—C10	−17.3 (3)	C7′—C8′—C9′—C10′	22.3 (3)
C7—C8—C9—C19	162.58 (19)	C7′—C8′—C9′—C19′	−158.11 (18)
C7—C8—C13—C14	65.5 (3)	C7′—C8′—C13′—C14′	104.8 (3)
C7—C8—C13—C18	−113.0 (2)	C7′—C8′—C13′—C18′	−75.2 (3)
C8—C7—P1—O1	31.62 (18)	C8′—C7′—P1′—O1′	−30.39 (18)
C8—C7—P1—O2	143.92 (16)	C8′—C7′—P1′—O2′	−143.25 (16)
C8—C7—P1—O3	−90.85 (18)	C8′—C7′—P1′—O3′	92.68 (18)
C8—C9—C10—C12	−176.4 (2)	C8′—C9′—C10′—C12′	175.5 (2)
C8—C9—C10—N1	5.4 (3)	C8′—C9′—C10′—N1′	−5.8 (3)
C8—C9—C19—O6	171.9 (2)	C8′—C9′—C19′—O6′	177.1 (2)
C8—C9—C19—O7	−9.2 (3)	C8′—C9′—C19′—O7′	−2.9 (3)
C8—C13—C14—C15	−178.2 (2)	C8′—C13′—C14′—C15′	179.8 (3)
C8—C13—C18—C17	177.5 (3)	C8′—C13′—C18′—C17′	179.9 (3)
C9—C8—C13—C14	−58.8 (3)	C9′—C8′—C13′—C14′	−132.1 (3)
C9—C8—C13—C18	122.7 (2)	C9′—C8′—C13′—C18′	47.9 (3)
C9—C10—N1—C6	9.6 (3)	C9′—C10′—N1′—C6′	−13.9 (3)
C9—C19—O7—C20	174.9 (2)	C9′—C19′—O7′—C20′	178.61 (18)
C10—C9—C19—O6	−8.2 (4)	C10′—C9′—C19′—O6′	−3.4 (4)

C10—C9—C19—O7	170.7 (2)	C10′—C9′—C19′—O7′	176.62 (19)
C11—C6—C7—C8	178.1 (2)	C11′—C6′—C7′—C8′	−175.2 (2)
C11—C6—C7—P1	5.5 (4)	C11′—C6′—C7′—P1′	−2.6 (4)
C11—C6—N1—C10	167.7 (2)	C11′—C6′—N1′—C10′	−165.0 (2)
C12—C10—N1—C6	−168.7 (2)	C12′—C10′—N1′—C6′	165.0 (2)
C13—C8—C9—C10	107.0 (2)	C13′—C8′—C9′—C10′	−101.1 (2)
C13—C8—C9—C19	−73.1 (2)	C13′—C8′—C9′—C19′	78.4 (2)
C13—C14—C15—C16	0.5 (5)	C13′—C14′—C15′—C16′	0.3 (6)
C13—C14—C15—N2	179.7 (3)	C14′—C13′—C18′—C17′	−0.1 (4)
C14—C13—C18—C17	−1.0 (4)	C14′—C15′—C16′—C17′	0.0 (6)
C14—C15—C16—C17	−0.5 (6)	C15′—C16′—C17′—C18′	−0.4 (6)
C14—C15—N2—O4	−176.3 (5)	C15′—C16′—C17′—N2′	−178.4 (4)
C14—C15—N2—O5	5.1 (7)	C16′—C17′—C18′—C13′	0.5 (5)
C15—C16—C17—C18	−0.2 (6)	C16′—C17′—N2′—O4′	162.5 (6)
C16—C15—N2—O4	2.9 (7)	C16′—C17′—N2′—O5′	−9.5 (8)
C16—C15—N2—O5	−175.7 (5)	C18′—C13′—C14′—C15′	−0.2 (5)
C16—C17—C18—C13	1.0 (6)	C18′—C17′—N2′—O4′	−15.6 (8)
C18—C13—C14—C15	0.3 (4)	C18′—C17′—N2′—O5′	172.4 (6)
C19—C9—C10—C12	3.7 (4)	C19′—C9′—C10′—C12′	−4.0 (3)
C19—C9—C10—N1	−174.4 (2)	C19′—C9′—C10′—N1′	174.68 (19)
C20—C21—N3—C22	−74.5 (3)	C20′—C21′—N3′—C22′	85.9 (3)
C20—C21—N3—C28	71.7 (3)	C20′—C21′—N3′—C28′	−98.0 (3)
C21—C20—O7—C19	−100.7 (2)	C21′—C20′—O7′—C19′	78.5 (3)
C22—C23—C24—C25	0.8 (4)	C22′—C23′—C24′—C25′	1.0 (5)
C23—C22—C27—C26	−0.4 (4)	C23′—C22′—C27′—C26′	−0.4 (5)
C23—C22—N3—C21	−33.9 (3)	C23′—C22′—N3′—C21′	−2.9 (4)
C23—C22—N3—C28	−179.4 (2)	C23′—C22′—N3′—C28′	−178.7 (3)
C23—C24—C25—C26	−0.2 (5)	C23′—C24′—C25′—C26′	0.4 (5)
C24—C25—C26—C27	−0.6 (6)	C24′—C25′—C26′—C27′	−1.9 (6)
C25—C26—C27—C22	1.0 (5)	C25′—C26′—C27′—C22′	1.9 (6)
C27—C22—C23—C24	−0.4 (4)	C27′—C22′—C23′—C24′	−1.0 (4)
C27—C22—N3—C21	148.7 (2)	C27′—C22′—N3′—C21′	176.8 (3)
C27—C22—N3—C28	3.2 (3)	C27′—C22′—N3′—C28′	1.0 (4)
C28—C29—C30—C31	−177.3 (3)	C28′—C29′—C30′—C31′	−179.9 (4)
C28—C29—C34—C33	178.2 (3)	C28′—C29′—C34′—C33′	−177.5 (6)
C29—C28—N3—C21	40.6 (3)	C29′—C28′—N3′—C21′	−74.0 (3)
C29—C28—N3—C22	−173.1 (2)	C29′—C28′—N3′—C22′	102.0 (3)
C29—C30—C31—C32	−1.1 (6)	C29′—C30′—C31′—C32′	−5.8 (7)
C30—C29—C34—C33	−1.0 (5)	C30′—C29′—C34′—C33′	−4.9 (8)
C30—C31—C32—C33	−0.5 (7)	C30′—C31′—C32′—C33′	1.0 (9)
C31—C32—C33—C34	1.5 (7)	C31′—C32′—C33′—C34′	1.5 (11)
C32—C33—C34—C29	−0.7 (7)	C32′—C33′—C34′—C29′	0.5 (11)
C34—C29—C30—C31	1.9 (5)	C34′—C29′—C30′—C31′	7.6 (6)
N1—C6—C7—C8	−4.2 (3)	N1′—C6′—C7′—C8′	6.4 (3)
N1—C6—C7—P1	−176.74 (17)	N1′—C6′—C7′—P1′	179.00 (17)
N2—C15—C16—C17	−179.7 (4)	N2′—C17′—C18′—C13′	178.5 (4)
N3—C22—C23—C24	−178.0 (2)	N3′—C22′—C23′—C24′	178.7 (3)
N3—C22—C27—C26	177.1 (3)	N3′—C22′—C27′—C26′	179.9 (3)

N3—C28—C29—C30	65.9 (3)	N3′—C28′—C29′—C30′	−59.1 (4)
N3—C28—C29—C34	−113.2 (3)	N3′—C28′—C29′—C34′	113.3 (4)
O1—C1—C2—C3	−58.2 (3)	O1′—C1′—C2′—C3′	57.0 (3)
O1—C1—C2—C4	−175.2 (2)	O1′—C1′—C2′—C4′	−64.8 (3)
O1—C1—C2—C5	63.1 (3)	O1′—C1′—C2′—C5′	173.9 (2)
O6—C19—O7—C20	−6.1 (3)	O6′—C19′—O7′—C20′	−1.4 (3)
O7—C20—C21—N3	−170.3 (2)	O7′—C20′—C21′—N3′	65.8 (3)
P1—C7—C8—C9	−170.31 (15)	P1′—C7′—C8′—C9′	164.54 (15)
P1—C7—C8—C13	64.9 (2)	P1′—C7′—C8′—C13′	−71.2 (2)

Hydrogen-bond geometry (Å, º)

Cg4 and Cg9 are the centroids of the C22′–C27′ and C22–C27 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3′	0.86	2.04	2.847 (2)	155
N1′—H1′···O3^{i}	0.86	2.20	2.917 (2)	141
C1—H1*A*···O6^{ii}	0.97	2.54	3.456 (4)	157
C1′—H1′*B*···O6′^{iii}	0.97	2.42	3.346 (4)	160
C15′—H15′···O5	0.93	2.55	3.470 (7)	173
C37—H37*C*···*Cg*4^{iv}	0.96	2.88	3.667 (9)	139
C3′—H3′*B*···*Cg*9^{v}	0.97	2.66	3.599 (3)	163

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+1, −*y*+2, −*z*; (iii) −*x*+2, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*+1; (v) *x*+1, *y*−1, *z*.