Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diisopropyl {[(*R*)-2-(2-amino-6-chloro-9*H*-purin-9-yl)-1-methylethoxy]methyl}-phosphonate

Guobao Zhao, Xinhua He* and Bohua Zhong

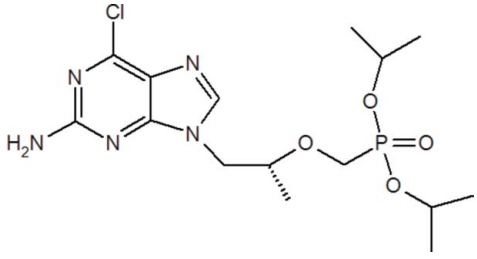
Beijing Institute of Pharmacology and Toxicology, Beijing 100850, People's Republic of China
Correspondence e-mail: hexinhua01@126.com

Received 26 January 2012; accepted 15 February 2012Superposition of the molecular conformations of the title compound (red) and its F-substituent (blue, Baszczyński *et al.*, 2011).single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.028; wR factor = 0.066; data-to-parameter ratio = 19.5.

In the title compound, $C_{15}H_{25}ClN_5O_4P$, the r.m.s. deviation for the purine ring system is 0.0165 Å. The coordination about the P atom is a distorted tetrahedron [O=P—O angles = 116.70 (6) and 109.87 (6)°]. In the crystal, molecules are linked by N—H···O hydrogen bonds, generating a three-dimensional network.

Related literature

For details of the synthesis, see: Yu *et al.* (1992). For the bioactivity of nucleoside analogues, see: Martin (1989). For reference bond lengths, see: Allen *et al.* (1987). For a related structure, see: Baszczyński *et al.* (2011).



Experimental

Crystal data

$C_{15}H_{25}ClN_5O_4P$
M_r = 405.82
Orthorhombic, $P2_12_12_1$
a = 7.7991 (12) Å
b = 13.950 (2) Å
c = 18.053 (3) Å
V = 1964.0 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 113 K
0.22 × 0.20 × 0.18 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.936, T_{max} = 0.947
24716 measured reflections
4669 independent reflections
4468 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.066
S = 1.05
4669 reflections
240 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Absolute structure: Flack (1983), 2007 Friedel pairs
Flack parameter: 0.02 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5A···O2^{i}	0.89	2.13	3.0185 (16)	174
N5—H5B···O2^{ii}	0.89	2.21	3.0920 (16)	172

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2005).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FK2051).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Baszczyński, O., Jansa, P., Dračínsky, M., Klepetářová, B., Holya, A., Votruba, I., de Clercq, E., Balzarini, J. & Janeba, Z. (2011). *Bioorg. Med. Chem.* **19**, 2114–2124.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Martin, J. C. (1989). Editor. *Nucleotide Analogs as Antiviral Agents*. Washington, DC: American Chemical Society.
Rigaku (2005). *CrystalClear* and *CrystalStructure*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yu, K.-L., Bronson, J. J., Yang, H., Patick, A., Alam, M., Brankovan, V., Datema, R., Hitchcock, M. J. M. & Martin, J. C. (1992). *J. Med. Chem.* **35**, 2958–2969.

supplementary materials

Acta Cryst. (2012). E**68**, o936 [doi:10.1107/S1600536812006757]

Diisopropyl {[(*R*)-2-(2-amino-6-chloro-9*H*-purin-9-yl)-1-methylethoxy]methyl}-phosphonate

Guobao Zhao, Xinhua He and Bohua Zhong

Comment

Nucleoside analogues are in the lead in research and application of the anti-HBV drugs. In our recent work, the title compound (I), Fig. 1, was synthetized according to Kuo-Long Yu *et al.* (1992). As known, the molecular conformation in single-crystal is low energy conformation, and is helpful to quantitative structure-activity relationship (QSAR) study, therefore this structure determination was undertaken. Though the molecular structure of OSOWUP (Baszczyński *et al.*, 2011) is similar to the title molecule, the molecular conformation is different (comparison is shown in Fig 3).

In (I), all bonds lengths and angles are normal (Allen *et al.*, 1987). Molecules are stacked along the *a* axis, and linked into a zigzag sheet propagating along the *c* axis by intermolecular N—H···O hydrogen bonds (Figure 2 and Table 2).

Experimental

The title compound was synthesized according to the procedure of Kuo-Long Yu *et al.* (1992). Colourless single crystals (m.p. 404–406 K) were obtained by slow evaporation of a solution in absolute ethanol.

Refinement

The H atoms linked to the C atoms were fixed geometrically and treated as riding with C—H = 0.95 Å (aromatic), 0.98Å (ethyl), 0.99 Å (methylene) with U_{iso}(H) =1.2–1.5Ueq(C). H atoms of the amino group were located in a difference Fourier map and also refined riding with N-H = 0.89 Å.

Computing details

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear* (Rigaku, 2005); data reduction: *CrystalClear* (Rigaku, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2005).

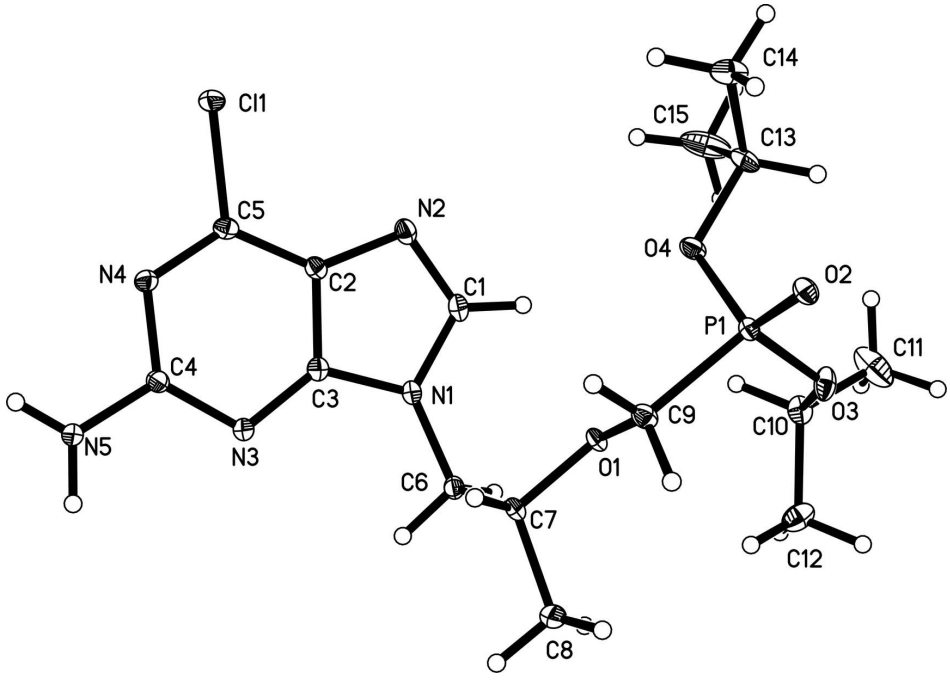


Figure 1

Molecular structure with displacement ellipsoids drawn at the 30% probability level and H atoms shown as small spheres of arbitrary radii.

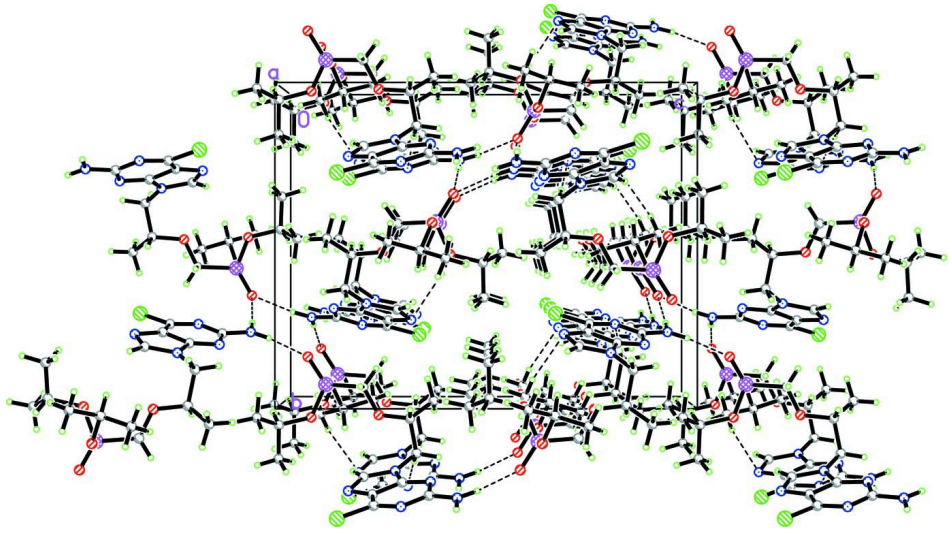


Figure 2

The crystal packing of (I) with hydrogen bonds drawn as dashed lines.

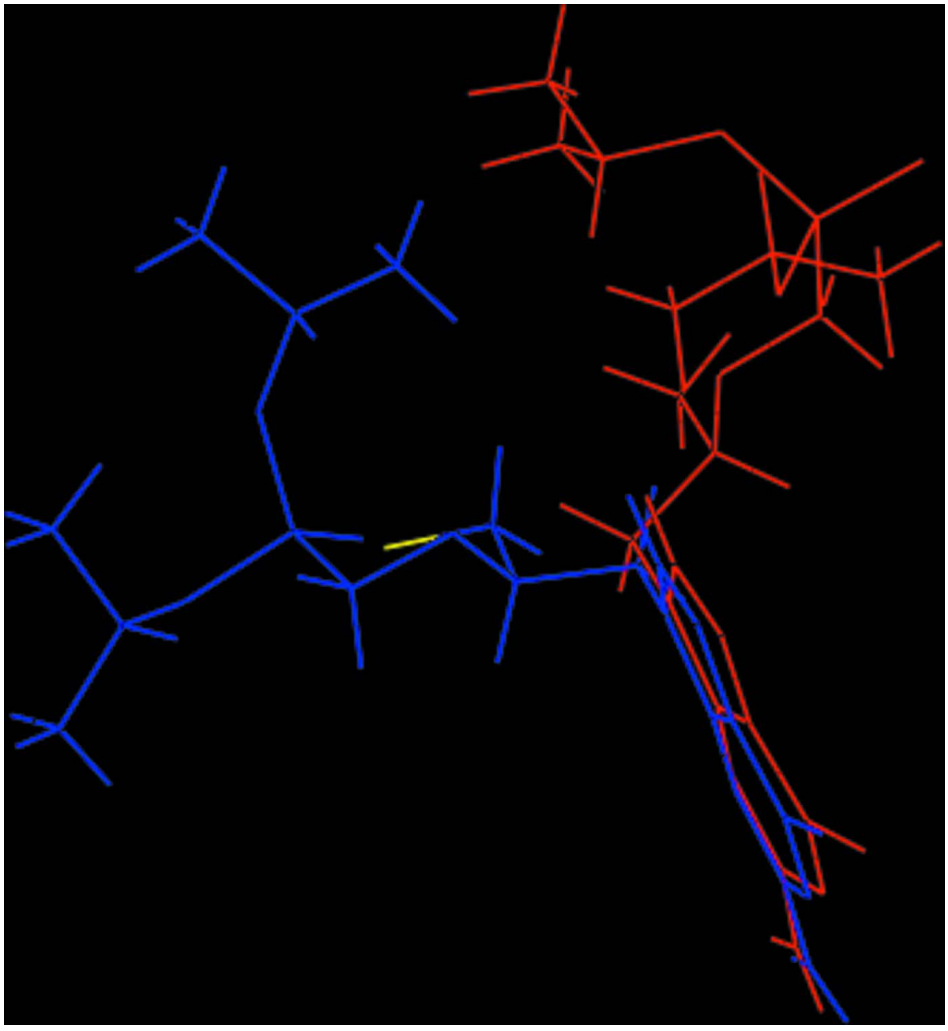


Figure 3

Superposition of the molecular conformations of the title compound (red) and its F-substituent (blue, Baszczyński *et al.*, 2011).

Diisopropyl {[(*R*)-2-(2-Amino-6-chloro-9*H*-purin-9-yl)- 1-methylethoxy]methyl}phosphonate

Crystal data

$C_{15}H_{25}ClN_5O_4P$
M_r = 405.82
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
a = 7.7991 (12) Å
b = 13.950 (2) Å
c = 18.053 (3) Å
V = 1964.0 (6) Å^3
Z = 4
F(000) = 856
D_x = 1.372 Mg m^{-3}
Melting point: 404 K
Mo $K\alpha$ radiation, λ = 0.71070 Å
Cell parameters from 7255 reflections
θ = 1.8–27.9°
μ = 0.31 mm^{-1}
T = 113 K
Block, colourless
0.22 × 0.20 × 0.18 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Radiation source: rotating anode
Confocal monochromator
Detector resolution: 7.31 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.936, T_{max} = 0.947
24716 measured reflections
4669 independent reflections
4468 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 27.9°, θ_{min} = 1.8°
h = −10→10
k = −18→18
l = −21→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.066
S = 1.05
4669 reflections
240 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0412P)^2 + 0.0557P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Absolute structure: Flack (1983), 2007 Friedel pairs
Flack parameter: 0.02 (4)

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.70932 (5)	0.28859 (3)	0.167353 (19)	0.02209 (9)
P1	−0.06920 (4)	−0.07232 (3)	0.118252 (19)	0.01452 (8)
O1	−0.02385 (12)	0.01978 (7)	0.24534 (5)	0.0159 (2)
O2	−0.01664 (13)	−0.15893 (7)	0.07748 (5)	0.0181 (2)
O3	−0.27016 (12)	−0.06894 (7)	0.12487 (6)	0.0235 (2)
O4	−0.00844 (13)	0.02658 (7)	0.08574 (5)	0.0196 (2)
N1	0.18098 (14)	0.18007 (8)	0.28806 (6)	0.0161 (2)
N2	0.30287 (16)	0.23315 (8)	0.18180 (6)	0.0194 (3)
N3	0.42068 (14)	0.19898 (8)	0.37275 (6)	0.0160 (2)
N4	0.67530 (15)	0.25616 (9)	0.30921 (6)	0.0175 (2)
N5	0.67325 (16)	0.23154 (9)	0.43524 (6)	0.0239 (3)
H5A	0.6250	0.2149	0.4780	0.029*
H5B	0.7770	0.2581	0.4341	0.029*
C1	0.16466 (18)	0.19896 (10)	0.21332 (8)	0.0192 (3)
H1	0.0612	0.1880	0.1868	0.023*

C2	0.41989 (18)	0.23658 (9)	0.23985 (7)	0.0162 (3)
C3	0.34601 (17)	0.20501 (9)	0.30642 (7)	0.0152 (3)
C4	0.58455 (17)	0.22921 (10)	0.37114 (7)	0.0168 (3)
C5	0.59151 (18)	0.25824 (9)	0.24618 (7)	0.0167 (3)
C6	0.05519 (17)	0.13378 (10)	0.33578 (8)	0.0175 (3)
H6A	−0.0582	0.1641	0.3282	0.021*
H6B	0.0882	0.1433	0.3882	0.021*
C7	0.04188 (18)	0.02758 (10)	0.31995 (7)	0.0176 (3)
H7	0.1582	−0.0023	0.3227	0.021*
C8	−0.0777 (2)	−0.02117 (12)	0.37504 (8)	0.0301 (4)
H8B	−0.1886	0.0119	0.3753	0.045*
H8C	−0.0270	−0.0185	0.4247	0.045*
H8A	−0.0944	−0.0882	0.3606	0.045*
C9	0.02123 (19)	−0.06768 (11)	0.20997 (7)	0.0187 (3)
H9B	−0.0218	−0.1224	0.2396	0.022*
H9A	0.1476	−0.0730	0.2069	0.022*
C10	−0.36850 (19)	0.01452 (11)	0.15103 (8)	0.0212 (3)
H10	−0.2899	0.0705	0.1578	0.025*
C11	−0.4980 (3)	0.03695 (17)	0.09230 (11)	0.0483 (6)
H11A	−0.4388	0.0548	0.0464	0.072*
H11C	−0.5704	0.0903	0.1087	0.072*
H11B	−0.5696	−0.0196	0.0833	0.072*
C12	−0.4493 (2)	−0.01170 (11)	0.22435 (9)	0.0287 (4)
H12B	−0.5299	−0.0648	0.2171	0.043*
H12C	−0.5107	0.0439	0.2443	0.043*
H12A	−0.3596	−0.0312	0.2593	0.043*
C13	−0.0413 (2)	0.05138 (11)	0.00761 (8)	0.0237 (3)
H13	−0.1452	0.0161	−0.0101	0.028*
C14	0.1104 (2)	0.02249 (12)	−0.03813 (9)	0.0306 (4)
H14C	0.2119	0.0579	−0.0215	0.046*
H14B	0.0881	0.0372	−0.0903	0.046*
H14A	0.1305	−0.0465	−0.0325	0.046*
C15	−0.0760 (3)	0.15761 (14)	0.00579 (10)	0.0476 (6)
H15C	−0.1792	0.1717	0.0348	0.071*
H15A	−0.0933	0.1782	−0.0456	0.071*
H15B	0.0220	0.1920	0.0270	0.071*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.02487 (18)	0.02488 (17)	0.01653 (16)	−0.00578 (14)	0.00178 (13)	0.00367 (14)
P1	0.01522 (16)	0.01520 (16)	0.01314 (16)	0.00033 (13)	−0.00102 (14)	−0.00204 (13)
O1	0.0198 (5)	0.0169 (5)	0.0112 (4)	0.0001 (4)	−0.0030 (4)	−0.0028 (4)
O2	0.0199 (5)	0.0185 (5)	0.0160 (5)	0.0024 (4)	−0.0008 (4)	−0.0038 (4)
O3	0.0156 (5)	0.0207 (5)	0.0341 (6)	0.0004 (4)	−0.0005 (4)	−0.0124 (5)
O4	0.0278 (5)	0.0184 (5)	0.0126 (5)	−0.0008 (4)	−0.0008 (4)	0.0019 (4)
N1	0.0153 (6)	0.0163 (5)	0.0165 (6)	−0.0005 (5)	−0.0027 (5)	−0.0019 (4)
N2	0.0219 (6)	0.0180 (6)	0.0183 (6)	−0.0012 (5)	−0.0055 (5)	0.0011 (4)
N3	0.0155 (5)	0.0169 (6)	0.0155 (6)	−0.0012 (5)	−0.0009 (5)	−0.0006 (4)
N4	0.0168 (6)	0.0190 (6)	0.0168 (5)	−0.0013 (5)	0.0003 (5)	0.0033 (5)

N5	0.0177 (6)	0.0374 (7)	0.0166 (6)	−0.0083 (5)	−0.0022 (5)	0.0061 (5)
C1	0.0197 (7)	0.0174 (7)	0.0204 (7)	−0.0005 (6)	−0.0063 (6)	−0.0020 (5)
C2	0.0197 (7)	0.0139 (6)	0.0151 (6)	0.0001 (5)	−0.0020 (6)	0.0003 (5)
C3	0.0166 (6)	0.0110 (6)	0.0182 (6)	0.0009 (5)	−0.0011 (5)	−0.0012 (5)
C4	0.0171 (7)	0.0185 (7)	0.0148 (6)	0.0006 (5)	−0.0002 (6)	0.0004 (5)
C5	0.0218 (7)	0.0120 (6)	0.0162 (6)	0.0002 (5)	0.0013 (6)	0.0021 (5)
C6	0.0141 (6)	0.0228 (7)	0.0157 (6)	−0.0016 (5)	0.0003 (6)	−0.0043 (5)
C7	0.0186 (7)	0.0226 (7)	0.0116 (6)	−0.0020 (6)	−0.0030 (5)	−0.0016 (5)
C8	0.0366 (9)	0.0367 (9)	0.0168 (7)	−0.0163 (8)	0.0018 (7)	−0.0008 (7)
C9	0.0255 (7)	0.0153 (7)	0.0154 (7)	0.0006 (6)	−0.0012 (5)	0.0000 (6)
C10	0.0180 (7)	0.0207 (7)	0.0250 (8)	0.0058 (6)	0.0001 (6)	−0.0067 (6)
C11	0.0364 (10)	0.0772 (16)	0.0314 (10)	0.0307 (10)	−0.0098 (8)	−0.0162 (10)
C12	0.0283 (8)	0.0192 (8)	0.0385 (9)	0.0006 (6)	0.0108 (7)	0.0004 (7)
C13	0.0300 (8)	0.0298 (8)	0.0114 (7)	0.0036 (6)	−0.0026 (6)	0.0024 (6)
C14	0.0405 (10)	0.0264 (8)	0.0250 (8)	0.0026 (7)	0.0116 (7)	0.0028 (7)
C15	0.0765 (15)	0.0412 (11)	0.0250 (9)	0.0284 (11)	0.0135 (10)	0.0143 (8)

Geometric parameters (Å, º)

Cl1—C5	1.7460 (14)	C6—H6B	0.9900
P1—O2	1.4729 (10)	C7—C8	1.523 (2)
P1—O4	1.5724 (11)	C7—H7	1.0000
P1—O3	1.5726 (10)	C8—H8B	0.9800
P1—C9	1.8009 (14)	C8—H8C	0.9800
O1—C9	1.4213 (17)	C8—H8A	0.9800
O1—C7	1.4453 (16)	C9—H9B	0.9900
O3—C10	1.4720 (16)	C9—H9A	0.9900
O4—C13	1.4748 (17)	C10—C11	1.498 (2)
N1—C3	1.3738 (17)	C10—C12	1.511 (2)
N1—C1	1.3806 (18)	C10—H10	1.0000
N1—C6	1.4566 (18)	C11—H11A	0.9800
N2—C1	1.3088 (19)	C11—H11C	0.9800
N2—C2	1.3904 (17)	C11—H11B	0.9800
N3—C3	1.3341 (17)	C12—H12B	0.9800
N3—C4	1.3462 (17)	C12—H12C	0.9800
N4—C5	1.3124 (17)	C12—H12A	0.9800
N4—C4	1.3756 (17)	C13—C14	1.498 (2)
N5—C4	1.3486 (17)	C13—C15	1.507 (2)
N5—H5A	0.8900	C13—H13	1.0000
N5—H5B	0.8901	C14—H14C	0.9800
C1—H1	0.9500	C14—H14B	0.9800
C2—C5	1.377 (2)	C14—H14A	0.9800
C2—C3	1.4038 (19)	C15—H15C	0.9800
C6—C7	1.5123 (19)	C15—H15A	0.9800
C6—H6A	0.9900	C15—H15B	0.9800
O2—P1—O4	116.70 (6)	H8B—C8—H8C	109.5
O2—P1—O3	109.87 (6)	C7—C8—H8A	109.5
O4—P1—O3	107.60 (6)	H8B—C8—H8A	109.5
O2—P1—C9	112.33 (6)	H8C—C8—H8A	109.5

O4—P1—C9	101.17 (6)	O1—C9—P1	110.30 (9)
O3—P1—C9	108.63 (6)	O1—C9—H9B	109.6
C9—O1—C7	113.30 (10)	P1—C9—H9B	109.6
C10—O3—P1	124.57 (9)	O1—C9—H9A	109.6
C13—O4—P1	120.69 (9)	P1—C9—H9A	109.6
C3—N1—C1	105.90 (11)	H9B—C9—H9A	108.1
C3—N1—C6	126.91 (12)	O3—C10—C11	106.83 (12)
C1—N1—C6	126.91 (11)	O3—C10—C12	107.87 (12)
C1—N2—C2	103.04 (11)	C11—C10—C12	112.93 (15)
C3—N3—C4	112.04 (11)	O3—C10—H10	109.7
C5—N4—C4	117.03 (12)	C11—C10—H10	109.7
C4—N5—H5A	121.4	C12—C10—H10	109.7
C4—N5—H5B	117.2	C10—C11—H11A	109.5
H5A—N5—H5B	120.9	C10—C11—H11C	109.5
N2—C1—N1	114.73 (12)	H11A—C11—H11C	109.5
N2—C1—H1	122.6	C10—C11—H11B	109.5
N1—C1—H1	122.6	H11A—C11—H11B	109.5
C5—C2—N2	135.10 (12)	H11C—C11—H11B	109.5
C5—C2—C3	113.37 (12)	C10—C12—H12B	109.5
N2—C2—C3	111.41 (12)	C10—C12—H12C	109.5
N3—C3—N1	127.56 (13)	H12B—C12—H12C	109.5
N3—C3—C2	127.52 (13)	C10—C12—H12A	109.5
N1—C3—C2	104.91 (12)	H12B—C12—H12A	109.5
N3—C4—N5	118.43 (12)	H12C—C12—H12A	109.5
N3—C4—N4	126.27 (12)	O4—C13—C14	109.06 (12)
N5—C4—N4	115.27 (12)	O4—C13—C15	106.42 (13)
N4—C5—C2	123.45 (12)	C14—C13—C15	113.22 (14)
N4—C5—Cl1	116.74 (10)	O4—C13—H13	109.4
C2—C5—Cl1	119.80 (10)	C14—C13—H13	109.4
N1—C6—C7	111.64 (11)	C15—C13—H13	109.4
N1—C6—H6A	109.3	C13—C14—H14C	109.5
C7—C6—H6A	109.3	C13—C14—H14B	109.5
N1—C6—H6B	109.3	H14C—C14—H14B	109.5
C7—C6—H6B	109.3	C13—C14—H14A	109.5
H6A—C6—H6B	108.0	H14C—C14—H14A	109.5
O1—C7—C6	105.91 (11)	H14B—C14—H14A	109.5
O1—C7—C8	110.96 (11)	C13—C15—H15C	109.5
C6—C7—C8	110.85 (12)	C13—C15—H15A	109.5
O1—C7—H7	109.7	H15C—C15—H15A	109.5
C6—C7—H7	109.7	C13—C15—H15B	109.5
C8—C7—H7	109.7	H15C—C15—H15B	109.5
C7—C8—H8B	109.5	H15A—C15—H15B	109.5
C7—C8—H8C	109.5		

O2—P1—O3—C10	−169.42 (10)	C5—N4—C4—N3	4.4 (2)
O4—P1—O3—C10	−41.40 (12)	C5—N4—C4—N5	−177.53 (13)
C9—P1—O3—C10	67.35 (12)	C4—N4—C5—C2	1.1 (2)
O2—P1—O4—C13	52.62 (12)	C4—N4—C5—Cl1	−177.90 (10)
O3—P1—O4—C13	−71.35 (11)	N2—C2—C5—N4	−179.99 (14)

C9—P1—O4—C13	174.81 (10)	C3—C2—C5—N4	−4.5 (2)
C2—N2—C1—N1	0.42 (16)	N2—C2—C5—Cl1	−1.0 (2)
C3—N1—C1—N2	0.27 (16)	C3—C2—C5—Cl1	174.40 (10)
C6—N1—C1—N2	−173.85 (13)	C3—N1—C6—C7	−100.58 (15)
C1—N2—C2—C5	174.56 (15)	C1—N1—C6—C7	72.34 (17)
C1—N2—C2—C3	−0.96 (15)	C9—O1—C7—C6	154.99 (11)
C4—N3—C3—N1	179.73 (13)	C9—O1—C7—C8	−84.65 (15)
C4—N3—C3—C2	1.00 (19)	N1—C6—C7—O1	−64.84 (14)
C1—N1—C3—N3	−179.77 (13)	N1—C6—C7—C8	174.73 (12)
C6—N1—C3—N3	−5.7 (2)	C7—O1—C9—P1	178.87 (9)
C1—N1—C3—C2	−0.82 (14)	O2—P1—C9—O1	176.25 (9)
C6—N1—C3—C2	173.30 (12)	O4—P1—C9—O1	51.07 (10)
C5—C2—C3—N3	3.5 (2)	O3—P1—C9—O1	−62.00 (11)
N2—C2—C3—N3	−179.91 (13)	P1—O3—C10—C11	125.75 (14)
C5—C2—C3—N1	−175.42 (11)	P1—O3—C10—C12	−112.57 (13)
N2—C2—C3—N1	1.13 (15)	P1—O4—C13—C14	−92.90 (14)
C3—N3—C4—N5	176.77 (12)	P1—O4—C13—C15	144.64 (13)
C3—N3—C4—N4	−5.24 (19)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5*A*···O2^{i}	0.89	2.13	3.0185 (16)	174
N5—H5*B*···O2^{ii}	0.89	2.21	3.0920 (16)	172

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