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Ammonium hydrogen (*RS*)-[(5-methyl-2-oxo-1,3-oxazolidin-3-yl)methyl]-phosphonate

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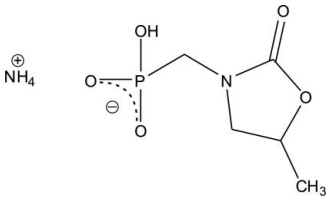
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(O–C) = 0.003 Å; disorder in main residue; R factor = 0.035; wR factor = 0.097; data-to-parameter ratio = 11.7.

In the title compound, $NH_4^+\cdot C_5H_9NO_5P^-$, the five-membered methyloxazolidin-2-one unit is disordered over two positions, the major component having a site occupancy of 0.832 (9). A three-dimensional network of O—H···O and N—H···O hydrogen bonds stabilizes the crystal structure.

Related literature

For general background of the use of phosphonic and aminophosphonic acids as chelating agents in metal extraction and as medicinal compounds, see: Metlushka *et al.* (2009); Naydenova *et al.* (2009); Matczak-Jon & Videnova-Adrabinska (2005). For related structures, see: Dudko *et al.* (2009); Shivachev *et al.* (2005); Todorov *et al.* (2006); Ying *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$NH_4^+\cdot C_5H_9NO_5P^-$
M_r = 212.14
Triclinic, $P\overline{1}$
a = 6.471 (3) Å
b = 8.801 (3) Å
c = 9.427 (4) Å
α = 70.76 (2)°
β = 70.658 (18)°
γ = 89.363 (16)°
V = 475.4 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 290 K
0.30 × 0.28 × 0.21 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
3673 measured reflections
1855 independent reflections
1606 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
3 standard reflections
frequency: 120 min
intensity decay: −1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.097
S = 1.05
1855 reflections
159 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H*N*1···O1	0.85	1.94	2.789 (2)	177
O2—H1*A*···O3^{i}	1.07	1.53	2.5770 (19)	166
N2—H*N*2···O1^{ii}	0.86	1.93	2.772 (2)	165
N2—H*N*3···O3^{iii}	0.89	1.93	2.793 (2)	161
N2—H*N*4···O4^{iv}	0.97	1.88	2.827 (2)	167

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2491).

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supporting information

Acta Cryst. (2010). E**66**, o6 [doi:10.1107/S1600536809050338]

Ammonium hydrogen (*RS*)-[(5-methyl-2-oxo-1,3-oxazolidin-3-yl)methyl]-phosphonate

Petar Todorov, Emilia Naydenova, Rositsa P. Nikolova and Boris L. Shivachev

S1. Comment

Phosphonic and aminophosphonic derivatives have a high potential for biological activity. These derivatives have been widely used in the manufacture of herbicides, as chelating agents in metal extraction and as medicinal compounds (Metlushka *et al.*, 2009; Naydenova *et al.*, 2009; Matczak-Jon & Videnova-Adrabinska, 2005). As part of our ongoing studies of the structure-activity relationships for phosphonic acid derivatives (Todorov *et al.*, 2006; Shivachev *et al.*, 2005) herein we report the structure of the titled compound.

The asymmetric unit of the title compound (Fig. 1) contains one molecule, with a proton transferred from the phosphonic group to the ammonia group. The ammonium cation attendant in structure neutralizes the negatively charged phosphonic acid residue. In the crystal structure, the methyloxazolidin-2-one moiety is disordered over two positions. In one of them (major occupancy) the oxazolidine ring (N1/C2/C3/O5/c4) is almost planar [r.m.s. of 0.017 (2) Å] while in the other one it adopts an envelope conformation, with atom C22 deviating within 0.367 (33) Å from the plane defined by the other four atoms [N1/C4/O25/C23 with r.m.s. 0.006 (5) Å]. Bond lengths and angles have normal values and compare well with related structures (Allen *et al.*, 1987; Dudko *et al.*, 2009; Ying *et al.*, 2007; Todorov *et al.*, 2006). The phosphorus atom displays a slightly distorted tetrahedral geometry provided by three oxygen atoms and one carbon atom.

The crystal structure of title compound shows three-dimensional network of O—H···O and N—H···O hydrogen bonds which additionally stabilize the structure (Table 1 and Fig. 2).

S2. Experimental

The title compound, $NH_4^+.C_5H_{10}N_2O_5P^-$, was obtained from the reaction of 5-methyloxazolidin-2-one with formaldehyde and phosphorus trichloride in glacial acetic acid. The solution was left at room temperature. Colorless crystals of the title compound were obtained after several days staying.

S3. Refinement

The hydroxy and ammonium H atoms were located in a difference map. H atoms bonded to C were placed in idealized positions (C—H = 0.97 Å for CH_3, C—H = 0.96 Å for CH_2 and C—H = 0.98 Å for CH). All H atoms were constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C, O) and U_{iso}(H) = 1.5U_{eq}(methyl C). The U_{iso}(H) values of N-bound H atoms were freely refined.

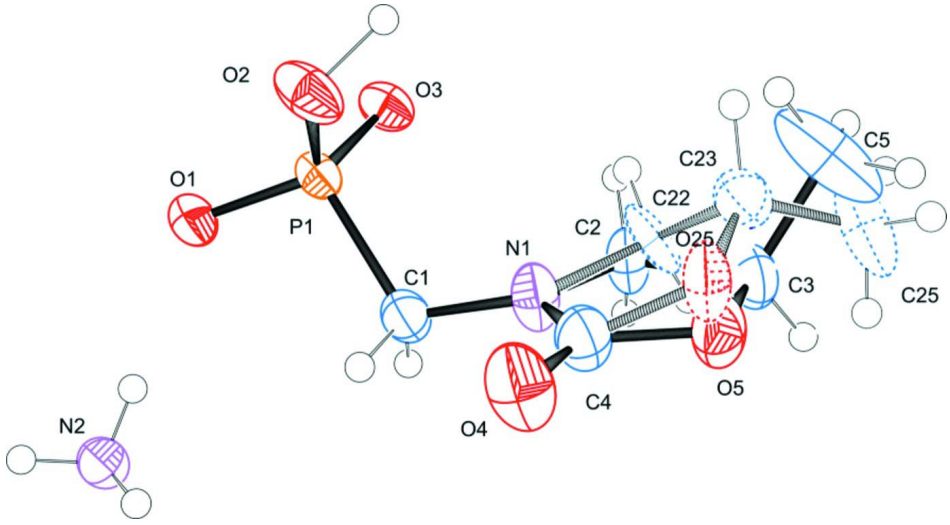

Figure 1

The asymmetric unit of title compound with the atom numbering scheme showing 50% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii. Minor occupancy disorder component is represented with dashed lines.

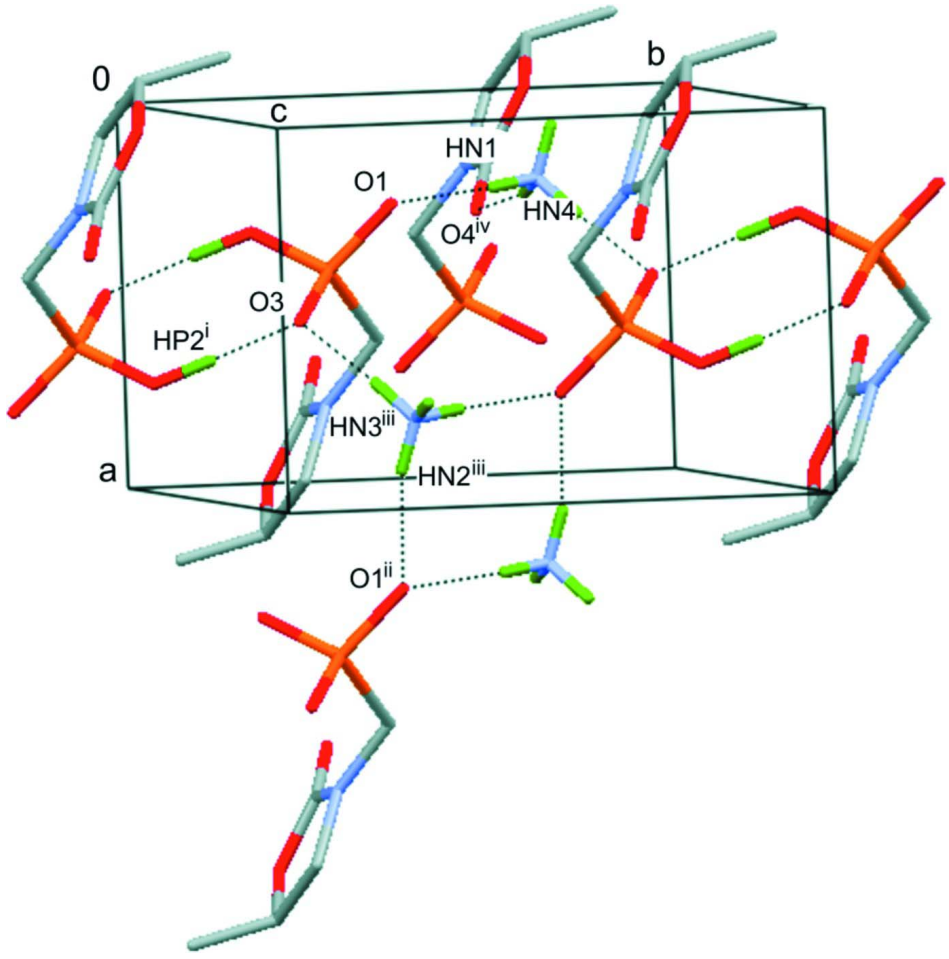

Figure 2

A view of the molecular packing in the title compound. All H atoms not involved in the short contact interactions have been omitted for clarity. [Symmetry codes: (i) -*x* + 1, -*y*, *z* + 1; (ii) 1 + *x*, -*y* + 1, -*z* + 1; (iii) -*x* + 1, -*y* + 1, -*z* + 1; (iv) -*x* + 1, -*y* + 1, -*z*.]

Ammonium hydrogen (*RS*)-[(5-methyl-2-oxo-1,3-oxazolidin-3-yl)methyl]phosphonate

Crystal data

$NH_4^+ \cdot C_5H_9NO_5P^-$
$M_r = 212.14$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.471\ (3)$ Å
$b = 8.801\ (3)$ Å
$c = 9.427\ (4)$ Å
$\alpha = 70.76\ (2)°$
$\beta = 70.658\ (18)°$
$\gamma = 89.363\ (16)°$
$V = 475.4\ (3)$ Å^3
$Z = 2$
$F(000) = 224$
$D_x = 1.482$ Mg m^{-3}
Melting point: not measured K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 22 reflections
$\theta = 18.2–19.9°$
$\mu = 0.29$ mm^{-1}
$T = 290$ K
Prismatic, pale yellow
0.30 × 0.28 × 0.21 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
3673 measured reflections
1855 independent reflections
1606 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.4°$
$h = -7\rightarrow7$
$k = -10\rightarrow10$
$l = -11\rightarrow11$
3 standard reflections every 120 min
intensity decay: −1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.097$
$S = 1.05$
1855 reflections
159 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
$w = 1/[\sigma^2(F_o^2) + (0.0517P)^2 + 0.1432P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
P1	0.41857 (7)	0.24449 (5)	0.45738 (5)	0.02797 (16)	
O3	0.5389 (2)	0.15751 (15)	0.56719 (15)	0.0337 (3)	
O1	0.2459 (2)	0.34533 (16)	0.51681 (16)	0.0398 (3)	
O4	0.6905 (3)	0.3598 (2)	−0.03575 (18)	0.0551 (4)	
O2	0.3153 (2)	0.12049 (16)	0.40620 (19)	0.0451 (4)	
H1A	0.3957	0.0129	0.4192	0.054*	
N1	0.7900 (3)	0.3121 (2)	0.18552 (19)	0.0384 (4)	
C4	0.8154 (3)	0.3152 (3)	0.0385 (2)	0.0409 (5)	
C1	0.6134 (3)	0.3843 (2)	0.2730 (2)	0.0344 (4)	
H1B	0.5331	0.4384	0.2035	0.041*	
H1C	0.6778	0.4664	0.2985	0.041*	
N2	0.2060 (2)	0.66240 (18)	0.34358 (18)	0.0328 (4)	
HN2	0.0704	0.6790	0.3837	0.045 (6)*	
HN1	0.2222	0.5670	0.3972	0.052 (7)*	
HN3	0.3009	0.7318	0.3485	0.056 (7)*	
HN4	0.2541	0.6712	0.2322	0.054 (7)*	

C2	0.9747 (8)	0.2620 (6)	0.2347 (6)	0.0391 (10)	0.832 (9)
H2A	0.9323	0.1667	0.3309	0.047*	0.832 (9)
H2B	1.0433	0.3480	0.2527	0.047*	0.832 (9)
O5	1.0145 (8)	0.2687 (6)	−0.0269 (6)	0.0502 (9)	0.832 (9)
C5	1.1711 (12)	0.0514 (6)	0.1183 (8)	0.094 (2)	0.832 (9)
H5A	1.2641	0.0400	0.0200	0.141*	0.832 (9)
H5B	1.0342	−0.0159	0.1578	0.141*	0.832 (9)
H5C	1.2432	0.0191	0.1961	0.141*	0.832 (9)
C3	1.1272 (5)	0.2245 (4)	0.0887 (3)	0.0421 (10)	0.832 (9)
H3	1.2677	0.2932	0.0443	0.050*	0.832 (9)
C22	0.988 (5)	0.221 (3)	0.217 (3)	0.039 (5)	0.168 (9)
H22A	1.1119	0.2984	0.1918	0.047*	0.168 (9)
H22B	0.9459	0.1536	0.3292	0.047*	0.168 (9)
O25	0.957 (3)	0.209 (3)	−0.005 (3)	0.043 (4)	0.168 (9)
C25	1.273 (4)	0.128 (3)	0.054 (3)	0.070 (7)	0.168 (9)
H25A	1.3078	0.0833	−0.0305	0.105*	0.168 (9)
H25B	1.3286	0.0648	0.1352	0.105*	0.168 (9)
H25C	1.3404	0.2376	0.0112	0.105*	0.168 (9)
C23	1.047 (3)	0.125 (2)	0.1196 (16)	0.041 (5)	0.168 (9)
H23	0.9758	0.0133	0.1781	0.049*	0.168 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0290 (3)	0.0249 (2)	0.0322 (3)	0.00831 (17)	−0.01321 (19)	−0.01013 (19)
O3	0.0414 (7)	0.0289 (6)	0.0372 (7)	0.0081 (5)	−0.0215 (6)	−0.0115 (6)
O1	0.0367 (7)	0.0324 (7)	0.0418 (8)	0.0125 (6)	−0.0063 (6)	−0.0097 (6)
O4	0.0615 (10)	0.0769 (11)	0.0407 (8)	0.0307 (9)	−0.0294 (8)	−0.0266 (8)
O2	0.0516 (8)	0.0327 (7)	0.0715 (10)	0.0147 (6)	−0.0440 (8)	−0.0214 (7)
N1	0.0343 (8)	0.0544 (10)	0.0328 (8)	0.0181 (8)	−0.0147 (7)	−0.0202 (8)
C4	0.0418 (11)	0.0482 (12)	0.0313 (10)	0.0140 (9)	−0.0122 (9)	−0.0129 (9)
C1	0.0363 (10)	0.0335 (9)	0.0314 (9)	0.0108 (8)	−0.0100 (8)	−0.0107 (8)
N2	0.0338 (9)	0.0310 (8)	0.0338 (8)	0.0066 (6)	−0.0128 (7)	−0.0108 (7)
C2	0.0315 (15)	0.054 (3)	0.0355 (17)	0.0178 (18)	−0.0107 (12)	−0.0209 (18)
O5	0.046 (2)	0.065 (2)	0.0321 (13)	0.0220 (15)	−0.0070 (15)	−0.0147 (17)
C5	0.158 (7)	0.063 (3)	0.130 (5)	0.064 (3)	−0.111 (5)	−0.059 (3)
C3	0.0309 (14)	0.045 (2)	0.0543 (17)	0.0107 (13)	−0.0152 (12)	−0.0220 (14)
C22	0.059 (9)	0.041 (11)	0.044 (8)	0.037 (8)	−0.042 (7)	−0.037 (8)
O25	0.034 (9)	0.067 (12)	0.035 (8)	0.023 (7)	−0.013 (7)	−0.025 (9)
C25	0.066 (14)	0.087 (18)	0.104 (19)	0.049 (11)	−0.050 (13)	−0.073 (16)
C23	0.045 (8)	0.037 (9)	0.043 (7)	0.009 (7)	−0.015 (6)	−0.016 (6)

Geometric parameters (Å, º)

P1—O1	1.4969 (14)	C2—C3	1.539 (5)
P1—O3	1.5041 (13)	C2—H2A	0.9700
P1—O2	1.5645 (14)	C2—H2B	0.9700
P1—C1	1.816 (2)	O5—C3	1.454 (6)

O4—C4	1.218 (2)	C5—C3	1.497 (6)
O2—H1A	1.0666	C5—H5A	0.9600
N1—C4	1.332 (3)	C5—H5B	0.9600
N1—C2	1.435 (6)	C5—H5C	0.9600
N1—C1	1.447 (2)	C3—H3	0.9800
N1—C22	1.56 (2)	C22—C23	1.41 (2)
C4—O5	1.355 (5)	C22—H22A	0.9700
C4—O25	1.36 (2)	C22—H22B	0.9700
C1—H1B	0.9700	O25—C23	1.46 (3)
C1—H1C	0.9700	C25—C23	1.39 (3)
N2—HN2	0.8645	C25—H25A	0.9600
N2—HN1	0.8517	C25—H25B	0.9600
N2—HN3	0.8934	C25—H25C	0.9600
N2—HN4	0.9676	C23—H23	0.9800

O1—P1—O3	117.20 (8)	H2A—C2—H2B	109.3
O1—P1—O2	109.29 (9)	C4—O5—C3	109.8 (4)
O3—P1—O2	109.68 (8)	C3—C5—H5A	109.5
O1—P1—C1	104.86 (8)	C3—C5—H5B	109.5
O3—P1—C1	109.63 (9)	H5A—C5—H5B	109.5
O2—P1—C1	105.49 (10)	C3—C5—H5C	109.4
P1—O2—H1A	112.0	H5A—C5—H5C	109.5
C4—N1—C2	114.0 (2)	H5B—C5—H5C	109.5
C4—N1—C1	122.16 (16)	O5—C3—C5	108.1 (3)
C2—N1—C1	122.7 (2)	O5—C3—C2	104.9 (3)
C4—N1—C22	101.9 (8)	C5—C3—C2	115.8 (4)
C1—N1—C22	135.9 (8)	O5—C3—H3	109.2
O4—C4—N1	127.90 (19)	C5—C3—H3	109.2
O4—C4—O5	122.2 (3)	C2—C3—H3	109.3
N1—C4—O5	109.8 (3)	C23—C22—N1	108.1 (16)
O4—C4—O25	116.8 (9)	C23—C22—H22A	110.5
N1—C4—O25	111.6 (10)	N1—C22—H22A	110.4
N1—C1—P1	115.39 (13)	C23—C22—H22B	109.8
N1—C1—H1B	108.4	N1—C22—H22B	109.7
P1—C1—H1B	108.4	H22A—C22—H22B	108.3
N1—C1—H1C	108.4	C4—O25—C23	112.2 (16)
P1—C1—H1C	108.4	C23—C25—H25A	109.5
H1B—C1—H1C	107.5	C23—C25—H25B	109.5
HN2—N2—HN1	108.1	H25A—C25—H25B	109.5
HN2—N2—HN3	112.5	C23—C25—H25C	109.4
HN1—N2—HN3	108.1	H25A—C25—H25C	109.5
HN2—N2—HN4	115.2	H25B—C25—H25C	109.5
HN1—N2—HN4	107.4	C25—C23—C22	112 (2)
HN3—N2—HN4	105.2	C25—C23—O25	110.4 (17)
N1—C2—C3	101.4 (3)	C22—C23—O25	100.2 (16)
N1—C2—H2A	111.6	C25—C23—H23	111.1
C3—C2—H2A	111.5	C22—C23—H23	111.5
N1—C2—H2B	111.5	O25—C23—H23	111.2

C3—C2—H2B	111.4		
C2—N1—C4—O4	−176.3 (3)	O4—C4—O5—C3	179.2 (2)
C1—N1—C4—O4	−8.3 (4)	N1—C4—O5—C3	2.6 (4)
C22—N1—C4—O4	172.4 (11)	O25—C4—O5—C3	−96 (3)
C2—N1—C4—O5	0.1 (3)	C4—O5—C3—C5	120.3 (5)
C1—N1—C4—O5	168.1 (3)	C4—O5—C3—C2	−3.9 (4)
C22—N1—C4—O5	−11.2 (11)	N1—C2—C3—O5	3.7 (4)
C2—N1—C4—O25	26.4 (9)	N1—C2—C3—C5	−115.5 (5)
C1—N1—C4—O25	−165.6 (9)	C4—N1—C22—C23	−25 (2)
C22—N1—C4—O25	15.1 (13)	C2—N1—C22—C23	−165 (6)
C4—N1—C1—P1	117.3 (2)	C1—N1—C22—C23	156.3 (11)
C2—N1—C1—P1	−75.7 (3)	O4—C4—O25—C23	−161.7 (9)
C22—N1—C1—P1	−63.7 (15)	N1—C4—O25—C23	−1.7 (15)
O1—P1—C1—N1	−175.71 (13)	O5—C4—O25—C23	89 (3)
O3—P1—C1—N1	57.66 (16)	N1—C22—C23—C25	140 (2)
O2—P1—C1—N1	−60.36 (15)	N1—C22—C23—O25	22 (2)
C4—N1—C2—C3	−2.4 (4)	C4—O25—C23—C25	−132 (2)
C1—N1—C2—C3	−170.3 (2)	C4—O25—C23—C22	−14 (2)
C22—N1—C2—C3	41 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H*N*1···O1	0.85	1.94	2.789 (2)	177
O2—H1*A*···O3^{i}	1.07	1.53	2.5770 (19)	166
N2—H*N*2···O1^{ii}	0.86	1.93	2.772 (2)	165
N2—H*N*3···O3^{iii}	0.89	1.93	2.793 (2)	161
N2—H*N*4···O4^{iv}	0.97	1.88	2.827 (2)	167

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