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Supporting information for article:

Ganciclovir polymorph I

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Crystal structure of Ganciclovir polymorph I

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Computing details

Data Collection: Bruker-AXS (2015) *APEX3* Ver. 2015.9-0 (Bruker-AXS, 2015), *SAINT*+ Ver. 2015.9-0 (Bruker-AXS, 2015), Krause, (2015). Program(s) used to solve structure *SHELX* (Sheldrick, 2013a); *XPREP* (Sheldrick, 2013b); *XT* (Sheldrick, 2015a), *XL* (Sheldrick, 2015b), *OLEX2* (Dolomanov *et al.*, 2009); Guzei, I. A. (2007-2013).

2-amino-9-{[(1,3-dihydroxypropan-2-yl)oxy]methyl}-6,9-dihydro-3H-purin-6-one

Table S1

Crystal data	GCV Form I
Chemical formula	$C_9H_{13}N_5O_4$
M_r	255.24
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	4.6448 (10), 15.632 (3), 14.130 (3)
β (°)	91.632 (10)
V (Å^3)	1025.5 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.13
Crystal size (mm)	0.58 × 0.1 × 0.1
Data collection	
Diffractometer	Bruker *SMART APEX2* area detector
Absorption correction	Multi-scan TWINABS-2012/1 (Bruker,2012) was used for absorption correction. For component 2: wR2(int) was 0.1538 before and 0.0967 after correction. The Ratio of minimum to maximum transmission not present. The λ/2 correction factor is Not present
T_{min}, T_{max}	0.54, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	45424, 45424, 38287
R_{int}	---
(sin θ/λ)$_{max}$ (Å^{-1})	0.715
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.151, 1.02
No. of reflections	45424
No. of parameters	184
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.29

Computer programs: *APEX3* Ver. 2015.9-0 (Bruker-AXS, 2015), *SAINT*+ Ver. 2015.9-0 (Bruker-AXS, 2015), XT (Sheldrick, 2015a), XL (Sheldrick, 2015b), OLEX2 (Dolomanov *et al.*, 2009).

Experimental details

Refinement. The systematic absences in the diffraction data were uniquely consistent for the space group $P2_1/c$ that yielded chemically reasonable and computationally stable results of refinement.

A successful solution by the direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms participating in hydrogen bonding interactions were found in the difference Fourier map and refined independently, other H atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

The crystal chosen for the single-crystal X-ray diffraction experiment proved to be a non-merohedral twin with a 48.10(16)% second component contribution. The twin components are related by a 180.0° rotation about reciprocal axis [001].

The final least-squares refinement of 184 parameters against 45424 data resulted in residuals *R* (based on F^2 for $I \geq 2\sigma$) and *wR* (based on F^2 for all data) of 0.0535 and 0.1510, respectively. The final difference Fourier map was featureless.

Table S2

Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for GCV Form I. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*X*	*y*	*z*	U(eq)
O1	-8794(3)	-2959.6(9)	-6766.3(10)	16.3(3)
O2	-4005(3)	-4072.6(9)	-2511.3(9)	14.4(3)
O4	-2212(3)	-3827.8(9)	22.8(9)	15.6(3)
O3	-5480(3)	-5521.9(9)	-1646(1)	15.8(3)
N5	-1570(3)	-4914.4(11)	-6255.5(12)	14.7(3)
N1	-5152(3)	-3907.9(11)	-6440.8(12)	12.7(3)
N3	-8130(3)	-2473.5(10)	-4648.1(11)	13.2(3)
N4	-4703(3)	-3141.6(10)	-3778.7(11)	12.6(3)
N2	-2822(3)	-4126(1)	-4941.4(11)	11.9(3)
C1	-3186(4)	-4313.7(12)	-5851.7(13)	12.0(3)
C4	-7116(4)	-3281.7(12)	-6174.3(13)	12.6(3)
C3	-6763(4)	-3084.2(12)	-5194.8(13)	12.5(3)
C5	-6837(4)	-2527.7(12)	-3813.2(13)	13.6(4)
C2	-4636(4)	-3499.6(12)	-4667.6(12)	11.5(3)
C6	-2863(4)	-3345.0(12)	-2971.9(13)	13.8(4)
C7	-2467(4)	-4257.7(12)	-1634.9(13)	12.3(3)
C9	-3819(4)	-3743.4(13)	-846.7(13)	15.6(4)
C8	-2598(4)	-5215.3(12)	-1481.1(13)	14.1(4)

Table S3

Anisotropic Displacement Parameters ($Å^2×10^3$) for GCV Form I. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	16.6(7)	19.2(7)	13.0(6)	2.6(5)	-1.9(5)	2.3(5)
O2	17.6(7)	14.2(7)	11.1(6)	3.1(5)	-2.9(5)	-3.6(5)
O4	19.6(7)	17.0(7)	10.2(6)	0.6(5)	-2.2(5)	-3.2(5)
O3	16.8(7)	17.4(7)	13.4(7)	1.4(5)	0.1(5)	-4.3(5)
N5	14.8(8)	16.3(8)	12.8(7)	-1.9(6)	-1.8(6)	2.3(6)
N1	13.4(8)	15.0(8)	9.6(7)	-0.8(6)	-0.5(5)	0.8(5)
N3	14.3(8)	12.6(7)	12.7(7)	0.4(6)	2.5(5)	-0.4(5)
N4	14.7(8)	12.4(7)	10.7(7)	-0.1(6)	-0.2(5)	-0.7(5)
N2	12.5(7)	12.1(7)	11.1(7)	0.0(6)	-0.7(5)	-0.8(5)
C1	11.2(8)	12.5(8)	12.4(8)	1.0(7)	0.0(6)	-2.0(6)
C4	12.6(8)	11.8(8)	13.4(8)	1.7(7)	0.3(6)	-1.5(6)
C3	12.7(8)	12.6(8)	12.1(8)	0.8(7)	1.0(6)	-0.6(6)
C5	16.0(9)	11.3(8)	13.4(8)	0.5(7)	2.3(6)	-0.5(6)
C2	12.9(8)	11.5(8)	10.2(8)	0.4(6)	0.7(6)	-2.8(6)
C6	15.7(9)	14.3(9)	11.4(8)	1.4(7)	-1.5(6)	-3.6(6)
C7	13.2(9)	13.2(8)	10.5(7)	0.6(6)	-1.9(6)	0.5(6)
C9	18.6(9)	17.3(9)	10.8(8)	-1.3(7)	-2.5(6)	3.5(7)
C8	14.1(9)	13.3(8)	14.8(8)	0.2(7)	-0.9(6)	0.3(6)

Table S4

Bond lengths for GCV Form I.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C4	1.234(2)	N4	C5	1.380(2)
O2	C6	1.421(2)	N4	C2	1.376(2)
O2	C7	1.441(2)	N4	C6	1.440(2)
O4	C9	1.425(2)	N2	C1	1.326(2)
O3	C8	1.435(2)	N2	C2	1.355(2)
N5	C1	1.340(2)	C4	C3	1.423(3)
N1	C1	1.373(2)	C3	C2	1.382(2)
N1	C4	1.397(2)	C7	C9	1.523(3)
N3	C3	1.393(2)	C7	C8	1.514(3)
N3	C5	1.311(2)			

Table S5

Bond Angles for GCV Form I.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C6	O2	C7	111.84(13)	N3	C3	C4	130.29(17)
C1	N1	C4	126.04(16)	C2	C3	N3	110.68(16)
C5	N3	C3	104.51(15)	C2	C3	C4	118.89(17)
C5	N4	C6	126.23(16)	N3	C5	N4	112.77(17)

C2	N4	C5	106.57(15)	N4	C2	C3	105.47(16)
C2	N4	C6	127.18(16)	N2	C2	N4	125.76(16)
C1	N2	C2	111.93(15)	N2	C2	C3	128.77(17)
N5	C1	N1	115.89(16)	O2	C6	N4	108.58(14)
N2	C1	N5	120.71(17)	O2	C7	C9	108.53(15)
N2	C1	N1	123.39(17)	O2	C7	C8	107.51(14)
O1	C4	N1	120.52(17)	C8	C7	C9	113.43(16)
O1	C4	C3	128.58(18)	O4	C9	C7	111.39(15)
N1	C4	C3	110.86(16)	O3	C8	C7	110.37(15)

Table S6

Hydrogen Bonds for GCV Form I.

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
O3—H3···N3^{i}	0.89 (3)	1.93 (3)	2.811 (2)	172 (3)
O4—H4···O3^{ii}	0.85 (3)	1.91 (4)	2.754 (2)	176 (3)
N1—H1A···N5^{iii}	0.86 (3)	2.15 (3)	3.012 (2)	179 (3)
N1—H1B···O2^{iv}	0.88 (3)	2.34 (3)	3.093 (2)	143 (2)
N2—H2···O4^{iv}	0.80 (3)	2.07 (3)	2.869 (2)	172 (3)

Symmetry code(s): (i) *x*−1, −*y*+1/2, *z*−1/2; (ii) −*x*+1, −*y*+1, −*z*; (iii) −*x*, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*+1.

Table S7

Torsion Angles for GCV Form I.

A B C D	**Angle/°**	**A B C D**	**Angle/°**
O1 C4 C3 N3	-1.7(3)	C5 N3 C3 C4	-175.54(19)
O1 C4 C3 C2	-176.87(18)	C5 N3 C3 C2	-0.1(2)
O2 C7 C9 O4	-173.90(14)	C5 N4 C2 N2	179.39(17)
O2 C7 C8 O3	-46.58(19)	C5 N4 C2 C3	-0.39(19)
N1 C4 C3 N3	176.04(18)	C5 N4 C6 O2	98.1(2)
N1 C4 C3 C2	0.9(2)	C2 N4 C5 N3	0.4(2)
N3 C3 C2 N4	0.3(2)	C2 N4 C6 O2	-83.8(2)
N3 C3 C2 N2	-179.48(17)	C2 N2 C1 N5	179.50(17)
C1 N1 C4 O1	-179.91(17)	C2 N2 C1 N1	0.8(2)
C1 N1 C4 C3	2.1(3)	C6 O2 C7 C9	87.48(18)
C1 N2 C2 N4	-177.25(17)	C6 O2 C7 C8	-149.46(15)
C1 N2 C2 C3	2.5(3)	C6 N4 C5 N3	178.82(17)
C4 N1 C1 N5	178.02(17)	C6 N4 C2 N2	1.0(3)
C4 N1 C1 N2	-3.2(3)	C6 N4 C2 C3	-178.81(17)
C4 C3 C2 N4	176.35(16)	C7 O2 C6 N4	-173.40(14)
C4 C3 C2 N2	-3.4(3)	C9 C7 C8 O3	73.42(19)
C3 N3 C5 N4	-0.2(2)	C8 C7 C9 O4	66.7(2)

Table S8

Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for GCV Form I.

Atom	***x***	***y***	***z***	**U(eq)**
H11	-940(70)	-3400(20)	70(20)	47(9)
H8	-6170(60)	-5750(20)	-1160(20)	42(9)
H10	-320(50)	-5186(17)	-5910(20)	24(7)
H9	-2200(60)	-5137(19)	-6800(20)	29(7)
H1	-5100(50)	-4037(17)	-6990(20)	24(7)
H4	-7318.99	-2181.49	-3288.32	16
H2	-888.43	-3468.04	-3179.95	17
H3	-2772.69	-2853.81	-2529.84	17
H5	-410.25	-4080.77	-1691.45	15
H7	-3904.02	-3132.59	-1030.46	19
H6	-5814.61	-3944.53	-758.5	19
H12	-1283.09	-5505.13	-1917.65	17
H13	-1955.64	-5351.55	-824.18	17