Table 2. *Bond distances* (Å), *bond angles* (°), *torsion angles* (°) *and hydrogen-bond geometry*

O—N	1·410 (2)	C(4)—C(5)	1·496 (4)
N—C(7)	1·272 (3)	C(4)—C(8)	1·512 (5)
C(1)—C)2)	1·323 (3)	C(5)—C(6)	1·518 (4)
C(1)—C(6)	1·499 (3)	C(8)—C(9)	1·301 (8)
C(1)—C(7)	1·451 (3)	C(8)—C(10)	1·538 (9)
C(2)—C(3)	1·494 (3)	O—H(991)	0·84 (3)
C(3)—C(4)	1·521 (4)		

O—N—C(7)	111·8 (2)	C(5)—C(4)—C(8)	116·4 (3)
C(2)—C(1)—C(6)	121·5 (2)	C(4)—C(5)—C(6)	111·6 (2)
C(2)—C(1)—C(7)	120·1 (2)	C(1)—C(6)—C(5)	112·0 (2)
C(6)—C(1)—C(7)	118·5 (2)	N—C(7)—C(1)	120·7 (2)
C(1)—C(2)—C(3)	125·0 (2)	C(4)—C(8)—C(9)	120·9 (5)
C(2)—C(3)—C(4)	111·6 (2)	C(4)—C(8)—C(10)	120·9 (4)
C(3)—C(4)—C(5)	110·1 (2)	C(9)—C(8)—C(10)	118·2 (5)
C(3)—C(4)—C(8)	112·0 (3)	N—O—H(991)	98 (2)

O—N—C(7)—C(1)	178·4 (2)	C(2)—C(3)—C(4)—C(8)	−175·4 (3)
C(6)—C(1)—C(2)—C(3)	1·0 (3)	C(3)—C(4)—C(5)—C(6)	61·9 (4)
C(7)—C(1)—C(2)—C(3)	−179·0 (2)	C(8)—C(4)—C(5)—C(6)	−169·3 (3)
C(2)—C(1)—C(6)—C(5)	14·9 (3)	C(3)—C(4)—C(8)—C(9)	−107·7 (5)
C(7)—C(1)—C(6)—C(5)	−165·2 (2)	C(3)—C(4)—C(8)—C(10)	71·0 (5)
C(2)—C(1)—C(7)—N	177·5 (2)	C(5)—C(4)—C(8)—C(9)	124·4 (5)
C(6)—C(1)—C(7)—N	−2·4 (3)	C(5)—C(4)—C(8)—C(10)	−56·9 (6)
C(1)—C(2)—C(3)—C(4)	14·0 (3)	C(4)—C(5)—C(6)—C(1)	−46·2 (4)
C(2)—C(3)—C(4)—C(5)	−44·3 (3)	H(991)—O—N—C(7)	173 (2)

Oonk, Baert & Fouret, 1976). Indeed a comparable substitution disorder is found in the crystal structure of a mixed (+) and (±) carvoxime crystal (Baert, Fouret, Oonk & Kroon, 1978).

The molecules are connected in the structure by two symmetry-related O—H···N-type hydrogen bonds, O···N 2·830 (2) Å, O—H···N 159 (3)°. In both carvoxime structures mentioned above and in the structure of racemic carvoxime (Oonk & Kroon, 1976) the same six-membered cyclic hydrogen-bonded dimer is reported.

In order to identify the origin of the sweet taste in terms of the so-called *A*H—*B* model of Shallenberger & Acree (1967), a systematic search of possible hydrogen-bond donors and acceptors was performed. This revealed the C7H—O moiety with a C···O distance of 2·22 Å as the only candidate.

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References

Baert, F., Fouret, R., Oonk, H. A. J. & Kroon, J. (1978). *Acta Cryst.* **B34**, 222–226.

Beets, M. G. J. (1978). In *Structure-Activity Relationships in Human Chemoreception.* Applied Science Publishers.

Boer, J. L. de & Duisenberg, A. J. M. (1984). *Acta Cryst.* **A40**, C410.

Cromer, D. T. & Liberman, D. (1970). *J. Chem. Phys.* **53**, 1891–1898.

Cromer, D. T. & Mann, J. B. (1968). *Acta Cryst.* **A24**, 321–324.

Heijden, A. van der, van der Wel, H. & Peer, H. G. (1985). *Chem. Senses*, **10**, 57–72.

Kroon, J., van Gurp, P. R. E., Oonk, H. A. J., Baert, F. & Fouret, R. (1976). *Acta Cryst.* **B32**, 2561–2564.

McCandlish, L. E., Stout, G. H. & Andrews, L. C. (1975). *Acta Cryst.* **A31**, 245–249.

McPherson, A. Jr (1976). In *Methods of Biochemical Analysis*, Vol. 23, edited by D. Glick, p. 277. New York: Wiley–Interscience.

Oonk, H. A. J. & Kroon, J. (1976). *Acta Cryst.* **B32**, 500–504.

Shallenberger, R. S. & Acree, T. E. (1967). *Nature* (*London*), **216**, 480–482.

Sheldrick, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.

Sheldrick, G. M. (1986). *SHELX86*. Program for crystal structure determination. Univ. of Göttingen, Federal Republic of Germany.

Spek, A. L. (1982). *The EUCLID package*. In *Computational Crystallography*, edited by D. Sayre, p. 528. Oxford: Clarendon Press.

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Structure of 5′-*O*-Sulfamoylribavirin, an Antiparasitic Agent

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Abstract. 1-(5-*O*-Sulfamoyl-β-D-ribofuranosyl)-1*H*-1,2,4-triazole-3-carboxamide, $C_8H_{13}N_5O_7S$, $M_r = 323{\cdot}28$, monoclinic, $P2_1$, $a = 4{\cdot}9405\,(4)$, $b = 9{\cdot}1804\,(11)$, $c = 14{\cdot}124\,(2)$ Å, $\beta = 93{\cdot}973\,(6)°$, $V = 639{\cdot}06\,(13)$ Å^3, $Z = 2$, $D_x = 1{\cdot}680$ g cm^{-3}, Cu $K\alpha$ ($\lambda = 1{\cdot}54178$ Å), $\mu = 26{\cdot}573$ cm^{-1}, $F(000) = 336$, $T = 295$ K, $R = 0{\cdot}0224$ for 2629 reflections ($F \geq 4\sigma_F$). The sugar conformation and puckering parameters are $^3T_2$ (C3′-*endo*/C2′-*exo*), $P = 2{\cdot}6°$ and $\tau_m = 40{\cdot}2°$. The C5′—O5′ side-chain orientation is *gauche*$^-$–*gauche*$^+$ [$\varphi_{OO} = -60{\cdot}9\,(2)$; $\varphi_{CO} = 57{\cdot}4\,(2)°$]. The glycosylic torsion angle (N2—N1—C1′—O4′) is

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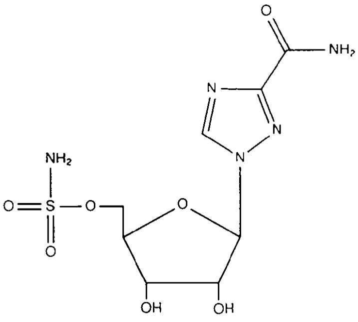
174·98 (12)° (*anti* conformation). The triazole ring is planar [r.m.s. deviation: 0·0015 (14) Å]; the dihedral angle between the carboxamide plane and the triazole ring is 13·70 (6)°. The carboxamide nitrogen is *cis* to N2 of the triazole. All possible hydrogen donors participate in hydrogen bonding [range of H···*A* distances is 1·88 (3)–2·49 (3) Å]. The sulfonamide amino group, which is above the furanose ring, is nonplanar; the N atom is displaced from the plane of the three adjoining atoms by 0·197 (2) Å.

Experimental. The title compound (1) was synthesized from ribavirin (1-β-D-ribofuranosyl-1*H*-1,2,4-triazole-3-carboxamide) as previously described (Kini, Henry, Robins, Larson, Marr, Berens, Bacchi, Nathan & Keithly, 1990). Colorless, transparent, prismatic crystals grew from a slowly cooled water/ethanol solution. Table 1 summarizes data collection and refinement. Unit-cell parameters were obtained by least-squares refinement of the setting angles of 25 reflections with $74·9 < 2\theta < 97·6°$. An Enraf–Nonius CAD-4 diffractometer with a graphite monochromator was used for all measurements. Data reduction, which included Lorentz, polarization, decay and absorption corrections, was accomplished with the *SDP-Plus* software (Frenz, 1985). Crystal and instrument stability were monitored by remeasurement of three check reflections every hour. A linear fit of the intensities of these reflections was used to correct the data. Absorption corrections, based on crystal-face measurements, were applied. The function minimized was $\sum w(|F_o| - |F_c|)^2$, where $w^{-1} = (\sigma_F{}^2 + 0·0004F^2)$, $\sigma_F = F\sigma_I/2I$, and $\sigma_I = (N_{\rm pk} + N_{\rm bg1} + N_{\rm bg2})^{1/2}$.



(1)

Table 1. *Summary of data collection and refinement for* (1)

(*a*) Data collection (295 K)	
Mode	ω–2θ scan
Scan range (°)	$0·80 + 0·15 \tan\theta$
Background	Scan 0·25 times scan range before and after scan
Scan rate (° min^{-1})	1·4–16·49
Exposure time (h)	65·1
Stability correction range on *I*	1·000–1·009
Check reflections	$2,4,\overline{10}$, 443, $1,\bar{6},\overline{10}$
2θ range (°)	3·0–152·0
Range in *hkl*, min.	−6, −11, −17
max.	6,11,17
Total reflections, measured, unique	5306, 2658
$R_{\rm int}$	0·0198
Crystal dimensions (mm)	0·28 × 0·25 × 0·08
Crystal volume (mm^3)	0·00553
Crystal faces	{001}; {021}; {$10\bar{2}$}
Transmission-factor range	0·530–0·822
(*b*) Structure refinement	
Reflections used ($F \geq 4\sigma_F$)	2629
No. of variables	242
Extinction parameter	5·6 (2) × 10^{-6}
Goodness of fit, *S*	1·498
R, *wR*	0·0224, 0·0336
R for all data	0·0226
Max., av. Δ/σ	0·009, 0·0009
Max., min. $\Delta\rho$ in ΔF map (e Å^{-3})	0·37, −0·36

Table 2. *Positional and isotropic thermal parameters for all atoms in* (1)

For non-H atoms, $U_{\rm eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i{}^*a_j{}^*\mathbf{A}_{ij}$, where $\mathbf{A}_{ij}$ is the dot product of the *i*th and *j*th direct-space unit-cell vectors.

	x	*y*	*z*	$U_{\rm eq}/U_{\rm iso}$(Å^2)
N1	0·4024 (2)	0·62748 (13)	0·79951 (8)	0·0269 (3)
N2	0·5963 (2)	0·72562 (15)	0·82707 (8)	0·0282 (3)
C3	0·6829 (3)	0·6767 (2)	0·91205 (9)	0·0265 (4)
N4	0·5578 (3)	0·55370 (15)	0·93971 (9)	0·0351 (4)
C5	0·3816 (3)	0·5264 (2)	0·86677 (11)	0·0347 (4)
C6	0·8928 (3)	0·7516 (2)	0·97549 (10)	0·0270 (4)
O7	0·9207 (2)	0·7160 (2)	1·05984 (7)	0·0391 (3)
N8	1·0385 (3)	0·8537 (2)	0·93630 (11)	0·0368 (4)
C1′	0·2309 (3)	0·6497 (2)	0·71030 (9)	0·0271 (4)
C2′	0·4042 (3)	0·6603 (2)	0·62546 (10)	0·0279 (4)
C3′	0·4406 (3)	0·4991 (2)	0·60324 (10)	0·0258 (4)
C4′	0·1597 (3)	0·4395 (2)	0·61828 (9)	0·0266 (3)
C5′	0·1474 (3)	0·2796 (2)	0·64116 (12)	0·0352 (4)
O2′	0·2484 (3)	0·72284 (14)	0·54776 (8)	0·0399 (3)
O3′	0·5271 (3)	0·4719 (2)	0·51162 (8)	0·0384 (3)
O4′	0·0659 (2)	0·52525 (13)	0·69606 (7)	0·0300 (3)
O5′	0·3250 (3)	0·25369 (12)	0·72593 (8)	0·0391 (3)
S6′	0·41508 (6)	0·090082	0·74513 (2)	0·02694 (9)
O7′	0·5924 (3)	0·0504 (2)	0·67451 (8)	0·0501 (4)
O8′	0·1765 (2)	0·00603 (13)	0·75412 (9)	0·0423 (4)
N9′	0·5788 (3)	0·0997 (2)	0·84487 (9)	0·0366 (4)
H5	0·280 (5)	0·443 (3)	0·858 (2)	0·056 (7)
H8*A*	1·150 (5)	0·911 (3)	0·972 (2)	0·045 (5)
H8*B*	1·003 (6)	0·877 (4)	0·887 (2)	0·063 (8)
H1′	0·115 (4)	0·721 (2)	0·7216 (13)	0·029 (4)
H2′	0·577 (4)	0·698 (2)	0·6442 (12)	0·024 (4)
H3′	0·559 (5)	0·472 (3)	0·648 (2)	0·042 (6)
H4′	0·026 (4)	0·456 (2)	0·5562 (14)	0·031 (4)
H5′*A*	0·194 (4)	0·224 (3)	0·587 (2)	0·042 (5)
H5′*B*	−0·007 (6)	0·252 (3)	0·664 (2)	0·065 (8)
HO2′	0·330 (5)	0·801 (3)	0·538 (2)	0·045 (6)
HO3′	0·430 (6)	0·500 (3)	0·476 (2)	0·062 (8)
H9′*A*	0·715 (5)	0·140 (3)	0·849 (2)	0·049 (6)
H9′*B*	0·476 (5)	0·113 (3)	0·890 (2)	0·059 (7)

The atomic coordinates of 19 non-H atoms were determined by direct methods [*SHELXS*86 (Sheldrick, 1986)]; a ΔF map afforded the coordinates of the remaining two non-H atoms. All H atoms were located in a difference map as peaks of density 0·51–1·00 e Å^{-3} at $R = 0·067$. All positional parameters, anisotropic thermal parameters for non-H atoms, isotropic thermal parameters for H atoms and an extinction parameter were refined with *SHELX*76 (Sheldrick, 1976). Scattering factors and

Table 3. *Bond lengths* (Å) *and bond angles* (°) *in* (1)

1	2	3	1—2	1—2—3
N2	N1	C5	1·352 (2)	110·23 (11)
C5	N1	C1′	1·337 (2)	129·15 (12)
C1′	N1	N2	1·483 (2)	120·31 (11)
C3	N2	N1	1·325 (2)	102·29 (11)
N4	C3	C6	1·358 (2)	121·49 (12)
N4	C3	N2		114·70 (12)
C6	C3	N2	1·491 (2)	123·76 (13)
C5	N4	C3	1·326 (2)	102·78 (12)
N1	C5	N4		110·00 (14)
O7	C6	N8	1·234 (2)	124·25 (14)
O7	C6	C3		118·98 (13)
N8	C6	C3	1·326 (2)	116·77 (13)
C2′	C1′	O4′	1·523 (2)	106·89 (11)
C2′	C1′	N1		110·98 (11)
O4′	C1′	N1	1·410 (2)	107·49 (11)
C3′	C2′	O2′	1·526 (2)	107·42 (11)
C3′	C2′	C1′		100·41 (12)
O2′	C2′	C1′	1·418 (2)	109·29 (12)
C4′	C3′	O3′	1·520 (2)	113·67 (12)
C4′	C3′	C2′		101·41 (12)
O3′	C3′	C2′	1·413 (2)	114·02 (12)
C5′	C4′	O4′	1·506 (2)	110·26 (12)
C5′	C4′	C3′		115·55 (12)
O4′	C4′	C3′	1·453 (2)	104·65 (11)
O5′	C5′	C4′	1·454 (2)	107·77 (12)
C1′	O4′	C4′		109·59 (10)
S6′	O5′	C5′	1·5846 (11)	116·25 (10)
O7′	S6′	O8′	1·4202 (13)	118·62 (8)
O7′	S6′	N9′		109·79 (8)
O7′	S6′	O5′		107·63 (8)
O8′	S6′	N9′	1·4218 (13)	109·13 (8)
O8′	S6′	O5′		107·76 (7)
N9′	S6′	O5′	1·5775 (13)	102·72 (8)

Table 4. *Hydrogen bonding in* (1)

D—	H···	*A*	Symmetry of *A* relative to *D*	*d*(*D*···*A*) (Å)	*d*(H···*A*) (Å)	∠(*D*—H···*A*) (°)
N8	H8*A*	N4	2·0 − *x*, 0·5 + *y*, 2·0 − *z*	3·152 (2)	2·26 (2)	178· (2)
N8	H8*B*	O8′	1·0 + *x*, 1·0 + *y*, *z*	3·048 (2)	2·42 (3)	143· (3)
O2′	HO2′	O3′	1·0 − *x*, 0·5 + *y*, 1·0 − *z*	2·701 (2)	1·88 (3)	167· (2)
O3′	HO3′	O2′	*x*, *y*, *z*	2·750 (2)	2·48 (3)	104· (3)
O3′	HO3′	O7′	1·0 − *x*, 0·5 + *y*, 1·0 − *z*	2·751 (2)	2·17 (3)	139· (3)
N9′	H9′*A*	O7	2·0 − *x*, *y* − 0·5, 2·0 − *z*	2·934 (2)	2·25 (3)	148· (2)
N9′	H9′*B*	O7	1·0 − *x*, *y* − 0·5, 2·0 − *z*	3·083 (2)	2·33 (3)	148· (2)
N9′	H9′*B*	N4	1·0 − *x*, *y* − 0·5, 2·0 − *z*	3·190 (2)	2·49 (3)	141· (2)

anomalous-dispersion corrections were taken from *International Tables for X-ray Crystallography* (1974) except those of H which were taken from Stewart, Davidson & Simpson (1965). Least-squares-planes program from Cordes (1983); figures were drawn with *ORTEP*II (Johnson, 1976); parameter and geometry tables were produced with *FUER* and structure-factor-amplitude tables were produced with *LISTFC* (Larson, 1980). The atomic coordinates are listed in Table 2. Bond lengths and bond angles are given in Table 3. Hydrogen bonding is detailed in Table 4. Fig. 1 illustrates the atom labeling and molecular conformation; Fig. 2 illustrates the unit-cell packing and hydrogen bonding.*

Related literature. The title compound (1) has shown significant antiparasitic activity (Kini *et al.*, 1990). The general conformational features (*i.e.* glycosylic torsion angle, disposition of the carboxamide moiety, sugar conformation, and C5′—O5′ orientation) are extremely similar to those of ribavirin (form VI) (Prusiner & Sundaralingam, 1976). Several other triazole nucleosides have been reported (Haines, Leonard & Wiemer, 1982; Sanghvi, Hanna, Larson, Fujitaki, Willis, Smith, Robins & Revankar, 1988; Hanna, Dimitrijevich, Larson, Robins & Revankar, 1988; Larson, Henry, Kini & Robins, 1990; Larson, Kini & Robins, 1990). A search of the Cambridge Structural Database (1989) revealed no structures

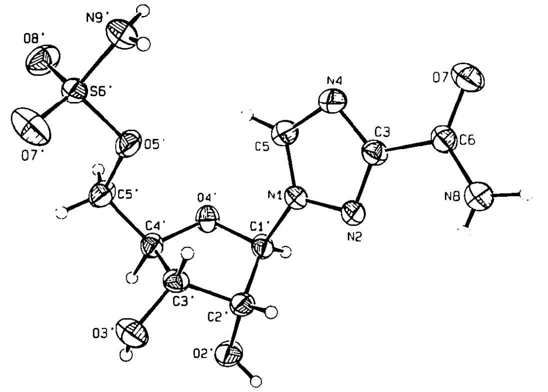


Fig. 1. Thermal-ellipsoid plot of (1) illustrating atom labeling and molecular conformation. The ellipsoids are drawn at the 50% probability level.

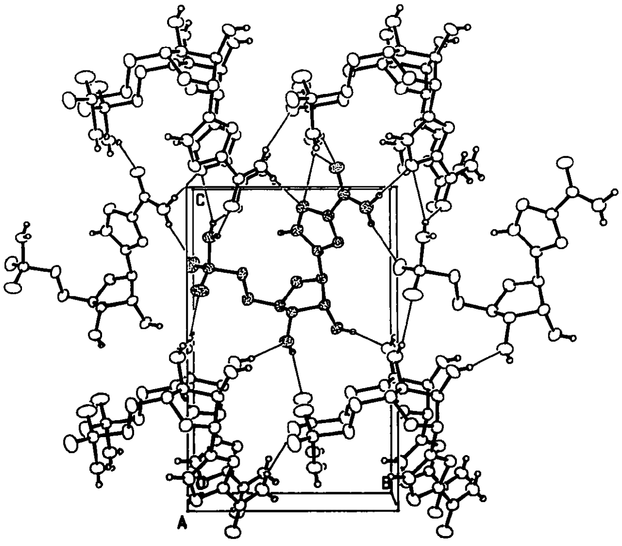


Fig. 2. Crystal packing diagram of (1) viewed along the *a* axis. C—H H atoms of the sugar moiety have been omitted. Hydrogen bonds are drawn as thin lines. All hydrogen bonds involving the shaded molecule are indicated. There are no interactions between molecules related by translation along the *a* axis. There is no base stacking.

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* Tables of anisotropic thermal parameters, bond lengths and angles involving H atoms, torsion angles, least-squares planes and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52435 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

containing the 5-*O*-sulfamoylribose moiety. Conformational parameters follow the conventions of Altona & Sundaralingam (1972).

References

Altona, C. & Sundaralingam, M. (1972). *J. Am. Chem. Soc.* **94**, 8205–8212.

Cambridge Structural Database (1989). Univ. Chemical Laboratory, Lensfield Road, Cambridge, England.

Cordes, A. W. (1983). Personal communication.

Frenz, B. A. (1985). *Enraf–Nonius SDP-Plus Structure Determination Package*. Version 3.0. Enraf–Nonius, Delft, The Netherlands.

Haines, D. R., Leonard, N. J. & Wiemer, D. F. (1982). *J. Org. Chem.* **47**, 474–482.

Hanna, N. B., Dimitrijevich, S. D., Larson, S. B., Robins, R. K. & Revankar, G. R. (1988). *J. Heterocycl. Chem.* **25**, 1857–1868.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Kini, G. D., Henry, E. M., Robins, R. K., Larson, S. B., Marr, J. J., Berens, R. L., Bacchi, C. J., Nathan, H. C. & Keithly, J. S. (1990). *J. Med. Chem.* **33**, 121–128.

Larson, S. B. (1980). PhD Dissertation, Brigham Young Univ., Provo, Utah, USA.

Larson, S. B., Henry, E. M., Kini, G. D. & Robins, R. K. (1990). *Acta Cryst.* **C46**, 1138–1141.

Larson, S. B., Kini, G. D. & Robins, R. K. (1990). *Acta Cryst.* **C46**, 1141–1143.

Prusiner, P. & Sundaralingam, M. (1976). *Acta Cryst.* **B32**, 419–426.

Sanghvi, Y. S., Hanna, N. B., Larson, S. B., Fujitaki, J. M., Willis, R. C., Smith, R. A., Robins, R. K. & Revankar, G. R. (1988). *J. Med. Chem.* **31**, 330–335.

Sheldrick, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.

Sheldrick, G. M. (1986). *SHELXS86*. Program for crystal structure solution. Univ. of Göttingen, Federal Republic of Germany.

Stewart, R. F., Davidson, E. R. & Simpson, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

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Structure of 1-(5-*O*-Sulfamoyl-*β*-D-ribofuranosyl)-1*H*-1,2,4-triazole-3-thiocarboxamide

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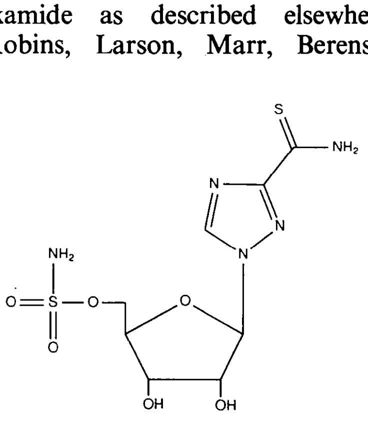
Abstract. $C_8H_{13}N_5O_6S_2$, M_r = 339·34, orthorhombic, $P2_12_12_1$, a = 8·5583 (10), b = 9·0779 (11), c = 17·360 (3) Å, V = 1348·7 (3) Å^3, Z = 4, D_x = 1·671 g cm^{-3}, Cu $K\alpha$ (λ = 1·54178 Å), μ = 38·925 cm^{-1}, $F(000)$ = 704, T = 295 K, R = 0·0243 for 2701 reflections ($F \geq 4\sigma_F$). The nucleoside has a *syn* conformation [χ_{CN}(N2—N1—C1′—O4′) = 50·6 (2)°]. The C5′—O5′ orientation is *gauche*$^-$–*gauche*$^+$ [φ_{OO} = −72·4 (2); φ_{CO} = 47·4 (2)°] which places the sulfamoyl group (especially NH_2) over the ribofuranose ring, resulting in the formation of an intramolecular hydrogen bond to N2 of the triazole ring [d(H···N) = 2·39 (4) Å; ∠N—H···N = 166 (3)°]. The sugar conformation and puckering parameters are C2′-*endo* ($^2T_1$), P = 155·9° and τ_m = 36·4°. All atoms in the triazole ring are within 0·0035 Å of their mean plane and the thiocarboxamide group is twisted out of this plane by 21·88 (6)°. The thiocarboxamide nitrogen is *cis* to N4 of the triazole. All possible hydrogen donors participate in hydrogen bonding [range for H···A distances is 2·07 (4)–2·65 (4) Å]. The sulfonamide amino group is nonplanar; the N atom is displaced from the plane of the three adjoining atoms by 0·230 (2) Å. There is no base stacking in the crystal structure.

Experimental. The title compound (1) was synthesized from 1-*β*-D-ribofuranosyl-1*H*-1,2,4-triazole-3-thiocarboxamide as described elsewhere (Kini, Henry, Robins, Larson, Marr, Berens, Bacchi,



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