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SUPPLEMENTARY MATERIAL

X-Ray Studies of FAST-4 (R=H, B=C^{Bz}) and FAST-5 (R=Px, B=Thy)

The crystal and molecular structures of both molecules **FAST-4** and **FAST-5** were determined using data collected at room temperature on a CAD4 diffractometer with graphite monochromatized CuKα radiation. The crystal data and experimental details are shown in Table 1. The lattice constants were refined by least-squares fit of 25 reflections in the θ range 15.34°-28.69° for **4** and 15.41°-27.46° for compound **5**. The decline in intensity of three control reflections (2,-2,-5; 3,2,-3; 2,3,-2) was 1.0% during 98.0 hours of exposure time for **4** and (5,3,-6; -4,-1,-6; -1,1,-8) was 11.2% during 329.8 hours of exposure time for **5**. An empirical absorption correction was applied by the use of the ψ-scan method (EAC program).[1,2] A total of 4038 reflections with $I>0\sigma(I)$ were used to solve the structure **4** by direct methods and to refine it by full matrix least-squares using F^2, and 6979 reflections with $I>0\sigma(I)$ for **5**. Hydrogen atoms of hydroxyl group in **4** (H5'1 at O5'), methyl group (H71, H72, H73 at C7) and phenyl ring (H121 at C12) were placed geometrically at idealized positions, allowed to ride on the parent atom X, rotate about the Y-X bond for hydroxyl and methyl groups, and refined isotropically. For compound **5** hydrogen atoms were placed geometrically, and set as riding with fixed thermal parameters equal to 1.33 times of the equivalent isotropic thermal parameter of the parent atom. For the base molecules the C-H distances were free to refine, and for methylene groups the rotation about Y-C bond was allowed. All others H-atoms were found on difference Fourier map and refined isotropically. Anisotropic thermal parameters were applied for all nonhydrogen atoms. The absolute configuration was determined by the Flack method[3] with result $\chi=0.00(3)$ for compound **4**, and $\chi=0.01(3)$ for crystal **5**. Data collection and cell refinement: *CAD*-4.[4] Absorption correction: *EAC*.[2] Structure solution: *SHELXS*-86[5]; structure refinement: *SHELXL*-93.

RESULTS

FIGURE 2 FIGURE 3 FIGURE 4

The molecular structures of methanephosphonoselenoloester **FAST-4 (R=H, B=C^{Bz})** and methanephosphonothioloester **FAST-5 (R=Px, B=Thy)** were determined by single crystal X-ray analysis and are presented on Figures 2 [**FAST-4 (R=H, B=C^{Bz})**], 3, and 4

[**FAST-5 (R=Px, B=Thy)**].

The compound **FAST-4 (R=H, B=C^{Bz})** consists of one molecule in the independent part of the elemental cell, while **FAST-5 (R=Px, B=Thy)** consists of two formal molecules in the independent part of elemental cell, both possessing the absolute configuration at the chiral centers identical with the configuration of **FAST-4 (R=H, B=C^{Bz})** and determined as $R_{C1'}$, $S_{C3'}$, R_{C4}, and S_{P1}. The substitution of selenium for sulfur atom changes significantly the structure of the elemental cell, thus creating enough space for four molecules of hexane to co-crystallize inside the elemental cell [structure **FAST-5 (R=Px, B=Thy)**]. The accurate positions of molecules in the elemental cells, together with inter- and intramolecular hydrogen bonds are presented as stereo-views in Figures 5 and 6.

FIGURE 5 FIGURE 6

Four molecules of hexane co-crystalize with four molecules of **FAST-5 (R=Px, B=Thy)** in the independent cell and are localized in a hydrophobic tunnel. They are partially delocalized and have no direct contacts with molecules **FAST-5 (R=Px, B=Thy)** (see Figure 6).

Two intramolecular hydrogen bonds of length 2.24Å and 2.25Å (N4-H4N···N3, and C1'-H1'1···O2, respectively) stabilize the structure of molecule **FAST-4 (R=H, B=C^{Bz})**, together with intermolecular hydrogen bonds of 2.11-2.20 Å (C5'-H5'2···O5'^{ii}, O5'-H5O'···O1'^{iii}; N4-H4N···O2) linking neighboring, perpendicular chains. Each molecule of compound **FAST-5** (**a** and **b** in the independent elemental cell) forms three intramolecular hydrogen bonds (C1'-H1'1···O2, C3'-H3'1···O5' and C24-H241···O5') of lengths 2.31-2.43 Å and one relatively short intermolecular hydrogen bond with the neighboring molecule (N3-H3N···O1^{ii}) of length 2.05 Å.

The comparison of bond distances and valence angles of analogous fragments of deoxyribose rings in compounds **FAST-4 (R=H, B=C^{Bz})** and **FAST-5** (Tables 2, 3, 4, and 5) demonstrate that in the sugar parts of these molecules the largest shifts do not exceed 3σ, so they can be considered as identical. However, the conformations of both rings are different. The asymmetry parameters calculated from the torsion angles show that **FAST-4 (R=H, B=C^{Bz})** has the conformation of an open envelope with C2' atom at the flat position, while **FAST-5 (R=Px, B=Thy)** (both **a** and **b** molecules) have a twisted (half-chair) conformation.[6,7]

The discrimination of geometry was achieved on the basis of the calculated dihedral

angles between appropriate planes. The rotation about the exocyclic C4'-C5' bond allows the O5' atom to assume different positions relative to furanose. The orientation about this bond is significantly influenced by the presence of the 5'-*O*-protecting group. For 5'-*O*-non-protected **FAST-4 (R=H, B=C^{Bz})** the values of torsion angles are Φ_{oo}=-68.7(7)° and Φ_{oc}=51.0(7)°, while for 5'-*O*-pixyl **FAST-5 (R=Px, B=Thy)** they are Φ_{oo}(a)=-72.2(6)°, Φ_{oo}(b)=-76.9(6)° and Φ_{oc}(a)=46.9(6)°, Φ_{oc}(b)=41.8(7)°, respectively.

The planar character of six-membered pyrimidine ring suggests values of valence angles close to 120°. However, the shifts from theoretical value 120° are bigger for molecule **FAST-5** and are caused by different arrangement of substituents. In both cases the orientation about the glycosidic C1'-N1 link (defined by O4'-C1'-N1-C2 torsion angle) is *high anti* (-sc).

The amino group of cytosine (**FAST-4**) is integrated into the resonance system as can be seen from exocyclic N4-C4 (1.317(5) Å) distances and N3-C4 (1.389(6) Å) which are shorter than for the single aliphatic N-C bond. They show a partial double-bond character, as those found in other conjugated heterocyclic systems. The partial double bond forces the amidine-like group to be coplanar with the attached heterocycle (see Figure 2). The exocyclic C4-O4 bond of **FAST-5 (R=Px, B=Thy)** displays a double bond character and reflects the presence of the lactam tautomeric form.

FIGURE 7 FIGURE 8

Figures 7 and 8 represent the Newman projection of the molecules along P1···C3' bond. They demonstrate the orientation of the deoxyribose moiety in relation to methanephosphonate group. Atom C2' is placed *synclinically* towards selenium atom in compound **FAST-4 (R=H, B=C^{Bz})**, but in compound **FAST-5** atom C2' is located *synperiplanally* in relation to sulfur.

The authors have deposited the complete set of data for all atoms of presented structures in Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, United Kingdom.

References

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Figure captions

Fig.5. Stereo view of the crystal packing diagram for **FAST-4 (R=H, B=C^{Bz})**. Hydrogen atoms, except H5'2, H5'O and H4N are omitted for clarity.

Fig.6. Stereo view of the crystal packing diagram for **FAST-5 (R=Px, B=Thy)**. Hydrogen atoms, except H3N and H3N are omitted for clarity.

Fig.7. The Newman projection of **FAST-4 (R=H, B=C^{Bz})**, perpendicular to the P1···C3' line.

Fig.8. The Newman projection of **FAST-5 (R=Px, B=Thy)**, perpendicular to the P1···C3' line.

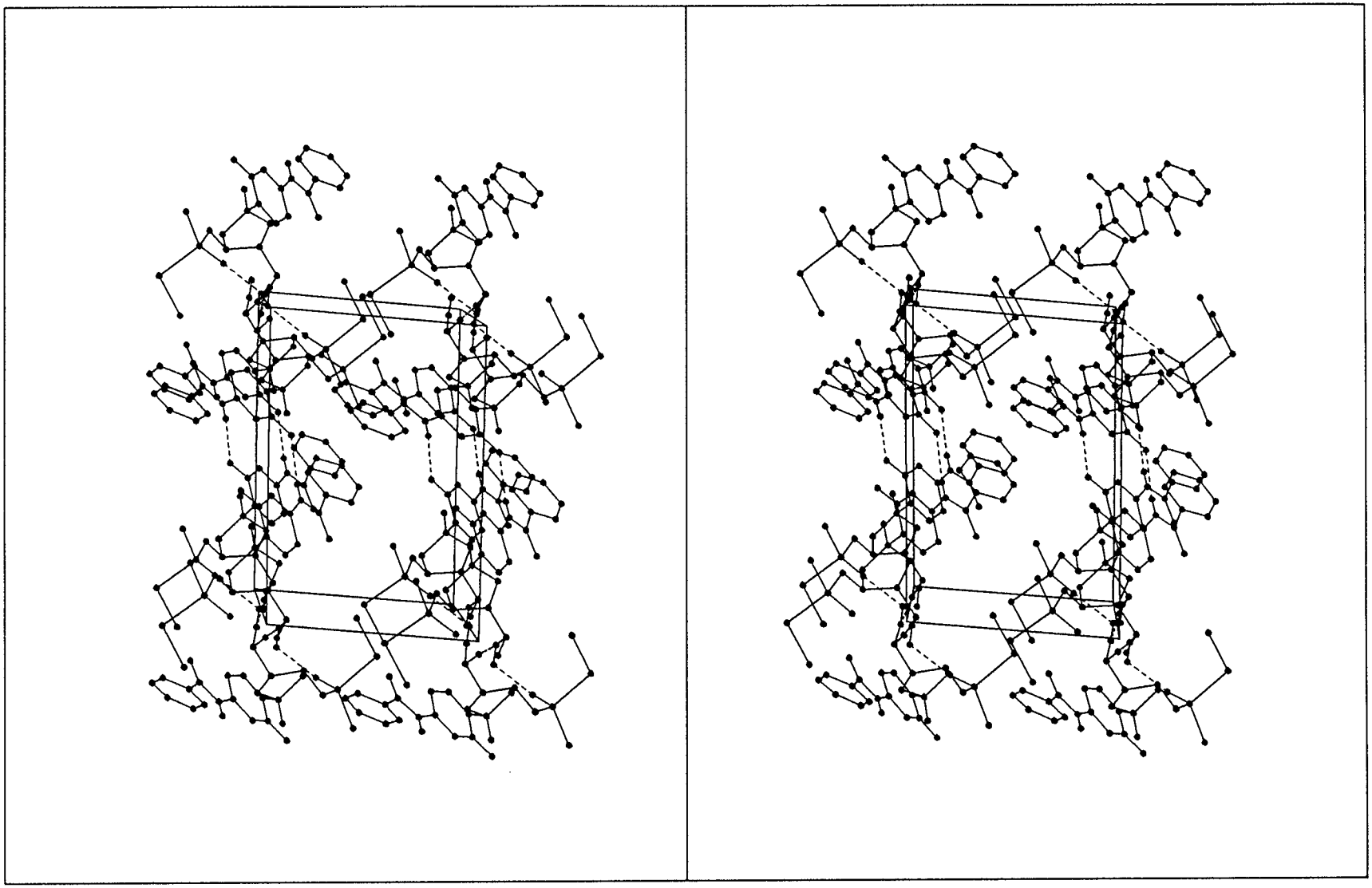


FIGURE 5

FIGURE 6

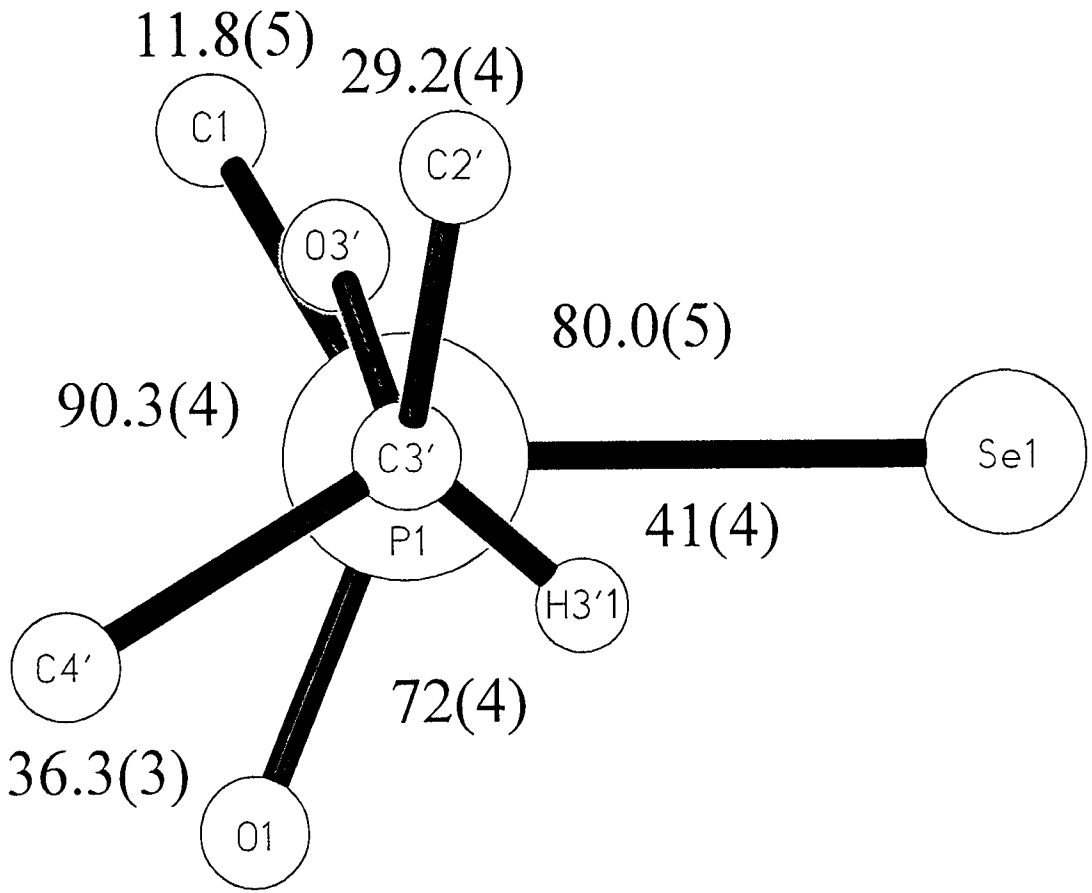
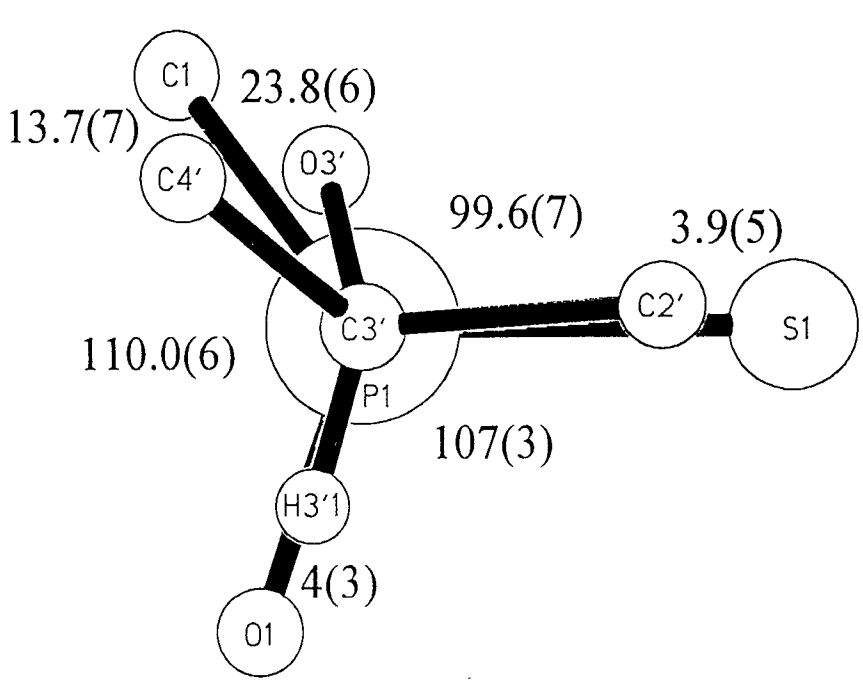


FIGURE 2


C1
23.8(6)
13.7(7)
C4'
O3'
99.6(7)
3.9(5)
C2'
S1
C3'
110.0(6)
P1
107(3)
H3'1
4(3)
O1

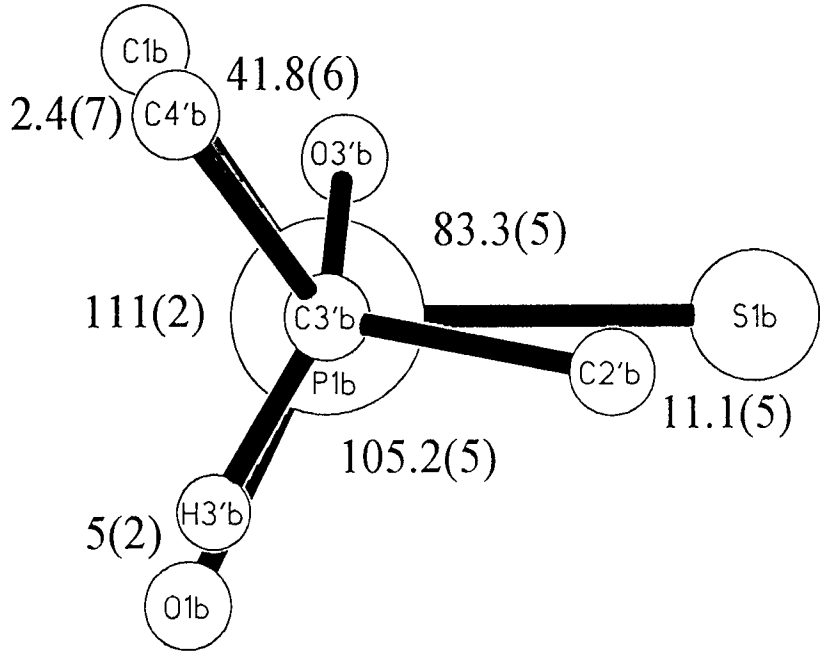

C1b
41.8(6)
2.4(7)
C4'b
O3'b
83.3(5)
111(2)
C3'b
S1b
C2'b
11.1(5)
P1b
105.2(5)
H3'b
5(2)
O1b

FIGURE 8

Crystal data and experimental details for **FAST-4 (R=H,B=C^{Bz})**

Molecular formula		$C_{18}H_{22}N_3O_6PSe$
Formula_weight		486.32
Crystallographic system		monoclinic
Space group		$P2_1$
a (Å)		9.419(2)
b (Å)		7.991(2)
c (Å)		13.668(3)
β (°)		94.69(3)
V (Å^3)		1025.3(4)
Z		2
D_c (g/cm^3)		1.575
μ [cm^{-1}]		35.81
Crystal dimensions (mm)		0.12 x0.16x0.32
Maximum 2θ (°)		150
Radiation, λ (Å)		CuKα, 1.54184
Scan mode		ω/2θ
Scan width (°)		1.27+0.14·tanθ
hkl ranges:	*h* =	-11 11
	k =	-10 10
	l =	-17 0
EAC correction:	min:	0.8731
	max:	1.0000
	ave:	0.9328
No. of reflections:	unique	4217
	refine with $I>0\sigma(I)$	4038
	observed with $I>2\sigma(I)$	3742
No. of parameters refined		337
No. of restraints		0
Largest diff. peak (eÅ^{-3})		0.423
Largest diff. hole (eÅ^{-3})		-1.193
R_{obs}		0.0576
wR_{obs}		0.1434
weighting coeff.*	m	0.1156
S_{obs}		1.088
shift/esd max		-0.001
R_{int}		0.0530
$T_{meas.}$		293(2)
F_000		496
Absolute structure		$R_{C1'}$, $S_{C3'}$, $R_{C4'}$, $\mathbf{S}_{P1}$
Flack parameter χ		0.00(3)

* weighting scheme $w=[\sigma^2(Fo^2)+(mP)^2]^{-1}$ where $P=(Fo^2+2Fc^2)/3$

Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) *for non-H atoms in* **FAST-4 (R=H,B=C^{Bz})**

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i \mathbf{a}_j$

	x	*y*	*z*	U_{eq}
P1	0.32278(12)	0.2744	0.84070(8)	0.0438(2)
Se1	0.50780(6)	0.3276(2)	0.94769(4)	0.0641(2)
O1	0.2127(4)	0.1766(5)	0.8855(3)	0.0617(9)
C1	0.3906(8)	0.1822(8)	0.7361(5)	0.0627(13)
C1'	0.0759(5)	0.7337(5)	0.7319(3)	0.0446(9)
C2'	0.1936(5)	0.7333(6)	0.8145(4)	0.0502(10)
C3'	0.1839(5)	0.5570(6)	0.8550(3)	0.0443(9)
O3'	0.2683(4)	0.4490(4)	0.7967(2)	0.0508(7)
C4'	0.0260(5)	0.5131(6)	0.8359(3)	0.0448(9)
O4'	-0.0308(4)	0.6279(5)	0.7629(3)	0.0558(8)
C5'	-0.0602(7)	0.5214(8)	0.9225(5)	0.0669(15)
O5'	-0.0362(7)	0.6786(8)	0.9688(5)	0.097(2)
N1	0.0112(4)	0.8979(5)	0.7107(3)	0.0417(7)
C2	0.0428(4)	0.9828(5)	0.6254(3)	0.0402(8)
O2	0.1327(4)	0.9209(5)	0.5751(3)	0.0570(9)
N3	-0.0242(4)	1.1289(5)	0.6026(3)	0.0414(7)
C4	-0.1168(4)	1.1901(5)	0.6604(3)	0.0388(8)
N4	-0.1790(4)	1.3399(5)	0.6279(3)	0.0435(7)
C5	-0.1490(6)	1.1093(6)	0.7480(3)	0.0491(10)
C6	-0.0810(6)	0.9651(7)	0.7702(3)	0.0511(10)
C7	0.4099(9)	0.3047(12)	1.0663(5)	0.080(2)
C8	-0.2742(5)	1.4369(6)	0.6736(3)	0.0443(9)
O8	-0.3225(4)	1.3910(5)	0.7508(3)	0.0629(9)
C9	-0.3197(5)	1.5969(6)	0.6271(3)	0.0443(9)
C10	-0.2377(6)	1.6868(6)	0.5653(3)	0.0498(10)
C11	-0.2889(7)	1.8390(9)	0.5274(4)	0.0631(12)
C12	-0.4214(8)	1.8989(9)	0.5513(5)	0.075(2)
C13	-0.5014(7)	1.8083(9)	0.6098(5)	0.071(2)
C14	-0.4521(6)	1.6592(8)	0.6501(4)	0.0598(12)

Fractional atomic coordinates and isotropic thermal parameters ($Å^2$) *for H atoms in* **FAST-4 (R=H,B=C^{Bz})**

	x	*y*	*z*	U_{iso}
H11	0.4250(94)	0.0775(129)	0.7494(67)	0.093(26)
H12	0.4416(99)	0.2435(128)	0.7094(68)	0.097(29)
H13	0.3284(96)	0.1615(118)	0.6868(71)	0.095(29)
H1'1	0.0941(57)	0.6890(72)	0.6625(44)	0.050(14)
H2'1	0.3020(67)	0.7721(84)	0.7893(48)	0.063(17)
H2'2	0.1702(59)	0.8096(95)	0.8674(43)	0.058(15)
H3'1	0.2141(59)	0.5344(74)	0.9152(46)	0.047(14)
H4'1	0.0147(55)	0.4143(76)	0.8135(39)	0.043(13)
H5'1	-0.1651(81)	0.4839(99)	0.9062(54)	0.074(20)
H5'2	-0.0106(79)	0.4153(106)	0.9688(51)	0.073(20)
H5O'	-0.0258(192)	0.6656(26)	1.0284(9)	0.248(106)
H4N	-0.1607(85)	1.3564(119)	0.5785(61)	0.092(26)
H51	-0.2090(65)	1.1381(80)	0.7787(47)	0.049(14)
H61	-0.0956(50)	0.9030(65)	0.8182(36)	0.035(11)
H71	0.4605(40)	0.3425(71)	1.1134(28)	0.176(52)
H72	0.3934(56)	0.2048(57)	1.0759(24)	0.152(49)
H73	0.3341(54)	0.3571(69)	1.0601(17)	0.058(17)
H101	-0.1434(64)	1.6539(83)	0.5527(44)	0.053(15)
H111	-0.2250(69)	1.8860(89)	0.5027(49)	0.062(19)
H121	-0.4545(8)	2.0015(9)	0.5268(5)	0.103(29)
H131	-0.5893(76)	1.8712(95)	0.6147(52)	0.076(20)
H141	-0.5053(61)	1.5883(76)	0.6892(44)	0.048(14)

Anisotropic displacement coefficients ($Å^2$) *for non-hydrogen atoms in* **FAST-4 (R=H,B=C^{Bz})**

P1	0.0484(5)	0.0383(5)	0.0458(5)	0.0029(4)	0.0106(4)	0.0027(4)
Se1	0.0589(3)	0.0694(4)	0.0630(3)	0.0004(3)	-0.0008(2)	0.0006(3)
O1	0.068(2)	0.055(2)	0.064(2)	0.008(2)	0.018(2)	-0.009(2)
C1	0.069(3)	0.056(3)	0.065(3)	-0.006(3)	0.019(3)	0.005(3)
C1'	0.054(2)	0.037(2)	0.043(2)	0.006(2)	0.008(2)	0.006(2)
C2'	0.045(2)	0.041(2)	0.065(3)	-0.001(2)	0.003(2)	-0.002(2)
C3'	0.048(2)	0.046(2)	0.038(2)	0.002(2)	0.001(2)	0.006(2)
O3'	0.058(2)	0.048(2)	0.048(2)	0.0071(13)	0.0108(14)	0.0111(14)
C4'	0.055(2)	0.036(2)	0.045(2)	0.005(2)	0.011(2)	0.003(2)
O4'	0.052(2)	0.048(2)	0.065(2)	0.018(2)	-0.0102(15)	-0.0061(15)
C5'	0.074(4)	0.064(3)	0.067(3)	0.001(3)	0.030(3)	-0.003(3)
O5'	0.114(4)	0.094(4)	0.089(3)	-0.039(3)	0.055(3)	-0.025(3)
N1	0.054(2)	0.039(2)	0.033(2)	0.0028(13)	0.0115(14)	0.0040(15)
C2	0.044(2)	0.038(2)	0.039(2)	0.008(2)	0.009(2)	0.003(2)
O2	0.071(2)	0.055(2)	0.049(2)	0.0086(15)	0.026(2)	0.023(2)
N3	0.049(2)	0.038(2)	0.039(2)	0.0052(13)	0.0128(14)	0.0049(14)
C4	0.043(2)	0.039(2)	0.036(2)	-0.0001(15)	0.0088(15)	0.000(2)
N4	0.051(2)	0.041(2)	0.040(2)	0.003(2)	0.0145(13)	0.008(2)
C5	0.057(3)	0.051(2)	0.042(2)	0.005(2)	0.020(2)	0.009(2)
C6	0.065(3)	0.051(3)	0.039(2)	0.007(2)	0.015(2)	0.009(2)
C7	0.092(4)	0.085(5)	0.062(3)	-0.003(3)	0.002(3)	0.003(4)
C8	0.044(2)	0.044(2)	0.046(2)	0.000(2)	0.012(2)	0.003(2)
O8	0.068(2)	0.064(2)	0.061(2)	0.010(2)	0.032(2)	0.011(2)
C9	0.046(2)	0.046(2)	0.041(2)	-0.006(2)	0.000(2)	0.006(2)
C10	0.062(3)	0.046(2)	0.042(2)	-0.003(2)	0.003(2)	0.010(2)
C11	0.087(3)	0.052(3)	0.050(2)	0.002(2)	-0.002(2)	0.001(3)
C12	0.095(4)	0.056(3)	0.069(3)	-0.010(3)	-0.019(3)	0.029(3)
C13	0.072(3)	0.059(3)	0.080(4)	-0.017(3)	0.000(3)	0.026(3)
C14	0.056(3)	0.063(3)	0.061(3)	-0.008(2)	0.010(2)	0.012(2)

The form of the anisotropic displacement parameter is: $\exp[-2\pi^2 h^2 a^2 U_{11} + k^2 b^2 U_{22} + l^2 c^2 U_{33} + 2hkab U_{12} + 2hlac U_{13} + 2klbc U_{23})]$ where a, b, c are reciprocal lattice constants.

Bond lengths (Å) *for non-hydrogen atoms in* **FAST-4 (R=H,B=C^{Bz})**

P1	O1	1.471(4)
P1	O3'	1.588(3)
P1	C1	1.773(6)
P1	Se1	2.2225(15)
Se1	C7	1.938(7)
C1'	O4'	1.405(6)
C1'	N1	1.466(5)
C1'	C2'	1.517(7)
C2'	C3'	1.519(6)
C3'	O3'	1.454(5)
C3'	C4'	1.529(7)
C4'	O4'	1.427(5)
C4'	C5'	1.490(7)
C5'	O5'	1.416(8)
N1	C2	1.401(5)
N1	C6	1.349(6)
C2	O2	1.237(5)
C2	N3	1.352(5)
N3	C4	1.317(5)
C4	N4	1.389(6)
C4	C5	1.415(6)
C5	C6	1.341(7)
N4	C8	1.374(5)
O8	C8	1.239(6)
C8	C9	1.476(6)
C9	C10	1.390(7)
C9	C14	1.402(7)
C10	C11	1.392(8)
C11	C12	1.399(9)
C12	C13	1.353(11)
C13	C14	1.377(9)

Bond lengths (Å) *involving hydrogen atoms in* **FAST-4 (R=H,B=C^{Bz})**

C1	H11	0.91(10)
C1	H12	0.80(10)
C1	H13	0.87(10)
C1'	H1'1	1.04(6)
C2'	H2'1	1.15(6)
C2'	H2'2	0.98(7)
C3'	H3'1	0.87(6)
C4'	H4'1	0.85(6)
C5'	H5'1	1.04(8)
C5'	H5'2	1.14(8)
O5'	H5O'	0.82
N4	H4N	0.72(8)
C5	H51	0.77(7)
C6	H61	0.84(5)
C7	H71	0.83(5)
C7	H72	0.83(5)
C7	H73	0.83(5)
C10	H101	0.96(6)
C11	H111	0.81(7)
C12	H121	0.93
C13	H131	0.98(7)
C14	H141	0.95(6)

Bond angles (°) for non-hydrogen atoms in **FAST-4 (R=H,B=C^{Bz})**

O1	P1	O3'	114.1(2)
O1	P1	C1	115.3(3)
O3'	P1	C1	100.7(3)
O1	P1	Se1	111.6(2)
O3'	P1	Se1	107.02(15)
C1	P1	Se1	107.2(3)
C7	Se1	P1	97.5(2)
O4'	C1'	N1	107.6(3)
O4'	C1'	C2'	105.8(3)
N1	C1'	C2'	114.6(4)
C1'	C2'	C3'	102.1(4)
O3'	C3'	C2'	107.4(4)
O3'	C3'	C4'	109.8(4)
C2'	C3'	C4'	103.7(4)
C3'	O3'	P1	119.2(3)
O4'	C4'	C5'	109.2(4)
O4'	C4'	C3'	106.0(4)
C5'	C4'	C3'	116.1(5)
C1'	O4'	C4'	111.2(3)
O5'	C5'	C4'	108.5(5)
C2	N1	C6	120.0(4)
C2	N1	C1'	119.0(3)
C6	N1	C1'	121.0(4)

O2	C2	N3	123.1(4)
O2	C2	N1	118.1(4)
N3	C2	N1	118.8(4)
C4	N3	C2	120.2(4)
N3	C4	N4	114.2(3)
N4	C4	C5	123.4(4)
N3	C4	C5	122.4(4)
C6	C5	C4	117.0(4)
C5	C6	N1	121.6(4)
C8	N4	C4	127.9(4)
O8	C8	N4	121.3(4)
O8	C8	C9	120.6(4)
N4	C8	C9	118.1(4)
C10	C9	C14	120.1(5)
C10	C9	C8	123.6(4)
C14	C9	C8	116.3(5)
C9	C10	C11	119.0(5)
C10	C11	C12	120.0(6)
C13	C12	C11	120.3(6)
C12	C13	C14	120.9(6)
C13	C14	C9	119.6(6)

Bond angles (°) *involving hydrogen atoms in* **FAST-4 (R=H,B=C^{Bz})**

P1	C1	H11	111.5(58)
P1	C1	H12	112.6(69)
H11	C1	H12	116.1(87)
P1	C1	H13	116.0(58)
H11	C1	H13	100.7(80)
H12	C1	H13	98.9(82)
O4'	C1'	H1'1	104.1(31)
N1	C1'	H1'1	102.9(32)
C2'	C1'	H1'1	120.9(31)
C1'	C2'	H2'1	113.0(33)
C3'	C2'	H2'1	116.2(33)
C1'	C2'	H2'2	110.6(33)
C3'	C2'	H2'2	106.5(40)
H2'1	C2'	H2'2	108.2(48)
O3'	C3'	H3'1	104.2(39)
C2'	C3'	H3'1	120.9(40)
C4'	C3'	H3'1	110.7(37)
O4'	C4'	H4'1	108.4(36)
C5'	C4'	H4'1	105.5(36)
C3'	C4'	H4'1	111.5(35)
O5'	C5'	H5'1	117.8(43)
C4'	C5'	H5'1	112.8(41)
O5'	C5'	H5'2	111.8(39)
C4'	C5'	H5'2	100.5(37)
H5'1	C5'	H5'2	104.1(58)
N1	C6	H61	112.9(34)
C5	C6	H61	125.3(34)
Se1	C7	H71	109.5(2)
Se1	C7	H72	109.5(3)
H71	C7	H72	109.5
Se1	C7	H73	109.5(3)
H71	C7	H73	109.5
H72	C7	H73	109.47(8)
C5'	O5'	H5O'	109.5(4)
C4	N4	H4N	109.3(74)
C8	N4	H4N	122.4(73)
C4	C5	H51	123.0(47)
C6	C5	H51	119.6(47)
C9	C10	H101	122.5(38)
C11	C10	H101	118.2(39)
C10	C11	H111	108.4(49)
C12	C11	H111	130.4(49)
C11	C12	H121	119.8(4)
C13	C12	H121	119.8(3)
C12	C13	H131	106.4(42)
C14	C13	H131	132.7(42)
C9	C14	H141	115.8(36)
C13	C14	H141	124.4(36)

Torsional angles (°) for non-hydrogen atoms in **FAST-4 (R=H,B=C^{Bz})**

O1	P1	Se1	C7	-23.3(3)
O3'	P1	Se1	C7	102.2(3)
C1	P1	Se1	C7	-150.4(4)
O4'	C1'	C2'	C3'	32.8(5)
N1	C1'	C2'	C3'	151.1(4)
C1'	C2'	C3'	O3'	85.7(4)
C1'	C2'	C3'	C4'	-30.5(4)
C2'	C3'	O3'	P1	159.4(3)
C4'	C3'	O3'	P1	-88.4(4)
O1	P1	O3'	C3'	46.6(4)
C1	P1	O3'	C3'	170.8(4)
Se1	P1	O3'	C3'	-77.4(3)
O3'	C3'	C4'	O4'	-96.1(4)
C2'	C3'	C4'	O4'	18.4(5)
O3'	C3'	C4'	C5'	142.5(4)
C2'	C3'	C4'	C5'	-103.0(5)
C5'	C4'	O4'	C1'	128.1(5)
C3'	C4'	O4'	C1'	2.4(5)
N1	C1'	O4'	C4'	-145.3(4)
C2'	C1'	O4'	C4'	-22.4(5)
O4'	C4'	C5'	O5'	-68.7(7)
C3'	C4'	C5'	O5'	51.0(7)
O4'	C1'	N1	C2	-136.2(4)
C2'	C1'	N1	C2	106.5(5)
O4'	C1'	N1	C6	41.7(6)
C2'	C1'	N1	C6	-75.5(5)
C6	N1	C2	O2	176.7(5)
C1'	N1	C2	O2	-5.3(6)
C6	N1	C2	N3	-2.3(7)
C1'	N1	C2	N3	175.6(4)
O2	C2	N3	C4	-178.5(5)
N1	C2	N3	C4	0.5(6)
C2	N3	C4	N4	-179.3(4)
C2	N3	C4	C5	0.8(7)
N4	C4	C5	C6	179.9(5)
N3	C4	C5	C6	-0.3(7)
C4	C5	C6	N1	-1.6(8)
C2	N1	C6	C5	2.9(8)
C1'	N1	C6	C5	-175.0(5)
C8	N4	C4	N3	-177.2(4)
C8	N4	C4	C5	2.6(7)
C4	N4	C8	O8	-4.4(8)
C4	N4	C8	C9	176.6(4)
O8	C8	C9	C10	155.0(5)
N4	C8	C9	C10	-25.9(7)
O8	C8	C9	C14	-23.6(7)
N4	C8	C9	C14	155.4(5)
C14	C9	C10	C11	0.3(7)
C8	C9	C10	C11	-178.2(5)
C9	C10	C11	C12	-0.3(8)
C10	C11	C12	C13	-1.1(9)
C11	C12	C13	C14	2.6(9)
C12	C13	C14	C9	-2.6(9)
C8	C9	C14	C13	179.8(5)
C10	C9	C14	C13	1.1(8)

Hydrogen-bonding geometry (Å, °) *in* **FAST-4 (R=H,B=C^{Bz})**

D–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
C1'–H1'1···O2	1.041(6)	2.25(6)	2.703(6)	104(4)
C2'–H2'2···O5'	0.984(7)	2.69(6)	3.173(9)	111(4)
C3'–H3'1···O5'	0.877(6)	2.78(6)	2.861(8)	87(4)
C4'–H4'1···O1	0.850(6)	2.78(6)	3.253(6)	116(4)
C4'–H4'1···O3'	0.850(6)	2.43(5)	2.441(6)	80(4)
C5'–H5'1···O8^{i}	1.040(8)	2.60(7)	3.428(8)	137(6)
C5'–H5'2···O5^{ii}	1.145(8)	2.11(8)	3.212(9)	164(6)
O5'–H5O'···O1^{iii}	0.820(2)	2.20(10)	2.697(8)	119(9)
C1–H12···O8^{iv}	0.805(10)	2.54(9)	3.169(8)	137(9)
N4–H4N···O2^{v}	0.722(8)	2.20(8)	2.916(5)	173(9)
N4–H4N···N3	0.722(8)	2.24(9)	2.273(5)	84(7)
C5–H51···O8	0.777(6)	2.30(6)	2.784(7)	122(6)
C6–H61···O4'	0.842(5)	2.42(5)	2.739(7)	103(4)
C6–H61···O5'	0.842(5)	2.75(5)	3.549(8)	158(4)
C10–H101···O2^{v}	0.965(6)	2.56(6)	3.080(6)	114(4)
C10–H101···N4	0.965(6)	2.74(6)	2.940(7)	92(4)
C10–H101···N3^{vi}	0.965(6)	2.76(6)	3.535(6)	139(5)
C13–H131···O2^{vii}	0.985(7)	2.66(7)	3.556(7)	153(6)
C14–H141···O8	0.950(6)	2.43(6)	2.776(7)	101(4)

Symmetry codes: (i) x, -1 + y, z; (ii) -x, -0.5 + y, 2 - z; (iii) -x, 0.5 + y, 2 - z; (iv) 1 + x, -1 + y, z; (v) -x, 0.5 + y, 1 - z; (vi) -x, 0.5 + y, 1 - z; (vii) -1 + x, 1 + y, z.

Asymmetry parameters of five-membered ring: C1',C2',C3',C4',O4' *in* **FAST-4 (R=H,B=C^{Bz})**

$\Delta C_s^{(C1')}$	21.2(9)
$\Delta C_s^{(C2')}$	3.3(9)
$\Delta C_s^{(C3')}$	26.3(9)
$\Delta C_s^{(C4')}$	40.2(9)
$\Delta C_s^{(O4')}$	38.9(9)
$\Delta C_2^{(C1'-C2')}$	12.7(9)
$\Delta C_2^{(C2'-C3')}$	20.3(9)
$\Delta C_2^{(C3'-C4')}$	45.4(9)
$\Delta C_2^{(C4'-O4')}$	53.3(9)
$\Delta C_2^{(O4'-C1')}$	40.7(9)

Dihedral angles between least-squares planes in **FAST-4 (R=H,B=C^{Bz})**:

Plane1: C1',C3',C4',O4'
Plane2: C1',C2',C3'
Plane3: N1,C2,N3,C4,C5,C6
Plane4: C9,C10,C11,C12,C13,C14

Plane1/Plane2	32.4(3)
Plane1/Plane3	60.0(2)
Plane2/Plane3	89.4(2)
Plane1/Plane4	39.4(2)
Plane2/Plane4	67.0(2)
Plane3/Plane4	24.8(1)

Crystal data and Structure Solution and Refinement for **FAST-5 (R=Px,B=Thy)**

Molecular formula		$C_{37}H_{45}N_2O_7PS$
Formula_weight		692.78
Crystallographic system		monoclinic
Space group		$P2_1$
a (Å)		18.828(10)
b (Å)		9.007(4)
c (Å)		23.899(9)
β (°)		105.89(3)
V (Å^3)		3897.9(31)
Z		4
D_c (g/cm^3)		1.181
μ [cm^{-1}]		15.06
Crystal dimensions (mm)		0.03x0.28x0.65
Maximum 2θ (°)		146
Radiation, λ (Å)		CuKα, 1.54178
Scan mode		ω/2θ
Scan width (°)		1.25+0.14·tanθ
hkl ranges:	*h* =	-23 23
	k =	-11 0
	l =	-29 29
DECAY correction:	min:	1.00008
	max:	1.06098
	ave:	1.02954
EAC correction:	min:	0.9026
	max:	0.9994
	ave:	0.9782
No. of reflections:	unique	8256
	refine with $I>0\sigma(I)$	6979
	observed with $I>2\sigma(I)$	4267
No. of parameters refined		858
No. of restraints		18
Largest diff. peak (eÅ^{-3})		0.430
Largest diff. hole (eÅ^{-3})		-0.252
R_{obs}		0.0626
wR_{obs}		0.1379
weighting coeff.*	m	0.0782
extinction coeff.**	k	0.00085(12)
S_{obs}		1.144
shift/esd max		-0.001
R_{int}		0.0873
$T_{meas.}$		293(2)
F_000		1472
Absolute structure		$R_{C1'}$, $S_{C3'}$, $R_{C4'}$, S_{P1}
Flack parameter x		0.01(3)

* weighting scheme $w=[\sigma^2(Fo^2)+(mP)^2]^{-1}$ where $P=(Fo^2+2Fc^2)/3$

** extinction method SHELXL, extinction expression $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Fractional atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) *for non-H atoms in molecules* **a** *of* **FAST-5 (R=Px,B=Thy)**

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i \mathbf{a}_j$

	x	*y*	*z*	U_{eq} or [U_{iso}]
P1	-0.20412(10)	0.3042	-0.68878(7)	0.0689(5)
S1	-0.2596(2)	0.3014(4)	-0.62605(11)	0.1130(8)
O1	-0.1632(3)	0.4457(6)	-0.6837(2)	0.075(2)
C1	-0.2648(4)	0.2673(12)	-0.7577(3)	0.106(4)
C1'	-0.0079(4)	0.0113(9)	-0.5614(2)	0.057(2)
C2'	-0.0820(4)	0.0910(9)	-0.5809(3)	0.061(2)
C3'	-0.0826(3)	0.1536(8)	-0.6398(2)	0.052(2)
O3'	-0.1545(2)	0.1592(6)	-0.6808(2)	0.0613(13)
C4'	-0.0364(3)	0.0412(8)	-0.6614(2)	0.048(2)
O4'	0.0184(2)	-0.0020(5)	-0.6113(2)	0.0556(11)
C5'	-0.0019(4)	0.0919(8)	-0.7073(2)	0.055(2)
O5'	0.0316(2)	0.2332(5)	-0.6887(2)	0.0535(11)
N1	0.0500(3)	0.0901(6)	-0.5171(2)	0.0514(13)
C2	0.0663(4)	0.0390(8)	-0.4612(3)	0.058(2)
O2	0.0313(3)	-0.0610(7)	-0.4467(2)	0.080(2)
N3	0.1222(3)	0.1115(7)	-0.4228(2)	0.061(2)
C4	0.1645(4)	0.2244(9)	-0.4355(3)	0.062(2)
O4	0.2143(3)	0.2757(7)	-0.3961(2)	0.087(2)
C5	0.1452(4)	0.2717(8)	-0.4951(3)	0.057(2)
C6	0.0907(4)	0.2050(8)	-0.5327(3)	0.059(2)
C7	-0.3033(6)	0.1195(15)	-0.6373(6)	0.146(5)
C8	0.1872(5)	0.3939(10)	-0.5132(3)	0.086(3)
C9	0.0607(4)	0.3086(8)	-0.7308(2)	0.057(2)
C10	0.0042(4)	0.3281(8)	-0.7879(3)	0.059(2)
C11	-0.0677(5)	0.3750(9)	-0.7892(3)	0.075(2)
C12	-0.1216(5)	0.3931(9)	-0.8411(4)	0.086(3)
C13	-0.1045(7)	0.3651(10)	-0.8927(4)	0.091(3)
C14	-0.0353(6)	0.3164(10)	-0.8932(3)	0.082(2)
C15	0.0178(5)	0.2979(9)	-0.8399(3)	0.066(2)
O16	0.0859(3)	0.2525(7)	-0.8440(2)	0.0795(15)
C17	0.1351(4)	0.2024(9)	-0.7944(3)	0.068(2)
C18	0.1262(4)	0.2233(8)	-0.7394(3)	0.060(2)
C19	0.1783(5)	0.1654(11)	-0.6923(4)	0.081(2)
C20	0.2398(6)	0.0915(13)	-0.7005(5)	0.105(3)
C21	0.2494(6)	0.0766(13)	-0.7549(6)	0.113(4)
C22	0.1964(6)	0.1298(11)	-0.8023(5)	0.096(3)
C23	0.0853(4)	0.4627(8)	-0.7033(3)	0.065(2)
C24	0.0521(5)	0.5230(9)	-0.6653(3)	0.077(2)
C25	0.0701(6)	0.6680(10)	-0.6432(4)	0.096(3)
C26	0.1248(6)	0.7451(11)	-0.6598(4)	0.097(3)
C27	0.1587(6)	0.6803(11)	-0.6975(5)	0.105(4)
C28	0.1399(5)	0.5409(10)	-0.7198(3)	0.079(2)
C1"	0.3190(26)	-0.2100(53)	-0.5319(20)	[0.568(34)]
C2"	0.2925(20)	-0.0441(48)	-0.5187(16)	[0.421(21)]
C3"	0.3769(29)	0.0182(58)	-0.5036(23)	[0.603(40)]
C4"	0.3857(30)	0.1252(67)	-0.4550(22)	[0.603(41)]
C5"	0.4408(37)	0.2478(71)	-0.4599(27)	[0.697(50)]
C6"	0.4443(38)	0.3524(72)	-0.4051(23)	[0.735(55)]

Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) *for non-H atoms in molecules* **b** *of* **FAST-5 (R=Px,B=Thy)**

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i \mathbf{a}_j$

	x	*y*	*z*	U_{eq} or $[U_{iso}]$
P1b	0.70593(9)	-0.2130(3)	0.19576(6)	0.0574(5)
S1b	0.62388(13)	-0.1858(4)	0.23652(10)	0.0985(7)
O1b	0.6993(3)	-0.3453(6)	0.1592(2)	0.0667(13)
C1b	0.7925(4)	-0.1990(11)	0.2487(3)	0.079(2)
C1'b	0.5805(3)	0.1037(9)	0.0301(3)	0.058(2)
C2'b	0.5876(4)	0.0167(9)	0.0864(3)	0.064(2)
C3'b	0.6651(3)	-0.0441(8)	0.1014(2)	0.0482(15)
O3'b	0.7000(3)	-0.0591(6)	0.1624(2)	0.0599(13)
C4'b	0.7064(3)	0.0778(8)	0.0778(2)	0.0463(14)
O4'b	0.6527(2)	0.1289(5)	0.0265(2)	0.0565(11)
C5'b	0.7762(4)	0.0347(7)	0.0647(3)	0.053(2)
O5'b	0.7637(2)	-0.1064(5)	0.0371(2)	0.0497(10)
N1b	0.5402(3)	0.0277(7)	-0.0241(2)	0.0559(14)
C2b	0.4700(4)	0.0746(9)	-0.0508(3)	0.061(2)
O2b	0.4385(3)	0.1689(8)	-0.0293(2)	0.087(2)
N3b	0.4373(3)	0.0086(7)	-0.1022(2)	0.064(2)
C4b	0.4678(4)	-0.0999(9)	-0.1297(3)	0.062(2)
O4b	0.4324(3)	-0.1466(7)	-0.1769(2)	0.096(2)
C5b	0.5414(4)	-0.1445(8)	-0.0992(3)	0.055(2)
C6b	0.5730(4)	-0.0812(8)	-0.0484(3)	0.056(2)
C7b	0.6373(6)	-0.3548(14)	0.2811(4)	0.122(4)
C8b	0.5772(5)	-0.2648(10)	-0.1251(4)	0.087(3)
C9b	0.8255(3)	-0.1666(7)	0.0201(2)	0.0445(14)
C10b	0.8931(3)	-0.1665(7)	0.0709(3)	0.052(2)
C11b	0.8940(4)	-0.2431(9)	0.1220(3)	0.061(2)
C12b	0.9528(5)	-0.2384(9)	0.1712(3)	0.077(2)
C13b	1.0146(5)	-0.1527(9)	0.1691(4)	0.075(2)
C14b	1.0162(4)	-0.0776(9)	0.1199(3)	0.068(2)
C15b	0.9561(3)	-0.0844(8)	0.0706(3)	0.058(2)
O16b	0.9634(3)	-0.0059(6)	0.0240(2)	0.0719(14)
C17b	0.9053(4)	-0.0035(8)	-0.0248(3)	0.059(2)
C18b	0.8396(4)	-0.0746(7)	-0.0293(3)	0.052(2)
C19b	0.7845(4)	-0.0617(8)	-0.0803(3)	0.061(2)
C20b	0.7946(5)	0.0238(10)	-0.1266(3)	0.076(2)
C21b	0.8621(5)	0.0940(9)	-0.1201(4)	0.079(2)
C22b	0.9156(5)	0.0813(9)	-0.0707(4)	0.070(2)
C23b	0.8031(3)	-0.3261(7)	-0.0005(2)	0.0466(14)
C24b	0.7419(4)	-0.3917(8)	0.0096(3)	0.063(2)
C25b	0.7226(5)	-0.5381(9)	-0.0099(3)	0.074(2)
C26b	0.7646(5)	-0.6133(9)	-0.0388(3)	0.071(2)
C27b	0.8260(6)	-0.5490(9)	-0.0470(3)	0.079(2)
C28b	0.8459(5)	-0.4047(9)	-0.0283(3)	0.066(2)
C1"b	0.5815(15)	0.2674(39)	-0.1343(12)	[0.351(15)]
C2"b	0.6033(18)	0.2819(40)	-0.1883(13)	[0.351(15)]
C3"b	0.5916(21)	0.1167(43)	-0.2125(13)	[0.381(18)]
C4"b	0.6006(26)	0.1045(51)	-0.2709(17)	[0.511(30)]
C5"b	0.6017(31)	-0.0553(68)	-0.2901(25)	[0.657(45)]
C6"b	0.5219(29)	-0.1268(63)	-0.3110(21)	[0.605(37)]

Fractional atomic coordinates and isotropic thermal parameters ($Å^2$) *for H atoms in molecules* **a** *of* **FAST-5 (R=Px,B=Thy)**

	x	*y*	*z*	U_{iso}
H11	-0.2833(37)	0.1851(68)	-0.7575(11)	0.141
H12	-0.2420(18)	0.2692(94)	-0.7823(17)	0.141
H13	-0.2974(35)	0.3302(68)	-0.7654(17)	0.141
H1'1	-0.0147(7)	-0.0809(83)	-0.5480(12)	0.076
H2'1	-0.1204(21)	0.0260(35)	-0.5839(3)	0.081
H2'2	-0.0850(4)	0.1654(41)	-0.5554(14)	0.081
H3'1	-0.0620(18)	0.2397(76)	-0.6362(4)	0.070
H4'1	-0.0646(23)	-0.0374(64)	-0.6749(11)	0.064
H5'1	0.0373(17)	0.0169(34)	-0.7119(4)	0.073
H5'2	-0.0412(17)	0.1020(8)	-0.7465(18)	0.073
H3N	0.1322(9)	0.0839(23)	-0.3867(29)	0.081
H61	0.0787(10)	0.2351(24)	-0.5710(29)	0.078
H71	-0.3324(42)	0.1062(41)	-0.6107(31)	0.195
H72	-0.2662(24)	0.0444(52)	-0.6310(35)	0.195
H73	-0.3342(42)	0.1126(37)	-0.6762(28)	0.195
H81	0.1880(26)	0.4702(43)	-0.4911(19)	0.114
H82	0.1661(21)	0.4177(46)	-0.5489(19)	0.114
H83	0.2318(23)	0.3649(26)	-0.5101(22)	0.114
H111	-0.0794(11)	0.3945(19)	-0.7536(30)	0.100
H121	-0.1747(48)	0.4276(32)	-0.8414(4)	0.114
H131	-0.1417(37)	0.3800(18)	-0.9292(35)	0.121
H141	-0.0241(13)	0.2963(22)	-0.9283(32)	0.109
H191	0.1715(7)	0.1774(14)	-0.6483(34)	0.107
H201	0.2816(38)	0.0439(45)	-0.6623(35)	0.140
H211	0.2978(55)	0.0239(60)	-0.7606(8)	0.151
H221	0.2019(7)	0.1166(17)	-0.8410(40)	0.127
H241	0.0144(34)	0.4648(53)	-0.6527(12)	0.103
H251	0.0413(26)	0.7186(44)	-0.6134(26)	0.128
H261	0.1383(17)	0.8400(119)	-0.6455(18)	0.129
H271	0.1886(47)	0.7224(66)	-0.7063(14)	0.140
H281	0.1595(23)	0.5062(40)	-0.7414(24)	0.105
H1"1	0.2768(26)	-0.2746(53)	-0.5426(20)	0.755
H1"2	0.3537(26)	-0.2479(53)	-0.4976(20)	0.755
H1"3	0.3419(26)	-0.2051(53)	-0.5631(20)	0.755
H2"1	0.2596(20)	0.0028(48)	-0.5525(16)	0.559
H2"2	0.2717(20)	-0.0408(48)	-0.4858(16)	0.559
H3"1	0.4118(29)	-0.0628(58)	-0.4922(23)	0.802
H3"2	0.3855(29)	0.0670(58)	-0.5373(23)	0.802
H4"1	0.4036(30)	0.0738(67)	-0.4182(22)	0.803
H4"2	0.3383(30)	0.1693(67)	-0.4563(22)	0.803
H5"1	0.4232(37)	0.3024(71)	-0.4961(27)	0.927
H5"2	0.4889(37)	0.2062(71)	-0.4579(27)	0.927
H6"1	0.4779(38)	0.4329(72)	-0.4047(23)	0.978
H6"2	0.4612(38)	0.2958(72)	-0.3700(23)	0.978
H6"3	0.3960(38)	0.3913(72)	-0.4078(23)	0.978

Fractional atomic coordinates and isotropic thermal parameters (Å^2) *for H atoms in molecules* **b** *of* **FAST-5 (R=Px,B=Thy)**

	x	*y*	*z*	U_{iso}
H1B	0.7900(10)	-0.1209(51)	0.2770(19)	0.105
H1C	0.8310(18)	-0.1736(60)	0.2295(9)	0.105
H1D	0.8046(15)	-0.2947(46)	0.2691(17)	0.105
H1'B	0.5558(20)	0.2029(79)	0.0327(3)	0.077
H2'B	0.5812(5)	0.0781(34)	0.1155(16)	0.086
H2'C	0.5534(19)	-0.0590(43)	0.0806(4)	0.086
H3'B	0.6666(3)	-0.1440(66)	0.0799(14)	0.064
H4'B	0.7172(8)	0.1596(57)	0.1061(20)	0.062
H5'B	0.7897(8)	0.1096(33)	0.0384(11)	0.070
H5'C	0.8174(19)	0.0286(7)	0.1014(16)	0.070
H3NB	0.3935(40)	0.0364(26)	-0.1194(15)	0.085
H6B	0.6254(36)	-0.1158(25)	-0.0259(16)	0.075
H7B	0.6023(33)	-0.3565(41)	0.3038(27)	0.163
H7C	0.6867(31)	-0.3561(41)	0.3066(27)	0.163
H7D	0.6300(39)	-0.4407(52)	0.2561(14)	0.163
H8B	0.5425(19)	-0.3536(45)	-0.1353(21)	0.116
H8C	0.6252(26)	-0.2964(44)	-0.0959(15)	0.116
H8D	0.5885(26)	-0.2262(25)	-0.1619(20)	0.116
H11B	0.8533(35)	-0.2994(49)	0.1227(3)	0.082
H12B	0.9515(5)	-0.2982(48)	0.2101(31)	0.102
H13B	1.0584(36)	-0.1467(10)	0.2045(29)	0.100
H14B	1.0610(38)	-0.0169(52)	0.1191(3)	0.091
H19B	0.7346(37)	-0.1163(40)	-0.0848(4)	0.081
H20B	0.7503(32)	0.0351(13)	-0.1670(29)	0.101
H21B	0.8707(9)	0.1561(54)	-0.1536(29)	0.105
H22B	0.9621(41)	0.1313(43)	-0.0667(5)	0.094
H24B	0.7118(24)	-0.3373(44)	0.0302(17)	0.084
H25B	0.6860(39)	-0.5782(42)	-0.0037(7)	0.098
H26B	0.7498(14)	-0.7173(97)	-0.0542(14)	0.094
H27B	0.8527(29)	-0.5974(52)	-0.0639(18)	0.105
H28B	0.8943(38)	-0.3554(39)	-0.0354(6)	0.088
H1"B	0.5862(15)	0.3619(39)	-0.1150(12)	0.467
H1"C	0.6129(15)	0.1963(39)	-0.1094(12)	0.467
H1"D	0.5312(15)	0.2346(39)	-0.1431(12)	0.467
H2"B	0.6544(18)	0.3129(40)	-0.1809(13)	0.467
H2"C	0.5719(18)	0.3515(40)	-0.2149(13)	0.467
H3"B	0.6269(21)	0.0519(43)	-0.1866(13)	0.507
H3"C	0.5425(21)	0.0836(43)	-0.2130(13)	0.507
H4"B	0.6465(26)	0.1522(51)	-0.2720(17)	0.679
H4"C	0.5604(26)	0.1564(51)	-0.2980(17)	0.679
H5"B	0.6315(31)	-0.1132(68)	-0.2580(25)	0.874
H5"C	0.6248(31)	-0.0602(68)	-0.3217(25)	0.874
H6"B	0.5259(29)	-0.2278(63)	-0.3226(21)	0.805
H6"C	0.4924(29)	-0.0715(63)	-0.3434(21)	0.805
H6"D	0.4991(29)	-0.1244(63)	-0.2797(21)	0.805

Anisotropic displacement coefficients ($Å^2$) *for non-hydrogen atoms for non-H atoms in molecule* **a** *of* **FAST-5 (R=Px,B=Thy)**

P1	0.0705(11)	0.0650(12)	0.0569(9)	-0.0119(10)	-0.0067(8)	0.0181(11)
S1	0.121(2)	0.105(2)	0.124(2)	-0.017(2)	0.051(2)	0.016(2)
O1	0.097(4)	0.053(3)	0.058(3)	-0.010(2)	-0.007(3)	0.008(3)
C1	0.084(6)	0.095(7)	0.103(6)	-0.031(6)	-0.036(5)	0.014(6)
C1'	0.068(4)	0.053(4)	0.041(3)	0.004(3)	-0.002(3)	-0.004(3)
C2'	0.064(4)	0.068(5)	0.050(4)	-0.001(3)	0.013(3)	-0.006(4)
C3'	0.060(4)	0.043(4)	0.048(3)	-0.003(3)	0.005(3)	-0.002(3)
O3'	0.058(3)	0.057(3)	0.054(3)	-0.010(2)	-0.009(2)	0.009(2)
C4'	0.055(4)	0.037(3)	0.046(3)	-0.003(3)	0.001(3)	0.001(3)
O4'	0.067(3)	0.050(3)	0.045(2)	0.002(2)	0.005(2)	0.008(2)
C5'	0.073(4)	0.040(4)	0.045(3)	0.000(3)	0.007(3)	0.009(3)
O5'	0.078(3)	0.037(2)	0.044(2)	-0.004(2)	0.015(2)	-0.011(2)
N1	0.065(3)	0.048(3)	0.036(2)	0.006(2)	0.004(2)	-0.005(3)
C2	0.079(5)	0.050(4)	0.040(3)	0.003(3)	0.010(3)	0.009(4)
O2	0.103(4)	0.074(4)	0.056(3)	0.019(3)	0.009(3)	-0.028(3)
N3	0.076(4)	0.061(4)	0.036(3)	0.006(3)	-0.001(2)	-0.012(3)
C4	0.072(4)	0.055(4)	0.053(4)	-0.002(3)	0.004(3)	-0.001(4)
O4	0.099(4)	0.079(4)	0.066(3)	0.000(3)	-0.006(3)	-0.022(4)
C5	0.064(4)	0.049(4)	0.054(3)	0.004(3)	0.009(3)	-0.002(4)
C6	0.076(5)	0.052(4)	0.050(3)	0.014(3)	0.019(3)	0.002(4)
C7	0.123(9)	0.129(11)	0.202(13)	0.015(10)	0.069(9)	-0.005(9)
C8	0.104(6)	0.079(6)	0.068(5)	0.006(4)	0.015(4)	-0.018(5)
C9	0.077(4)	0.041(4)	0.048(3)	-0.002(3)	0.011(3)	0.000(4)
C10	0.081(5)	0.039(4)	0.053(3)	0.008(3)	0.013(3)	-0.001(4)
C11	0.097(6)	0.059(5)	0.064(4)	0.010(4)	0.010(4)	0.002(4)
C12	0.088(6)	0.053(5)	0.097(6)	0.023(5)	-0.005(5)	-0.010(4)
C13	0.128(9)	0.054(5)	0.069(5)	0.022(4)	-0.008(6)	-0.020(5)
C14	0.123(7)	0.062(5)	0.056(4)	0.005(4)	0.016(4)	-0.018(6)
C15	0.095(5)	0.050(4)	0.047(3)	-0.005(4)	0.011(3)	-0.016(4)
O16	0.105(4)	0.079(4)	0.059(3)	-0.005(3)	0.029(3)	-0.017(3)
C17	0.081(5)	0.056(5)	0.075(5)	-0.009(4)	0.032(4)	-0.013(4)
C18	0.067(4)	0.057(4)	0.057(4)	0.002(3)	0.018(3)	0.001(4)
C19	0.076(5)	0.089(6)	0.076(5)	-0.002(5)	0.019(4)	0.012(5)
C20	0.100(7)	0.102(8)	0.107(7)	0.002(6)	0.019(6)	0.017(6)
C21	0.094(7)	0.098(8)	0.153(10)	-0.032(8)	0.042(7)	0.018(7)
C22	0.107(8)	0.087(7)	0.108(7)	-0.036(6)	0.055(6)	-0.027(6)
C23	0.090(5)	0.043(4)	0.051(4)	0.006(3)	0.001(4)	-0.004(4)
C24	0.114(7)	0.045(4)	0.078(5)	-0.008(4)	0.037(5)	-0.007(5)
C25	0.152(9)	0.048(5)	0.089(6)	-0.011(4)	0.035(6)	0.008(6)
C26	0.118(8)	0.045(5)	0.111(7)	0.003(5)	0.001(6)	-0.009(5)
C27	0.125(9)	0.065(6)	0.128(8)	-0.002(6)	0.037(7)	-0.032(6)
C28	0.099(6)	0.063(5)	0.076(5)	-0.008(4)	0.026(4)	-0.014(5)

The form of the anisotropic displacement parameter is: $\exp[-2\pi^2 h^2 a^2 U_{11} + k^2 b^2 U_{22} + l^2 c^2 U_{33} + +2hkab U_{12} + 2hlac U_{13} + 2klbc U_{23})]$ where a, b, c are reciprocal lattice constants.

Anisotropic displacement coefficients (Å^2) *for non-hydrogen atoms for non-H atoms in molecule* **b** *of* **FAST-5 (R=Px,B=Thy)**

P1b	0.0588(9)	0.0581(11)	0.0479(8)	0.0007(9)	0.0023(7)	-0.0065(10)
S1b	0.0964(15)	0.110(2)	0.0977(14)	0.013(2)	0.0417(12)	0.007(2)
O1b	0.064(3)	0.061(3)	0.064(3)	-0.005(2)	-0.002(2)	-0.009(3)
C1b	0.077(5)	0.076(5)	0.065(4)	-0.003(4)	-0.012(3)	-0.009(5)
C1'b	0.043(4)	0.061(4)	0.061(4)	-0.008(3)	0.000(3)	0.013(3)
C2'b	0.060(4)	0.074(5)	0.054(4)	-0.010(4)	0.007(3)	0.009(4)
C3'b	0.044(3)	0.053(4)	0.043(3)	-0.006(3)	0.004(2)	0.001(3)
O3'b	0.077(3)	0.053(3)	0.039(2)	-0.001(2)	-0.001(2)	-0.009(2)
C4'b	0.050(3)	0.042(3)	0.043(3)	-0.002(3)	0.006(3)	-0.003(3)
O4'b	0.058(3)	0.049(3)	0.054(2)	0.009(2)	0.002(2)	0.004(2)
C5'b	0.058(4)	0.033(3)	0.063(4)	-0.009(3)	0.009(3)	-0.011(3)
O5'b	0.049(2)	0.034(2)	0.067(3)	-0.008(2)	0.017(2)	-0.003(2)
N1b	0.044(3)	0.057(3)	0.060(3)	-0.004(3)	0.002(2)	0.013(3)
C2b	0.051(4)	0.070(5)	0.055(4)	-0.004(4)	0.005(3)	0.015(4)
O2b	0.069(3)	0.100(4)	0.083(3)	-0.018(3)	0.004(3)	0.036(3)
N3b	0.057(3)	0.064(4)	0.060(3)	0.002(3)	-0.005(3)	0.006(3)
C4b	0.052(4)	0.067(5)	0.059(4)	-0.005(4)	0.001(3)	0.001(4)
O4b	0.076(3)	0.101(5)	0.087(3)	-0.028(3)	-0.017(3)	0.013(3)
C5b	0.058(4)	0.052(4)	0.053(3)	-0.002(3)	0.008(3)	-0.002(3)
C6b	0.050(4)	0.055(4)	0.063(4)	-0.007(3)	0.014(3)	0.010(3)
C7b	0.152(10)	0.124(9)	0.109(7)	0.022(7)	0.066(7)	-0.020(8)
C8b	0.070(5)	0.079(6)	0.102(6)	-0.029(5)	0.006(4)	0.014(4)
C9b	0.047(3)	0.033(3)	0.054(3)	-0.003(3)	0.015(3)	-0.001(3)
C10b	0.054(4)	0.042(4)	0.060(4)	-0.009(3)	0.017(3)	0.000(3)
C11b	0.056(4)	0.052(4)	0.070(4)	0.001(3)	0.007(3)	0.004(3)
C12b	0.096(6)	0.054(5)	0.066(4)	0.000(4)	-0.002(4)	0.009(5)
C13b	0.067(5)	0.060(5)	0.081(5)	-0.025(4)	-0.010(4)	0.013(4)
C14b	0.057(4)	0.059(5)	0.081(5)	-0.018(4)	0.008(4)	0.000(4)
C15b	0.053(4)	0.047(4)	0.071(4)	-0.023(3)	0.013(3)	-0.001(3)
O16b	0.061(3)	0.074(4)	0.083(3)	-0.001(3)	0.022(3)	-0.022(3)
C17b	0.064(4)	0.043(4)	0.081(5)	-0.008(4)	0.039(4)	-0.005(3)
C18b	0.060(4)	0.033(3)	0.068(4)	0.002(3)	0.024(3)	-0.001(3)
C19b	0.062(4)	0.049(4)	0.073(4)	0.006(4)	0.022(4)	-0.002(4)
C20b	0.085(6)	0.064(5)	0.076(5)	0.014(4)	0.019(4)	0.001(5)
C21b	0.119(7)	0.051(4)	0.076(5)	-0.003(4)	0.044(5)	-0.002(5)
C22b	0.082(5)	0.045(4)	0.098(6)	-0.005(4)	0.048(5)	-0.011(4)
C23b	0.051(4)	0.038(3)	0.049(3)	0.002(3)	0.009(3)	0.001(3)
C24b	0.063(4)	0.038(4)	0.096(5)	-0.005(4)	0.032(4)	-0.004(3)
C25b	0.071(5)	0.042(4)	0.103(6)	0.008(4)	0.015(4)	-0.009(4)
C26b	0.106(6)	0.038(4)	0.062(4)	-0.003(3)	0.011(4)	-0.006(4)
C27b	0.128(7)	0.046(4)	0.075(5)	-0.011(4)	0.047(5)	-0.002(5)
C28b	0.087(5)	0.048(4)	0.070(4)	0.000(4)	0.034(4)	0.000(4)

The form of the anisotropic displacement parameter is: $\exp[-2\pi^2 h^2 a^2 U_{11} + k^2 b^2 U_{22} + l^2 c^2 U_{33} + 2hkab U_{12} + 2hlac U_{13} + 2klbc U_{23})]$ where a, b, c are reciprocal lattice constants.

Bond lengths (Å) *for non-H atoms in* **FAST-5 (R=Px,B=Thy)**

		a	b
P1	O1	1.477(6)	1.462(5)
P1	O3'	1.587(5)	1.588(5)
P1	C1	1.760(7)	1.773(6)
P1	S1	2.048(3)	2.054(3)
S1	C7	1.820(13)	1.835(11)
C1'	O4'	1.417(7)	1.405(8)
C1'	N1	1.476(7)	1.477(8)
C1'	C2'	1.523(10)	1.531(9)
C2'	C3'	1.514(8)	1.506(9)
C3'	O3'	1.437(7)	1.433(6)
C3'	C4'	1.514(9)	1.539(9)
C4'	O4'	1.406(6)	1.434(6)
C4'	C5'	1.490(8)	1.483(9)
C5'	O5'	1.435(7)	1.422(7)
N1	C2	1.367(7)	1.367(8)
N1	C6	1.398(8)	1.370(8)
C2	O2	1.220(8)	1.226(8)
C2	N3	1.359(8)	1.353(8)
N3	C4	1.376(9)	1.388(9)
C4	O4	1.223(7)	1.217(7)
C4	C5	1.436(8)	1.434(9)
C5	C6	1.309(8)	1.326(8)
C5	C8	1.486(10)	1.498(10)
O5'	C9	1.441(7)	1.439(7)
C9	C10	1.493(8)	1.498(8)
C9	C18	1.514(10)	1.525(8)
C9	C23	1.551(9)	1.539(8)
C10	C15	1.364(9)	1.398(9)
C10	C11	1.411(10)	1.399(9)
C11	C12	1.381(10)	1.379(9)
C12	C13	1.379(12)	1.410(11)
C13	C14	1.378(12)	1.364(11)
C14	C15	1.397(10)	1.394(9)
C15	O16	1.374(9)	1.358(8)
O16	C17	1.366(9)	1.362(8)
C17	C18	1.382(9)	1.371(9)
C17	C22	1.383(12)	1.394(9)
C18	C19	1.378(10)	1.373(9)
C19	C20	1.395(13)	1.403(10)
C20	C21	1.368(13)	1.389(11)
C21	C22	1.375(13)	1.331(10)
C23	C24	1.349(10)	1.374(9)
C23	C28	1.389(11)	1.372(9)
C24	C25	1.415(11)	1.412(10)
C25	C26	1.387(13)	1.364(11)
C26	C27	1.368(13)	1.355(11)
C27	C28	1.372(12)	1.392(11)
C1"	C2"	1.63(4)	1.46(3)
C2"	C3"	1.63(4)	1.59(3)
C3"	C4"	1.48(4)	1.46(4)
C4"	C5"	1.54(5)	1.51(4)
C5"	C6"	1.60(4)	1.58(4)

Bond lengths (Å) *involving H atoms in* **FAST-5 (R=Px,B=Thy)**

		a	b
C1	H11	0.82(5)	0.99(4)
C1	H12	0.82(5)	0.99(4)
C1	H13	0.82(5)	0.99(4)
C1'	H1'1	0.91(8)	1.02(8)
C2'	H2'1	0.92(5)	0.92(5)
C2'	H2'2	0.92(5)	0.92(5)
C3'	H3'1	0.86(7)	1.04(7)
C4'	H4'1	0.89(7)	0.98(7)
C5'	H5'1	1.03(4)	1.00(4)
C5'	H5'2	1.03(4)	1.00(4)
N3	H3N	0.87(7)	0.85(7)
C6	H61	0.92(7)	1.03(7)
C7	H71	0.95(6)	0.96(5)
C7	H72	0.95(6)	0.96(5)
C7	H73	0.95(6)	0.96(5)
C8	H81	0.86(4)	1.02(4)
C8	H82	0.86(4)	1.02(4)
C8	H83	0.86(4)	1.02(4)
C11	H111	0.95(8)	0.92(8)
C12	H121	1.05(9)	1.08(8)
C13	H131	0.97(9)	1.01(8)
C14	H141	0.93(8)	1.01(8)
C19	H191	1.10(8)	1.04(7)
C20	H201	1.12(10)	1.09(7)
C21	H211	1.07(12)	1.03(8)
C22	H221	0.96(9)	0.96(8)
C24	H241	0.99(9)	0.98(8)
C25	H251	1.11(9)	0.83(8)
C26	H261	0.93(11)	1.02(9)
C27	H271	0.75(11)	0.85(9)
C28	H281	0.78(9)	1.07(8)
C1"	H1"1	0.96	0.96
C1"	H1"2	0.96	0.96
C1"	H1"3	0.96	0.96
C2"	H2"1	0.97	0.97
C2"	H2"2	0.97	0.97
C3"	H3"1	0.97	0.97
C3"	H3"2	0.97	0.97
C4"	H4"1	0.97	0.97
C4"	H4"2	0.97	0.97
C5"	H5"1	0.97	0.97
C5"	H5"2	0.97	0.97
C6"	H6"1	0.96	0.96
C6"	H6"2	0.96	0.96
C6"	H6"3	0.96	0.96

Bond angles (°) for non-H atoms in **FAST-5 (R=Px,B=Thy)**

			a	b
O1	P1	O3'	115.1(3)	115.4(2)
O1	P1	C1	115.5(4)	113.3(4)
O3'	P1	C1	99.6(4)	102.7(3)
O1	P1	S1	108.0(2)	115.4(2)
O3'	P1	S1	107.7(2)	100.1(2)
C1	P1	S1	110.6(3)	108.5(3)
C7	S1	P1	101.7(4)	100.0(4)
O4'	C1'	N1	106.5(5)	107.1(5)
O4'	C1'	C2'	106.5(5)	106.4(5)
N1	C1'	C2'	115.3(6)	115.7(6)
C3'	C2'	C1'	103.5(5)	104.0(5)
O3'	C3'	C2'	114.4(5)	114.9(5)
O3'	C3'	C4'	108.2(5)	107.6(4)
C2'	C3'	C4'	102.1(5)	102.0(5)
C3'	O3'	P1	121.6(4)	122.9(4)
O4'	C4'	C5'	110.2(5)	111.2(5)
O4'	C4'	C3'	104.5(4)	103.5(4)
C5'	C4'	C3'	116.9(5)	117.1(5)
C4'	O4'	C1'	110.5(5)	111.3(4)
O5'	C5'	C4'	106.7(5)	106.8(5)
C2	N1	C6	121.2(5)	120.9(5)
C2	N1	C1'	117.6(5)	117.6(5)
C6	N1	C1'	121.1(5)	121.4(5)
O2	C2	N3	122.8(6)	122.2(6)
O2	C2	N1	122.1(6)	122.4(6)
N3	C2	N1	115.1(6)	115.4(6)
C2	N3	C4	126.4(6)	126.6(6)
O4	C4	N3	118.5(6)	119.3(6)
O4	C4	C5	125.8(7)	125.6(7)
N3	C4	C5	115.7(6)	115.1(6)
C6	C5	C4	118.9(6)	118.3(6)
C5	C6	N1	122.7(6)	123.7(6)
C6	C5	C8	121.3(6)	123.3(6)
C4	C5	C8	119.8(6)	118.3(6)
C5'	O5'	C9	114.9(4)	115.2(4)
O5'	C9	C10	112.4(5)	110.2(4)
O5'	C9	C18	109.6(5)	109.8(5)
C10	C9	C18	109.8(5)	109.7(5)
O5'	C9	C23	104.6(5)	105.7(5)
C10	C9	C23	109.7(5)	111.0(5)
C18	C9	C23	110.7(6)	110.5(5)
C15	C10	C11	117.2(7)	117.2(6)
C15	C10	C9	123.0(7)	122.0(6)
C11	C10	C9	119.8(6)	120.7(6)
C12	C11	C10	121.4(8)	123.0(7)
C13	C12	C11	119.1(10)	117.6(8)
C14	C13	C12	121.3(9)	121.0(7)
C13	C14	C15	118.1(8)	120.2(8)
C10	C15	O16	122.4(6)	123.8(6)
C10	C15	C14	122.8(8)	120.8(7)
O16	C15	C14	114.7(7)	115.4(6)
C17	O16	C15	117.4(5)	118.1(5)
O16	C17	C18	123.4(7)	123.8(6)
O16	C17	C22	115.5(8)	115.5(7)
C18	C17	C22	121.1(8)	120.7(7)
C19	C18	C17	118.8(7)	118.5(6)
C19	C18	C9	120.3(6)	119.0(6)
C17	C18	C9	120.9(6)	122.5(6)
C18	C19	C20	119.8(8)	120.9(7)
C21	C20	C19	120.8(10)	118.6(8)
C20	C21	C22	119.6(10)	120.5(8)
C21	C22	C17	119.8(9)	120.7(8)
C24	C23	C28	120.1(7)	119.6(6)
C24	C23	C9	120.4(7)	121.0(6)
C28	C23	C9	119.4(7)	119.4(6)
C23	C24	C25	121.0(9)	119.7(7)
C26	C25	C24	118.4(9)	119.9(8)
C27	C26	C25	119.4(9)	119.8(7)
C26	C27	C28	121.9(10)	121.1(8)
C27	C28	C23	119.2(9)	119.7(8)
C1"	C2"	C3"	91.6(27)	101.1(26)
C2"	C3"	C4"	106.9(38)	112.3(30)
C3"	C4"	C5"	109.8(40)	112.1(39)
C4"	C5"	C6"	103.8(35)	113.1(42)

Bond angles (°) involving H atoms in **FAST-5 (R=Px,B=Thy)**

			a	b
P1	C1	H11	109.5(4)	109.5(3)
P1	C1	H12	109.5(3)	109.5(3)
H11	C1	H12	109.47(6)	109.5
P1	C1	H13	109.5(3)	109.5(3)
H11	C1	H13	109.47(8)	109.5
H12	C1	H13	109.5	109.5
O4'	C1'	H1'1	109.4(4)	109.1(4)
N1	C1'	H1'1	109.4(3)	109.1(3)
C2'	C1'	H1'1	109.4(4)	109.1(4)
C1'	C2'	H2'1	111.1(4)	111.0(4)
C3'	C2'	H2'1	111.1(4)	111.0(3)
C1'	C2'	H2'2	111.1(4)	111.0(4)
C3'	C2'	H2'2	111.1(4)	111.0(4)
H2'1	C2'	H2'2	109.0	109.0
O3'	C3'	H3'1	110.6(3)	110.6(3)
C2'	C3'	H3'1	110.6(4)	110.6(4)
C4'	C3'	H3'1	110.6(4)	110.6(3)
O4'	C4'	H4'1	108.3(3)	108.2(3)
C5'	C4'	H4'1	108.3(3)	108.2(3)
C3'	C4'	H4'1	108.3(4)	108.2(3)
O5'	C5'	H5'1	110.4(3)	110.4(3)
C4'	C5'	H5'1	110.4(3)	110.4(3)
O5'	C5'	H5'2	110.4(3)	110.4(3)
C4'	C5'	H5'2	110.4(3)	110.4(3)
H5'1	C5'	H5'2	108.6	108.6
N1	C6	H61	118.6(3)	118.2(3)
C5	C6	H61	118.6(4)	118.2(4)
S1	C7	H71	109.5(4)	109.5(3)
S1	C7	H72	109.5(4)	109.5(4)
H71	C7	H72	109.5	109.5
S1	C7	H73	109.5(4)	109.5(4)
H71	C7	H73	109.5	109.5
H72	C7	H73	109.5	109.5
C2	N3	H3N	116.8(4)	116.7(4)
C4	N3	H3N	116.8(3)	116.7(3)
C5	C8	H81	109.5(4)	109.5(4)
C5	C8	H82	109.5(4)	109.5(4)
H81	C8	H82	109.5	109.5
C5	C8	H83	109.5(4)	109.5(5)
H81	C8	H83	109.5	109.5
H82	C8	H83	109.5	109.5
C10	C11	H111	119.3(4)	118.5(4)
C12	C11	H111	119.3(6)	118.5(5)
C11	C12	H121	120.4(6)	121.2(5)
C13	C12	H121	120.4(6)	121.2(5)
C12	C13	H131	119.3(6)	119.5(5)
C14	C13	H131	119.3(5)	119.5(5)
C13	C14	H141	120.9(5)	119.9(5)
C15	C14	H141	120.9(6)	119.9(5)
C18	C19	H191	120.1(5)	119.5(4)
C20	C19	H191	120.1(6)	119.5(5)
C19	C20	H201	119.6(6)	120.7(5)
C21	C20	H201	119.6(7)	120.7(5)
C20	C21	H211	120.2(7)	119.7(5)
C22	C21	H211	120.2(6)	119.7(5)
C17	C22	H221	120.1(6)	119.6(5)
C21	C22	H221	120.1(6)	119.6(5)
C23	C24	H241	119.5(5)	120.1(4)
C25	C24	H241	119.5(6)	120.1(5)
C24	C25	H251	120.8(6)	120.0(5)
C26	C25	H251	120.8(6)	120.0(5)
C25	C26	H261	120.3(6)	120.1(5)
C27	C26	H261	120.3(6)	120.1(5)
C26	C27	H271	119.1(6)	119.4(5)
C28	C27	H271	119.1(7)	119.4(5)
C23	C28	H281	120.4(5)	120.1(4)
C27	C28	H281	120.4(7)	120.1(5)
C2"	C1"	H1"1	109.5(23)	109.5(20)
C2"	C1"	H1"2	109.5(24)	109.5(19)
H1"1	C1"	H1"2	109.47(7)	109.5
C2"	C1"	H1"3	109.5(26)	109.5(18)
H1"1	C1"	H1"3	109.5	109.5
H1"2	C1"	H1"3	109.5	109.5
C1"	C2"	H2"1	113.4(24)	111.5(18)
C3"	C2"	H2"1	113.4(28)	111.5(21)
C1"	C2"	H2"2	113.4(26)	111.5(19)
C3"	C2"	H2"2	113.4(24)	111.5(19)
H2"1	C2"	H2"2	110.7	109.4
C4"	C3"	H3"1	110.3(40)	109.2(26)
C2"	C3"	H3"1	110.3(25)	109.2(19)
C4"	C3"	H3"2	110.3(30)	109.2(26)
C2"	C3"	H3"2	110.3(27)	109.2(21)
H3"1	C3"	H3"2	108.6	107.9
C3"	C4"	H4"1	109.7(37)	109.2(25)
C5"	C4"	H4"1	109.7(42)	109.2(31)
C3"	C4"	H4"2	109.7(35)	109.2(27)
C5"	C4"	H4"2	109.7(40)	109.2(33)
H4"1	C4"	H4"2	108.2	107.9
C4"	C5"	H5"1	111.0(43)	109.0(33)
C6"	C5"	H5"1	111.0(43)	109.0(35)
C4"	C5"	H5"2	111.0(39)	109.0(30)
C6"	C5"	H5"2	111.0(45)	109.0(29)
H5"1	C5"	H5"2	109.0	107.8
C5"	C6"	H6"1	109.5(27)	109.5(26)
C5"	C6"	H6"2	109.5(42)	109.5(35)
H6"1	C6"	H6"2	109.5	109.5
C5"	C6"	H6"3	109.5(45)	109.5(30)
H6"1	C6"	H6"3	109.47(7)	109.47(5)
H6"2	C6"	H6"3	109.5	109.5

Torsional angles (°) for non-H atoms in **FAST-5 (R=Px,B=Thy)**

				a	b
O1	P1	S1	C7	-178.2(5)	61.2(4)
O3'	P1	S1	C7	-53.3(5)	-174.3(4)
C1	P1	S1	C7	54.6(6)	-67.1(5)
O4'	C1'	C2'	C3'	-14.5(7)	-17.9(7)
N1	C1'	C2'	C3'	103.4(6)	100.9(6)
C1'	C2'	C3'	O3'	146.7(5)	148.1(5)
C1'	C2'	C3'	C4'	30.1(7)	32.0(6)
C2'	C3'	O3'	P1	94.1(7)	100.4(6)
C4'	C3'	O3'	P1	-152.8(4)	-146.8(5)
O1	P1	O3'	C3'	36.4(5)	21.9(5)
C1	P1	O3'	C3'	160.6(6)	145.7(5)
S1	P1	O3'	C3'	-84.0(5)	-102.6(5)
O3'	C3'	C4'	O4'	-157.0(5)	-156.4(5)
C2'	C3'	C4'	O4'	-36.0(6)	-35.2(6)
O3'	C3'	C4'	C5'	80.9(7)	80.9(6)
C2'	C3'	C4'	C5'	-158.1(5)	-157.9(5)
C5'	C4'	O4'	C1'	154.9(5)	152.1(5)
C3'	C4'	O4'	C1'	28.4(7)	25.5(7)
N1	C1'	O4'	C4'	-132.3(5)	-129.4(5)
C2'	C1'	O4'	C4'	-8.7(7)	-5.1(7)
O4'	C4'	C5'	O5'	-72.2(6)	-76.9(6)
C3'	C4'	C5'	O5'	46.9(6)	41.8(7)
O4'	C1'	N1	C2	-137.5(6)	-136.4(6)
C2'	C1'	N1	C2	104.6(7)	105.1(7)
O4'	C1'	N1	C6	37.5(8)	40.5(8)
C2'	C1'	N1	C6	-80.4(7)	-78.0(8)
C6	N1	C2	O2	179.8(6)	178.0(7)
C1'	N1	C2	O2	-5.2(10)	-5.1(10)
C6	N1	C2	N3	2.2(9)	-1.2(10)
C1'	N1	C2	N3	177.2(6)	175.7(6)
O2	C2	N3	C4	179.6(7)	-179.3(7)
N1	C2	N3	C4	-2.8(10)	-0.1(10)
C2	N3	C4	O4	-178.0(7)	-178.1(7)
C2	N3	C4	C5	2.1(10)	0.4(10)
O4	C4	C5	C6	179.4(7)	178.9(8)
N3	C4	C5	C6	-0.8(9)	0.5(10)
C4	C5	C6	N1	0.5(10)	-1.8(10)
C2	N1	C6	C5	-1.3(10)	2.3(10)
C1'	N1	C6	C5	-176.1(7)	-174.6(6)
O4	C4	C5	C8	-0.4(11)	-3.6(11)
N3	C4	C5	C8	179.5(7)	178.0(7)
C4'	C5'	O5'	C9	-173.1(5)	179.2(5)
C8	C5	C6	N1	-179.8(7)	-179.2(7)
C5'	O5'	C9	C10	55.0(7)	52.4(6)
C5'	O5'	C9	C18	-67.3(6)	-68.5(6)
C5'	O5'	C9	C23	174.0(5)	172.3(4)
O5'	C9	C10	C15	-133.8(7)	-117.7(6)
C18	C9	C10	C15	-11.6(9)	3.2(8)
C23	C9	C10	C15	110.2(8)	125.6(6)
O5'	C9	C10	C11	43.9(8)	58.8(7)
C18	C9	C10	C11	166.2(6)	179.7(6)
C23	C9	C10	C11	-72.0(8)	-57.9(8)
C15	C10	C11	C12	-1.6(11)	1.2(10)
C9	C10	C11	C12	-179.5(7)	-175.5(6)
C10	C11	C12	C13	-0.2(11)	-0.4(11)
C11	C12	C13	C14	1.5(12)	-0.2(11)
C12	C13	C14	C15	-0.9(12)	0.1(11)
C9	C10	C15	O16	-2.7(11)	-4.1(9)
C11	C10	C15	O16	179.5(7)	179.3(6)
C9	C10	C15	C14	-180.0(7)	175.3(6)
C11	C10	C15	C14	2.2(11)	-1.3(9)
C13	C14	C15	C10	-1.0(11)	0.7(10)
C13	C14	C15	O16	-178.5(7)	-179.8(6)
C10	C15	O16	C17	16.0(10)	2.0(9)
C14	C15	O16	C17	-166.5(6)	-177.5(6)
C15	O16	C17	C18	-13.7(10)	0.6(10)
C15	O16	C17	C22	167.2(7)	178.7(6)
O16	C17	C18	C19	178.6(7)	178.8(6)
C22	C17	C18	C19	-2.4(11)	0.8(10)
O16	C17	C18	C9	-1.7(11)	-1.1(10)
C22	C17	C18	C9	177.3(7)	-179.1(6)
O5'	C9	C18	C17	137.4(6)	120.4(6)
C10	C9	C18	C17	13.6(9)	-0.8(8)
C23	C9	C18	C17	-107.7(7)	-123.4(6)
O5'	C9	C18	C19	-42.8(9)	-59.5(7)
C10	C9	C18	C19	-166.7(7)	179.3(6)
C23	C9	C18	C19	72.0(9)	56.7(7)
C17	C18	C19	C20	2.0(13)	-0.9(10)
C9	C18	C19	C20	-177.7(8)	179.0(6)
C18	C19	C20	C21	0.5(15)	0.9(11)
C19	C20	C21	C22	-2.6(17)	-0.7(12)
C20	C21	C22	C17	2.2(15)	0.5(12)
O16	C17	C22	C21	179.4(8)	-178.7(7)
C18	C17	C22	C21	0.3(12)	-0.6(11)
O5'	C9	C23	C24	-27.2(8)	-11.9(7)
C10	C9	C23	C24	93.5(8)	107.5(7)
C18	C9	C23	C24	-145.2(7)	-130.6(6)
O5'	C9	C23	C28	155.4(6)	169.6(5)
C10	C9	C23	C28	-83.9(8)	-71.0(7)
C18	C9	C23	C28	37.4(8)	50.9(7)
C28	C23	C24	C25	2.1(12)	-1.5(10)
C9	C23	C24	C25	-175.3(7)	180.0(6)
C23	C24	C25	C26	-2.2(13)	-0.3(11)
C24	C25	C26	C27	0.9(14)	2.2(11)
C25	C26	C27	C28	0.4(15)	-2.3(12)
C26	C27	C28	C23	-0.6(14)	0.5(11)
C24	C23	C28	C27	-0.7(12)	1.4(10)
C9	C23	C28	C27	176.7(7)	180.0(6)
C1"	C2"	C3"	C4"	-142.9(48)	172.5(33)
C2"	C3"	C4"	C5"	-148.4(53)	170.8(40)
C3"	C4"	C5"	C6"	-179.8(58)	78.9(66)

Hydrogen-bonding geometry (Å, °) *for* **FAST-5 (R=Px,B=Thy)**

D–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
C1–H13···O4b^{i}	0.81(7)	2.56(7)	3.210(9)	138(6)
C1'–H1'1···O2	0.91(7)	2.34(2)	2.716(7)	104(3)
C2'–H2'2···O2^{i}	0.92(3)	2.66(3)	3.290(10)	126(2)
C3'–H3'1···O1	0.86(7)	2.68(6)	3.074(9)	109(4)
C3'–H3'1···O5'	0.86(7)	2.43(3)	2.805(8)	107(4)
C3'–H3'1···O2^{i}	0.86(7)	2.61(5)	3.276(9)	134(4)
N3–H3N···O1^{ii}	0.86(7)	2.05(6)	2.869(7)	158(4)
C6–H61···O4'	0.92(7)	2.49(3)	2.731(8)	95(3)
C6–H61···O5'	0.92(7)	2.71(7)	3.596(8)	162(4)
C7–H72···O4^{ii}	0.96(4)	2.62(5)	3.507(14)	154(5)
C8–H81···O4	0.86(4)	2.80(4)	2.906(9)	88(3)
C11–H111···O1	0.94(7)	2.65(6)	3.532(11)	157(4)
C11–H111···O5'	0.94(7)	2.67(3)	2.905(8)	95(3)
C19–H191···O5'	1.11(7)	2.59(2)	2.853(11)	92(2)
C24–H241···O5'	1.00(5)	2.31(4)	2.675(9)	100(3)
C24–H241···O2^{i}	1.00(5)	2.75(4)	3.536(11)	136(3)
C25–H251···O4'^{iii}	1.12(7)	2.55(4)	3.282(11)	122(4)
C1b–H1D···O1^{iv}	0.99(5)	2.59(4)	3.579(11)	177(4)
C1'b–H1'B···O2b	1.02(7)	2.32(3)	2.726(8)	102(3)
C2'b–H2'C···O2b^{v}	0.93(4)	2.77(3)	3.399(11)	126(2)
C3'b–H3'B···O1b	1.04(6)	2.57(5)	3.032(9)	106(3)
C3'b–H3'B···O5'b	1.04(6)	2.35(2)	2.772(8)	103(3)
C3'b–H3'B···O2b^{v}	1.04(6)	2.63(4)	3.408(9)	131(3)
N3b–H3NB···O1b^{vi}	0.84(7)	2.06(6)	2.878(7)	166(5)
C6b–H6B···O4'b	1.03(6)	2.52(3)	2.751(8)	92(3)
C6b–H6B···O5'b	1.03(6)	2.64(6)	3.620(8)	160(4)
C6b–H6B···O2b^{v}	1.03(6)	2.79(5)	2.963(10)	89(3)
C7b–H7C···O4^{v}	0.97(5)	2.69(5)	3.541(11)	147(4)
C7b–H7D···O4b^{v}	0.97(4)	2.68(4)	3.612(12)	162(4)
C8b–H8B···O4b	1.02(4)	2.77(4)	2.874(10)	85(2)
C14b–H14B···O16^{vii}	1.01(7)	2.58(4)	3.269(10)	125(4)
C24b–H24B···O5'b	0.97(5)	2.28(4)	2.656(9)	102(3)

Symmetry codes: (i) $-x$, $0.5+y$, $-1-z$; (ii) $-x$, $-0.5+y$, $-1-z$; (iii) x, $1+y$, z; (iv) $1+x$, $-1+y$, $1+z$; (v) $1-x$, $-0.5+y$, $-z$; (vi) $1-x$, $0.5+y$, $-z$; (vii) $1+x$, y, $1+z$.

Asymmetry parameters of five-membered ring: C1',C2',C3',C4',O4' *in* **FAST-5 (R=Px,B=Thy)**

	a	b
$\Delta C_s^{(C1')}$	44.5(12)	43.8(12)
$\Delta C_s^{(C2')}$	33.5(12)	30.2(12)
$\Delta C_s^{(C3')}$	10.7(12)	5.8(12)
$\Delta C_s^{(C4')}$	16.0(12)	20.2(12)
$\Delta C_s^{(O4')}$	38.3(12)	40.2(12)
$\Delta C_2^{(C1'-C2')}$	53.2(13)	50.3(13)
$\Delta C_2^{(C2'-C3')}$	30.3(13)	24.9(12)
$\Delta C_2^{(C3'-C4')}$	4.2(11)	10.1(12)
$\Delta C_2^{(C4'-O4')}$	37.0(13)	41.1(12)
$\Delta C_2^{(O4'-C1')}$	55.7(13)	56.5(13)

Dihedral angles between least-squares planes in **FAST-5 (R=Px,B=Thy)**:

Plane1: C1',C2',C4',O4'
Plane2: C2',C3',C4'
Plane3: N1,C2,N3,C4,C5,C6
Plane4: C10,C11,C12,C13,C14,C15
Plane5: C17,C18,C19,C20,C21,C22
Plane6: C23,C24,C25,C26,C27,C28

	a	b
Plane1/Plane2	34.9(4)	35.0(4)
Plane1/Plane3	70.0(2)	71.4(2)
Plane2/Plane3	84.3(3)	83.6(3)
Plane1/Plane4	10.5(3)	22.1(2)
Plane2/Plane4	44.7(4)	47.3(3)
Plane3/Plane4	66.4(2)	81.7(2)
Plane1/Plane5	6.2(3)	19.0(3)
Plane2/Plane5	30.9(3)	44.3(3)
Plane3/Plane5	76.1(2)	81.2(2)
Plane4/Plane5	13.9(2)	3.4(2)
Plane1/Plane6	86.0(3)	87.8(3)
Plane2/Plane6	60.6(3)	53.4(3)
Plane3/Plane6	61.4(2)	60.1(2)
Plane4/Plane6	75.6(2)	80.4(2)
Plane5/Plane6	88.9(3)	83.1(2)