Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

A diisopropoxyphosphonate disulfone

Jessica H. Wong, Marilyn M. Olmstead,* James C. Fettinger and Jacquelyn Gervay-Hague

Department of Chemistry, University of California, One Shields Avenue, Davis, CA 95616, USA
Correspondence e-mail: olmstead@chem.ucdavis.edu

Received 16 May 2007; accepted 22 May 2007

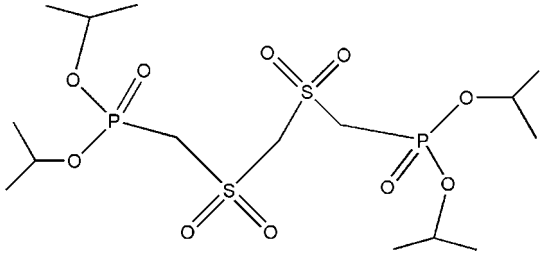
Key indicators: single-crystal X-ray study; T = 180 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.041; wR factor = 0.117; data-to-parameter ratio = 22.5.

The title molecule, diisopropyl (diisopropoxyphosphoryl-methylsulfonylmethylsulfonylmethyl)phosphonate, $C_{15}H_{34}O_{10}P_2S_2$, represents a disulfone of a phosphate ester that has been investigated as a target for chemotherapy. The disulfone has four half-molecules with crystallographic twofold symmetry in the asymmetric unit. The S═O, P═O and P—O bonds average 1.439, 1.472 and 1.567 Å, respectively. Three isopropyl groups are each disordered over two sites, two of them in a 2:1 ratio and the other in a 3:2 ratio.

Related literature

Theoretical and conformational studies of related molecules, together with the crystal structure of a sulfonylphosphonate, have been reported by Olivato *et al.* (2001). Studies related to chemotherapeutic uses of disulfones have been reported by Meadows *et al.* (2005, 2007) and Meadows & Gervay-Hague (2006).

For related literature, see: Hadd *et al.* (2001); Wong *et al.* (2007).



Experimental

Crystal data

$C_{15}H_{34}O_{10}P_2S_2$
M_r = 500.50
Monoclinic, $P2/n$
a = 21.7314 (17) Å
b = 10.2307 (8) Å
c = 21.8150 (17) Å
β = 92.922 (5)°
V = 4843.8 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 180 (2) K
0.40 × 0.25 × 0.13 mm

Data collection

Bruker SMART APEX II diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2005)
T_{min} = 0.857, T_{max} = 0.950
53365 measured reflections
14085 independent reflections
12471 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.117
S = 1.08
14085 reflections
627 parameters
9 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 1994); software used to prepare material for publication: *SHELXL97*.

The authors thank the University AIDS research Program (D02-0-400) and Tobacco-Related Disease Research Program (12RT-0294H) for partial support of this research. The Bruker SMART 1000 diffractometer was funded in part by NSF Instrumentation grant CHE-9808259.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2026).

References

Bruker (2005). *SAINT*. Version 7.23. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2006). *APEX2*. Version 2.0-2. Bruker AXS Inc., Madison, Wisconsin, USA.
Hadd, M. J., Smith, M. A. & Gervay-Hague, J. (2001). *Tetrahedron Lett.* **42**, 5137–5140.
Meadows, D. C. & Gervay-Hague, J. (2006). *ChemMedChem*, **1**, 16–29.
Meadows, D. C., Mathews, T. B., North, T. W., Hadd, M. J., Kuo, C. L., Neamati, N. & Gervay-Hague, J. (2005). *J. Med. Chem.* **48**, 4526–4534.
Meadows, D. C., Sanchez, T., Neamati, N., North, T. W. & Gervay-Hague, J. (2007). *Bioorg. Med. Chem.* **15**, 1127–1137.
Olivato, P. R., Filho, R. R., Zukerman-Schpector, J., Colle, M. D. & Distefano, G. (2001). *J. Chem. Soc. Perkin Trans. 2*, pp. 97–102.
Sheldrick, G. M. (1994). *SHELXTL*. Version 5.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2005). *SADABS*. Version 2.10. University of Göttingen, Germany.
Wong, J. H., Olmstead, M. M. & Gervay-Hague, J. (2007). *Acta Cryst.* E**63**, o3045.

  doi:10.1107/S160053680702507X

supplementary materials

Acta Cryst. (2007). E**63**, o3046 [**doi:10.1107/S160053680702507X**]

A diisopropoxyphosphonate disulfone

J. H. Wong, M. M. Olmstead, J. C. Fettinger and J. Gervay-Hague

Comment

Organophosphates are ubiquitous in nature as substrates for key enzymes including glycosyltransferases, RNA/DNA polymerases, HIV-1 integrase and kinases. Inhibitors of these enzymes have proven useful as probes for biomechanistic elucidation and represent important targets for chemotherapeutic intervention. In continuation of the synthesis of enzyme substrate analogs and screening of compounds for inhibition against relevant enzymes, the disulfone reagent (I) has been developed and extensively used in the Gervay-Hague laboratories (Hadd *et al.*, 2001, Meadows *et al.*, 2005, Meadows & Gervay-Hague, 2006, Meadows *et al.*, 2007).

Disulfone (I), has *Z*'=2; however, there are four half-molecules in the asymmetric unit. A crystallographic twofold axis passes through the central carbon atom in each of the four molecules in the structure (Fig. 1). The differences among the molecules are slight, as can be seen by their common orientations in the figure. Three of the four have varying degrees of disorder in one of the isopropyl groups. There are only minor conformational differences in the isopropyl groups that distinguish one molecule from another. Values of the individual bonds show good internal consistency and also agree with those of the mono-sulfone (Wong *et al.*, 2007). The average S=O, P=O, and P—O distances, together with their average deviations in square brackets are 1.439[3] Å, 1.472[1] Å, and 1.567[2] Å, respectively. There are no short intermolecular interactions. The phosphoryl and sulfonyl intramolecular interactions follow the trend P···O=S < S···O=S < S···O=P with average values and average deviations in square brackets of 3.209[24] Å < 3.270[6] Å < 3.330[12] Å, respectively. These values compare well with those described by Olivato *et al.* (2001). The P—C—S—C backbone has average torsion angles of −71.9[17]° whereas that of the C—S—C—S backbone is −68.1[5]°.

Experimental

The synthesis of (I) was reported earlier (Hadd *et al.*, 2001). Crystals were grown from diethyl ether.

Refinement

The methyl H atoms were constrained to an ideal geometry with C—H distances of 0.98 \%A and *U*ĩso~(H) = 1.5*U*~eq~(C), and each group was allowed to rotate freely about its C—C bond. Other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances in the range 0.99–1.00 \%A and *U*ĩso~(H) = 1.2*U*~eq~(C). The structure was refined as a pseudomerohedral twin, twin law (0 0 − 1 0 − 1 0 − 1 0 0) and twin parameter 0.1098 (6). Three isopropyl groups suffer rotational disorder and were modeled with split positions. The occupancies were fixed in the final cycles of refinement.

Figures

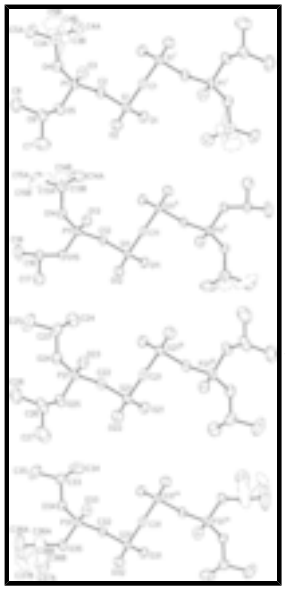


Fig. 1. A view of the four molecules of (I) in a common orientation. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms have been omitted for clarity. Symmetry codes: i = 1/2 − *x*, *y*, 1/2 − *z*; ii = 1.5 − *x*, *y*, 1.5 − *z*; iii = 1/2 − *x*, *y*, 1.5 − *z*; iv = 1.5 − *x*, *y*, 1/2 − *z*.

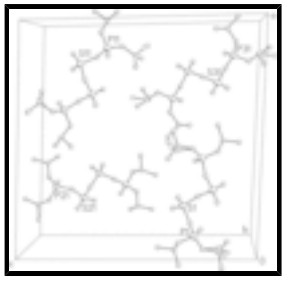


Fig. 2. A view of the four molecules of (I) projected along the b-direction.

diisopropyl (diisopropoxyphosphorylmethylsulfonylmethylsulfonylmethyl)phosphonate

Crystal data

$C_{15}H_{34}O_{10}P_2S_2$	F_{000} = 2128
M_r = 500.50	D_x = 1.373 Mg m^{-3}
Monoclinic, *P*2/*n*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2yac	Cell parameters from 7807 reflections
a = 21.7314 (17) Å	θ = 2.9–30.5º
b = 10.2307 (8) Å	μ = 0.40 mm^{-1}
c = 21.8150 (17) Å	*T* = 180 (2) K
β = 92.922 (5)º	Block, colorless
V = 4843.8 (7) Å^3	0.40 × 0.25 × 0.13 mm
Z = 8	

Data collection

Bruker SMART APEX II diffractometer	14085 independent reflections

Radiation source: fine-focus sealed tube
Monochromator: graphite
Detector resolution: 8.3 pixels mm^{-1}
T = 180(2) K
ω and φ scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2005)
T_{min} = 0.857, T_{max} = 0.950
53365 measured reflections
12471 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 30.0º
θ_{min} = 2.9º
h = −30→30
k = −14→14
l = −30→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.117
S = 1.08
14085 reflections
627 parameters
9 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
$w = 1/[\sigma^2(F_o^2) + (0.0753P)^2 + 0.8408P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.026
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}
Extinction correction: none

Special details

Experimental. The data collection temperature of 180 K was used due to an apparent destructive phase transition as the temperature was further lowered to 90 K.

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 $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
P1	0.085776 (19)	0.12874 (4)	0.26172 (2)	0.02586 (9)	
S1	0.217544 (18)	0.10297 (4)	0.310518 (18)	0.02721 (8)	
O1	0.26109 (6)	0.00310 (15)	0.32980 (6)	0.0377 (3)	
O2	0.19921 (6)	0.19881 (14)	0.35408 (6)	0.0404 (3)	
O3	0.10166 (6)	0.25460 (11)	0.23388 (6)	0.0317 (2)	

O4	0.03976 (6)	0.04176 (12)	0.22177 (6)	0.0337 (3)	
O5	0.05649 (6)	0.13298 (12)	0.32571 (6)	0.0333 (3)	
C1	0.2500	0.1938 (2)	0.2500	0.0256 (4)	
H1	0.2816	0.2494	0.2680	0.031*	
C2	0.15125 (7)	0.02299 (15)	0.27774 (8)	0.0281 (3)	
H2A	0.1390	−0.0468	0.3061	0.034*	
H2B	0.1623	−0.0194	0.2390	0.034*	
C3A	0.0269 (2)	0.0588 (4)	0.1572 (2)	0.0368 (9)	0.57
H3A	0.0264	0.1537	0.1461	0.044*	0.57
C4A	0.0772 (2)	−0.0128 (8)	0.1250 (2)	0.0779 (17)	0.57
H4AA	0.1166	0.0320	0.1333	0.117*	0.57
H4AB	0.0673	−0.0137	0.0806	0.117*	0.57
H4AC	0.0802	−0.1028	0.1402	0.117*	0.57
C5A	−0.03493 (17)	−0.0028 (7)	0.1420 (2)	0.0652 (13)	0.57
H5AA	−0.0668	0.0440	0.1635	0.098*	0.57
H5AB	−0.0341	−0.0945	0.1550	0.098*	0.57
H5AC	−0.0442	0.0019	0.0976	0.098*	0.57
C3B	0.0476 (3)	0.0236 (6)	0.1535 (3)	0.0359 (12)	0.43
H3B	0.0925	0.0282	0.1454	0.043*	0.43
C4B	0.0240 (3)	−0.1129 (5)	0.1378 (3)	0.0572 (14)	0.43
H4BA	0.0222	−0.1249	0.0932	0.086*	0.43
H4BB	−0.0174	−0.1238	0.1531	0.086*	0.43
H4BC	0.0518	−0.1780	0.1571	0.086*	0.43
C5B	0.0147 (4)	0.1294 (6)	0.1186 (3)	0.0661 (17)	0.43
H5BA	0.0302	0.2144	0.1332	0.099*	0.43
H5BB	−0.0295	0.1234	0.1249	0.099*	0.43
H5BC	0.0218	0.1201	0.0748	0.099*	0.43
C6	0.01642 (8)	0.24022 (18)	0.34433 (9)	0.0361 (4)	
H6	0.0306	0.3241	0.3262	0.043*	
C7	0.02495 (14)	0.2464 (3)	0.41301 (11)	0.0635 (7)	
H7A	0.0690	0.2523	0.4248	0.095*	
H7B	0.0078	0.1674	0.4309	0.095*	
H7C	0.0037	0.3235	0.4281	0.095*	
C8	−0.04901 (10)	0.2129 (3)	0.32162 (13)	0.0566 (6)	
H8A	−0.0511	0.2082	0.2767	0.085*	
H8B	−0.0759	0.2833	0.3349	0.085*	
H8C	−0.0625	0.1296	0.3385	0.085*	
P11	0.882618 (18)	0.37244 (4)	0.659619 (18)	0.02439 (8)	
S11	0.816104 (16)	0.40065 (4)	0.777057 (16)	0.02385 (8)	
O11	0.79536 (5)	0.50171 (14)	0.81719 (5)	0.0351 (3)	
O12	0.86010 (6)	0.30603 (15)	0.80066 (6)	0.0393 (3)	
O13	0.84913 (6)	0.24861 (12)	0.64917 (6)	0.0325 (2)	
O14	0.88947 (6)	0.45678 (13)	0.60039 (5)	0.0353 (3)	
O15	0.95002 (5)	0.36449 (12)	0.68835 (5)	0.0300 (2)	
C11	0.7500	0.3085 (2)	0.7500	0.0229 (4)	
H11	0.7379	0.2529	0.7827	0.027*	
C12	0.84566 (7)	0.47943 (15)	0.71235 (7)	0.0242 (3)	
H12A	0.8758	0.5465	0.7270	0.029*	
H12B	0.8114	0.5253	0.6898	0.029*	

C13A	0.8499 (4)	0.4293 (5)	0.5436 (3)	0.0325 (10)	0.68
H13A	0.8315	0.3400	0.5459	0.039*	0.68
C14A	0.80000 (19)	0.5314 (5)	0.54370 (17)	0.0664 (11)	0.68
H14A	0.7737	0.5154	0.5781	0.100*	0.68
H14B	0.7751	0.5270	0.5050	0.100*	0.68
H14C	0.8187	0.6182	0.5481	0.100*	0.68
C15A	0.8897 (3)	0.4383 (7)	0.4904 (3)	0.0649 (17)	0.68
H15A	0.9233	0.3747	0.4953	0.097*	0.68
H15B	0.9069	0.5266	0.4882	0.097*	0.68
H15C	0.8652	0.4194	0.4525	0.097*	0.68
C13B	0.8467 (8)	0.4713 (10)	0.5464 (6)	0.039 (3)	0.32
H13B	0.8065	0.4266	0.5527	0.047*	0.32
C14B	0.8369 (4)	0.6099 (8)	0.5236 (3)	0.0562 (19)	0.32
H14D	0.8138	0.6593	0.5532	0.084*	0.32
H14E	0.8138	0.6084	0.4838	0.084*	0.32
H14F	0.8770	0.6517	0.5188	0.084*	0.32
C15B	0.8838 (9)	0.3987 (11)	0.5009 (5)	0.090 (6)	0.32
H15D	0.8921	0.3098	0.5158	0.135*	0.32
H15E	0.9229	0.4443	0.4960	0.135*	0.32
H15F	0.8606	0.3948	0.4612	0.135*	0.32
C16	0.99712 (8)	0.28756 (18)	0.65737 (8)	0.0326 (3)	
H16	0.9763	0.2246	0.6280	0.039*	
C17	1.03399 (10)	0.2135 (2)	0.70582 (10)	0.0456 (5)	
H17A	1.0062	0.1608	0.7298	0.068*	
H17B	1.0565	0.2752	0.7330	0.068*	
H17C	1.0633	0.1560	0.6863	0.068*	
C18	1.03599 (10)	0.3813 (2)	0.62260 (12)	0.0549 (6)	
H18A	1.0102	0.4251	0.5906	0.082*	
H18B	1.0690	0.3331	0.6036	0.082*	
H18C	1.0540	0.4468	0.6510	0.082*	
P21	0.24751 (2)	0.86489 (4)	0.913720 (18)	0.02752 (9)	
S21	0.191320 (19)	0.89188 (4)	0.785262 (18)	0.02933 (9)	
O21	0.17004 (6)	0.99185 (15)	0.74286 (6)	0.0377 (3)	
O22	0.14858 (7)	0.79628 (15)	0.80573 (7)	0.0458 (3)	
O23	0.27713 (6)	0.74223 (12)	0.89584 (6)	0.0339 (3)	
O24	0.28696 (6)	0.95280 (13)	0.95945 (6)	0.0374 (3)	
O25	0.18443 (6)	0.85339 (13)	0.94472 (6)	0.0352 (3)	
C21	0.2500	0.8007 (2)	0.7500	0.0289 (4)	
H21	0.2305	0.7451	0.7194	0.035*	
C22	0.22707 (8)	0.97182 (16)	0.84988 (7)	0.0294 (3)	
H22A	0.1989	1.0402	0.8640	0.035*	
H22B	0.2648	1.0159	0.8370	0.035*	
C23	0.35436 (10)	0.95121 (19)	0.96529 (9)	0.0398 (4)	
H23	0.3701	0.8658	0.9502	0.048*	
C24	0.37912 (12)	1.0610 (2)	0.92810 (11)	0.0542 (5)	
H24A	0.3679	1.0465	0.8845	0.081*	
H24B	0.4241	1.0641	0.9342	0.081*	
H24C	0.3615	1.1439	0.9413	0.081*	
C25	0.37131 (14)	0.9660 (3)	1.03304 (10)	0.0633 (7)	

H25A	0.3520	0.8958	1.0558	0.095*	
H25B	0.3568	1.0508	1.0474	0.095*	
H25C	0.4162	0.9609	1.0398	0.095*	
C26	0.17096 (11)	0.74753 (19)	0.98726 (9)	0.0448 (5)	
H26	0.1911	0.6654	0.9737	0.054*	
C27	0.10246 (14)	0.7309 (3)	0.98155 (14)	0.0686 (8)	
H27A	0.0894	0.7178	0.9383	0.103*	
H27B	0.0825	0.8093	0.9971	0.103*	
H27C	0.0906	0.6548	1.0055	0.103*	
C28	0.19542 (14)	0.7815 (3)	1.05117 (10)	0.0619 (7)	
H28A	0.2404	0.7879	1.0518	0.093*	
H28B	0.1836	0.7133	1.0798	0.093*	
H28C	0.1782	0.8655	1.0634	0.093*	
P31	0.84281 (2)	0.63324 (4)	0.119898 (18)	0.02613 (9)	
S31	0.722851 (17)	0.60354 (4)	0.184137 (17)	0.02589 (8)	
O31	0.68284 (5)	0.50178 (14)	0.20468 (5)	0.0342 (2)	
O32	0.69880 (6)	0.69798 (14)	0.14054 (6)	0.0402 (3)	
O33	0.85417 (6)	0.75450 (12)	0.15487 (6)	0.0352 (3)	
O34	0.90134 (5)	0.54539 (12)	0.11237 (6)	0.0321 (2)	
O35	0.81563 (6)	0.64658 (14)	0.05247 (6)	0.0368 (3)	
C31	0.7500	0.6947 (2)	0.2500	0.0259 (4)	
H31	0.7172	0.7503	0.2620	0.031*	
C32	0.78787 (7)	0.52589 (15)	0.15428 (7)	0.0258 (3)	
H32A	0.7731	0.4616	0.1230	0.031*	
H32B	0.8096	0.4767	0.1879	0.031*	
C33	0.95852 (8)	0.5560 (2)	0.15169 (9)	0.0383 (4)	
H33	0.9611	0.6447	0.1709	0.046*	
C34	0.95734 (11)	0.4539 (2)	0.20065 (11)	0.0542 (6)	
H34A	0.9230	0.4711	0.2269	0.081*	
H34B	0.9962	0.4561	0.2255	0.081*	
H34C	0.9521	0.3676	0.1816	0.081*	
C35	1.01006 (11)	0.5392 (4)	0.10867 (14)	0.0830 (11)	
H35A	1.0074	0.6079	0.0773	0.125*	
H35B	1.0066	0.4534	0.0888	0.125*	
H35C	1.0498	0.5455	0.1319	0.125*	
C36A	0.8487 (5)	0.7282 (12)	0.0093 (4)	0.060 (3)	0.65
H36A	0.8823	0.7784	0.0317	0.072*	0.65
C37A	0.8027 (2)	0.8201 (5)	−0.0206 (3)	0.0573 (12)	0.65
H37A	0.7851	0.8754	0.0107	0.086*	0.65
H37B	0.7697	0.7698	−0.0419	0.086*	0.65
H37C	0.8231	0.8751	−0.0502	0.086*	0.65
C38A	0.8750 (4)	0.6385 (7)	−0.0356 (3)	0.113 (3)	0.65
H38A	0.9053	0.5811	−0.0144	0.169*	0.65
H38B	0.8952	0.6894	−0.0669	0.169*	0.65
H38C	0.8420	0.5855	−0.0552	0.169*	0.65
C36B	0.8490 (13)	0.7087 (18)	0.0041 (7)	0.050 (4)	0.35
H36B	0.8939	0.6990	0.0156	0.060*	0.35
C37B	0.8369 (6)	0.6380 (10)	−0.0574 (3)	0.070 (3)	0.35
H37D	0.8433	0.5439	−0.0516	0.105*	0.35

H37E	0.8653	0.6710	−0.0873	0.105*	0.35
H37F	0.7944	0.6540	−0.0726	0.105*	0.35
C38B	0.8366 (10)	0.8457 (11)	−0.0001 (7)	0.129 (8)	0.35
H38D	0.8464	0.8869	0.0398	0.193*	0.35
H38E	0.7930	0.8594	−0.0119	0.193*	0.35
H38F	0.8621	0.8847	−0.0311	0.193*	0.35

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.02296 (18)	0.02212 (17)	0.0326 (2)	−0.00184 (13)	0.00276 (14)	−0.00063 (14)
S1	0.02454 (18)	0.03144 (19)	0.02572 (18)	0.00067 (14)	0.00205 (13)	−0.00022 (13)
O1	0.0299 (6)	0.0471 (7)	0.0360 (6)	0.0053 (5)	0.0004 (5)	0.0141 (6)
O2	0.0374 (7)	0.0495 (8)	0.0346 (6)	−0.0019 (6)	0.0058 (5)	−0.0155 (6)
O3	0.0331 (6)	0.0227 (5)	0.0393 (6)	−0.0031 (4)	0.0013 (5)	0.0012 (4)
O4	0.0309 (6)	0.0335 (6)	0.0365 (6)	−0.0089 (5)	0.0001 (5)	−0.0007 (5)
O5	0.0328 (6)	0.0307 (6)	0.0372 (6)	0.0057 (5)	0.0089 (5)	0.0005 (5)
C1	0.0236 (9)	0.0224 (9)	0.0309 (10)	0.000	0.0013 (8)	0.000
C2	0.0242 (7)	0.0232 (7)	0.0371 (8)	−0.0006 (5)	0.0039 (6)	0.0000 (6)
C3A	0.048 (3)	0.0241 (19)	0.0377 (19)	0.0003 (15)	−0.0046 (18)	−0.0018 (15)
C4A	0.046 (2)	0.147 (5)	0.041 (2)	0.012 (3)	0.0058 (18)	−0.017 (3)
C5A	0.0305 (17)	0.111 (4)	0.053 (2)	−0.006 (2)	−0.0097 (15)	−0.019 (3)
C3B	0.046 (3)	0.027 (3)	0.035 (2)	−0.006 (2)	0.003 (2)	−0.005 (2)
C4B	0.077 (4)	0.038 (2)	0.055 (3)	0.001 (2)	−0.011 (3)	−0.014 (2)
C5B	0.100 (5)	0.046 (3)	0.050 (3)	0.001 (3)	−0.014 (3)	0.008 (2)
C6	0.0325 (8)	0.0344 (8)	0.0421 (9)	0.0092 (7)	0.0083 (7)	0.0002 (7)
C7	0.0773 (18)	0.0703 (16)	0.0431 (12)	0.0337 (14)	0.0063 (11)	−0.0090 (11)
C8	0.0305 (10)	0.0675 (15)	0.0716 (16)	0.0085 (10)	0.0020 (9)	0.0118 (12)
P11	0.02121 (18)	0.02863 (19)	0.02384 (18)	−0.00176 (14)	0.00612 (13)	−0.00264 (13)
S11	0.01977 (16)	0.03162 (18)	0.02031 (16)	−0.00039 (13)	0.00258 (12)	−0.00054 (12)
O11	0.0302 (6)	0.0473 (7)	0.0282 (6)	−0.0065 (5)	0.0067 (4)	−0.0148 (5)
O12	0.0268 (6)	0.0555 (8)	0.0353 (6)	0.0076 (6)	0.0001 (5)	0.0145 (6)
O13	0.0317 (6)	0.0299 (6)	0.0364 (6)	−0.0036 (5)	0.0066 (5)	−0.0081 (5)
O14	0.0294 (6)	0.0523 (8)	0.0245 (5)	−0.0064 (5)	0.0043 (4)	0.0062 (5)
O15	0.0218 (5)	0.0395 (6)	0.0291 (6)	0.0031 (4)	0.0055 (4)	−0.0048 (5)
C11	0.0217 (9)	0.0220 (9)	0.0253 (9)	0.000	0.0058 (7)	0.000
C12	0.0219 (6)	0.0246 (6)	0.0266 (7)	−0.0028 (5)	0.0062 (5)	−0.0002 (5)
C13A	0.0372 (17)	0.035 (2)	0.0257 (17)	−0.002 (2)	0.0016 (12)	−0.0004 (18)
C14A	0.064 (2)	0.079 (3)	0.054 (2)	0.029 (2)	−0.0243 (17)	−0.0062 (19)
C15A	0.063 (3)	0.108 (5)	0.026 (2)	−0.017 (3)	0.0141 (17)	−0.007 (3)
C13B	0.040 (5)	0.056 (7)	0.022 (3)	−0.016 (6)	0.002 (3)	−0.003 (5)
C14B	0.060 (5)	0.067 (5)	0.040 (4)	0.027 (4)	−0.006 (3)	−0.005 (3)
C15B	0.204 (18)	0.040 (5)	0.023 (5)	0.010 (7)	−0.013 (6)	−0.003 (3)
C16	0.0264 (7)	0.0397 (9)	0.0324 (8)	0.0063 (6)	0.0085 (6)	−0.0043 (6)
C17	0.0440 (11)	0.0479 (11)	0.0454 (10)	0.0156 (9)	0.0077 (8)	0.0055 (8)
C18	0.0374 (11)	0.0641 (14)	0.0657 (15)	0.0142 (10)	0.0264 (10)	0.0232 (11)
P21	0.0373 (2)	0.02489 (18)	0.02055 (18)	−0.00273 (15)	0.00356 (15)	−0.00162 (13)
S21	0.0305 (2)	0.0330 (2)	0.02438 (18)	−0.00355 (15)	0.00056 (14)	0.00304 (14)

O21	0.0367 (6)	0.0460 (7)	0.0303 (6)	0.0092 (6)	0.0008 (5)	0.0067 (5)
O22	0.0445 (8)	0.0541 (9)	0.0389 (7)	−0.0219 (7)	0.0019 (6)	0.0052 (6)
O23	0.0420 (7)	0.0285 (6)	0.0311 (6)	0.0017 (5)	0.0007 (5)	−0.0029 (4)
O24	0.0466 (7)	0.0363 (6)	0.0292 (6)	−0.0050 (5)	0.0018 (5)	−0.0085 (5)
O25	0.0428 (7)	0.0324 (6)	0.0314 (6)	−0.0025 (5)	0.0113 (5)	0.0040 (5)
C21	0.0405 (12)	0.0239 (9)	0.0218 (9)	0.000	−0.0021 (8)	0.000
C22	0.0380 (8)	0.0272 (7)	0.0232 (7)	−0.0022 (6)	0.0043 (6)	−0.0002 (5)
C23	0.0459 (10)	0.0366 (9)	0.0361 (9)	−0.0067 (8)	−0.0066 (7)	0.0008 (7)
C24	0.0525 (13)	0.0592 (13)	0.0511 (12)	−0.0067 (11)	0.0039 (10)	0.0196 (10)
C25	0.0864 (18)	0.0602 (15)	0.0407 (11)	−0.0310 (13)	−0.0218 (11)	0.0125 (10)
C26	0.0655 (13)	0.0310 (8)	0.0402 (10)	−0.0037 (8)	0.0233 (9)	0.0055 (7)
C27	0.0712 (17)	0.0718 (17)	0.0648 (16)	−0.0309 (14)	0.0225 (13)	−0.0053 (13)
C28	0.0781 (18)	0.0714 (17)	0.0367 (11)	0.0045 (14)	0.0095 (11)	0.0169 (11)
P31	0.0284 (2)	0.02564 (18)	0.02487 (19)	0.00070 (14)	0.00601 (14)	−0.00023 (13)
S31	0.02421 (18)	0.03015 (18)	0.02341 (17)	0.00079 (13)	0.00221 (13)	0.00124 (13)
O31	0.0290 (6)	0.0402 (6)	0.0337 (6)	−0.0092 (5)	0.0046 (4)	−0.0030 (5)
O32	0.0389 (7)	0.0492 (8)	0.0324 (6)	0.0130 (6)	0.0009 (5)	0.0106 (6)
O33	0.0403 (7)	0.0253 (5)	0.0408 (7)	−0.0026 (5)	0.0106 (5)	−0.0044 (5)
O34	0.0275 (6)	0.0364 (6)	0.0324 (6)	0.0044 (5)	0.0027 (4)	−0.0065 (5)
O35	0.0371 (7)	0.0477 (7)	0.0260 (6)	0.0036 (6)	0.0050 (5)	0.0080 (5)
C31	0.0299 (10)	0.0223 (9)	0.0262 (9)	0.000	0.0078 (8)	0.000
C32	0.0277 (7)	0.0254 (7)	0.0246 (7)	0.0004 (5)	0.0050 (5)	−0.0024 (5)
C33	0.0288 (8)	0.0432 (10)	0.0427 (10)	−0.0040 (7)	0.0009 (7)	−0.0058 (8)
C34	0.0490 (12)	0.0518 (13)	0.0599 (14)	0.0010 (10)	−0.0148 (10)	0.0068 (10)
C35	0.0319 (11)	0.143 (3)	0.0760 (18)	−0.0151 (15)	0.0172 (11)	−0.024 (2)
C36A	0.044 (4)	0.093 (7)	0.043 (4)	−0.010 (4)	0.005 (3)	0.037 (4)
C37A	0.072 (3)	0.042 (2)	0.058 (3)	0.0094 (19)	0.012 (2)	0.0191 (19)
C38A	0.159 (7)	0.102 (4)	0.085 (4)	0.069 (5)	0.086 (5)	0.039 (4)
C36B	0.072 (9)	0.045 (5)	0.033 (5)	−0.002 (4)	0.012 (5)	−0.001 (4)
C37B	0.108 (8)	0.077 (6)	0.025 (3)	0.023 (5)	0.008 (4)	−0.009 (3)
C38B	0.25 (2)	0.050 (6)	0.098 (11)	0.035 (10)	0.110 (13)	0.012 (6)

Geometric parameters (Å, °)

P1—O3	1.4722 (12)	C17—H17B	0.9800
P1—O5	1.5640 (13)	C17—H17C	0.9800
P1—O4	1.5693 (12)	C18—H18A	0.9800
P1—C2	1.8074 (16)	C18—H18B	0.9800
S1—O2	1.4359 (13)	C18—H18C	0.9800
S1—O1	1.4407 (13)	P21—O23	1.4721 (13)
S1—C2	1.7751 (16)	P21—O25	1.5635 (14)
S1—C1	1.7884 (12)	P21—O24	1.5658 (13)
O4—C3A	1.433 (5)	P21—C22	1.8085 (16)
O4—C3B	1.520 (6)	S21—O22	1.4355 (14)
O5—C6	1.471 (2)	S21—O21	1.4394 (13)
C1—S1^{i}	1.7884 (12)	S21—C22	1.7742 (16)
C1—H1	0.9601	S21—C21	1.7857 (12)
C2—H2A	0.9900	O24—C23	1.464 (2)
C2—H2B	0.9900	O25—C26	1.465 (2)

C3A—C5A	1.505 (6)	C21—S21^{iii}	1.7857 (12)
C3A—C4A	1.519 (6)	C21—H21	0.9601
C3A—H3A	1.0000	C22—H22A	0.9900
C4A—H4AA	0.9800	C22—H22B	0.9900
C4A—H4AB	0.9800	C23—C24	1.501 (3)
C4A—H4AC	0.9800	C23—C25	1.512 (3)
C5A—H5AA	0.9800	C23—H23	1.0000
C5A—H5AB	0.9800	C24—H24A	0.9800
C5A—H5AC	0.9800	C24—H24B	0.9800
C3B—C5B	1.484 (8)	C24—H24C	0.9800
C3B—C4B	1.521 (7)	C25—H25A	0.9800
C3B—H3B	1.0000	C25—H25B	0.9800
C4B—H4BA	0.9800	C25—H25C	0.9800
C4B—H4BB	0.9800	C26—C27	1.497 (4)
C4B—H4BC	0.9800	C26—C28	1.507 (3)
C5B—H5BA	0.9800	C26—H26	1.0000
C5B—H5BB	0.9800	C27—H27A	0.9800
C5B—H5BC	0.9800	C27—H27B	0.9800
C6—C7	1.502 (3)	C27—H27C	0.9800
C6—C8	1.508 (3)	C28—H28A	0.9800
C6—H6	1.0000	C28—H28B	0.9800
C7—H7A	0.9800	C28—H28C	0.9800
C7—H7B	0.9800	P31—O33	1.4706 (13)
C7—H7C	0.9800	P31—O35	1.5629 (13)
C8—H8A	0.9800	P31—O34	1.5728 (12)
C8—H8B	0.9800	P31—C32	1.8127 (15)
C8—H8C	0.9800	S31—O32	1.4355 (13)
P11—O13	1.4729 (12)	S31—O31	1.4423 (13)
P11—O15	1.5656 (13)	S31—C32	1.7735 (15)
P11—O14	1.5671 (12)	S31—C31	1.7879 (12)
P11—C12	1.8058 (15)	O34—C33	1.477 (2)
S11—O12	1.4374 (13)	O35—C36B	1.46 (2)
S11—O11	1.4419 (12)	O35—C36A	1.473 (10)
S11—C12	1.7740 (14)	C31—S31^{iv}	1.7879 (12)
S11—C11	1.7929 (11)	C31—H31	0.9598
O14—C13B	1.470 (16)	C32—H32A	0.9900
O14—C13A	1.498 (8)	C32—H32B	0.9900
O15—C16	1.4814 (19)	C33—C34	1.495 (3)
C11—S11^{ii}	1.7929 (11)	C33—C35	1.507 (3)
C11—H11	0.9600	C33—H33	1.0000
C12—H12A	0.9900	C34—H34A	0.9800
C12—H12B	0.9900	C34—H34B	0.9800
C13A—C15A	1.487 (7)	C34—H34C	0.9800
C13A—C14A	1.505 (7)	C35—H35A	0.9800
C13A—H13A	1.0000	C35—H35B	0.9800
C14A—H14A	0.9800	C35—H35C	0.9800
C14A—H14B	0.9800	C36A—C38A	1.478 (13)
C14A—H14C	0.9800	C36A—C37A	1.498 (10)

C15A—H15A	0.9800	C36A—H36A	1.0000
C15A—H15B	0.9800	C37A—H37A	0.9800
C15A—H15C	0.9800	C37A—H37B	0.9800
C13B—C15B	1.507 (13)	C37A—H37C	0.9800
C13B—C14B	1.515 (12)	C38A—H38A	0.9800
C13B—H13B	1.0000	C38A—H38B	0.9800
C14B—H14D	0.9800	C38A—H38C	0.9800
C14B—H14E	0.9800	C36B—C38B	1.429 (19)
C14B—H14F	0.9800	C36B—C37B	1.536 (15)
C15B—H15D	0.9800	C36B—H36B	1.0000
C15B—H15E	0.9800	C37B—H37D	0.9800
C15B—H15F	0.9800	C37B—H37E	0.9800
C16—C17	1.499 (3)	C37B—H37F	0.9800
C16—C18	1.508 (3)	C38B—H38D	0.9800
C16—H16	1.0000	C38B—H38E	0.9800
C17—H17A	0.9800	C38B—H38F	0.9800
O3—P1—O5	117.30 (7)	C16—C18—H18C	109.5
O3—P1—O4	115.03 (7)	H18A—C18—H18C	109.5
O5—P1—O4	103.57 (7)	H18B—C18—H18C	109.5
O3—P1—C2	113.86 (7)	O23—P21—O25	117.09 (8)
O5—P1—C2	101.31 (7)	O23—P21—O24	115.20 (8)
O4—P1—C2	103.95 (7)	O25—P21—O24	103.38 (7)
O2—S1—O1	119.43 (8)	O23—P21—C22	113.90 (7)
O2—S1—C2	109.54 (8)	O25—P21—C22	101.09 (8)
O1—S1—C2	107.34 (8)	O24—P21—C22	104.37 (7)
O2—S1—C1	105.49 (9)	O22—S21—O21	119.48 (9)
O1—S1—C1	107.82 (7)	O22—S21—C22	109.34 (8)
C2—S1—C1	106.54 (6)	O21—S21—C22	107.24 (8)
C3A—O4—P1	124.3 (2)	O22—S21—C21	105.40 (9)
C3B—O4—P1	120.9 (2)	O21—S21—C21	107.91 (7)
C6—O5—P1	122.74 (11)	C22—S21—C21	106.84 (6)
$S1^{i}$—C1—S1	117.41 (12)	C23—O24—P21	124.19 (12)
$S1^{i}$—C1—H1	108.0	C26—O25—P21	122.50 (13)
S1—C1—H1	107.9	$S21^{iii}$—C21—S21	116.99 (12)
S1—C2—P1	114.63 (9)	$S21^{iii}$—C21—H21	108.1
S1—C2—H2A	108.6	S21—C21—H21	108.0
P1—C2—H2A	108.6	S21—C22—P21	114.42 (9)
S1—C2—H2B	108.6	S21—C22—H22A	108.7
P1—C2—H2B	108.6	P21—C22—H22A	108.7
H2A—C2—H2B	107.6	S21—C22—H22B	108.7
O4—C3A—C5A	107.0 (4)	P21—C22—H22B	108.7
O4—C3A—C4A	106.7 (3)	H22A—C22—H22B	107.6
C5A—C3A—C4A	110.6 (4)	O24—C23—C24	109.23 (17)
O4—C3A—H3A	110.8	O24—C23—C25	106.07 (18)
C5A—C3A—H3A	110.8	C24—C23—C25	112.17 (18)
C4A—C3A—H3A	110.8	O24—C23—H23	109.8
C5B—C3B—O4	109.7 (5)	C24—C23—H23	109.8
C5B—C3B—C4B	114.0 (5)	C25—C23—H23	109.8

O4—C3B—C4B	106.2 (4)	C23—C24—H24A	109.5
C5B—C3B—H3B	109.0	C23—C24—H24B	109.5
O4—C3B—H3B	109.0	H24A—C24—H24B	109.5
C4B—C3B—H3B	109.0	C23—C24—H24C	109.5
C3B—C4B—H4BA	109.5	H24A—C24—H24C	109.5
C3B—C4B—H4BB	109.5	H24B—C24—H24C	109.5
H4BA—C4B—H4BB	109.5	C23—C25—H25A	109.5
C3B—C4B—H4BC	109.5	C23—C25—H25B	109.5
H4BA—C4B—H4BC	109.5	H25A—C25—H25B	109.5
H4BB—C4B—H4BC	109.5	C23—C25—H25C	109.5
C3B—C5B—H5BA	109.5	H25A—C25—H25C	109.5
C3B—C5B—H5BB	109.5	H25B—C25—H25C	109.5
H5BA—C5B—H5BB	109.5	O25—C26—C27	105.1 (2)
C3B—C5B—H5BC	109.5	O25—C26—C28	110.05 (18)
H5BA—C5B—H5BC	109.5	C27—C26—C28	113.92 (19)
H5BB—C5B—H5BC	109.5	O25—C26—H26	109.2
O5—C6—C7	105.20 (15)	C27—C26—H26	109.2
O5—C6—C8	109.44 (17)	C28—C26—H26	109.2
C7—C6—C8	113.71 (19)	C26—C27—H27A	109.5
O5—C6—H6	109.5	C26—C27—H27B	109.5
C7—C6—H6	109.5	H27A—C27—H27B	109.5
C8—C6—H6	109.5	C26—C27—H27C	109.5
C6—C7—H7A	109.5	H27A—C27—H27C	109.5
C6—C7—H7B	109.5	H27B—C27—H27C	109.5
H7A—C7—H7B	109.5	C26—C28—H28A	109.5
C6—C7—H7C	109.5	C26—C28—H28B	109.5
H7A—C7—H7C	109.5	H28A—C28—H28B	109.5
H7B—C7—H7C	109.5	C26—C28—H28C	109.5
C6—C8—H8A	109.5	H28A—C28—H28C	109.5
C6—C8—H8B	109.5	H28B—C28—H28C	109.5
H8A—C8—H8B	109.5	O33—P31—O35	117.38 (8)
C6—C8—H8C	109.5	O33—P31—O34	114.90 (7)
H8A—C8—H8C	109.5	O35—P31—O34	102.73 (7)
H8B—C8—H8C	109.5	O33—P31—C32	113.16 (7)
O13—P11—O15	117.52 (7)	O35—P31—C32	102.53 (7)
O13—P11—O14	114.40 (7)	O34—P31—C32	104.49 (7)
O15—P11—O14	103.43 (7)	O32—S31—O31	119.12 (8)
O13—P11—C12	112.81 (7)	O32—S31—C32	109.16 (8)
O15—P11—C12	102.35 (7)	O31—S31—C32	107.16 (8)
O14—P11—C12	104.81 (7)	O32—S31—C31	105.98 (9)
O12—S11—O11	119.22 (8)	O31—S31—C31	107.85 (7)
O12—S11—C12	109.26 (7)	C32—S31—C31	107.01 (6)
O11—S11—C12	107.12 (8)	C33—O34—P31	123.92 (11)
O12—S11—C11	105.72 (8)	C36B—O35—P31	122.8 (8)
O11—S11—C11	107.88 (6)	C36A—O35—P31	118.6 (4)
C12—S11—C11	107.06 (6)	S31—C31—S31^{iv}	117.09 (12)
C13B—O14—P11	129.3 (6)	S31—C31—H31	108.0
C13A—O14—P11	120.2 (2)	S31^{iv}—C31—H31	108.0

C16—O15—P11	119.94 (11)	S31—C32—P31	115.75 (8)
S11^{ii}—C11—S11	116.55 (11)	S31—C32—H32A	108.3
S11^{ii}—C11—H11	108.2	P31—C32—H32A	108.3
S11—C11—H11	108.1	S31—C32—H32B	108.3
S11—C12—P11	114.98 (8)	P31—C32—H32B	108.3
S11—C12—H12A	108.5	H32A—C32—H32B	107.4
P11—C12—H12A	108.5	O34—C33—C34	108.60 (16)
S11—C12—H12B	108.5	O34—C33—C35	105.06 (18)
P11—C12—H12B	108.5	C34—C33—C35	113.9 (2)
H12A—C12—H12B	107.5	O34—C33—H33	109.7
C15A—C13A—O14	107.6 (6)	C34—C33—H33	109.7
C15A—C13A—C14A	113.9 (5)	C35—C33—H33	109.7
O14—C13A—C14A	104.6 (4)	C33—C34—H34A	109.5
C15A—C13A—H13A	110.2	C33—C34—H34B	109.5
O14—C13A—H13A	110.2	H34A—C34—H34B	109.5
C14A—C13A—H13A	110.2	C33—C34—H34C	109.5
O14—C13B—C15B	98.0 (11)	H34A—C34—H34C	109.5
O14—C13B—C14B	115.5 (9)	H34B—C34—H34C	109.5
C15B—C13B—C14B	108.3 (9)	C33—C35—H35A	109.5
O14—C13B—H13B	111.4	C33—C35—H35B	109.5
C15B—C13B—H13B	111.4	H35A—C35—H35B	109.5
C14B—C13B—H13B	111.4	C33—C35—H35C	109.5
C13B—C14B—H14D	109.5	H35A—C35—H35C	109.5
C13B—C14B—H14E	109.5	H35B—C35—H35C	109.5
H14D—C14B—H14E	109.5	O35—C36A—C38A	106.8 (8)
C13B—C14B—H14F	109.5	O35—C36A—C37A	107.3 (7)
H14D—C14B—H14F	109.5	C38A—C36A—C37A	111.9 (7)
H14E—C14B—H14F	109.5	O35—C36A—H36A	110.2
C13B—C15B—H15D	109.5	C38A—C36A—H36A	110.2
C13B—C15B—H15E	109.5	C37A—C36A—H36A	110.2
H15D—C15B—H15E	109.5	C38B—C36B—O35	112.1 (16)
C13B—C15B—H15F	109.5	C38B—C36B—C37B	112.5 (14)
H15D—C15B—H15F	109.5	O35—C36B—C37B	111.0 (14)
H15E—C15B—H15F	109.5	C38B—C36B—H36B	107.0
O15—C16—C17	107.69 (14)	O35—C36B—H36B	107.0
O15—C16—C18	108.01 (15)	C37B—C36B—H36B	107.0
C17—C16—C18	112.54 (17)	C36B—C37B—H37D	109.5
O15—C16—H16	109.5	C36B—C37B—H37E	109.5
C17—C16—H16	109.5	H37D—C37B—H37E	109.5
C18—C16—H16	109.5	C36B—C37B—H37F	109.5
C16—C17—H17A	109.5	H37D—C37B—H37F	109.5
C16—C17—H17B	109.5	H37E—C37B—H37F	109.5
H17A—C17—H17B	109.5	C36B—C38B—H38D	109.5
C16—C17—H17C	109.5	C36B—C38B—H38E	109.5
H17A—C17—H17C	109.5	H38D—C38B—H38E	109.5
H17B—C17—H17C	109.5	C36B—C38B—H38F	109.5
C16—C18—H18A	109.5	H38D—C38B—H38F	109.5
C16—C18—H18B	109.5	H38E—C38B—H38F	109.5

H18A—C18—H18B	109.5		
O3—P1—O4—C3A	17.8 (3)	C13A—O14—C13B—C14B	−161 (3)
O5—P1—O4—C3A	147.1 (2)	P11—O14—C13B—C14B	135.4 (7)
C2—P1—O4—C3A	−107.4 (2)	P11—O15—C16—C17	−137.88 (14)
O3—P1—O4—C3B	44.4 (3)	P11—O15—C16—C18	100.33 (17)
O5—P1—O4—C3B	173.7 (3)	O23—P21—O24—C23	25.61 (16)
C2—P1—O4—C3B	−80.7 (3)	O25—P21—O24—C23	154.60 (14)
O3—P1—O5—C6	32.28 (16)	C22—P21—O24—C23	−100.03 (14)
O4—P1—O5—C6	−95.61 (14)	O23—P21—O25—C26	36.62 (17)
C2—P1—O5—C6	156.86 (14)	O24—P21—O25—C26	−91.20 (15)
O2—S1—C1—S1^{i}	176.09 (6)	C22—P21—O25—C26	160.95 (14)
O1—S1—C1—S1^{i}	47.44 (7)	O22—S21—C21—S21^{iii}	176.05 (7)
C2—S1—C1—S1^{i}	−67.53 (6)	O21—S21—C21—S21^{iii}	47.33 (7)
O2—S1—C2—P1	39.36 (12)	C22—S21—C21—S21^{iii}	−67.70 (6)
O1—S1—C2—P1	170.43 (8)	O22—S21—C22—P21	40.73 (13)
C1—S1—C2—P1	−74.28 (11)	O21—S21—C22—P21	171.65 (9)
O3—P1—C2—S1	42.99 (12)	C21—S21—C22—P21	−72.86 (11)
O5—P1—C2—S1	−83.87 (10)	O23—P21—C22—S21	44.75 (12)
O4—P1—C2—S1	168.90 (8)	O25—P21—C22—S21	−81.72 (10)
C3B—O4—C3A—C5A	113.5 (10)	O24—P21—C22—S21	171.21 (9)
P1—O4—C3A—C5A	−157.8 (3)	P21—O24—C23—C24	97.35 (18)
C3B—O4—C3A—C4A	−4.9 (8)	P21—O24—C23—C25	−141.56 (15)
P1—O4—C3A—C4A	83.8 (4)	P21—O25—C26—C27	−152.51 (16)
C3A—O4—C3B—C5B	17.7 (7)	P21—O25—C26—C28	84.4 (2)
P1—O4—C3B—C5B	−88.2 (5)	O33—P31—O34—C33	18.92 (16)
C3A—O4—C3B—C4B	−105.9 (11)	O35—P31—O34—C33	147.58 (14)
P1—O4—C3B—C4B	148.3 (4)	C32—P31—O34—C33	−105.67 (14)
P1—O5—C6—C7	−151.72 (17)	O33—P31—O35—C36B	64.7 (10)
P1—O5—C6—C8	85.76 (19)	O34—P31—O35—C36B	−62.3 (10)
O13—P11—O14—C13B	33.8 (6)	C32—P31—O35—C36B	−170.6 (10)
O15—P11—O14—C13B	162.9 (5)	O33—P31—O35—C36A	55.6 (6)
C12—P11—O14—C13B	−90.3 (5)	O34—P31—O35—C36A	−71.5 (6)
O13—P11—O14—C13A	16.2 (3)	C32—P31—O35—C36A	−179.7 (6)
O15—P11—O14—C13A	145.3 (3)	O32—S31—C31—S31^{iv}	174.83 (6)
C12—P11—O14—C13A	−107.9 (3)	O31—S31—C31—S31^{iv}	46.22 (6)
O13—P11—O15—C16	57.69 (14)	C32—S31—C31—S31^{iv}	−68.78 (6)
O14—P11—O15—C16	−69.41 (13)	O32—S31—C32—P31	45.23 (12)
C12—P11—O15—C16	−178.15 (12)	O31—S31—C32—P31	175.50 (8)
O12—S11—C11—S11^{ii}	175.24 (6)	C31—S31—C32—P31	−69.04 (10)
O11—S11—C11—S11^{ii}	46.65 (6)	O33—P31—C32—S31	41.17 (12)
C12—S11—C11—S11^{ii}	−68.35 (6)	O35—P31—C32—S31	−86.24 (10)
O12—S11—C12—P11	42.73 (11)	O34—P31—C32—S31	166.86 (8)
O11—S11—C12—P11	173.17 (8)	P31—O34—C33—C34	97.55 (18)
C11—S11—C12—P11	−71.32 (10)	P31—O34—C33—C35	−140.2 (2)
O13—P11—C12—S11	41.33 (11)	C36B—O35—C36A—C38A	−10 (8)
O15—P11—C12—S11	−85.91 (9)	P31—O35—C36A—C38A	110.2 (6)
O14—P11—C12—S11	166.40 (8)	C36B—O35—C36A—C37A	110 (8)

C13B—O14—C13A—C15A	95 (3)	P31—O35—C36A—C37A	−129.6 (5)
P11—O14—C13A—C15A	−137.8 (4)	C36A—O35—C36B—C38B	−26 (7)
C13B—O14—C13A—C14A	−26 (2)	P31—O35—C36B—C38B	−90.2 (18)
P11—O14—C13A—C14A	100.7 (4)	C36A—O35—C36B—C37B	−153 (10)
C13A—O14—C13B—C15B	−47 (2)	P31—O35—C36B—C37B	143.0 (10)
P11—O14—C13B—C15B	−109.8 (8)		

Symmetry codes: (i) −*x*+1/2, *y*, −*z*+1/2; (ii) −*x*+3/2, *y*, −*z*+3/2; (iii) −*x*+1/2, *y*, −*z*+3/2; (iv) −*x*+3/2, *y*, −*z*+1/2.

Fig. 1

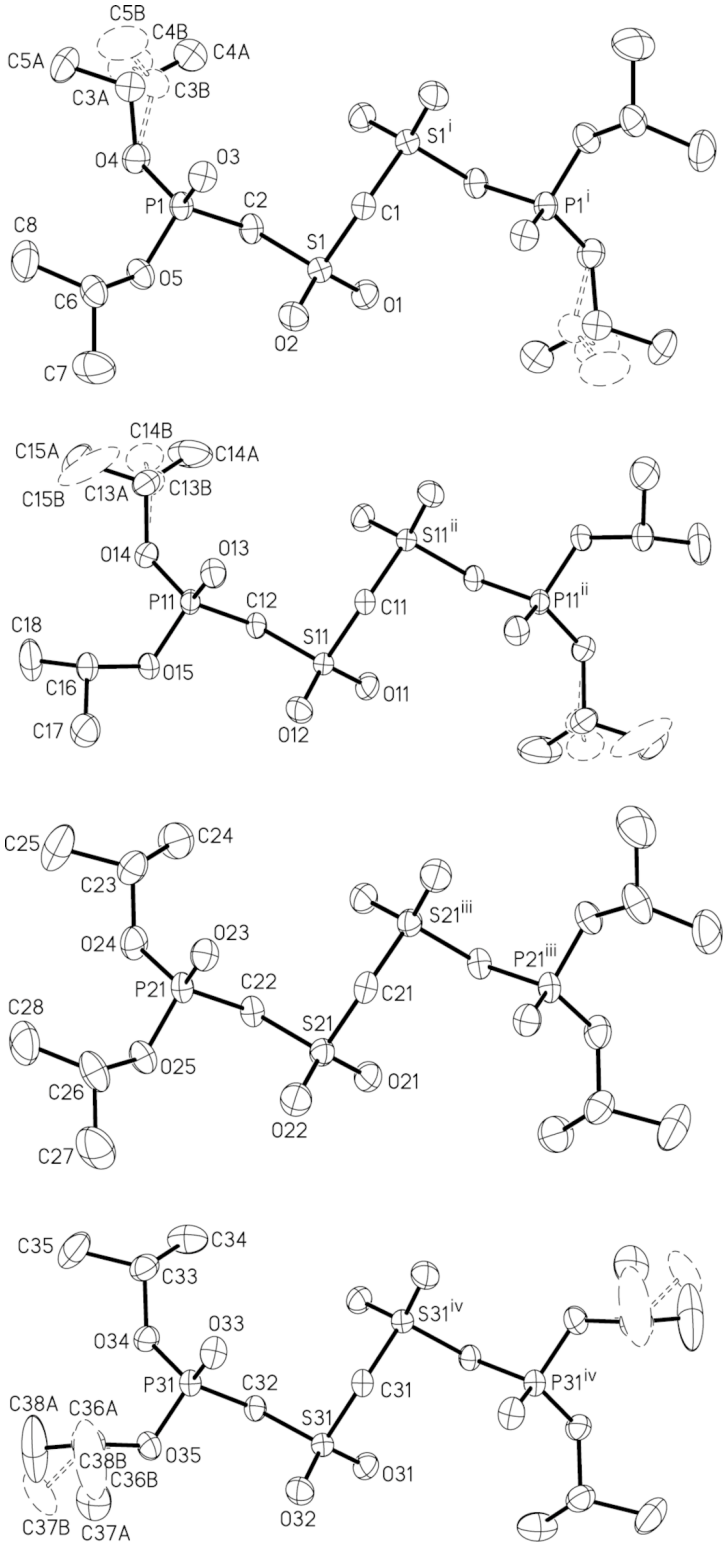

C5B
C4B
C4A
C5A
C3A
C3B
O4
O3
P1
C2
S1
C1
S1i
P1i
C8
O5
C6
C7
O1
O2
C14B
C15A
C14A
C15B
C13A
C13B
O14
O13
P11
C12
S11
C11
S11ii
P11ii
C18
O15
C16
C17
O11
O12
C25
C24
C23
O24
O23
P21
C22
S21
C21
S21iii
P21iii
C28
O25
C26
C27
O21
O22
C35
C34
C33
O34
O33
P31
C32
S31
C31
S31iv
P31iv
C38A
C36A
C38B
O35
C36B
C37B
C37A
O31
O32

Fig. 2