Table 1. Fractional atomic coordinates and equivalent isotropic thermal parameters (Å²)

$B_{eq} = \frac{4}{3} \sum_{i} \sum_{j} \beta_{ij} \mathbf{a}_{i} \cdot \mathbf{a}_{j}.$					
	x	у	z	B_{eq}	
S	0.5601 (2)	0.0197 (2)	0.2767 (2)	4.69 (5)	
O(1)	0.8645 (7)	0.3186 (5)	0.6945 (5)	5.9 (2)	
O(2)	0.7407 (6)	0.3856 (4)	0.4186 (5)	5.2 (2)	
O(3)	0.9372 (6)	0.4063 (4)	0.3798 (5)	5.6 (2)	
N	0.8686 (8)	-0.0645 (5)	0.5359 (7)	5.6 (2)	
C(1)	0.7915 (8)	0.2601 (6)	0.6217(7)	4.1 (2)	
C(2)	0.8430 (7)	0.2051 (6)	0.5368 (6)	3.3 (2)	
C(3)	0.7001 (7)	0.1589 (6)	0.4446 (6)	3.1(1)	
C(4)	0.6090 (8)	0.1385 (6)	0.5191 (6)	3.9 (2)	
C(5)	0.6404 (9)	0.2278 (7)	0.6008 (8)	4.9 (2)	
C(6)	0.9321 (8)	0.2663 (6)	0.4861 (6)	3.6 (2)	
C(7)	0.8525 (8)	0.3581 (6)	0.4234 (6)	3.6 (2)	
C(8)	0.883 (1)	0.4976 (8)	0.3232 (8)	6.2 (2)	
C(9)	0.7300 (8)	0.0690 (6)	0.3820 (6)	3.4 (2)	
C(10)	0.8093 (8)	-0.0069 (6)	0.4690 (6)	3.7 (2)	
C(11)	0.6263 (8)	-0.0745 (6)	0.2129 (7)	3.8 (2)	
C(12)	0.664 (1)	-0.0544 (7)	0.1174 (8)	5.8 (2)	
C(13)	0.719(1)	-0.1300 (9)	0.0719 (9)	9.2 (3)	
C(14)	0.738(1)	-0.2217 (8)	0.121(1)	8.1 (3)	
C(15)	0.701(1)	-0.2403 (7)	0.214(1)	7.1 (3)	
C(16)	0.644 (1)	-0.1670 (7)	0.2617 (8)	5.4 (3)	

Table 2. Selected bond distances (Å) and angles (°)

S-C(9)	1.812(7)	C(3)—C(4)	1.54 (1)
S-C(11)	1.769 (9)	C(3) - C(9)	1.54(1)
O(1) - C(1)	1.208 (9)	C(4)C(5)	1.53 (1)
O(2) - C(7)	1.16(1)	C(6)-C(7)	1.53 (1)
O(3)-C(7)	1.34(1)	C(11)-C(12)	1.38 (1)
O(3)-C(8)	1.43 (1)	C(11)-C(16)	1.39(1)
N-C(10)	1.13(1)	C(12)-C(13)	1.39 (2)
C(1)-C(2)	1.53 (1)	C(13)—C(14)	1.38 (2)
C(1)C(5)	1.50(1)	C(14)—C(15)	1.36 (2)
C(2)—C(3)	1.566 (9)	C(15)-C(16)	1.39 (2)
C(2)—C(6)	1.52 (1)	C(9)—C(10)	1.48 (1)
C(9)—S—C(11)	100.1 (4)	O(2)—C(7)—C(6)	126.7 (8)
C(7)—O(3)—C(8)	116.3 (7)	O(3) - C(7) - C(6)	108.6 (7)
O(1) - C(1) - C(2)	124.0 (8)	S-C(9)-C(3)	109.8 (5)
O(1) - C(1) - C(5)	127.0 (9)	S-C(9)-C(10)	109.5 (5)
C(2) - C(1) - C(5)	109.0 (6)	C(3) - C(9) - C(10)	111.5 (6)
C(1) - C(2) - C(3)	103.3 (6)	N - C(10) - C(9)	1 79 (1)
C(1) - C(2) - C(6)	114.2 (6)	S-C(11)-C(12)	119.7 (7)
C(3) - C(2) - C(6)	116.7 (6)	S-C(11)-C(16)	119.3 (8)
C(2) - C(3) - C(4)	103.7 (5)	C(12) - C(11) - C(16)	121.0 (9)
C(2) - C(3) - C(9)	112.3 (5)	C(11) - C(12) - C(13)	117.9 (9)
C(4) - C(3) - C(9)	114.8 (6)	C(12)-C(13)-C(14)	121(1)
C(3)C(4)C(5)	102.6 (7)	C(13) - C(14) - C(15)	120(1)
C(1) - C(5) - C(4)	106.5 (8)	C(14)-C(15)-C(16)	120(1)
C(2) - C(6) - C(7)	112.7 (6)	C(11)—C(16)—C(15)	119 (1)
O(2)-C(7)-O(3)	124.5 (7)		

The title compound was prepared by Michael addition of lithiated phenylthioacetonitrile to 2-cyclopentenone followed by methyl bromoacetate alkylation. After the usual treatment of the reaction medium, the residue was dissolved in the minimum amount of ether. After 48 h at room temperature, a solid had precipitated; crystals were grown by slow evaporation of an etheral solution at room temperature; m.p. 382 K.

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A Chiral Tetrahydro- γ -pyranonecarboxylate Ester for Asymmetric Nazarov Cyclization

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Abstract

(1S,2-exo)-1-[(N,N-Dicyclohexylamino)sulfonylmethyl]-7,7-dimethylbicyclo[2.2.1]heptan-2-yl [$2R(2\alpha,-3\beta,5\beta,6\alpha)$]-tetrahydro-2,5,6-trimethyl-4-oxo-2*H*-pyran-3-carboxylate, C₃₁H₅₁NO₆S, has an asymmetric unit containing two unique but similarly conformed molecules (A and B). In molecule A the cyclohexyl rings are free to crystallize in either of the approximately coplanar conformations, whereas in molecule B only one conformation is allowed. The N atoms in

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71450 (9 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: DU1045]

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each molecule have approximately planar geometries, as expected from previous related structures. The tetrahydropyranone ring adopts the chair conformation with all substituents equatorial.

Comment

The compound is a precursor for a Nazarov cyclization (Santelli-Rouvier & Santelli, 1983) to give a substituted cyclopentenone (Andrews & Regan, 1991), using a chiral auxiliary attached to the tetrahydr: γ - γ -pyranone via an ester linkage. In order to produce enantiomerically pure cyclopentenones, this intermediate was prepared from a racemic ester (1) and Oppolzer's enantiomerically pure alcohol (2) (Oppolzer, 1987) yielding two diastereoisomers, (3a) and (3b). Either isomer could be treated with a suitable Lewis acid causing dehydration to give a divinylketone intermediate, which then undergoes Nazarov's cyclization to a cyclopentenone.





(3a) Major diastereoisomer

(3b) Minor diastereoisomer

The X-ray crystal structure of the major diastereoisomer was determined in order to establish the absolute stereochemical configuration and to examine the conformation of the chiral auxiliary group, following the structure determination of an ester produced from a different chiral auxiliary and the same racemic ester (Andrews, Regan, Wallis & Povey, 1992). The relative stereochemistry of the tetrahydropyranone ring of the major diastereoisomer was the same in both cases.

The two unique molecules have similar conformations in the lattice: the N atoms are both planar [sum of angles at N: molecule A 360 (3), molecule B $359 (3)^{\circ}$].

In molecule A there is freedom for the cyclohexyl rings to crystallize into either approximately coplanar position, while in B only one conformation is allowed. This is shown by the apparent planarity of the rings in the plot of A (Fig. 1) compared with the obvious puckering of the rings in the plot of B (Fig. 2). The extended ellipsoid shape in the *ORTEP* plot (Johnson, 1965) of some of the ring C atoms in molecule A, and the apparently larger cyclohexyl



Fig. 1. ORTEP drawing of molecule A showing the numbering scheme; ellipsoids are represented at the 30% probability level.



Fig. 2. ORTEP drawing of molecule B showing the numbering scheme; ellipsoids are represented at the 30% probability level.

N(1A)

C(1A)

C(2A)

C(3A)

C(4A)

C(5A)

0.4863 (7)

0.237(1)

0.097(1)

0.017(1)

0.058 (1)

0.199 (1)

-0.0076(4)

0.1885 (6)

0.1839 (5)

0.1989 (6)

0.2452 (6)

0.2391 (5)

0.6913 (7)

0.597 (1)

0.531(1)

0.603 (1)

0.684 (1)

0.741 (1)

bond angles in molecule A compared with molecule B, confirm this.

The molecules pack in a nose-to-tail fashion with the extra-annular ester carbonyl group extending towards the N atom in the gap between the cyclo-

towards the N atom in the gap between the cyclo-		C(6A)	0.064 (1)	0.1255 (6)	0.476(1)	5.9 (6)
hexyl rings.		C(7A)	0.313 (1)	0.1918 (7)	0.522 (1)	8.3 (7)
		C(8A)	0.253 (1)	0.2885 (7)	0.819(1)	10.1 (9)
		C(9A)	-0.012 (2)	0.2484 (8)	0.761 (1)	12.0(1)
		C(10A)	0.0596 (8)	0.0213 (5)	0.5046 (9)	5.8 (5)
Experimental		C(11A)	-0.0804 (8)	0.0098 (5)	0.476 (1)	6.6 (6)
Crystal data		C(12A)	-0.0887(9)	-0.0420 (6)	0.549(1)	/.5(0)
Crystat data		C(13A)	-0.043(1)	-0.0970(6)	0.501(1)	0.7(7)
$C_{31}H_{51}NO_6S$	Cu $K\alpha$ radiation	C(14A) C(15A)	0.1138 (8)	-0.0259(5)	0.5892 (8)	59(5)
$M_r = 565.81$	$\lambda = 1.54178 \text{ Å}$	C(15A)	0.019 (1)	-0.0310(6)	0.649 (1)	7.2 (6)
Monoclinic	Cell parameters from 20	C(17A)	-0.001(1)	0.0255 (8)	0.707 (1)	8.4 (7)
P).	reflections	C(18A)	0.042 (1)	-0.0821 (7)	0.732 (1)	9.3 (8)
r = 11524(6) Å	$A = 20.5 - 36.7^{\circ}$	C(19A)	0.2441 (8)	-0.0139 (5)	0.6624 (8)	5.9 (5)
a = 11.334 (0) A	0 - 29.3 - 30.7	C(20A)	0.535 (1)	0.0494 (7)	0.731 (1)	9.6 (9)
b = 22.224 (8) A	$\mu = 0.11/2 \text{ mm}^{-1}$	C(21A)	0.494 (1)	0.0809 (6)	0.812(1)	7.8 (7)
c = 13.295 (9) A	T = 294 (1) K	C(22A)	0.547 (2)	0.1393 (8)	0.851 (1)	12.0(1)
$\beta = 108.09 (5)^{\circ}$	Prism	C(23A)	0.644 (2)	0.1658 (8)	0.821 (2)	15.0(1)
$V = 3239 (3) \text{ Å}^3$	$0.30 \times 0.15 \times 0.15$ mm	C(24A)	0.682 (2)	0.1357(9)	0.740(2)	12.0(1)
7 = 2	Colourless	C(25A)	0.033(1)	0.0703(7)	0.099(1)	9.0(8)
$D = 1.158 \text{ Mg m}^{-3}$	concurrence	C(20A)	0.540(1)	-0.0851(6)	0.747(1) 0.714(1)	73(7)
$D_x = 1.150$ wig m		C(28A)	0.047(1) 0.717(1)	-0.1353(8)	0.776 (1)	10.1 (9)
D		C(29A)	0.676 (1)	-0.1670 (7)	0.851 (2)	11.0(1)
Data collection		C(30A)	0.580(1)	-0.1398 (6)	0.889(1)	8.3 (7)
Rigaku AFC-5R diffractome-	$\theta_{\rm max} = 60^{\circ}$	C(31A)	0.510(1)	-0.0891 (6)	0.828 (1)	7.8 (7)
ter	$h = -9 \rightarrow 12$	S(1 <i>B</i>)	0.2568 (2)	0.1241	0.0736 (2)	5.9(1)
ω 12A scans	$k = -15 \rightarrow 17$	O(1 <i>B</i>)	0.6768 (8)	-0.0697 (4)	0.3114 (8)	10.1 (5)
Absention consection:	l = 11 + 12	O(2 <i>B</i>)	0.3339 (7)	-0.1303 (4)	0.186(1)	7.7 (5)
Absorption correction:	$i = -11 \implies 13$	O(3 B)	0.6056 (7)	-0.0138 (5)	0.0612 (7)	9.0 (5)
none	3 standard reflections	O(4 <i>B</i>)	0.5202 (6)	0.0252 (4)	0.1770 (6)	6.5 (4)
4395 measured reflections	monitored every 150	O(5B)	0.2842 (6)	0.0768 (4)	0.0134 (6)	7.3(4)
4083 independent reflections	reflections	U(0 <i>B</i>)	0.2557 (6)	0.1843 (4)	0.0303 (0)	57(4)
3144 observed reflections	intensity variation:	C(1B)	0.1250(0)	-0.0800 (6)	0.0092(0)	67(6)
$[I > \sigma(I)]$	-11.8%	C(2B)	0.507(1)	-0.0785(6)	0.155 (1)	7.1 (7)
$P_{\rm r} = 0.076$		C(3B)	0.579(1)	-0.0931(5)	0.269 (1)	7.1 (6)
R _{int} = 0.070		C(4B)	0.528 (1)	-0.1402 (6)	0.327 (1)	7.2 (7)
Deferrent and		C(5B)	0.390(1)	-0.1298 (6)	0.299 (1)	7.4 (7)
Rejinemeni		C(6B)	0.552 (1)	-0.0202 (7)	0.124 (1)	7.1 (7)
Refinement on F^2	$w = 4F_o^2/\sigma^2(F_o)^2$	C(7 <i>B</i>)	0.297 (1)	-0.0818 (7)	0.021 (1)	9.4 (8)
R = 0.069	$(\Delta/\sigma)_{\rm max} < 0.029$	C(8B)	0.327 (1)	-0.1764 (8)	0.345 (1)	11.0(1)
$w \mathbf{R} = 0.080$	$\Lambda_{2} = 0.28 \circ \Lambda^{-3}$	C(9B)	0.594 (2)	-0.1368 (8)	0.445 (1)	11.0(1)
R = 1.22	$\Delta p_{\text{max}} = 0.28 \text{ e A}$	C(10B)	0.5597 (8)	0.0848 (0)	0.1334 (9)	9.1 (3) 9.1 (7)
5 = 1.55	$\Delta \rho_{\rm min} = -0.31 \ {\rm e \ A}$	C(11B)	0.099(1)	0.0933(7)	0.212(1) 0.282(1)	82(7)
3144 reflections	Atomic scattering factors	C(12B) C(13R)	0.661 (1)	0.1493(7) 0.2041(7)	0.202(1)	9.9 (9)
701 parameters	from Cromer & Waber	C(14B)	0.525(1)	0.1918 (6)	0.158 (1)	7.3 (6)
H atoms refined as riding	(1974)	C(15B)	0.5001 (8)	0.1322 (5)	0.2084 (9)	5.8 (5)
(Beurskens, 1984)	. ,	C(16B)	0.589 (1)	0.1377 (6)	0.320 (1)	7.5 (7)
Program(c) used to colve struc	ture: TEYSAN (Molecular Struc	C(17B)	0.599 (1)	0.0825 (8)	0.390 (1)	8.8 (8)
riogram(s) used to solve struc	UTUDII (Cilmono 1094) and	C(18B)	0.563 (1)	0.1914 (7)	0.382 (1)	9.8 (8)
ture Corporation, 1985), M	iinkil (Gimore, 1984) and	C(19 <i>B</i>)	0.3669 (8)	0.1200 (5)	0.2012 (8)	5.6 (5)
SHELXS86 (Sheldrick, 1986)	. Anomalous-dispersion effects	C(20 B)	0.0886 (9)	0.0473 (5)	0.0961 (8)	5.1 (5)
were included in F_c (Ibers & Hamilton, 1964). Molecular graph-		C(21 <i>B</i>)	0.089(1)	0.0273 (5)	0.203 (1)	6.3 (6)

C(22B)

C(23*B*)

C(24B)

C(25B)

C(26B)

C(27B)

C(28B)

C(29B)

C(30**B**)

C(31B)

Table 1. Fractional atomic coordinates and equivalent isotropic thermal parameters $(Å^2)$

ics: ORTEP (Johnson, 1965).

$B_{\rm eq} = (8\pi^2/3)\sum_i\sum_j U_{ij}a_i^*a_i^*\mathbf{a}_i.\mathbf{a}_j.$				
	x	у	z	B _{eq}
S(1A)	0.3599 (2)	-0.0138	0.5993 (2)	6.8 (2)
O(1A)	-0.0804(8)	0.1741 (5)	0.5847 (8)	9.8 (5)
O(2A)	0.2611 (7)	0.2394 (4)	0.6622 (6)	6.8 (4)
O(3A)	0.0133 (7)	0.1206 (4)	0.3837 (7)	6.7 (4)
O(4A)	0.0925 (6)	0.0814 (4)	0.5470 (6)	5.8 (4)
O(5A)	0.3450 (7)	0.0380 (6)	0.5343 (8)	11.6 (6)
O(6A)	0.3630 (8)	-0.0714 (6)	0.5553 (8)	12.2 (7

3.1 (7) .2 (7) .9 (9) .3 (6) .8 (5) .5 (7) .8 (8) .8 (8) .6 (5) 5.1 (5) 6.3 (6) 0.051 (1) -0.0377 (6) 0.206 (1) 7.9 (7) -0.074 (1) -0.0489(6)0.126 (2) 10.2 (9) -0.072 (1) -0.0292(7)0.019 (1) 9.6 (8) 0.015(1) 7.9(7) -0.037 (1) 0.0372 (6) 5.6 (5) 0.0498 (9) 0.1598 (5) 0.1128 (9) -0.015(1)0.1945 (6) 0.011 (1) 7.0 (6) 0.2385 (6) 0.031(1) 7.6 (6) -0.108(1)-0.050(1) 0.2798 (6) 0.125(1)7.8 (6) 0.2444 (5) 0.225(1)6.5 (5) 0.016(1) 0.1094 (9) 0.1997 (5) 0.2048 (9) 5.2 (5)

Table 2. Geometric parameters (Å, °)

S(1A) - O(5A)	1.42 (1)	S(1B) - O(5B)	1.416 (7)
S(1A) - O(6A)	1.41 (1)	S(1B) - O(6B)	1.429 (8)
S(1A) - N(1A)	1.591 (8)	S(1B) - N(1B)	1.628 (7)

6.0 (4)

6.3 (6)

6.1 (6)

7.1 (7)

7.6(7)

6.9 (6)

	1./8(1)	S(1B) - C(19B)	1.78(1)
O(1A) - C(3A)	1.21(1)	O(1B) - C(3B)	1.21 (1)
O(2A) - C(1A)	1.40(1)	O(2B) - C(1B)	1.40(1)
O(2A) - C(5A)	1.44 (1)	O(2B) - C(5B)	1.43 (1)
O(34) - C(64)	1.19(1)	O(3R) - C(6R)	1 20 (1)
$\Omega(4A) - C(6A)$	1 33 (1)	O(4R) - C(6R)	1 34 (1)
O(44) = C(104)	1.00(1)	O(4B) - C(10B)	1.34(1)
N(14) = C(204)	1.43 (1)	N(1B) = C(20B)	1.46(1)
N(1A) = C(2(A))	1.42(2)	N(1B) = C(20B)	1.40(1)
N(IA) = C(2bA)	1.40(1)	N(IB) - C(20B)	1.50(1)
C(IA) = C(2A)	1.59(1)	C(1B) = C(2B)	1.54 (2)
C(IA) - C(/A)	1.52(2)	C(1B) - C(7B)	1.52 (2)
C(2A) - C(3A)	1.57 (1)	C(2B) - C(3B)	1.53 (2)
C(2A) - C(6A)	1.48 (2)	C(2B) - C(6B)	1.50 (2)
C(3A) - C(4A)	1.45 (2)	C(3B) - C(4B)	1.52 (2)
C(4A) - C(5A)	1.57 (2)	C(4B) - C(5B)	1.54 (2)
C(4A) - C(9A)	1.49 (2)	C(4B) - C(9B)	1.52 (2)
C(5A) - C(8A)	1.51 (2)	C(5B) - C(8B)	1.50 (2)
C(10A) - C(11A)	1 56 (1)	C(10R) - C(11R)	1 57 (1)
C(104) - C(154)	1.50(1)	C(10B) - C(15B)	1.57(1)
C(114) = C(124)	1.52(1)	C(11B) = C(12B)	1.5+(1)
C(124) = C(124)	1.52(1)	C(12B) = C(12B)	1.51(2)
C(12A) = C(13A)	1.54 (2)	C(12B) = C(13B)	1.54 (2)
C(12A) - C(10A)	1.54 (2)	C(12B) - C(16B)	1.54 (1)
C(13A) - C(14A)	1.56 (2)	C(13B) - C(14B)	1.53 (2)
C(14A) - C(15A)	1.55 (1)	C(14B) - C(15B)	1.55 (2)
C(15A) - C(16A)	1.55 (1)	C(15B) - C(16B)	1.52 (2)
C(15A) - C(19A)	1.54 (1)	C(15B) - C(19B)	1.53(1)
C(16A) - C(17A)	1.53 (2)	C(16B) - C(17B)	1.52 (2)
C(164) - C(184)	1 55 (2)	C(16B) - C(18B)	1 54 (2)
C(20A) - C(21A)	147(2)	C(20B) - C(21B)	1 49 (1)
C(204) - C(254)	1.45(2)	C(20B) = C(25B)	1 53 (2)
C(20A) = C(23A)	1.45(2)	C(20B) = C(20B)	1.55(2)
C(21A) = C(22A)	1.40(2)	C(21B) = C(22B)	1.52(2)
C(22A) = C(23A)	1.42 (3)	C(22B) = C(23B)	1.52 (2)
C(23A) = C(24A)	1.44 (3)	C(23B) = C(24B)	1.50(2)
C(24A) = C(25A)	1.47(2)	C(24B) - C(25B)	1.53(2)
C(26A) - C(27A)	1.47 (2)	C(26B) - C(27B)	1.54 (2)
C(26A) - C(31A)	1.41 (2)	C(26B) - C(31B)	1.49 (1)
C(27A) - C(28A)	1.46 (2)	C(27B)-C(28B)	1.54 (2)
C(28A) - C(29A)	1.42 (2)	C(28B) = C(20B)	1.52 (2)
		C(20D) - C(29D)	
C(29A) - C(30A)	1.48 (2)	C(29B) - C(29B) C(29B) - C(30B)	1.53 (2)
C(29A) - C(30A) C(30A) - C(31A)	1.48 (2) 1.47 (2)	C(28B) - C(29B) C(29B) - C(30B) C(30B) - C(31B)	1.53 (2) 1.55 (1)
C(29A) - C(30A) C(30A) - C(31A)	1.48 (2) 1.47 (2)	C(29B) - C(29B) C(29B) - C(30B) C(30B) - C(31B)	1.53 (2) 1.55 (1)
C(29A) - C(30A) C(30A) - C(31A) O(5A) - S(1A) - O(6A)	1.48 (2) 1.47 (2) 119.8 (7)	C(29B)-C(29B) C(29B)-C(30B) C(30B)-C(31B) O(5B)-S(1B)-O(6B)	1.53 (2) 1.55 (1) 118.8 (5)
C(29A) - C(30A) C(30A) - C(31A) O(5A) - S(1A) - O(6A) O(5A) - S(1A) - N(1A)	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5)	C(28B)-C(29B) C(29B)-C(30B) C(30B)-C(31B) O(5B)-S(1B)-O(6B) O(5B)-S(1B)-N(1B)	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4)
C(29A) - C(30A) C(30A) - C(31A) O(5A) - S(1A) - O(6A) O(5A) - S(1A) - N(1A) O(5A) - S(1A) - C(19A) O(5A) - S(1A) - C(1A) - C(1A	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5)	C(29B) - C(30B) C(30B) - C(31B) O(5B) - S(1B) - O(6B) O(5B) - S(1B) - N(1B) O(5B) - S(1B) - C(19B)	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5)
C(29A)-C(30A) C(30A)-C(31A) O(5A)-S(1A)-O(6A) O(5A)-S(1A)-N(1A) O(5A)-S(1A)-C(19A) O(6A)-S(1A)-N(1A)	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 105.2 (5)	C(28b) = C(38b) C(29b) = C(30b) C(30b) = C(31b) O(5b) = S(1b) = O(6b) O(5b) = S(1b) = O(6b) O(5b) = S(1b) = C(19b) O(6b) = S(1b) = O(1b) O(1b) = O(1b) = O(1b) O(1b) = O(1b)	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 108.6 (5)
C(29A) - C(30A) C(30A) - C(31A) O(5A) - S(1A) - O(6A) O(5A) - S(1A) - N(1A) O(5A) - S(1A) - C(19A) O(6A) - S(1A) - N(1A) O(6A) - S(1A) - C(19A) O(7A) - C(19A) - C(19A) O(7A) - C(19A)	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 105.2 (5) 108.2 (6)	C(29B)-C(30B) C(30B)-C(31B) O(5B)-S(1B)-O(6B) O(5B)-S(1B)-N(1B) O(5B)-S(1B)-C(19B) O(6B)-S(1B)-N(1B) O(6B)-S(1B)-C(19B) O(6B)-S(1B)	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 108.6 (5) 107.8 (5)
C(29A) - C(30A) C(30A) - C(31A) O(5A) - S(1A) - O(6A) O(5A) - S(1A) - N(1A) O(5A) - S(1A) - C(19A) O(6A) - S(1A) - C(19A) O(6A) - S(1A) - C(19A) N(1A) - S(1A) - C(19A) O(5A) - S(1A) - C(19A) - C(19A) O(5A) - S(1A) - C(19A) - C(19A) - C(19A) - C(19A) - C(19A)	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 105.2 (5) 108.2 (6) 106.2 (5)	C(29B) - C(39B) C(30B) - C(31B) O(5B) - S(1B) - O(6B) O(5B) - S(1B) - N(1B) O(5B) - S(1B) - C(19B) O(6B) - S(1B) -	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 108.6 (5) 107.8 (5) 106.7 (4)
C(29A)-C(30A)C(30A)-C(31A)O(5A)-S(1A)-O(6A)O(5A)-S(1A)-N(1A)O(5A)-S(1A)-C(19A)O(6A)-S(1A)-C(19A)O(6A)-S(1A)-C(19A)N(1A)-S(1A)-C(19A)	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 105.2 (5) 108.2 (6) 106.2 (5)	C(29B) - C(30B) C(30B) - C(31B) O(5B) - S(1B) - O(6B) O(5B) - S(1B) - N(1B) O(5B) - S(1B) - C(19B) O(6B) - S(1B) - C(19B) O(6B) - S(1B) - C(19B) N(1B) - C(19B)	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 108.6 (5) 107.8 (5) 106.7 (4)
C(29A)-C(30A)C(30A)-C(31A)O(5A)-S(1A)-O(6A)O(5A)-S(1A)-N(1A)O(5A)-S(1A)-C(19A)O(6A)-S(1A)-C(19A)N(1A)-S(1A)-C(19A)N(1A)-S(1A)-C(19A)C(1A)-O(2A)-C(5A)C(1A)-O(2A)-C(5A)	1.48 (2) 1.47 (2) 107.9 (5) 108.7 (5) 108.2 (5) 108.2 (6) 106.2 (5) 113.5 (8)	C(29B)-C(30B)C(30B)-C(31B)O(5B)-S(1B)-O(6B)O(5B)-S(1B)-N(1B)O(5B)-S(1B)-C(19B)O(6B)-S(1B)-C(19B)O(6B)-S(1B)-C(19B)N(1B)-C(1B)-C(19B)C(1B)-O(2B)-C(5B)C(1B)-O(2B)-C(5B)	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 108.6 (5) 107.8 (5) 106.7 (4) 112 (1)
$\begin{array}{c} C(29A) - C(30A) \\ C(30A) - C(31A) \\ O(5A) - S(1A) - O(6A) \\ O(5A) - S(1A) - N(1A) \\ O(5A) - S(1A) - C(19A) \\ O(6A) - S(1A) - C(19A) \\ O(6A) - S(1A) - C(19A) \\ O(1A) - S(1A) - C(19A) \\ C(1A) - O(2A) - C(5A) \\ C(6A) - O(4A) - C(10A) \\ \end{array}$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 105.2 (5) 106.2 (5) 113.5 (8) 115.3 (9)	C(28b) - C(29b) - C(30b) - C(30b) - C(30b) - C(30b) - C(31b) - C(30b) - C(31b) - C(30b) - C	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 108.6 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9)
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ C(14)-O(24)-C(54)\\ C(64)-O(44)-C(104)\\ S(14)-N(14)-C(204)\\ \end{array}$	1.48 (2) 1.47 (2) 119,8 (7) 107,9 (5) 108,7 (5) 105,2 (5) 106,2 (5) 113,5 (8) 115,3 (9) 122 (1)	C(28b) - C(29b) - C(29b) - C(30b) - C(10b) - C(20b) - C	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 108.6 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6)
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ C(14)-O(24)-C(54)\\ C(64)-O(44)-C(104)\\ S(14)-N(14)-C(204)\\ S(14)-N(14)-C(264)\\ \end{array}$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 105.2 (5) 108.2 (6) 106.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9)	C(28b) - C(29b) - C(30b) - C(30b) - C(30b) - C(30b) - C(31b) - C(30b) - C(31b) - C(31b) - C(3b) - C(1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 108.6 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7)
$\begin{array}{c} C(29A)-C(30A) \\ C(30A)-C(31A) \\ \hline \\ O(5A)-S(1A)-O(6A) \\ O(5A)-S(1A)-N(1A) \\ O(5A)-S(1A)-C(19A) \\ O(6A)-S(1A)-C(19A) \\ O(6A)-S(1A)-C(19A) \\ N(1A)-S(1A)-C(19A) \\ C(1A)-O(2A)-C(5A) \\ C(6A)-O(4A)-C(10A) \\ S(1A)-N(1A)-C(20A) \\ S(1A)-N(1A)-C(26A) \\ C(20A)-N(1A)-C(26A) \end{array}$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 108.2 (5) 108.2 (6) 106.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1)	C(28b)-C(28b) - C(28b) - C(30B) - C(30B) - C(30B) - C(31B) - C(30B) - C(31B) - C(30B) - C(31B) - C(30B) - C(3	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 108.6 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7)
$\begin{array}{c} C(29A)-C(30A) \\ C(30A)-C(31A) \\ O(5A)-S(1A)-O(6A) \\ O(5A)-S(1A)-N(1A) \\ O(5A)-S(1A)-C(19A) \\ O(6A)-S(1A)-C(19A) \\ O(6A)-S(1A)-C(19A) \\ O(1A)-S(1A)-C(19A) \\ C(1A)-O(2A)-C(5A) \\ C(1A)-O(2A)-C(5A) \\ C(6A)-O(4A)-C(10A) \\ S(1A)-N(1A)-C(26A) \\ C(20A)-N(1A)-C(26A) \\ C(20A)-C(1A)-C(2A) \\ \end{array}$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 105.2 (5) 106.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9)	C(28b) - C(28b) C(29B) - C(30B) C(30B) - C(31B) O(5B) - S(1B) - O(6B) O(5B) - S(1B) - N(1B) O(5B) - S(1B) - C(19B) O(6B) - S(1B) - C(19B) O(6B) - S(1B) - C(19B) C(1B) - O(2B) - C(5B) C(6B) - O(4B) - C(10B) S(1B) - N(1B) - C(20B) S(1B) - N(1B) - C(26B) C(20B) - N(1B) - C(26B) O(2B) - C(1B) - C(2B) (C(2B) - C(2B) (1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 107.8 (5) 107.8 (5) 107.8 (5) 107.8 (5) 107.8 (5) 107.8 (5) 107.8 (5) 107.9 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 112 (1)
$\begin{array}{l} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ N(14)-O(24)-C(54)\\ C(64)-O(44)-C(104)\\ S(14)-N(14)-C(264)\\ S(14)-N(14)-C(264)\\ C(204)-N(14)-C(264)\\ O(24)-C(14)-C(74)\\ \end{array}$	1.48 (2) 1.47 (2) 1.9,8 (7) 107,9 (5) 105,2 (5) 106,2 (5) 106,2 (5) 113,5 (8) 115,3 (9) 122 (1) 119,8 (9) 118 (1) 111,5 (9) 109 (1)	C(28b) - C(28b) C(29b) - C(30b) C(30b) - C(31b) O(5b) - S(1b) - O(6b) O(5b) - S(1b) - N(1b) O(5b) - S(1b) - C(19b) O(6b) - S(1b) - C(19b) O(6b) - S(1b) - C(19b) C(1b) - O(2b) - C(5b) C(6b) - O(4b) - C(10b) S(1b) - N(1b) - C(26b) S(1b) - N(1b) - C(26b) O(2b) - C(1b) - C(2b) O(2b) - C(2b) - C(2b) - C(2b) O(2b) - C(2b) -	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 119.6 (7) 112 (1) 108 (1)
$\begin{array}{l} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ C(14)-O(24)-C(54)\\ C(64)-O(44)-C(104)\\ S(14)-N(14)-C(264)\\ S(14)-N(14)-C(264)\\ C(204)-N(14)-C(264)\\ O(24)-C(14)-C(24)\\ O(24)-C(14)-C(74)\\ \end{array}$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 108.2 (5) 108.2 (6) 106.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1)	C(28b)-C(28b) = C(28b) = C(30B) = C(20B) = C(2	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 119.6 (7) 112 (1) 108 (1) 110 (1)
$\begin{array}{c} C(294)-C(30A) \\ C(30A)-C(31A) \\ O(5A)-S(1A)-O(6A) \\ O(5A)-S(1A)-N(1A) \\ O(5A)-S(1A)-C(19A) \\ O(6A)-S(1A)-C(19A) \\ O(6A)-S(1A)-C(19A) \\ N(1A)-S(1A)-C(19A) \\ C(1A)-O(2A)-C(5A) \\ C(6A)-O(4A)-C(10A) \\ S(1A)-N(1A)-C(26A) \\ C(20A)-N(1A)-C(26A) \\ C(20A)-N(1A)-C(26A) \\ O(24)-C(1A)-C(2A) \\ O(24)-C(1A)-C(2A) \\ O(24)-C(1A)-C(7A) \\ C(2A)-C(1A)-C(7A) \\ C(2A)-C(1A)-C(7A) \\ C(2A)-C(1A)-C(7A) \\ C(2A)-C(1A)-C(7A) \\ C(2A)-C(2A)-C(3A) \\ \end{array}$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 108.2 (6) 108.2 (6) 108.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1)	C(28b) - C(28b) - C(28b) - C(30B) - C(20B) - C	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 112 (1) 108 (1) 110 (1) 111 (1)
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ C(14)-O(24)-C(54)\\ C(64)-O(14)-C(104)\\ S(14)-N(14)-C(264)\\ O(24)-C(14)-C(24)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(14)-C(24)-C(34)\\ C(14)-C(24)-C(14)\\ C(14)-C(24)\\ C(14)-C(24)-C($	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 105.2 (5) 106.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1) 110 (1) 113 (1)	C(28b) - C(28b) C(29b) - C(30b) C(29b) - C(30b) C(30b) C(30b) - C(31b) C(5b) - S(1b) - N(1b) O(5b) - S(1b) - N(1b) O(5b) - S(1b) - N(1b) O(6b) - S(1b) - N(1b) O(6b) - S(1b) - N(1b) O(6b) - S(1b) - C(19b) N(1b) - C(2b) - C(5b) C(6b) - O(4b) - C(10b) S(1b) - N(1b) - C(2cb) S(1b) - N(1b) - C(2cb) C(2b) - C(1b) - C(2cb) C(2b) - C(1b) - C(2cb) O(2b) - C(1b) - C(2cb) C(2b) - C	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 107.8 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 119.6 (7) 119 (1) 110 (1) 111 (1) 115 (1)
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ C(14)-O(24)-C(54)\\ C(64)-O(44)-C(104)\\ S(14)-N(14)-C(264)\\ C(204)-N(14)-C(264)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(14)-C(24)-C(54)\\ C(14)$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 105.2 (5) 106.2 (5) 113.5 (8) 115.3 (9) 112 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1) 110 (1) 113 (1) 112 (1)	C(28b) - C(28b) C(29b) - C(30b) C(30b) - C(31b) O(5b) - S(1b) - O(6b) O(5b) - S(1b) - N(1b) O(5b) - S(1b) - C(19b) O(6b) - S(1b) - C(19b) O(6b) - S(1b) - C(19b) C(1b) - O(2b) - C(5b) C(2b) - O(4b) - C(10b) S(1b) - N(1b) - C(26b) C(2b) - C(1b) - C(2b) O(2b) - C(1b) - C(2b) O(2b) - C(1b) - C(7b) C(2b) - C(1b) - C(7b) C(2b) - C(2b) - C(6b) C(1b) - C(2b) - C(6b) C(2b) - C(2b) - C(b) C(2b) - C(2b) - C(b) C(2b) - C(b) - C(b) C(b) - C(b) - C(b) - C(b) C(b) - C(b)	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 108.4 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 119.6 (7) 119.6 (7) 119.1 (1) 110 (1) 111 (1) 115 (1) 108 (1)
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ C(14)-O(24)-C(54)\\ C(54)-O(44)-C(104)\\ S(14)-N(14)-C(264)\\ O(24)-C(14)-C(264)\\ O(24)-C(14)-C(264)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(14)-C(24)-C(54)\\ C(14)-C(24)-C(54)\\ C(14)-C(24)-C(54)\\ C(34)-C(24)-C(64)\\ C(34)-C(24)-C(24)\\ C(34)-C(24)-C(24)\\ C(34)-C(24)-C(24)\\ C(34)-C(24)-C(24)\\ C(34)-C(24)-C(24)\\ C(34)-C(24)-C(24)\\ C(34)-C(24)-C(24)\\ C(34)-C(24)-C(24)\\ C(34)-C(24)-C(24)\\ C(34)-C(24)\\ C(34)\\ C(34)-C(24)\\ C(34)\\ C(34)-C(24)\\ C(34)\\ C(34)-C(24)\\ C(34)\\ C(34)$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 108.2 (5) 108.2 (6) 106.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1) 113 (1) 112 (1) 112 (1) 112 (1)	C(28b) - C(28b) - C(28b) - C(30B) - C(26B) - C	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 108.6 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 112 (1) 108 (1) 115 (1) 108 (1) 201 (1)
$\begin{array}{c} C(294) - C(30A) \\ C(30A) - C(31A) \\ O(5A) - S(1A) - O(6A) \\ O(5A) - S(1A) - N(1A) \\ O(5A) - S(1A) - C(19A) \\ O(6A) - S(1A) - C(19A) \\ O(6A) - S(1A) - C(19A) \\ N(1A) - S(1A) - C(19A) \\ C(1A) - O(2A) - C(5A) \\ C(5A) - O(2A) - C(5A) \\ C(5A) - O(4A) - C(10A) \\ S(1A) - N(1A) - C(26A) \\ O(2A) - C(1A) - C(26A) \\ O(2A) - C(1A) - C(2A) \\ O(2A) - C(1A) - C(7A) \\ C(1A) - C(2A) - C(5A) \\ C(1A) - C(2A) - C(5A) \\ C(2A) - C(1A) - C(7A) \\ C(2A) - C(1A) - C(7A) \\ C(1A) - C(2A) - C(5A) \\ C(1A) - C(2A) - C(6A) \\ C(3A) - C(2A) - C(6A) \\ O(1A) - C(2A) - C(2A) \\ O(1A) - C(2A) - C(2A) \\ O(1A) - C(2A) - C(5A) \\ C(2A) - C(2A) - C(2A) \\ C(2A$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 108.2 (6) 108.2 (6) 108.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1) 113 (1) 112 (1) 118 (1) 112 (1)	C(28b) - C(28b) C(29b) - C(30b) C(29b) - C(30b) C(30b) C(30b) - C(31b) C(5b) - S(1b) - N(1b) O(5b) - S(1b) - N(1b) O(5b) - S(1b) - N(1b) O(6b) - S(1b) - N(1b) O(6b) - S(1b) - N(1b) C(19b) N(1b) - C(19b) C(1b) - O(2b) - C(5b) C(6b) - O(4b) - C(10b) S(1b) - N(1b) - C(20b) S(1b) - N(1b) - C(20b) S(1b) - N(1b) - C(20b) O(2b) - C(1b) - C(2b) C(2b) - C(1b) - C(2b) C(2b) - C(1b) - C(2b) C(2b) - C(2b) - C(2b) C(2b) - C(2b) - C(2b) C(2b) - C(2	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 108.6 (5) 107.8 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 119.6 (1) 119 (1) 111 (1) 108 (1) 121 (1) 121 (1) 121 (1) 121 (1)
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ N(14)-O(24)-C(54)\\ C(64)-O(44)-C(104)\\ S(14)-N(14)-C(264)\\ S(14)-N(14)-C(264)\\ O(24)-C(14)-C(74)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(14)-C(24)-C(34)\\ C(34)-C(24)-C(64)\\ O(14)-C(24)-C(24)\\ O(14)-C(24)\\ O(14$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 108.2 (6) 106.2 (5) 113.5 (8) 115.3 (9) 112 (1) 119.8 (9) 118 (1) 109 (1) 109 (1) 110 (1) 113 (1) 112 (1) 118 (1) 123 (1)	C(28b) - C(28b) C(29b) - C(30b) C(29b) - C(30b) C(30b) C(30b) - C(31b) C(5b) - S(1b) - N(1b) O(5b) - S(1b) - N(1b) O(5b) - S(1b) - N(1b) O(6b) - S(1b) - N(1b) O(6b) - S(1b) - N(1b) O(6b) - S(1b) - C(19b) N(1b) - C(2b) - C(5b) C(6b) - O(4b) - C(10b) S(1b) - N(1b) - C(2cb) C(2b) - C(1b) - C(2cb) C(2b) - C(1b) - C(2cb) O(2b) - C(1b) - C(2cb) C(2b) - C(1b) - C(2cb) - C(2cb) C(2cb) - C(2cb) - C(2cb) C(2cb) - C(2cb) - C(2cb) C(2cb) - C(2cb) O(1b) - C(2cb) - C(2cb) - C(2cb) O(1b) - C(2cb) -	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 119.6 (7) 119.6 (7) 119.1 (1) 110 (1) 111 (1) 115 (1) 108 (1) 121 (1) 121 (1)
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ C(14)-O(24)-C(54)\\ C(14)-O(24)-C(54)\\ C(24)-O(14)-C(204)\\ S(14)-N(14)-C(204)\\ S(14)-N(14)-C(264)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(14)-C(24)-C(54)\\ C(14)-C(24)-C(54)\\ C(14)-C(24)-C(54)\\ C(14)-C(24)-C(54)\\ C(34)-C(24)-C(64)\\ O(14)-C(24)-C(44)\\ C(24)-C(34)-C(44)\\ C(24)-C(34)-C(44)\\ C(24)-C(34)-C(44)\\ \end{array}$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 108.2 (5) 108.2 (6) 106.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 110 (1) 113 (1) 112 (1) 118 (1) 123 (1) 119 (1)	C(28b) - C(28b) - C(28b) - C(30B) - C(20B) - C(30B) - C(20B) - C(20B) - C(1B) - C(26B) - C(20B) - C(1B) - C(26B) - C(2B) - C(1B) - C(2B) - C(2B) - C(1B) - C(2B) - C(2B) - C(1B) - C(2B) - C(2B	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 112 (1) 108 (1) 111 (1) 115 (1) 108 (1) 121 (1) 1
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ C(14)-O(24)-C(54)\\ C(54)-O(44)-C(104)\\ S(14)-N(14)-C(264)\\ O(24)-C(14)-C(264)\\ O(24)-C(14)-C(264)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(14)-C(24)-C(54)\\ C(14)-C(24)-C(64)\\ C(14)-C(24)-C(64)\\ C(14)-C(24)-C(64)\\ O(14)-C(34)-C(44)\\ C(24)-C(34)-C(44)\\ C(24)-C(34)-C(44)\\ C(24)-C(34)-C(44)\\ C(34)-C(44)-C(54)\\ \end{array}$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 108.2 (5) 108.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1) 112 (1) 118 (1) 123 (1) 119 (1) 110 (1)	C(28b) - C(28b) - C(28b) - C(30B) - C(19B) - C(20B) - C	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 112 (1) 108 (1) 115 (1) 108 (1) 121 (1) 118 (1) 108 (1)
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ N(14)-S(14)-C(104)\\ S(14)-O(24)-C(54)\\ C(64)-O(44)-C(104)\\ S(14)-N(14)-C(264)\\ O(24)-C(14)-C(24)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(14)-C(24)-C(34)\\ C(14)-C(24)-C(64)\\ O(14)-C(24)-C(64)\\ O(14)-C(34)-C(24)\\ O(14)-C(34)-C(24)\\ C(24)-C(14)-C(24)\\ O(14)-C(34)-C(24)\\ C(24)-C(14)-C(24)\\ O(14)-C(34)-C(24)\\ O(14)-C(34)-C(24)\\ C(24)-C(34)-C(44)\\ C(23)-C(34)-C(44)\\ C(34)-C(34)-C(54)\\ C(34)-C$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 105.2 (5) 106.2 (5) 106.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 109 (1) 109 (1) 110 (1) 112 (1) 119 (1) 115 (1)	C(28b) - C(28b) = C(28b) = C(28b) = C(28b) = C(30B) = C	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 108.4 (5) 108.6 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 112 (1) 108 (1) 111 (1) 115 (1) 108 (1) 121 (1) 121 (1) 121 (1) 121 (1) 108 (1) 110 (1) 111 (1) 121 (1) 1
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ C(14)-O(24)-C(54)\\ C(64)-O(44)-C(104)\\ S(14)-N(14)-C(264)\\ C(204)-N(14)-C(264)\\ O(24)-C(14)-C(74)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(14)-C(24)-C(54)\\ C(34)-C(24)-C(64)\\ C(34)-C(24)-C(64)\\ C(34)-C(24)-C(64)\\ C(24)-C(34)-C(24)\\ C(34)-C(24)-C(54)\\ C(34)-C(34)-C(24)\\ C(34)-C(34)-C(34)\\ C(34)-C(34)\\ C(34)\\ C(34)-C(34)\\ C(34)\\ C(34)-C(34)\\ C(34)\\ C(34)-C(34$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 105.2 (5) 106.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 110 (1) 113 (1) 112 (1) 119 (1) 115 (1) 112 (1)	C(29B)-C(30B) = C(30B) = C(20B) = C(2	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 119.4 (6) 110 (1) 111 (1) 115 (1) 108 (1) 121 (1) 118 (1) 108 (1) 113 (1)
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ C(14)-O(24)-C(54)\\ C(64)-O(44)-C(104)\\ S(14)-N(14)-C(204)\\ S(14)-N(14)-C(204)\\ S(14)-N(14)-C(264)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(14)-C(24)-C(54)\\ C(24)-C(14)-C(74)\\ C(14)-C(24)-C(64)\\ C(34)-C(24)-C(64)\\ C(34)-C(44)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(44)-C(54)\\ C(54)-C(44)-C(54)\\ C(54)-C(44)-C(54)\\ C(54)-C(44)-C(54)\\ \end{array}$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 108.2 (5) 108.2 (6) 106.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 113 (1) 112 (1) 119 (1) 115 (1) 112 (1) 115 (1) 112 (1) 109 (1)	C(28b) - C(28b) - C(28b) - C(30B) - C(26B) - C(46B) - C(26B) - C(46B) - C(46B) - C(36B) - C(46B) - C(46B) - C(36B) - C(46B) - C(46B) - C(36B) - C(46B) - C(36B) - C(46B) - C(56B) - C(46) - C(56) - C(46) - C(56) - C(46) - C(56) - C(46) - C(56) - C(56) - C(56) - C(46) - C(56) - C(56) - C(46) - C(56) - C(46) - C(56) - C(46) - C(56) - C(46) - C(56) - C(56) - C(56) - C(46) - C(56) - C(56) - C(46) - C(56) - C	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 112 (1) 108 (1) 111 (1) 115 (1) 108 (1) 121 (1) 108 (1) 113 (1) 110 (1) 113 (1) 110 (1)
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(504)-C(314)\\ O(504)-S(14)-O(64)\\ O(504)-S(14)-N(14)\\ O(504)-S(14)-C(194)\\ O(604)-S(14)-C(194)\\ O(604)-S(14)-C(194)\\ C(14)-O(24)-C(50)\\ C(14)-O(24)-C(50)\\ C(14)-O(24)-C(104)\\ S(14)-N(14)-C(264)\\ C(204)-N(14)-C(264)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(34)-C(54)\\ C(34)-C(34)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(44)-C(54)\\ C(24)-C(54)-C(44)\\ O(24)-C(54)-C(64)\\ O(24)-C(54)\\ O(24)-C(54)-C(64)\\ O(24)-C(54)\\$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 108.2 (6) 108.2 (6) 108.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 110 (1) 113 (1) 112 (1) 118 (1) 123 (1) 115 (1) 115 (1) 112 (1) 109 (1) 109 (1) 109 (1) 109 (1) 109 (1) 109 (1) 109 (1) 109 (1) 108 (1) 108 (1)	C(28b) - C(29b) - C(30b) - C(40b) - C(50b) - C(50b) - C(40b) - C(50b) - C(50b) - C(40b) - C(50b) - C	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 107.8 (5) 107.8 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 112 (1) 108 (1) 111 (1) 108 (1) 108 (1) 108 (1) 110 (1) 113 (1) 100 (1) 110 (1) 110 (1) 108 (1) 100 (1) 100 (1) 108 (1) 100 (1) 100 (1) 100 (1) 108 (1) 100 (1) 100 (1) 100 (1) 108 (1) 100 (1) 100 (1) 100 (1) 108 (1) 100
$\begin{array}{c} C(294) - C(304) \\ C(304) - C(314) \\ O(54) - S(14) - O(64) \\ O(54) - S(14) - N(14) \\ O(54) - S(14) - C(194) \\ O(64) - S(14) - C(194) \\ O(64) - S(14) - C(194) \\ N(14) - S(14) - C(194) \\ N(14) - S(14) - C(194) \\ C(14) - O(24) - C(54) \\ C(64) - O(44) - C(104) \\ S(14) - N(14) - C(264) \\ O(24) - C(14) - C(24) \\ O(24) - C(14) - C(24) \\ O(24) - C(14) - C(74) \\ C(14) - C(24) - C(34) \\ C(34) - C(24) - C(64) \\ C(34) - C(34) - C(24) \\ C(34) - C(34) - C(24) \\ C(34) - C(34) - C(54) \\ C(34) - C(44) - C(54) \\ C(34) - C(54) - C(64) \\ O(24) - C(54) - C(64) \\ O(24) - C(54) - C(64) \\ C(24) - C(54) - C(64) \\ O(24) - C(54) - C(64) \\ C(24) - C(24) - C(24) \\ C(24$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 105.2 (5) 106.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1) 112 (1) 118 (1) 123 (1) 119 (1) 115 (1) 112 (1) 109 (1) 109 (1) 109 (1) 109 (1) 114 (1)	C(28b) - C(28b) = C(28b) = C(28b) = C(28b) = C(30B) = C	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 119.6 (7) 119.6 (7) 119.6 (7) 119.6 (1) 110 (1) 111 (1) 121 (1) 108 (1) 113 (1) 110 (1) 108 (1) 113 (1) 110 (1) 108 (1) 113 (1) 11
$\begin{array}{c} C(294) - C(304) \\ C(304) - C(314) \\ O(54) - S(14) - O(64) \\ O(54) - S(14) - N(14) \\ O(54) - S(14) - C(194) \\ O(64) - S(14) - C(194) \\ O(64) - S(14) - C(194) \\ O(64) - S(14) - C(194) \\ C(14) - O(24) - C(54) \\ C(64) - O(44) - C(104) \\ S(14) - N(14) - C(264) \\ O(24) - C(14) - C(264) \\ O(24) - C(14) - C(74) \\ C(24) - C(14) - C(74) \\ C(14) - C(24) - C(54) \\ C(34) - C(24) - C(64) \\ O(14) - C(24) - C(64) \\ O(14) - C(34) - C(24) \\ C(34) - C(44) - C(54) \\ C(54) - C(44) - C(94) \\ O(24) - C(54) - C(94) \\ O(24) - C(54) - C(64) \\ O(24) - C(64) - C(64) \\ O(24) - C(64) \\ O(24) - C(64) - C(64) \\ O(24) - C(64) \\ O(24$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 105.2 (5) 108.2 (6) 106.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1) 113 (1) 112 (1) 115 (1) 115 (1) 115 (1) 112 (1) 109 (1) 108 (1) 114 (1) 127 (1)	C(28b) - C(28b) - C(38b) - C(28b) - C	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 119.4 (6) 110 (1) 110 (1) 108 (1) 121 (1) 113 (1) 103 (1) 124 (1) 124 (1)
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ C(14)-O(24)-C(54)\\ C(14)-O(24)-C(54)\\ C(14)-O(24)-C(54)\\ C(14)-O(24)-C(264)\\ O(24)-C(14)-C(264)\\ O(24)-C(14)-C(264)\\ O(24)-C(14)-C(264)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(24)\\ O(24)-C(34)-C(64)\\ C(24)-C(34)-C(44)\\ C(24)-C(34)-C(44)\\ C(34)-C(44)-C(54)\\ C(54)-C(44)-C(54)\\ C(54)-C(64)-O(64)\\ O(24)-C(54)-C(64)\\ O(24)-C(54)-C(24)\\ O(24)-C(54)-C(24)\\ O(24)-C(54)-C(24)\\ O(24)-C(54)-C(24)\\ O(24)-C(54)-C(24)\\ O(24)-C(54)-C(24)\\ O(24)-C(54)-C(24)\\ O(24)-C(54)-C(24)\\ O(24)-C(54)-C(24)\\ O(24)-C(24)\\ O(24)-C(24)\\ O(24)-C(24)\\ O(24)-C(24)\\ O(24)-C(24)\\ O(24)-C(24)\\ O(24)$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 108.2 (6) 108.2 (6) 108.2 (6) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 110 (1) 113 (1) 112 (1) 115 (1) 115 (1) 115 (1) 115 (1) 114 (1) 127 (1) 124 (1)	$C(28b) - C(28b) \\ C(29b) - C(30b) \\ C(30b) - C(31b) \\ O(5b) - S(1b) - O(6b) \\ O(5b) - S(1b) - N(1b) \\ O(5b) - S(1b) - N(1b) \\ O(6b) - S(1b) - N(1b) \\ O(6b) - S(1b) - N(1b) \\ O(6b) - S(1b) - C(19b) \\ N(1b) - S(1b) - C(19b) \\ C(1b) - O(2b) - C(5b) \\ C(2b) - O(4b) - C(2b) \\ S(1b) - N(1b) - C(2cb) \\ S(1b) - N(1b) - C(2cb) \\ O(2b) - C(1b) - C(2b) \\ O(2b) - C(2b) - C(6b) \\ O(1b) - C(3b) - C(4b) \\ O(2b) - C(4b) - C(4b) \\ O(2b) - C(5b) - C(4b) \\ O(2b) - C(6b) - O(4b) \\ O(3b) - C(3b) - O(3b) \\ O(3b) - O(3b) - O(3b) - O(3b) \\ O(3b) - O(3b) - O(3b) - O(3b) \\ O(3b) - O(3b) - O(3b) \\ O(3b) - O(3b) - O(3b) \\ O($	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 108.6 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 119.6 (7) 112 (1) 108 (1) 111 (1) 108 (1) 113 (1) 108 (1) 113 (1) 108 (1) 113 (1) 124 (1) 127 (1)
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ C(14)-O(24)-C(54)\\ C(64)-O(44)-C(104)\\ S(14)-N(14)-C(264)\\ O(24)-C(14)-C(24)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(14)-C(24)-C(34)\\ C(14)-C(24)-C(64)\\ O(14)-C(34)-C(24)\\ O(14)-C(34)-C(24)\\ O(34)-C(44)-C(94)\\ C(34)-C(44)-C(94)\\ O(24)-C(54)-C(84)\\ O(24)-C(54)-C(84)\\ O(34)-C(64)-O(24)\\ O(34)-C(64)-C(24)\\ O(34)-C(24)\\ O(34)-C(24)\\ O(34)-C(24)\\ O(34)-C(24)\\ O(34)-C(24)\\ O(34)-C(24)\\ O(34)-C(24)\\ O(34)-C(24)$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 105.2 (5) 106.2 (5) 113.5 (8) 115.3 (9) 112 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1) 110 (1) 113 (1) 112 (1) 119 (1) 115 (1) 112 (1) 108 (1) 112 (1) 109 (1) 114 (1) 127 (1) 124 (1) 127 (1) 124 (1) 124 (1) 126 (1) 127 (1) 124 (1) 127 (1) 124 (1) 127 (1) 124 (1) 126 (1) 127 (1) 127 (1) 124 (1) 127 (1) 124 (1) 127 (1) 126 (1) 127 (1) 127 (1) 124 (1) 127 (1) 126 (1) 127 (1) 127 (1) 127 (1) 124 (1) 126 (1) 127 (1) 127 (1) 124 (1) 127 (1) 126 (1) 126 (1) 127 (1) 126 (1) 126 (1) 127 (1) 126 (1) 1	$C(28b) - C(28b) \\ C(29b) - C(30b) \\ C(30b) - C(31b) \\ C(30b) - C(31b) \\ O(5b) - S(1b) - N(1b) \\ O(5b) - S(1b) - N(1b) \\ O(5b) - S(1b) - N(1b) \\ O(6b) - S(1b) - C(19b) \\ O(6b) - S(1b) - C(19b) \\ O(6b) - S(1b) - C(19b) \\ C(1b) - O(2b) - C(5b) \\ C(6b) - O(4b) - C(10b) \\ S(1b) - N(1b) - C(2cb) \\ C(2b) - C(1b) - C(2cb) \\ O(2b) - C(1b) - C(2b) \\ C(2b) - C(1b) - C(2b) \\ C(2b) - C(1b) - C(2b) \\ C(2b) - C(2b) - C(6b) \\ C(1b) - C(2b) - C(6b) \\ O(1b) - C(2b) - C(6b) \\ O(1b) - C(3b) - C(2b) \\ O(2b) - C(4b) - C(5b) \\ C(3b) - C(4b) - C(5b) \\ C(3b) - C(4b) - C(5b) \\ C(3b) - C(4b) - C(6b) \\ O(2b) - C(5b) - C(4b) \\ O(2b) - C(5b) - C(4b) \\ O(2b) - C(5b) - C(4b) \\ O(2b) - C(6b) - O(4b) \\ O(3b) - C(6b) - O(4b) \\ O(4b) - C(6b) - C(2b) \\ O(4b) - C(6b) - O(4b) \\ O(4b) - C(6b) - O(4$	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 119.6 (7) 119.6 (7) 119.4 (1) 110 (1) 111 (1) 111 (1) 121 (1) 121 (1) 121 (1) 121 (1) 121 (1) 113 (1) 110 (1) 113 (1) 110 (1) 124 (1) 127 (1) 109 (1)
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ C(14)-O(24)-C(54)\\ C(64)-O(44)-C(104)\\ S(14)-N(14)-C(264)\\ C(204)-N(14)-C(264)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(14)-C(24)-C(34)\\ C(34)-C(24)-C(64)\\ C(34)-C(24)-C(64)\\ C(34)-C(24)-C(64)\\ C(34)-C(44)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(54)-C(44)\\ C(24)-C(54)-C(44)\\ C(24)-C(54)-C(64)\\ O(24)-C(54)-C(64)\\ O(24)-C(54)-C(64)\\ O(24)-C(54)-C(64)\\ O(24)-C(54)-C(64)\\ O(34)-C(64)-C(24)\\ O(34)-C(64)-C(24)\\ O(34)-C(64)-C(24)\\ O(44)-C(64)-C(24)\\ O(44)-C(64)-C(4)\\ O(44)-C(64)-C(4)\\ O(44)-C(64)-C(4)\\ O(44)-C(64)-C(4)\\ O(44)-C(64)-C(4)\\ O(44)-C(64)-C(4)\\ O(44)-C(64)-C(4)\\ O(44)-C(64)-C(4)\\ O(4)-C(4)-C(4)\\ O(4)-C(4)-C(4)\\ O(4)-C(4)-C(4)\\ O(4)-C(4)\\ O(4)-C(4)-C(4)\\ O(4)-C(4)-C(4)$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 105.2 (5) 105.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1) 113 (1) 112 (1) 118 (1) 112 (1) 115 (1) 115 (1) 115 (1) 112 (1) 109 (1) 109 (1) 109 (1) 109 (1) 110 (1) 112 (1) 110 (1) 124 (1) 127 (1) 124 (1) 110 (1) 111 (9)	$C(28b) - C(28b) \\ C(29B) - C(30B) \\ C(30B) - C(31B) \\ O(5B) - S(1B) - N(1B) \\ O(5B) - S(1B) - N(1B) \\ O(5B) - S(1B) - N(1B) \\ O(6B) - S(1B) - C(19B) \\ O(6B) - S(1B) - C(19B) \\ O(6B) - S(1B) - C(19B) \\ C(1B) - O(2B) - C(5B) \\ C(6B) - O(4B) - C(10B) \\ S(1B) - N(1B) - C(20B) \\ S(1B) - N(1B) - C(26B) \\ O(2B) - O(1B) - C(26B) \\ O(2B) - C(1B) - C(2B) \\ O(2B) - C(1B) - C(7B) \\ O(2B) - C(2B) - C(3B) \\ C(1B) - C(2B) - C(3B) \\ C(1B) - C(2B) - C(4B) \\ O(1B) - C(2B) - C(4B) \\ O(1B) - C(3B) - C(4B) \\ C(3B) - C(4B) - C(5B) \\ C(3B) - C(4B) - C(9B) \\ O(2B) - C(5B) - C(4B) \\ O(3B) - C(6B) - O(4B) \\ O(3B) - C(6B) - C(2B) \\ O(4B) - C(6B) -$	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 119.4 (6) 110 (1) 110 (1) 110 (1) 113 (1) 121 (1) 113 (1) 124 (1) 129 (1) 129 (1) 129 (1) 129 (1) 129 (1) 129 (1) 129 (1) 120 (1) 120 (1) 121 (1) 122 (1) 123 (1) 124 (1) 124 (1) 129 (1) 120 (1) 120 (1) 120 (1) 120 (1) 121 (1) 121 (1) 121 (1) 122 (1) 122 (1) 122 (1) 123 (1) 124 (1) 129 (1) 129 (1) 129 (1) 129 (1) 129 (1) 129 (1) 120 (1) 120 (1) 120 (1) 120 (1) 120 (1) 121 (1) 121 (1) 121 (1) 121 (1) 121 (1) 121 (1) 122 (1) 123 (1) 123 (1) 124 (1) 125 (1) 126
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ C(14)-O(24)-C(54)\\ C(14)-O(24)-C(54)\\ C(14)-O(24)-C(54)\\ C(204)-N(14)-C(204)\\ S(14)-N(14)-C(264)\\ C(204)-N(14)-C(264)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(14)-C(24)-C(54)\\ C(34)-C(24)-C(54)\\ C(34)-C(24)-C(54)\\ C(34)-C(24)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(54)-C(44)\\ O(24)-C(54)-C(44)\\ C(34)-C(54)-C(44)\\ O(24)-C(54)-C(44)\\ O(24)-C(54)-C(44)\\ O(24)-C(54)-C(44)\\ O(24)-C(54)-C(44)\\ O(24)-C(54)-C(44)\\ O(24)-C(54)-C(44)\\ O(24)-C(54)-C(44)\\ O(24)-C(54)-C(24)\\ O(34)-C(64)-C(24)\\ O(44)-C(24)-C(24)\\ O(44)-C(24)\\ O(44)-C(24)-C(24)\\ O(44)-C(24)-C(24)\\ O(44)-C(24)\\ O(44)-C(24)-C(24)\\ O(44)-C(24)\\ O(44)-C(24)-C(24)\\ O(44)-C(24)\\ O(44)-C(24)\\ O(44)-C(24)\\ O(44)-C(24)\\ O(44)-C(24$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 108.2 (5) 108.2 (6) 106.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 110 (1) 113 (1) 112 (1) 118 (1) 123 (1) 119 (1) 115 (1) 115 (1) 115 (1) 117 (1) 124 (1) 104 (1) 114 (1) 124 (1) 110 (1) 114 (1) 124 (1) 110 (1) 114 (1) 124 (1) 104 (1) 114 (1) 124 (1) 104 (1) 114 (1) 124 (1) 104 (1) 114 (1) 115 (1) 114 (1)	$C(28b) - C(28b) \\ C(29B) - C(30B) \\ C(30B) - C(31B) \\ O(5B) - S(1B) - O(6B) \\ O(5B) - S(1B) - N(1B) \\ O(5B) - S(1B) - C(19B) \\ O(6B) - S(1B) - C(19B) \\ O(6B) - S(1B) - C(19B) \\ C(1B) - O(2B) - C(5B) \\ C(6B) - O(4B) - C(10B) \\ S(1B) - N(1B) - C(26B) \\ C(2B) - O(4B) - C(2B) \\ O(2B) - C(1B) - C(2B) \\ O(2B) - C(2B) - C(3B) \\ C(2B) - C(2B) - C(4B) \\ C(3B) - C(2B) - C(4B) \\ C(3B) - C(4B) - C(2B) \\ O(1B) - C(3B) - C(4B) \\ C(3B) - C(4B) - C(5B) \\ C(3B) - C(4B) - C(5B) \\ C(3B) - C(4B) - C(5B) \\ C(4B) - C(5B) - C(4B) \\ O(2B) - C(5B) - C(4B) \\ O(2B) - C(5B) - C(4B) \\ O(3B) - C(6B) - O(2B) \\ O(4B) - C(2B) - C(2B) \\ O(4B) - C(2B) - C(2B) \\ O(4B) - C(1B) - C(1B) \\ O(4B) - C(1B) \\ O(4B) - C(1B) \\ O(4B) - C$	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 112 (1) 108 (1) 111 (1) 115 (1) 108 (1) 121 (1) 118 (1) 108 (1) 113 (1) 124 (1) 109 (1) 112 (4 (9) 109 (1) 1124 (9)
$\begin{array}{c} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ C(14)-O(24)-C(54)\\ C(14)-O(24)-C(54)\\ C(64)-O(44)-C(104)\\ S(14)-N(14)-C(264)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(14)-C(24)-C(54)\\ C(34)-C(24)-C(64)\\ O(14)-C(24)-C(64)\\ O(14)-C(24)-C(64)\\ O(14)-C(34)-C(24)\\ O(24)-C(14)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(54)-C(84)\\ O(24)-C(54)-C(84)\\ O(24)-C(54)-C(84)\\ O(24)-C(54)-C(84)\\ O(34)-C(54)-C(84)\\ O(34)-C(64)-C(24)\\ O(34)-C(64)-C(24)\\ O(34)-C(104)-C(114)\\ O(34)-C(104)-C(114)\\ O(34)-C(104)-C(114)\\ O(44)-C(104)-C(114)\\ O(44)-$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 108.2 (5) 108.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1) 112 (1) 118 (1) 112 (1) 115 (1) 115 (1) 115 (1) 115 (1) 117 (1) 108 (1) 114 (1) 127 (1) 124 (1) 111.6 (8) 110.4 (9)	$C(28b) - C(28b) \\ C(29b) - C(30b) \\ C(30b) - C(31b) \\ O(5b) - S(1b) - N(1b) \\ O(6b) - S(1b) - C(19b) \\ N(1b) - S(1b) - C(19b) \\ N(1b) - O(2b) - C(5b) \\ C(2b) - O(4b) - C(10b) \\ S(1b) - N(1b) - C(2cb) \\ O(2b) - C(1b) - C(2b) \\ O(2b) - C(2b) - C(4b) \\ C(2b) - C(3b) - C(4b) \\ O(2b) - C(3b) - C(4b) \\ O(2b) - C(4b) - C(5b) \\ O(2b) - C(4b) - C(2b) \\ O(2b) - C(5b) - C(4b) \\ O(4b) - C(10b) - C(1b) \\ O(4b) - C(10b) - C(1b) \\ O(4b) - C(10b) - C(15b) \\ O(4b) - C(10b) -$	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 119.6 (7) 119.6 (7) 119.6 (7) 119.6 (7) 119.6 (7) 119.1 (1) 110 (1) 111 (1) 115 (1) 108 (1) 121 (1) 121 (1) 133 (1) 110 (1) 113 (1) 113 (1) 112.4 (1) 124 (1) 124 (1) 124.4 (9) 108.6 (8) 105.5 (1) 105.5
$\begin{array}{l} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ N(14)-O(24)-C(54)\\ C(64)-O(44)-C(104)\\ S(14)-N(14)-C(264)\\ O(24)-C(14)-C(24)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(24)\\ O(24)-C(14)-C(24)\\ O(24)-C(14)-C(24)\\ C(34)-C(24)-C(64)\\ C(34)-C(24)-C(64)\\ C(34)-C(44)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(54)-C(84)\\ O(24)-C(54)-C(84)\\ O(24)-C(54)-C(84)\\ O(24)-C(54)-C(24)\\ O(24)-C(54)-C(24)\\ O(24)-C(54)-C(24)\\ O(24)-C(54)-C(24)\\ O(24)-C(54)-C(24)\\ O(24)-C(54)-C(24)\\ O(24)-C(54)-C(24)\\ O(34)-C(64)-C(24)\\ O(34)-C(64)-C(24)\\ O(44)-C(104)-C(114)\\ O(44)-C(104)-C(154)\\ C(114)-C(104)-C(154)\\ C(114)-C(104)-C(154)\\ \end{array}$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 105.2 (5) 105.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1) 110 (1) 113 (1) 112 (1) 118 (1) 123 (1) 119 (1) 110 (1) 115 (1) 112 (1) 109 (1) 109 (1) 109 (1) 110 (1) 115 (1) 112 (1) 116 (1) 116 (1) 117 (1) 124 (1) 110 (1) 111.6 (8) 110.4 (9) 102.9 (9) 102.9 (9)	$C(28b) - C(30B) \\ C(30B) - C(31B) \\ C(30B) - C(31B) \\ O(5B) - S(1B) - N(1B) \\ O(5B) - S(1B) - N(1B) \\ O(5B) - S(1B) - N(1B) \\ O(6B) - S(1B) - C(19B) \\ O(6B) - S(1B) - C(19B) \\ O(6B) - S(1B) - C(19B) \\ C(1B) - O(2B) - C(5B) \\ C(6B) - O(4B) - C(10B) \\ S(1B) - N(1B) - C(20B) \\ S(1B) - N(1B) - C(20B) \\ S(1B) - N(1B) - C(26B) \\ O(2B) - C(1B) - C(2B) \\ O(2B) - C(1B) - C(2B) \\ O(2B) - C(1B) - C(7B) \\ C(2B) - C(1B) - C(2B) \\ O(2B) - C(1B) - C(7B) \\ C(2B) - C(2B) - C(6B) \\ O(1B) - C(2B) - C(6B) \\ C(3B) - C(2B) - C(4B) \\ C(3B) - C(2B) - C(4B) \\ C(3B) - C(4B) - C(5B) \\ C(3B) - C(4B) - C(5B) \\ C(3B) - C(5B) - C(4B) \\ O(2B) - C(5B) - C(4B) \\ O(3B) - C(6B) - C(2B) \\ O(4B) - C(10B) - C(1B) \\ O(4B) - C(10B) - C(11B) \\ O(4B) - C(10B) - C(15B) \\ C(11B) - C(10B) - C(15B) \\ C(10B) - C(10B) - C(15B) \\ C(11B) - C(10B) - C(15B) \\ C(10B) - C(10B) - C(15B) \\ C(1B) - C(10B) - C(15B) \\ C(1B)$	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 119.6 (7) 119.6 (7) 112 (1) 108 (1) 121 (1) 108 (1) 121 (1) 113 (1) 110 (1) 113 (1) 110 (1) 113 (1) 110 (1) 124 (1
$\begin{array}{l} C(294)C(304)\\ C(304)C(314)\\ O(54)S(14)O(64)\\ O(54)S(14)N(14)\\ O(54)S(14)C(194)\\ O(64)S(14)C(194)\\ O(64)S(14)C(194)\\ C(14)O(24)C(54)\\ C(64)O(44)C(104)\\ S(14)N(14)C(264)\\ C(204)N(14)C(264)\\ C(204)C(14)C(74)\\ C(24)C(14)C(74)\\ C(24)C(14)C(74)\\ C(24)C(14)C(74)\\ C(24)C(14)C(74)\\ C(24)C(14)C(24)\\ O(14)C(24)-C(54)\\ C(34)C(24)-C(54)\\ C(34)C(24)-C(54)\\ C(34)C(24)-C(54)\\ C(34)C(24)-C(54)\\ C(34)C(24)-C(54)\\ C(34)C(24)-C(54)\\ C(34)C(54)-C(54)\\ C(34)C(54)-C(54)\\ C(34)C(54)C(54)\\ C(34)C(54)C(54)\\ C(34)C(54)C(24)\\ O(24)C(54)C(24)\\ O(24)C(54)C(24)\\ O(24)C(54)C(24)\\ O(24)C(54)C(24)\\ O(34)C(64)C(24)\\ O(34)C(104)C(114)\\ O(44)C(104)C(114)\\ O(44)C(104)C(154)\\ C(114)C(104)C(154)\\ C(104)C(114)C(124)\\ \end{array}$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 108.2 (6) 108.2 (6) 106.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1) 113 (1) 112 (1) 118 (1) 123 (1) 119 (1) 115 (1) 115 (1) 115 (1) 115 (1) 112 (1) 108 (1) 114 (1) 124 (1) 109 (1) 108 (1) 114 (1) 127 (1) 124 (1) 100 (1) 111.6 (8) 100.4 (9) 103.5 (8)	$C(28b) - C(28b) \\ C(29B) - C(30B) \\ C(30B) - C(31B) \\ O(5B) - S(1B) - N(1B) \\ O(5B) - S(1B) - N(1B) \\ O(5B) - S(1B) - N(1B) \\ O(6B) - S(1B) - C(19B) \\ O(6B) - S(1B) - C(19B) \\ O(6B) - S(1B) - C(19B) \\ C(1B) - O(2B) - C(5B) \\ C(6B) - O(4B) - C(10B) \\ S(1B) - N(1B) - C(26B) \\ C(2B) - N(1B) - C(26B) \\ O(2B) - C(1B) - C(2B) \\ O(2B) - C(2B) - C(3B) \\ C(2B) - C(2B) - C(4B) \\ C(3B) - C(2B) - C(4B) \\ C(3B) - C(4B) - C(2B) \\ O(3B) - C(5B) - C(4B) \\ O(2B) - C(5B) - C(4B) \\ O(2B) - C(5B) - C(4B) \\ O(2B) - C(5B) - C(4B) \\ O(3B) - C(6B) - O(2B) \\ O(4B) - C(2B) - C(2B) \\ O(4B) - C(1B) - C(1B) \\ O(4B) - C(10B) - C(11B) \\ O(4B) - C(11B) - C(12B) \\ C(10B) - C(11B) - C(12B) \\ C(11B) - $	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 119.4 (6) 110 (1) 110 (1) 110 (1) 113 (1) 121 (1) 113 (1) 124 (1) 108 (1) 113 (1) 124 (1) 108 (1) 113 (1) 124 (1) 109 (1) 112.4 (9) 102.9 (9)
$\begin{array}{l} C(294)-C(304)\\ C(304)-C(314)\\ O(504)-C(314)\\ O(504)-S(14)-O(64)\\ O(504)-S(14)-C(194)\\ O(504)-S(14)-C(194)\\ O(604)-S(14)-C(194)\\ O(604)-S(14)-C(194)\\ C(14)-O(24)-C(504)\\ C(14)-O(24)-C(504)\\ C(204)-O(14)-C(204)\\ S(14)-N(14)-C(204)\\ S(14)-N(14)-C(204)\\ C(204)-N(14)-C(204)\\ O(24)-C(14)-C(74)\\ C(204)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(34)-C(24)\\ O(24)-C(34)-C(24)\\ O(14)-C(34)-C(24)\\ C(34)-C(34)-C(44)\\ C(24)-C(34)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(54)-C(84)\\ O(24)-C(54)-C(84)\\ O(34)-C(64)-C(24)\\ O(34)-C(64)-C(24)\\ O(34)-C(104)-C(114)\\ O(44)-C(104)-C(114)\\ O(14)-C(104)-C(114)\\ C(114)-C(124)-C(124)\\ C(114)-C(124)-C(134)\\ \end{array}$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 108.2 (5) 108.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1) 113 (1) 112 (1) 118 (1) 123 (1) 119 (1) 115 (1) 119 (1) 115 (1) 112 (1) 108 (1) 114 (1) 127 (1) 124 (1) 110 (1) 114 (2) 111.6 (8) 100.4 (9) 102.9 (9) 103.5 (8) 105 (1)	$C(28b) - C(28b) \\ C(29B) - C(30B) \\ C(30B) - C(31B) \\ O(5B) - S(1B) - O(6B) \\ O(5B) - S(1B) - N(1B) \\ O(5B) - S(1B) - N(1B) \\ O(6B) - S(1B) - C(19B) \\ O(6B) - S(1B) - C(19B) \\ O(6B) - S(1B) - C(19B) \\ C(1B) - O(2B) - C(5B) \\ C(1B) - O(2B) - C(5B) \\ C(2B) - O(4B) - C(10B) \\ S(1B) - N(1B) - C(26B) \\ O(2B) - C(1B) - C(2B) \\ O(2B) - C(2B) - C(3B) \\ C(2B) - C(2B) - C(3B) \\ C(2B) - C(2B) - C(4B) \\ C(2B) - C(3B) - C(2B) \\ O(1B) - C(3B) - C(4B) \\ C(2B) - C(3B) - C(4B) \\ C(3B) - C(4B) - C(5B) \\ C(3B) - C(4B) - C(2B) \\ O(2B) - C(5B) - C(4B) \\ O(2B) - C(5B) - C(4B) \\ O(3B) - C(6B) - C(2B) \\ O(4B) - C(10B) - C(11B) \\ O(4B) - C(10B) - C(11B) \\ O(1B) - C(10B) - C(11B) \\ C(10B) - C(11B) - C(12B) \\ C(10B) - C(12B) - C(13B) \\ C(1B) - C(12B) - C(13B) \\ C(10B) - C(12B) - C(13B) \\ C(11B) - C(1$	$\begin{array}{c} 1.53 \ (2)\\ 1.55 \ (1)\\ 118.8 \ (5)\\ 107.9 \ (4)\\ 106.4 \ (5)\\ 107.9 \ (4)\\ 108.6 \ (5)\\ 108.6 \ (5)\\ 106.7 \ (4)\\ 112 \ (1)\\ 115.5 \ (9)\\ 119.4 \ (6)\\ 120.3 \ (7)\\ 119.6 \ (7)\\ 112 \ (1)\\ 120.3 \ (7)\\ 119.6 \ (7)\\ 112 \ (1)\\ 119.6 \ (7)\\ 112 \ (1)\\ 110 \ (1)\\ 111 \ (1)\\ 115 \ (1)\\ 108 \ (1)\\ 111 \ (1)\\ 118 \ (1)\\ 108 \ (1)\\ 113 \ (1)\\ 113 \ (1)\\ 113 \ (1)\\ 1124 \ (1)\\ 108 \ (1)\\ 113 \ (1)\\ 113 \ (1)\\ 1124 \ (1)\\ 108 \ (1)\\ 113 \ (1)\\ 113 \ (1)\\ 124 \ (1)\\ 127 \ (1)\\ 109 \ (1)\\ 112.4 \ (9)\\ 102.9 \ (9)\\ 102.9 \ (9)\\ 107 \ (1)\\ \end{array}$
$\begin{array}{l} C(294)C(304)\\ C(304)C(314)\\ O(54)S(14)O(64)\\ O(54)S(14)N(14)\\ O(54)S(14)C(194)\\ O(64)S(14)C(194)\\ O(64)S(14)C(194)\\ N(14)S(14)C(194)\\ N(14)S(14)C(194)\\ C(14)O(24)C(54)\\ C(64)O(44)C(104)\\ S(14)N(14)C(264)\\ O(24)C(14)C(74)\\ C(24)C(14)C(74)\\ C(24)C(14)C(74)\\ C(14)C(24)C(64)\\ O(14)C(24)C(64)\\ O(14)C(34)C(64)\\ O(14)C(34)C(64)\\ O(24)C(14)C(24)\\ O(24)C(14)C(24)\\ O(14)C(34)C(44)\\ C(24)C(34)C(44)\\ C(24)C(54)C(84)\\ O(24)C(54)C(84)\\ O(24)C(54)C(84)\\ O(24)C(54)C(84)\\ O(34)C(54)C(84)\\ O(34)C(64)C(24)\\ O(44)C(164)C(154)\\ C(114)C(104)C(154)\\ C(114)C(114)C(124)\\ C(114)C(124)C(154)\\ C(124)C(154)-C(154)\\ C(114)C(124)C(154)\\ C(124)C(154)-C(154)\\ C(124)C(154)\\ C(124)C(154)-C(154)\\ C(124)C(154)-C(154)\\ C(124)C(154)-C(154)\\ C(124)C(154)-C(154)\\ C(124)C(154)-C(154)\\ C(124)C(154)-C(154)\\ C(124)C(154)-C(154)\\ C(124)C(154)\\ C(124)C(154)-C(154)\\ C(124)C(154)-C(154)\\ C(124)C(154)\\ C(124)-C(154)-C(154)\\ C(124)C(154)\\ C(154)-C(154)-C(154)\\ C(154)-C(154)-C(154)\\ C(154)C(154)\\ C(154)-C(154)-C(154)\\ C(154)-C(154)\\ C(154)-C(154)\\ C(154)-C(1$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 105.2 (5) 106.2 (5) 113.5 (8) 115.3 (9) 112 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1) 110 (1) 113 (1) 112 (1) 118 (1) 123 (1) 119 (1) 115 (1) 112 (1) 108 (1) 112 (1) 109 (1) 108 (1) 114 (1) 127 (1) 124 (1) 101 (1) 114 (1) 127 (1) 124 (1) 102.9 (9) 103.5 (8) 103.8 (9)	$C(28b) - C(28b) \\ C(29b) - C(30b) \\ C(30b) - C(31b) \\ O(5b) - S(1b) - N(1b) \\ O(5b) - S(1b) - N(1b) \\ O(5b) - S(1b) - N(1b) \\ O(5b) - S(1b) - C(19b) \\ O(6b) - O(2b) - C(5b) \\ C(2b) - O(4b) - C(2b) \\ O(2b) - C(1b) - C(2b) \\ O(2b) - C(2b) - C(6b) \\ O(1b) - C(3b) - C(2b) \\ O(1b) - C(3b) - C(4b) \\ O(2b) - C(4b) - C(5b) \\ O(2b) - C(4b) - C(5b) \\ O(2b) - C(5b) - C(4b) \\ O(3b) - C(6b) - O(2b) \\ O(4b) - C(10b) - C(15b) \\ O(4b) - C(10b) - C(15b) \\ C(11b) - C(12b) - C(15b) \\ C(11b) $	$\begin{array}{c} 1.53\ (2)\\ 1.55\ (1)\\ \hline\\ 118.8\ (5)\\ 107.9\ (4)\\ 106.4\ (5)\\ 108.6\ (5)\\ 106.7\ (4)\\ 112\ (1)\\ 115.5\ (9)\\ 119.4\ (6)\\ 120.3\ (7)\\ 119.6\ (7)\\ 119.6\ (7)\\ 112\ (1)\\ 108\ (1)\\ 110\ (1)\\ 111\ (1)\\ 115\ (1)\\ 108\ (1)\\ 111\ (1)\\ 111\ (1)\\ 115\ (1)\\ 108\ (1)\\ 111\ (1)\\ 111\ (1)\\ 111\ (1)\\ 1121\ (1)\\ 124\ (1)\\ 124\ (1)\\ 124\ (1)\\ 124\ (1)\\ 124\ (1)\\ 124\ (1)\\ 124\ (1)\\ 124\ (1)\\ 124\ (1)\\ 109\ (1)\\ 112.4\ (9)\\ 108.6\ (8)\\ 102\ (1)\ (1)\\ 103\ (1)\\ 103\ (1)\\ 103\ (1)\\ 103\ (1)\\ 103\ (1)\\ 103\ (1)\\ 103\ (1)\\ 103\ (1)\\ 103\ (1)\\ 100\ (1)\\ 103\ (1)\\ 103\ (1)\\ 100\ (1)\\ 103\ (1)\\ 100\ (1)\\ 103\ (1)\\ 100\ (1)\ (1)\ (1)\ (1)\ (1)\ (1)\ (1)\ (1)$
$\begin{array}{l} C(294)-C(304)\\ C(304)-C(314)\\ O(54)-S(14)-O(64)\\ O(54)-S(14)-N(14)\\ O(54)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ O(64)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ N(14)-S(14)-C(194)\\ C(14)-O(24)-C(54)\\ C(64)-O(44)-C(104)\\ S(14)-N(14)-C(264)\\ C(204)-N(14)-C(264)\\ O(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(24)-C(14)-C(74)\\ C(34)-C(24)-C(64)\\ C(34)-C(24)-C(64)\\ C(34)-C(24)-C(64)\\ C(34)-C(24)-C(64)\\ C(34)-C(44)-C(54)\\ C(34)-C(44)-C(54)\\ C(34)-C(54)-C(84)\\ C(34)-C(54)-C(84)\\ C(34)-C(64)-C(24)\\ O(34)-C(64)-C(24)\\ O(34)-C(64)-C(24)\\ O(34)-C(64)-C(24)\\ O(34)-C(64)-C(24)\\ O(34)-C(104)-C(154)\\ C(114)-C(104)-C(154)\\ C(114)-C(104)-C(154)\\ C(114)-C(124)-C(154)\\ C(154)-C(124)-C(154)\\ C(154)-C(154)\\ C(154)-C$	1.48 (2) 1.47 (2) 119.8 (7) 107.9 (5) 108.7 (5) 105.2 (5) 105.2 (5) 113.5 (8) 115.3 (9) 122 (1) 119.8 (9) 118 (1) 111.5 (9) 109 (1) 109 (1) 109 (1) 110 (1) 113 (1) 112 (1) 118 (1) 123 (1) 119 (1) 109 (1) 109 (1) 110 (1) 115 (1) 112 (1) 109 (1) 109 (1) 109 (1) 108 (1) 112 (1) 115 (1) 112 (1) 109 (1) 109 (1) 109 (1) 105 (1) 112 (1) 109 (1) 105 (1) 114 (1) 127 (1) 124 (1) 110 (4) 110 (4) 110 (5) 103.8 (9) 103.8 (9) 102 (1)	$C(29B)-C(30B) \\ C(30B)-C(31B) \\ O(5B)-S(1B)-N(1B) \\ O(5B)-S(1B)-N(1B) \\ O(5B)-S(1B)-N(1B) \\ O(5B)-S(1B)-C(19B) \\ O(6B)-S(1B)-C(19B) \\ O(6B)-S(1B)-C(19B) \\ O(6B)-S(1B)-C(19B) \\ C(1B)-O(2B)-C(5B) \\ C(6B)-O(4B)-C(26B) \\ C(2B)-O(1B)-C(26B) \\ O(2B)-C(1B)-C(2B) \\ O(2B)-C(1B)-C(2B) \\ O(2B)-C(1B)-C(2B) \\ O(2B)-C(1B)-C(7B) \\ C(2B)-C(1B)-C(7B) \\ C(2B)-C(2B)-C(4B) \\ C(2B)-C(2B)-C(4B) \\ C(2B)-C(3B)-C(4B) \\ C(2B)-C(3B)-C(4B) \\ C(3B)-C(4B)-C(5B) \\ C(3B)-C(4B)-C(5B) \\ C(4B)-C(5B)-C(4B) \\ O(2B)-C(5B)-C(4B) \\ O(2B)-C(5B)-C(4B) \\ O(2B)-C(5B)-C(4B) \\ O(2B)-C(5B)-C(4B) \\ O(3B)-C(6B)-C(2B) \\ O(4B)-C(1B)-C(1B) \\ O(1B)-C(1B)-C(15B) \\ C(11B)-C(12B)-C(13B) \\ C(11B)-C(12B)-C(12B) \\ C(11B)-C(12B)-C(12B) \\ C(11B)-C(12B)-C(12B) \\ C(11B)-C(12B)-C(16B) \\ C(12B)-C(12B)-C(16B) \\ C(13B)-C(12B)-C(16B) \\ C(12B)-C(12B)-C(16B) \\ $	1.53 (2) 1.55 (1) 118.8 (5) 107.9 (4) 106.4 (5) 107.8 (5) 106.7 (4) 112 (1) 115.5 (9) 119.4 (6) 120.3 (7) 119.6 (7) 119.6 (7) 119.4 (6) 120.3 (7) 119.6 (7) 119.6 (7) 112 (1) 108 (1) 110 (1) 108 (1) 121 (1) 113 (1) 110 (1) 108 (1) 113 (1) 110 (1) 124 (1) 125 (1) 108 (1) 124 (1)

C(13A) - C(14A) - C(15A)	103 (1)	C(13B) - C(14B) - C(15B)	106 (1)
C(10A) - C(15A) - C(14A)	105.3 (9)	C(10B) - C(15B) - C(14B)	102.7 (8)
C(10A) - C(15A) - C(16A)	103.9 (8)	C(10B) - C(15B) - C(16B)	103.7 (8)
C(10A) - C(15A) - C(19A)	116.4 (9)	C(10B)-C(15B)-C(19B)	115.5 (9)
C(14A) - C(15A) - C(16A)	101 (1)	C(14B) - C(15B) - C(16B)	101 (1)
C(14A) - C(15A) - C(19A)	115.2 (9)	C(14B) - C(15B) - C(19B)	116.1 (8)
C(16A) - C(15A) - C(19A)	113.2 (9)	C(16B) - C(15B) - C(19B)	115.9 (9)
C(12A) - C(16A) - C(15A)	94 (1)	C(12B) - C(16B) - C(15B)	94 (1)
C(12A) - C(16A) - C(17A)	111 (1)	C(12B) - C(16B) - C(17B)	115(1)
C(12A) - C(16A) - C(18A)	115 (1)	C(12B) - C(16B) - C(18B)	112(1)
C(15A) - C(16A) - C(17A)	116(1)	C(15B) - C(16B) - C(17B)	115(1)
C(15A) - C(16A) - C(18A)	116 (1)	C(15B) - C(16B) - C(18B)	114 (1)
C(17A) - C(16A) - C(18A)	105 (1)	C(17B) - C(16B) - C(18B)	106 (1)
S(1A) - C(19A) - C(15A)	115.5 (7)	S(1B) - C(19B) - C(15B)	117.1 (7)
N(1A) - C(20A) - C(21A)	121 (1)	N(1B) - C(20B) - C(21B)	115.3 (9)
N(1A) - C(20A) - C(25A)	121 (1)	N(1B) - C(20B) - C(25B)	108.9 (9)
C(21A) - C(20A) - C(25A)	118 (1)	C(21B) - C(20B) - C(25B)	110(1)
C(20A) - C(21A) - C(22A)	119 (1)	C(20B) - C(21B) - C(22B)	114 (1)
C(21A) - C(22A) - C(23A)	123 (2)	C(21B) - C(22B) - C(23B)	111 (1)
C(22A) - C(23A) - C(24A)	117 (2)	C(22B) - C(23B) - C(24B)	109 (1)
C(23A) - C(24A) - C(25A)	121 (2)	C(23B) - C(24B) - C(25B)	113 (1)
C(20A) - C(25A) - C(24A)	120 (1)	C(20B) - C(25B) - C(24B)	109 (1)
N(1A) - C(26A) - C(27A)	116(1)	N(1B) - C(26B) - C(27B)	110.1 (9)
N(1A) - C(26A) - C(31A)	123 (1)	N(1B) - C(26B) - C(31B)	117.5 (8)
C(27A) - C(26A) - C(31A)	121 (1)	C(27B) - C(26B) - C(31B)	113 (1)
C(26A) - C(27A) - C(28A)	117 (1)	C(26B) - C(27B) - C(28B)	110(1)
C(27A) - C(28A) - C(29A)	122 (1)	C(27B) - C(28B) - C(29B)	112 (1)
C(28A) - C(29A) - C(30A)	119 (1)	C(28B) - C(29B) - C(30B)	112(1)
C(29A) - C(30A) - C(31A)	118 (1)	C(29B) - C(30B) - C(31B)	111 (1)
C(26A) - C(31A) - C(30A)	121 (1)	C(26B) - C(31B) - C(30B)	110.7 (9)

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Lists of structure factors, anisotropic thermal parameters and H-atom coordinates and crystal packing and molecular structure diagrams have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71427 (44 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: LI1056]

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