Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

threo-Diethyl 2-ethyl-2-hydroxy-3-(4-methylbenzenesulfonamido)succinate

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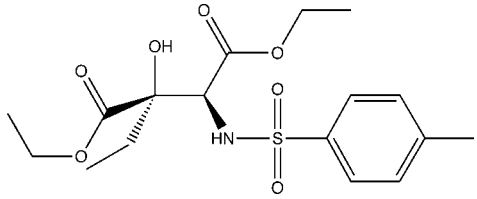
Received 11 July 2011; accepted 21 July 2011

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.040; wR factor = 0.114; data-to-parameter ratio = 13.3.

The asymmetric unit of the title compound, $C_{17}H_{25}NO_7S$, contains two independent molecules, which are enantiomers forming a hydrogen-bonded dimer associated with two $R_2^2(7)$ patterns. In each molecule, one ethyl group from the two available ethyl ester functional groups is disordered. In one molecule, the ethyl group of the ester function from an α-carboxylic acid is positionally disordered over two sets of sites with occupancies of 0.66:0.34. In the second molecule, it is the ethyl group in the γ-ester function that is disordered over two sets of sites with occupancies of 0.58:0.42.

Related literature

For our studies on optically pure β-substituted β-hydroxy aspartates as glutamate transporter blockers, see: Wehbe *et al.* (2003*a*,*b*,*c*); Mekki *et al.* (2011*a*,*b*). For hydrogen-bond motifs, see: Etter (1990); Bernstein *et al.* (1995). For the visualization of non-covalent interactions, see: Johnson *et al.* (2010); *Jmol* (2011). For a description of the *Jmol* toolkit for the preparation of enhanced figures, see: McMahon & Hanson (2008).



Experimental

Crystal data

$C_{17}H_{25}NO_7S$
M_r = 387.44
Triclinic, $P\overline{1}$
a = 9.5424 (3) Å
b = 12.2708 (4) Å
c = 18.2427 (5) Å
α = 90.800 (2)°
β = 91.153 (2)°
γ = 112.513 (3)°
V = 1972.36 (10) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 1.79 mm^{-1}
T = 173 K
0.27 × 0.24 × 0.12 mm

Data collection

Agilent Xcalibur Sapphire3 Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.110, T_{max} = 1.000
25194 measured reflections
6999 independent reflections
6214 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.114
S = 1.02
6999 reflections
527 parameters
81 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N11—H11···O32	0.84 (2)	2.23 (2)	3.0426 (18)	162 (2)
O31—H31···O22	0.80 (2)	2.10 (2)	2.7747 (17)	142 (2)
N12—H12···O31	0.86 (2)	2.19 (2)	3.019 (2)	161 (2)
O32—H32···O21	0.81 (2)	2.15 (2)	2.8321 (17)	142 (2)

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97*; molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *Jmol* (Jmol, 2011); software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

This work was supported by the Erasmus Mundus Averroés program.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2708).

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supporting information

Acta Cryst. (2011). E**67**, o2181–o2182 [doi:10.1107/S1600536811029527]

threo-Diethyl 2-ethyl-2-hydroxy-3-(4-methylbenzenesulfonamido)succinate

Sofiane Mekki, Valérie Rolland, Arie van der Lee and Marc Rolland

S1. Comment

In the present work, as a part of an on-going study of asymmetric syntheses of optically pure *β*-substituted *β*-hydroxy aspartates (Wehbe *et al.*, 2003*a*,*b*,*c*; Mekki *et al.*, 2011*a*,*b*), the structure of a new compound, *threo*-diethyl 2-ethyl-2-hydroxy-3-(4-methylphenylsulfonamido)succinate, is described. The key step of the synthesis is the regiospecific Sharpless aminohydroxylation on an ethyl fumarate derivative.

The crystal structure is made up by racemic dimers formed by two independent homochiral molecules ((2*S*,3*S*) and (2*R*,3*R*) for (I) and (II), respectively). They are bonded by non-covalent NH···O and OH···O hydrogen bonds (Fig. 1) forming two $R^2_2(7)$ patterns (Etter, 1990; Bernstein *et al.*, 1995), where the H···O distances range from 2.10 (2) Å to 2.232 (19) Å and the *D*—H···O angles from 142 (2) to 161.9 (18) ° (Table 1). In order to get an idea of the relative strength of the NH···O and OH···O hydrogen bonds the intersection of the Van der Waals surfaces of donor hydrogen and acceptor was calculated using the program *Jmol* (*Jmol*, 2011; 'contact′ command with 'full′ and 'hbond′ options). The resulting Fig. 2 shows clearly that the Van der Waals interaction zones between the hydroxyl groups and the carbonyl ester O atoms are more important than those between the hydroxyl groups and the secondary amine group. The latter interaction zones are much smaller than the former ones. A calculation based on the electron density and its derivatives (Johnson *et al.*, 2010; calculation done in *Jmol* using the 'contact′ command with 'nci′ and 'hbond′ as options) gives slightly different results (Fig. 3), in the sense that one of the OH···O interactions appears to be negligible. The relevant Van der Waals surfaces may be inspected in the enhanced *Jmol* picture in Fig. 4. This pictorial view of the non-covalent interaction regions is not completely in agreement with what could be concluded from the directionality of the interaction which is greater for nitrogen as hydrogen bond donor than for oxygen (Table 1). The dimeric structure bears much similarity with those reported recently for the two concomitant *β*-benzyl *β*-hydroxy aspartate analogue polymorphs (Mekki *et al.*, 2011*a*).

The two independent homochiral molecules are very approximately related by a local inversion center between the two molecules. That this local center is only very approximate, can be clearly seen in Fig. 5, which shows the best superposition of the (2*S*,3*S*) molecule (I) and the (2*S*,3*S*) inversion center related molecule (II) as calculated with *Olex2* (Dolomanov *et al.*, 2009). The root-mean-squared deviation (considering the majority disordered parts only) between the two molecules is 0.780 Å. The main conformational differences between molecules (I) and (II) stem from the orientation of the ethyl ester moiety in both residues. This is well illustrated by the torsion angles C9—O5—C4—C3 (-4.2 (2)° and 173.6 (3)° for molecules (I) and (II), respectively) and C1–01-C7—C8 (-165.5 (3)° and -88.6 (2)° for molecules (I) and (II), respectively).

In both molecules, the S1—N1(H1)—C2 pseudo-torsion angle [140.2 (1)° for (I) and -143.3 (1)° for (II)] implies a slight pyramidalization of the sulfonamide moiety.

S2. Experimental

A solution of (0.04 mmole, 14.7 mg) $K_2[OsO_2(OH)_4]$ in water (2.5 ml) and chloramine-T (1.5 mmole, 423 mg) was added to a solution of diethyl 2-ethylfumarate (20 mg, 0.1 mmole) and $(DHQD)_2PHAL$ (0.05 mmole, 39 mg) in CH_3CN (1.25 ml). After 1 h stirring at room temperature a second fraction of diethyl 2-ethylfumarate (180 mg, 0.9 mmole) in CH_3CN (1.25 ml) was added to the reaction mixture. After 5 h, a solution of Na_2SO_3 (357 mg) in water (5.4 ml) was added an the reaction mixture was extracted 3 times with AcOEt (5.4 ml). The fraction was then washed with brine and dried under $MgSO_4$. The solvent was removed and the title compound was recrystallized in cyclohexane by slow evaporation at ambient temperature yielding colourless crystals in the form of relatively large prisms.

S3. Refinement

All N-bound and O-bound H atoms were located in a difference Fourier maps and later restraint to a distance O–H = 0.82 (2) Å with U_{iso}(H)=1.5U_{eq}(O) and N–H = 0.88 (2) Å with U_{iso}(H)=1.2U_{eq}(N) in order to stabilize their coordinates during the final step of the refinement. All other H atoms were introduced at calculated positions and refined as riding atoms with C–H = 0.96–0.98 Å, with displacement parameters U_{iso}(H) equal to 1.5U_{eq}(C) for methyl and 1.2U_{eq}(C) for all other H atoms. Restraints (SADI, SIMU, DELU) were used to stabilize the refinement of the disordered diethyl groups. The occupancies of the disordered parts were fixed during the final cycles of the refinements.

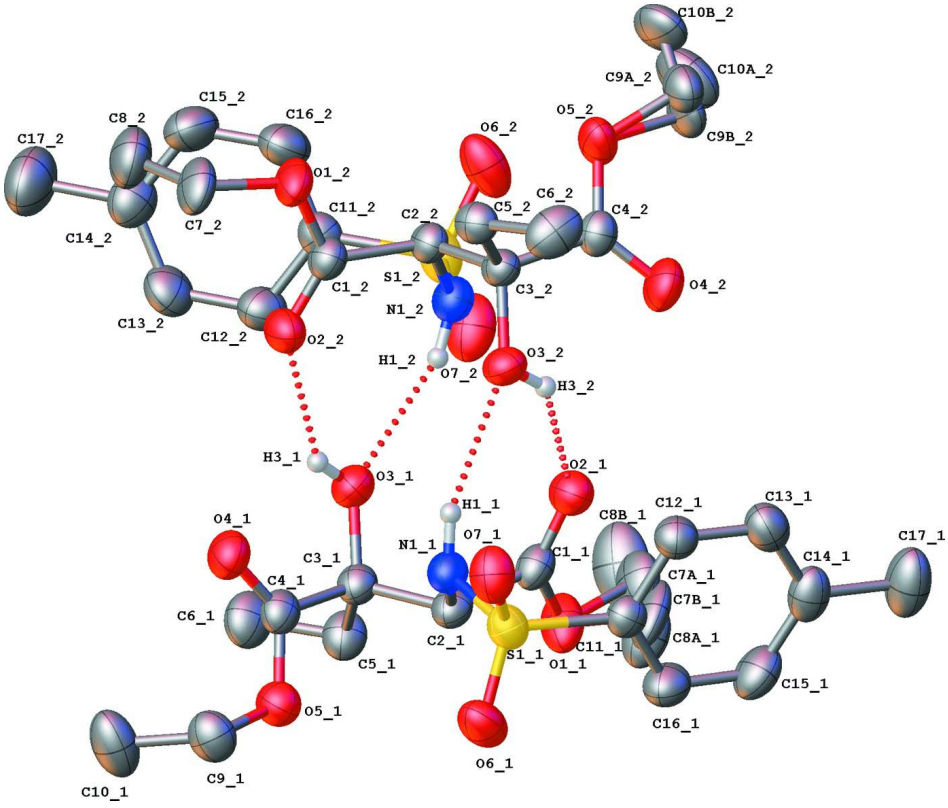

Figure 1

The asymmetric unit of the title compound with displacement ellipsoids for the non-hydrogen atoms drawn at the 50% probability level. Hydrogen bonds are indicated as dotted lines. Hydrogen atoms not involved in hydrogen bond interactions have been omitted for clarity.

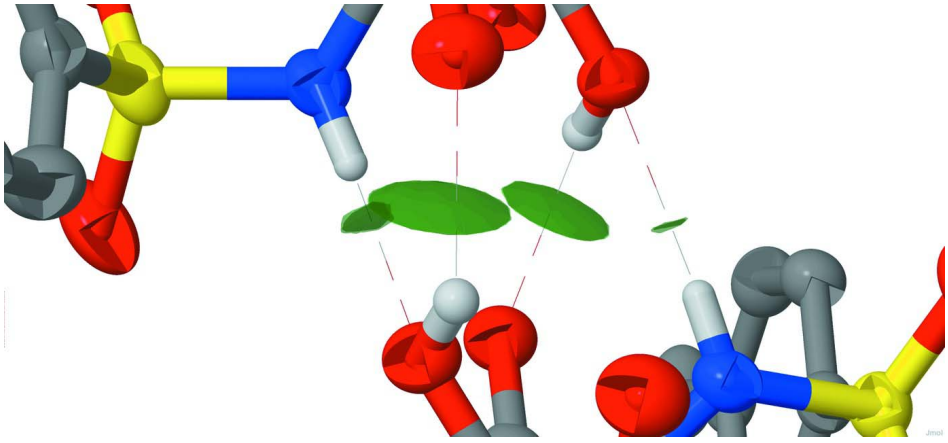

Figure 2

Van der Waals intersection surfaces (green) between nitrogen and oxygen hydrogen bond donors and oxygen acceptors of the two independent molecules in the asymmetric unit.

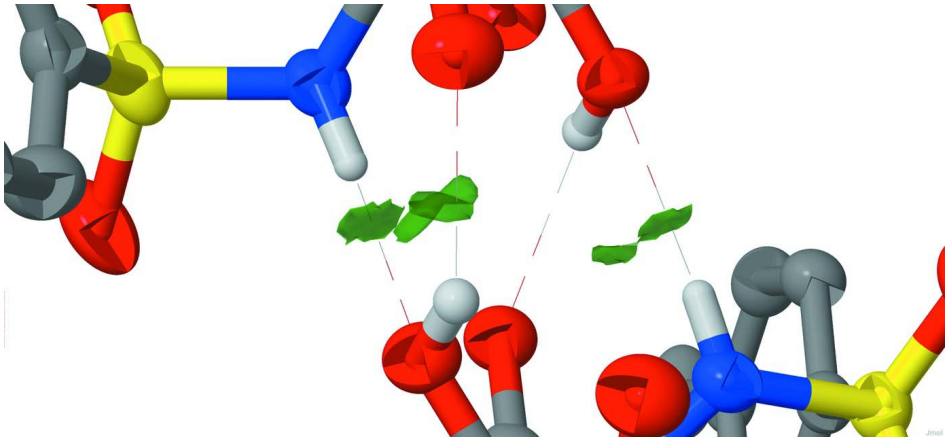

Figure 3

Non-covalent interaction surfaces (green) between nitrogen and oxygen hydrogen bond donors and oxygen acceptors of the two independent molecules in the asymmetric unit.

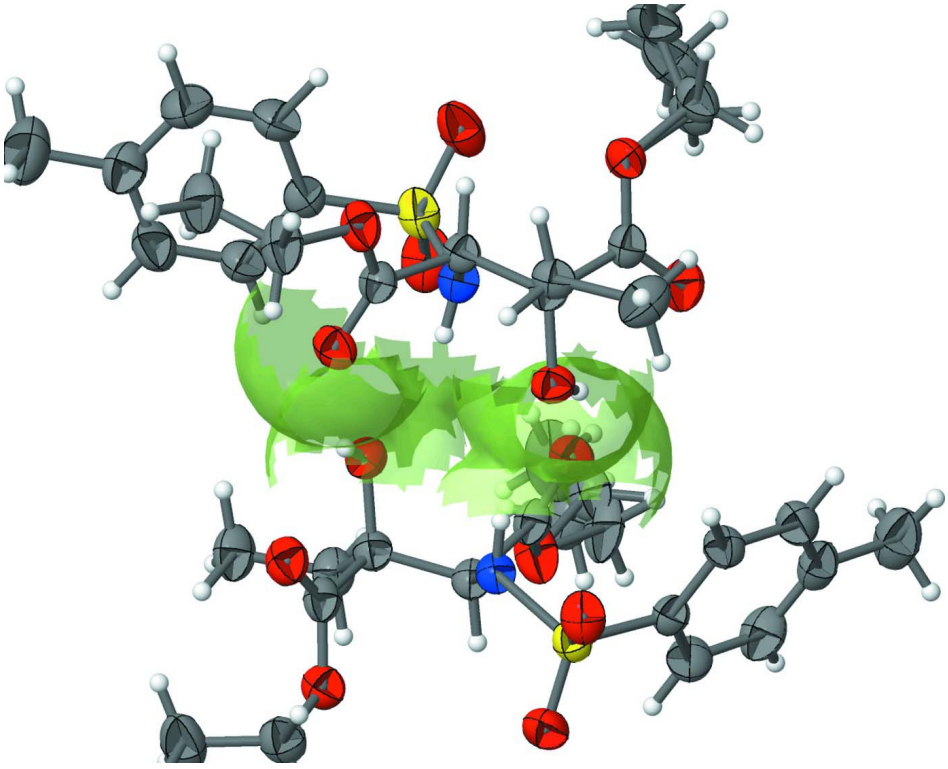

Figure 4

Enhanced *Jmol* view of the title compound showing displacement ellipsoids at the 50% probability level. Semi-translucent Van der Waals surfaces for donor H atoms and acceptors are displayed in green.

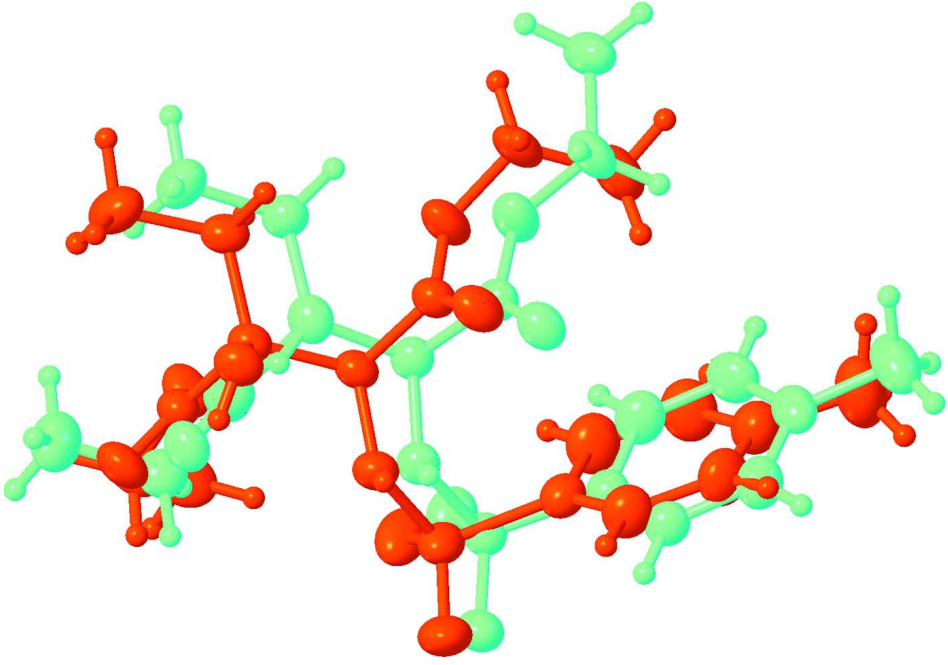

Figure 5

Best superposition of the two independent molecules in the asymmetric unit. Hydrogen bonds are omitted for clarity.

threo-Diethyl 2-ethyl-2-hydroxy-3-(4-methylbenzenesulfonamido)succinate

Crystal data

$C_{17}H_{25}NO_7S$
$M_r = 387.44$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.5424$ (3) Å
$b = 12.2708$ (4) Å
$c = 18.2427$ (5) Å
$\alpha = 90.800$ (2)°
$\beta = 91.153$ (2)°
$\gamma = 112.513$ (3)°
$V = 1972.36$ (10) Å^3
$Z = 4$
$F(000) = 824$
$D_x = 1.305$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 6999 reflections
$\theta = 4.6$–$67.3°$
$\mu = 1.79$ mm^{-1}
$T = 173$ K
Prism, colourless
0.27 × 0.24 × 0.12 mm

Data collection

Agilent Xcalibur Sapphire3 Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0143 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min} = 0.110$, $T_{max} = 1.000$
25194 measured reflections
6999 independent reflections
6214 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 67.3°$, $\theta_{min} = 4.6°$
$h = -11 \rightarrow 11$
$k = -14 \rightarrow 14$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.114$
$S = 1.02$
6999 reflections
527 parameters
81 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.066P)^2 + 0.4378P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

Special details

Experimental. *CrysAlis PRO* (Agilent, 2010); Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S11	0.49201 (5)	0.41250 (4)	0.16266 (2)	0.03996 (12)	
O11	0.36355 (15)	0.60190 (15)	0.33568 (7)	0.0597 (4)	
O21	0.48790 (14)	0.69378 (11)	0.23799 (7)	0.0461 (3)	
O31	0.77622 (13)	0.69982 (11)	0.32660 (7)	0.0436 (3)	
H31	0.852 (2)	0.702 (2)	0.3077 (13)	0.065*	
O41	0.90123 (14)	0.54137 (12)	0.31132 (7)	0.0494 (3)	
O51	0.69568 (14)	0.39398 (11)	0.35277 (7)	0.0455 (3)	
O61	0.43567 (17)	0.30752 (11)	0.20417 (8)	0.0552 (3)	
O71	0.57708 (15)	0.41810 (12)	0.09820 (7)	0.0516 (3)	
N11	0.60481 (15)	0.51686 (13)	0.21844 (7)	0.0377 (3)	
H11	0.656 (2)	0.5792 (15)	0.1966 (11)	0.045*	
C11	0.46431 (18)	0.61992 (16)	0.28350 (9)	0.0400 (4)	
C21	0.54737 (18)	0.53549 (15)	0.28902 (9)	0.0376 (3)	
H21	0.4746	0.4577	0.3062	0.045*	
C31	0.68397 (18)	0.58310 (15)	0.34482 (9)	0.0379 (3)	
C41	0.77443 (19)	0.50450 (16)	0.33431 (9)	0.0400 (4)	
C51	0.6352 (2)	0.58202 (18)	0.42443 (9)	0.0463 (4)	
H5A1	0.5827	0.6371	0.4301	0.056*	
H5B1	0.5622	0.5019	0.4355	0.056*	
C61	0.7683 (2)	0.6170 (2)	0.47904 (11)	0.0575 (5)	
H6A1	0.8154	0.5588	0.4767	0.086*	
H6B1	0.7321	0.6200	0.5286	0.086*	
H6C1	0.8431	0.6949	0.4670	0.086*	
C7A1	0.2915 (6)	0.6916 (5)	0.3353 (4)	0.0568 (13)	0.66
H7A1	0.3701	0.7717	0.3301	0.068*	0.66
H7B1	0.2179	0.6752	0.2935	0.068*	0.66
C8A1	0.2124 (4)	0.6844 (4)	0.40588 (19)	0.0621 (9)	0.66
H8A1	0.1381	0.6038	0.4117	0.093*	0.66
H8B1	0.1603	0.7394	0.4056	0.093*	0.66
H8C1	0.2869	0.7052	0.4467	0.093*	0.66
C7B1	0.2456 (11)	0.6449 (11)	0.3313 (8)	0.071 (3)	0.34
H7C1	0.1489	0.5876	0.3497	0.085*	0.34
H7D1	0.2295	0.6673	0.2808	0.085*	0.34
C8B1	0.3134 (11)	0.7484 (10)	0.3809 (5)	0.093 (3)	0.34
H8D1	0.3265	0.7224	0.4302	0.139*	0.34
H8E1	0.2465	0.7922	0.3827	0.139*	0.34
H8F1	0.4124	0.7996	0.3628	0.139*	0.34
C91	0.7677 (2)	0.30975 (18)	0.33901 (11)	0.0525 (4)	
H9A1	0.8184	0.3263	0.2913	0.063*	
H9B1	0.6889	0.2287	0.3362	0.063*	
C101	0.8821 (3)	0.3172 (2)	0.39851 (14)	0.0725 (7)	
H10A1	0.9676	0.3936	0.3967	0.109*	
H10B1	0.9188	0.2535	0.3913	0.109*	
H10C1	0.8347	0.3095	0.4463	0.109*	
C111	0.33817 (18)	0.45303 (14)	0.14075 (9)	0.0370 (3)	

C121	0.3501 (2)	0.52924 (16)	0.08434 (9)	0.0423 (4)	
H121	0.4370	0.5551	0.0547	0.051*	
C131	0.2333 (2)	0.56743 (17)	0.07165 (11)	0.0508 (4)	
H131	0.2408	0.6197	0.0327	0.061*	
C141	0.1055 (2)	0.53164 (17)	0.11419 (11)	0.0504 (4)	
C151	0.0970 (2)	0.4554 (2)	0.17044 (12)	0.0573 (5)	
H151	0.0105	0.4301	0.2004	0.069*	
C161	0.2117 (2)	0.41539 (18)	0.18398 (11)	0.0516 (4)	
H161	0.2039	0.3625	0.2226	0.062*	
C171	−0.0214 (3)	0.5743 (2)	0.10073 (16)	0.0741 (7)	
H17A1	−0.1189	0.5069	0.0997	0.111*	
H17B1	−0.0075	0.6141	0.0536	0.111*	
H17C1	−0.0201	0.6298	0.1402	0.111*	
S12	0.84903 (5)	1.02772 (4)	0.29860 (2)	0.04747 (13)	
O12	1.16142 (13)	0.94133 (13)	0.16081 (7)	0.0505 (3)	
O22	1.02729 (14)	0.80796 (11)	0.24124 (7)	0.0470 (3)	
O32	0.71903 (13)	0.74485 (10)	0.13370 (7)	0.0409 (3)	
H32	0.640 (2)	0.746 (2)	0.1483 (13)	0.061*	
O42	0.57282 (14)	0.88091 (13)	0.09183 (8)	0.0538 (3)	
O52	0.79035 (14)	1.03488 (11)	0.07151 (8)	0.0486 (3)	
O62	0.8723 (2)	1.12985 (13)	0.25634 (8)	0.0641 (4)	
O72	0.73105 (17)	0.98906 (16)	0.35091 (8)	0.0660 (4)	
N12	0.81369 (16)	0.91758 (14)	0.24099 (8)	0.0403 (3)	
H12	0.781 (2)	0.8512 (15)	0.2626 (11)	0.048*	
C12	1.03877 (18)	0.88414 (15)	0.19833 (9)	0.0376 (3)	
C22	0.91316 (17)	0.92874 (14)	0.17950 (9)	0.0353 (3)	
H22	0.9614	1.0140	0.1670	0.042*	
C32	0.81149 (17)	0.85996 (14)	0.11295 (9)	0.0340 (3)	
C42	0.70850 (18)	0.92560 (15)	0.09133 (9)	0.0381 (4)	
C52	0.90368 (19)	0.85057 (15)	0.04729 (9)	0.0389 (4)	
H5A2	0.9816	0.9296	0.0379	0.047*	
H5B2	0.9570	0.7979	0.0597	0.047*	
C62	0.8076 (2)	0.8036 (2)	−0.02228 (11)	0.0579 (5)	
H6A2	0.7248	0.7284	−0.0124	0.087*	
H6B2	0.8708	0.7914	−0.0607	0.087*	
H6C2	0.7651	0.8606	−0.0386	0.087*	
C72	1.2928 (2)	0.9086 (2)	0.17253 (11)	0.0564 (5)	
H7A2	1.3525	0.9224	0.1274	0.068*	
H7B2	1.2575	0.8236	0.1836	0.068*	
C82	1.3905 (2)	0.9804 (2)	0.23496 (14)	0.0684 (6)	
H8A2	1.4197	1.0645	0.2253	0.103*	
H8B2	1.4818	0.9626	0.2400	0.103*	
H8C2	1.3339	0.9612	0.2804	0.103*	
C9A2	0.7216 (7)	1.1129 (6)	0.0412 (3)	0.0498 (13)	0.58
H9A2	0.6213	1.0660	0.0182	0.060*	0.58
H9B2	0.7872	1.1633	0.0035	0.060*	0.58
C10A2	0.7047 (8)	1.1870 (5)	0.1027 (3)	0.0780 (14)	0.58
H10A2	0.6370	1.1364	0.1389	0.117*	0.58

H10B2	0.6617	1.2423	0.0839	0.117*	0.58
H10C2	0.8044	1.2313	0.1259	0.117*	0.58
C9B2	0.6878 (9)	1.1038 (7)	0.0679 (5)	0.0497 (18)	0.42
H9C2	0.6388	1.0954	0.0186	0.060*	0.42
H9D2	0.6080	1.0760	0.1049	0.060*	0.42
C10B2	0.7904 (7)	1.2279 (5)	0.0836 (4)	0.0624 (15)	0.42
H10D2	0.7326	1.2788	0.0802	0.094*	0.42
H10E2	0.8714	1.2524	0.0478	0.094*	0.42
H10F2	0.8351	1.2347	0.1331	0.094*	0.42
C112	1.0231 (2)	1.05241 (15)	0.34519 (9)	0.0417 (4)	
C122	1.0273 (2)	0.98059 (18)	0.40217 (10)	0.0511 (4)	
H122	0.9382	0.9163	0.4153	0.061*	
C132	1.1631 (3)	1.0037 (2)	0.43969 (11)	0.0589 (5)	
H132	1.1667	0.9545	0.4788	0.071*	
C142	1.2943 (2)	1.0971 (2)	0.42160 (11)	0.0571 (5)	
C152	1.2877 (3)	1.1647 (2)	0.36312 (13)	0.0642 (6)	
H152	1.3773	1.2276	0.3490	0.077*	
C162	1.1536 (3)	1.14287 (18)	0.32469 (12)	0.0576 (5)	
H162	1.1512	1.1900	0.2842	0.069*	
C172	1.4417 (3)	1.1235 (3)	0.46385 (17)	0.0910 (9)	
H17A2	1.4979	1.0804	0.4411	0.137*	
H17B2	1.4202	1.0988	0.5147	0.137*	
H17C2	1.5026	1.2084	0.4632	0.137*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S11	0.0442 (2)	0.0407 (2)	0.0390 (2)	0.02082 (18)	−0.00107 (16)	−0.00119 (16)
O11	0.0464 (7)	0.1004 (11)	0.0453 (7)	0.0415 (8)	0.0135 (6)	0.0136 (7)
O21	0.0424 (7)	0.0480 (7)	0.0516 (7)	0.0211 (6)	0.0082 (5)	0.0059 (6)
O31	0.0354 (6)	0.0449 (7)	0.0483 (7)	0.0129 (5)	0.0031 (5)	0.0038 (5)
O41	0.0380 (7)	0.0594 (8)	0.0538 (7)	0.0218 (6)	0.0046 (5)	0.0051 (6)
O51	0.0443 (7)	0.0473 (7)	0.0473 (7)	0.0199 (6)	0.0049 (5)	0.0043 (5)
O61	0.0664 (9)	0.0404 (7)	0.0598 (8)	0.0218 (6)	−0.0082 (7)	0.0038 (6)
O71	0.0541 (7)	0.0655 (8)	0.0453 (7)	0.0347 (7)	−0.0003 (6)	−0.0098 (6)
N11	0.0351 (7)	0.0436 (8)	0.0351 (7)	0.0157 (6)	0.0040 (5)	0.0029 (6)
C11	0.0298 (8)	0.0521 (10)	0.0372 (8)	0.0147 (7)	0.0026 (6)	−0.0017 (7)
C21	0.0331 (8)	0.0440 (9)	0.0343 (8)	0.0130 (7)	0.0048 (6)	0.0041 (7)
C31	0.0338 (8)	0.0430 (9)	0.0363 (8)	0.0137 (7)	0.0034 (6)	0.0041 (7)
C41	0.0370 (9)	0.0505 (10)	0.0329 (8)	0.0173 (8)	0.0003 (6)	0.0023 (7)
C51	0.0443 (9)	0.0598 (11)	0.0371 (9)	0.0225 (9)	0.0038 (7)	−0.0004 (8)
C61	0.0570 (12)	0.0768 (14)	0.0392 (9)	0.0267 (11)	−0.0043 (8)	−0.0029 (9)
C7A1	0.043 (3)	0.081 (3)	0.059 (3)	0.038 (3)	0.011 (3)	0.003 (3)
C8A1	0.0473 (18)	0.090 (3)	0.0539 (18)	0.0325 (18)	0.0016 (14)	−0.0199 (17)
C7B1	0.027 (5)	0.127 (10)	0.060 (5)	0.031 (5)	0.002 (4)	0.000 (6)
C8B1	0.101 (7)	0.148 (8)	0.064 (5)	0.087 (7)	0.004 (5)	−0.023 (5)
C91	0.0594 (11)	0.0510 (11)	0.0532 (10)	0.0282 (9)	−0.0003 (9)	−0.0025 (8)
C101	0.0917 (17)	0.0723 (15)	0.0710 (14)	0.0523 (14)	−0.0224 (13)	−0.0108 (11)

C111	0.0365 (8)	0.0381 (8)	0.0355 (8)	0.0136 (7)	−0.0009 (6)	−0.0028 (6)
C121	0.0421 (9)	0.0459 (9)	0.0391 (8)	0.0168 (8)	0.0035 (7)	0.0038 (7)
C131	0.0544 (11)	0.0487 (10)	0.0521 (10)	0.0233 (9)	−0.0060 (8)	0.0019 (8)
C141	0.0436 (10)	0.0522 (11)	0.0578 (11)	0.0224 (9)	−0.0107 (8)	−0.0171 (9)
C151	0.0368 (9)	0.0736 (14)	0.0580 (11)	0.0172 (9)	0.0078 (8)	−0.0025 (10)
C161	0.0446 (10)	0.0577 (11)	0.0478 (10)	0.0135 (9)	0.0059 (8)	0.0118 (8)
C171	0.0594 (13)	0.0789 (16)	0.0958 (18)	0.0416 (12)	−0.0172 (12)	−0.0252 (13)
S12	0.0538 (3)	0.0588 (3)	0.0417 (2)	0.0352 (2)	−0.00150 (18)	−0.00783 (19)
O12	0.0307 (6)	0.0710 (9)	0.0533 (7)	0.0228 (6)	0.0078 (5)	0.0169 (6)
O22	0.0410 (7)	0.0504 (7)	0.0556 (7)	0.0234 (6)	0.0064 (5)	0.0122 (6)
O32	0.0347 (6)	0.0384 (6)	0.0473 (6)	0.0110 (5)	0.0080 (5)	0.0058 (5)
O42	0.0334 (7)	0.0666 (9)	0.0657 (8)	0.0239 (6)	0.0021 (6)	0.0016 (7)
O52	0.0450 (7)	0.0396 (7)	0.0665 (8)	0.0227 (6)	−0.0096 (6)	0.0006 (6)
O62	0.0951 (11)	0.0635 (9)	0.0549 (8)	0.0549 (9)	−0.0132 (7)	−0.0097 (7)
O72	0.0586 (8)	0.1001 (12)	0.0516 (8)	0.0444 (8)	0.0058 (6)	−0.0156 (8)
N12	0.0361 (7)	0.0474 (8)	0.0401 (7)	0.0190 (7)	0.0050 (6)	−0.0018 (6)
C12	0.0312 (8)	0.0421 (9)	0.0405 (8)	0.0152 (7)	0.0031 (6)	0.0007 (7)
C22	0.0305 (8)	0.0386 (8)	0.0390 (8)	0.0157 (7)	0.0041 (6)	0.0022 (6)
C32	0.0304 (7)	0.0340 (8)	0.0383 (8)	0.0130 (6)	0.0046 (6)	0.0025 (6)
C42	0.0351 (9)	0.0446 (9)	0.0375 (8)	0.0187 (7)	0.0005 (6)	−0.0044 (7)
C52	0.0395 (9)	0.0386 (8)	0.0422 (9)	0.0186 (7)	0.0076 (7)	0.0013 (7)
C62	0.0553 (11)	0.0633 (12)	0.0468 (10)	0.0137 (10)	0.0076 (9)	−0.0129 (9)
C72	0.0330 (9)	0.0871 (15)	0.0577 (11)	0.0321 (10)	0.0067 (8)	0.0061 (10)
C82	0.0431 (11)	0.0901 (17)	0.0765 (15)	0.0310 (11)	−0.0062 (10)	0.0021 (13)
C9A2	0.044 (3)	0.056 (3)	0.058 (3)	0.029 (2)	0.004 (2)	0.011 (2)
C10A2	0.114 (5)	0.071 (3)	0.076 (3)	0.064 (3)	0.013 (3)	0.010 (3)
C9B2	0.046 (4)	0.043 (3)	0.073 (5)	0.031 (3)	0.001 (3)	0.010 (4)
C10B2	0.069 (4)	0.041 (3)	0.088 (4)	0.032 (3)	0.008 (3)	0.013 (3)
C112	0.0488 (10)	0.0419 (9)	0.0374 (8)	0.0210 (8)	0.0004 (7)	−0.0026 (7)
C122	0.0528 (11)	0.0497 (10)	0.0469 (10)	0.0149 (9)	0.0033 (8)	0.0080 (8)
C132	0.0656 (13)	0.0682 (13)	0.0451 (10)	0.0278 (11)	−0.0011 (9)	0.0123 (9)
C142	0.0537 (11)	0.0657 (13)	0.0493 (10)	0.0203 (10)	−0.0027 (9)	−0.0041 (9)
C152	0.0546 (12)	0.0539 (12)	0.0713 (14)	0.0064 (10)	0.0014 (10)	0.0090 (10)
C162	0.0643 (13)	0.0478 (11)	0.0568 (11)	0.0168 (10)	0.0002 (9)	0.0140 (9)
C172	0.0648 (15)	0.119 (2)	0.0807 (18)	0.0267 (16)	−0.0178 (13)	0.0017 (16)

Geometric parameters (Å, º)

S11—O61	1.4266 (14)	S12—O62	1.4266 (15)
S11—O71	1.4298 (13)	S12—O72	1.4318 (16)
S11—N11	1.6425 (15)	S12—N12	1.6252 (15)
S11—C111	1.7615 (16)	S12—C112	1.7675 (18)
O11—C11	1.326 (2)	O12—C12	1.322 (2)
O11—C7B1	1.415 (11)	O12—C72	1.469 (2)
O11—C7A1	1.504 (5)	O22—C12	1.202 (2)
O21—C11	1.197 (2)	O32—C32	1.4110 (19)
O31—C31	1.413 (2)	O32—H32	0.813 (16)
O31—H31	0.804 (16)	O42—C42	1.198 (2)

O41—C41	1.205 (2)	O52—C42	1.327 (2)
O51—C41	1.327 (2)	O52—C9A2	1.461 (6)
O51—C91	1.465 (2)	O52—C9B2	1.519 (7)
N11—C21	1.458 (2)	N12—C22	1.458 (2)
N11—H11	0.841 (15)	N12—H12	0.855 (15)
C11—C21	1.530 (2)	C12—C22	1.531 (2)
C21—C31	1.557 (2)	C22—C32	1.557 (2)
C21—H21	1.0000	C22—H22	1.0000
C31—C51	1.532 (2)	C32—C52	1.529 (2)
C31—C41	1.533 (2)	C32—C42	1.539 (2)
C51—C61	1.519 (3)	C52—C62	1.521 (3)
C51—H5A1	0.9900	C52—H5A2	0.9900
C51—H5B1	0.9900	C52—H5B2	0.9900
C61—H6A1	0.9800	C62—H6A2	0.9800
C61—H6B1	0.9800	C62—H6B2	0.9800
C61—H6C1	0.9800	C62—H6C2	0.9800
C7A1—C8A1	1.492 (7)	C72—C82	1.498 (3)
C7A1—H7A1	0.9900	C72—H7A2	0.9900
C7A1—H7B1	0.9900	C72—H7B2	0.9900
C8A1—H8A1	0.9800	C82—H8A2	0.9800
C8A1—H8B1	0.9800	C82—H8B2	0.9800
C8A1—H8C1	0.9800	C82—H8C2	0.9800
C7B1—C8B1	1.472 (13)	C9A2—C10A2	1.484 (8)
C7B1—H7C1	0.9900	C9A2—H9A2	0.9900
C7B1—H7D1	0.9900	C9A2—H9B2	0.9900
C8B1—H8D1	0.9800	C10A2—H10A2	0.9800
C8B1—H8E1	0.9800	C10A2—H10B2	0.9800
C8B1—H8F1	0.9800	C10A2—H10C2	0.9800
C91—C101	1.501 (3)	C9B2—C10B2	1.482 (10)
C91—H9A1	0.9900	C9B2—H9C2	0.9900
C91—H9B1	0.9900	C9B2—H9D2	0.9900
C101—H10A1	0.9800	C10B2—H10D2	0.9800
C101—H10B1	0.9800	C10B2—H10E2	0.9800
C101—H10C1	0.9800	C10B2—H10F2	0.9800
C111—C121	1.377 (2)	C112—C162	1.376 (3)
C111—C161	1.383 (3)	C112—C122	1.382 (3)
C121—C131	1.381 (3)	C122—C132	1.380 (3)
C121—H121	0.9500	C122—H122	0.9500
C131—C141	1.385 (3)	C132—C142	1.385 (3)
C131—H131	0.9500	C132—H132	0.9500
C141—C151	1.380 (3)	C142—C152	1.376 (3)
C141—C171	1.510 (3)	C142—C172	1.509 (3)
C151—C161	1.381 (3)	C152—C162	1.377 (3)
C151—H151	0.9500	C152—H152	0.9500
C161—H161	0.9500	C162—H162	0.9500
C171—H17A1	0.9800	C172—H17A2	0.9800
C171—H17B1	0.9800	C172—H17B2	0.9800
C171—H17C1	0.9800	C172—H17C2	0.9800

O61—S11—O71	120.91 (8)	O62—S12—O72	120.70 (10)
O61—S11—N11	106.45 (8)	O62—S12—N12	107.00 (8)
O71—S11—N11	105.62 (8)	O72—S12—N12	105.77 (9)
O61—S11—C111	107.85 (8)	O62—S12—C112	106.58 (9)
O71—S11—C111	109.08 (8)	O72—S12—C112	107.99 (9)
N11—S11—C111	105.98 (7)	N12—S12—C112	108.32 (8)
C11—O11—C7B1	122.2 (6)	C12—O12—C72	117.23 (14)
C11—O11—C7A1	112.3 (3)	C32—O32—H32	108.2 (17)
C7B1—O11—C7A1	22.5 (5)	C42—O52—C9A2	122.5 (3)
C31—O31—H31	110.7 (18)	C42—O52—C9B2	108.6 (4)
C41—O51—C91	116.00 (14)	C9A2—O52—C9B2	22.2 (3)
C21—N11—S11	118.55 (11)	C22—N12—S12	119.77 (12)
C21—N11—H11	114.8 (14)	C22—N12—H12	116.9 (14)
S11—N11—H11	113.0 (14)	S12—N12—H12	111.8 (14)
O21—C11—O11	124.05 (16)	O22—C12—O12	124.87 (15)
O21—C11—C21	124.23 (14)	O22—C12—C22	124.70 (14)
O11—C11—C21	111.71 (15)	O12—C12—C22	110.43 (13)
N11—C21—C11	111.84 (13)	N12—C22—C12	111.69 (13)
N11—C21—C31	108.01 (13)	N12—C22—C32	107.26 (12)
C11—C21—C31	111.30 (14)	C12—C22—C32	112.26 (13)
N11—C21—H21	108.5	N12—C22—H22	108.5
C11—C21—H21	108.5	C12—C22—H22	108.5
C31—C21—H21	108.5	C32—C22—H22	108.5
O31—C31—C51	109.13 (14)	O32—C32—C52	108.40 (13)
O31—C31—C41	108.78 (13)	O32—C32—C42	108.55 (12)
C51—C31—C41	110.99 (13)	C52—C32—C42	109.96 (13)
O31—C31—C21	108.75 (13)	O32—C32—C22	109.83 (12)
C51—C31—C21	113.07 (14)	C52—C32—C22	112.77 (13)
C41—C31—C21	105.98 (13)	C42—C32—C22	107.27 (12)
O41—C41—O51	125.60 (16)	O42—C42—O52	125.97 (16)
O41—C41—C31	122.53 (16)	O42—C42—C32	123.10 (16)
O51—C41—C31	111.87 (14)	O52—C42—C32	110.92 (13)
C61—C51—C31	112.68 (15)	C62—C52—C32	113.37 (14)
C61—C51—H5A1	109.1	C62—C52—H5A2	108.9
C31—C51—H5A1	109.1	C32—C52—H5A2	108.9
C61—C51—H5B1	109.1	C62—C52—H5B2	108.9
C31—C51—H5B1	109.1	C32—C52—H5B2	108.9
H5A1—C51—H5B1	107.8	H5A2—C52—H5B2	107.7
C51—C61—H6A1	109.5	C52—C62—H6A2	109.5
C51—C61—H6B1	109.5	C52—C62—H6B2	109.5
H6A1—C61—H6B1	109.5	H6A2—C62—H6B2	109.5
C51—C61—H6C1	109.5	C52—C62—H6C2	109.5
H6A1—C61—H6C1	109.5	H6A2—C62—H6C2	109.5
H6B1—C61—H6C1	109.5	H6B2—C62—H6C2	109.5
C8A1—C7A1—O11	108.3 (4)	O12—C72—C82	109.90 (17)
C8A1—C7A1—H7A1	110.0	O12—C72—H7A2	109.7
O11—C7A1—H7A1	110.0	C82—C72—H7A2	109.7

C8A1—C7A1—H7B1	110.0	O12—C72—H7B2	109.7
O11—C7A1—H7B1	110.0	C82—C72—H7B2	109.7
H7A1—C7A1—H7B1	108.4	H7A2—C72—H7B2	108.2
O11—C7B1—C8B1	98.3 (7)	C72—C82—H8A2	109.5
O11—C7B1—H7C1	112.1	C72—C82—H8B2	109.5
C8B1—C7B1—H7C1	112.1	H8A2—C82—H8B2	109.5
O11—C7B1—H7D1	112.1	C72—C82—H8C2	109.5
C8B1—C7B1—H7D1	112.1	H8A2—C82—H8C2	109.5
H7C1—C7B1—H7D1	109.7	H8B2—C82—H8C2	109.5
C7B1—C8B1—H8D1	109.5	O52—C9A2—C10A2	107.4 (4)
C7B1—C8B1—H8E1	109.5	O52—C9A2—H9A2	110.2
H8D1—C8B1—H8E1	109.5	C10A2—C9A2—H9A2	110.2
C7B1—C8B1—H8F1	109.5	O52—C9A2—H9B2	110.2
H8D1—C8B1—H8F1	109.5	C10A2—C9A2—H9B2	110.2
H8E1—C8B1—H8F1	109.5	H9A2—C9A2—H9B2	108.5
O51—C91—C101	111.26 (16)	C10B2—C9B2—O52	104.7 (6)
O51—C91—H9A1	109.4	C10B2—C9B2—H9C2	110.8
C101—C91—H9A1	109.4	O52—C9B2—H9C2	110.8
O51—C91—H9B1	109.4	C10B2—C9B2—H9D2	110.8
C101—C91—H9B1	109.4	O52—C9B2—H9D2	110.8
H9A1—C91—H9B1	108.0	H9C2—C9B2—H9D2	108.9
C91—C101—H10A1	109.5	C9B2—C10B2—H10D2	109.5
C91—C101—H10B1	109.5	C9B2—C10B2—H10E2	109.5
H10A1—C101—H10B1	109.5	H10D2—C10B2—H10E2	109.5
C91—C101—H10C1	109.5	C9B2—C10B2—H10F2	109.5
H10A1—C101—H10C1	109.5	H10D2—C10B2—H10F2	109.5
H10B1—C101—H10C1	109.5	H10E2—C10B2—H10F2	109.5
C121—C111—C161	120.69 (16)	C162—C112—C122	120.33 (18)
C121—C111—S11	119.56 (13)	C162—C112—S12	119.98 (14)
C161—C111—S11	119.56 (13)	C122—C112—S12	119.69 (15)
C111—C121—C131	118.78 (17)	C132—C122—C112	118.94 (19)
C111—C121—H121	120.6	C132—C122—H122	120.5
C131—C121—H121	120.6	C112—C122—H122	120.5
C121—C131—C141	121.85 (18)	C122—C132—C142	121.50 (19)
C121—C131—H131	119.1	C122—C132—H132	119.3
C141—C131—H131	119.1	C142—C132—H132	119.3
C151—C141—C131	118.05 (17)	C152—C142—C132	118.2 (2)
C151—C141—C171	120.1 (2)	C152—C142—C172	120.5 (2)
C131—C141—C171	121.8 (2)	C132—C142—C172	121.3 (2)
C141—C151—C161	121.24 (18)	C142—C152—C162	121.2 (2)
C141—C151—H151	119.4	C142—C152—H152	119.4
C161—C151—H151	119.4	C162—C152—H152	119.4
C151—C161—C111	119.39 (18)	C112—C162—C152	119.70 (18)
C151—C161—H161	120.3	C112—C162—H162	120.2
C111—C161—H161	120.3	C152—C162—H162	120.2
C141—C171—H17A1	109.5	C142—C172—H17A2	109.5
C141—C171—H17B1	109.5	C142—C172—H17B2	109.5
H17A1—C171—H17B1	109.5	H17A2—C172—H17B2	109.5

C141—C171—H17C1	109.5	C142—C172—H17C2	109.5
H17A1—C171—H17C1	109.5	H17A2—C172—H17C2	109.5
H17B1—C171—H17C1	109.5	H17B2—C172—H17C2	109.5
O61—S11—N11—C21	−52.11 (14)	O72—S12—N12—C22	179.32 (12)
O71—S11—N11—C21	178.20 (12)	C112—S12—N12—C22	−65.12 (14)
C111—S11—N11—C21	62.54 (13)	C72—O12—C12—O22	0.2 (3)
C7B1—O11—C11—O21	17.8 (6)	C72—O12—C12—C22	−179.84 (15)
C7A1—O11—C11—O21	−4.9 (3)	S12—N12—C22—C12	92.68 (15)
C7B1—O11—C11—C21	−162.6 (5)	S12—N12—C22—C32	−143.93 (11)
C7A1—O11—C11—C21	174.6 (3)	O22—C12—C22—N12	29.4 (2)
S11—N11—C21—C11	−86.97 (16)	O12—C12—C22—N12	−150.56 (14)
S11—N11—C21—C31	150.22 (11)	O22—C12—C22—C32	−91.1 (2)
O21—C11—C21—N11	−25.6 (2)	O12—C12—C22—C32	88.93 (17)
O11—C11—C21—N11	154.86 (15)	N12—C22—C32—O32	−51.41 (16)
O21—C11—C21—C31	95.31 (19)	C12—C22—C32—O32	71.63 (16)
O11—C11—C21—C31	−84.23 (17)	N12—C22—C32—C52	−172.42 (13)
N11—C21—C31—O31	70.63 (16)	C12—C22—C32—C52	−49.38 (17)
C11—C21—C31—O31	−52.50 (17)	N12—C22—C32—C42	66.37 (15)
N11—C21—C31—C51	−167.99 (14)	C12—C22—C32—C42	−170.59 (13)
C11—C21—C31—C51	68.88 (18)	C9A2—O52—C42—O42	−5.3 (4)
N11—C21—C31—C41	−46.18 (17)	C9B2—O52—C42—O42	14.0 (4)
C11—C21—C31—C41	−169.31 (13)	C9A2—O52—C42—C32	173.6 (3)
C91—O51—C41—O41	−4.2 (2)	C9B2—O52—C42—C32	−167.1 (4)
C91—O51—C41—C31	175.19 (14)	O32—C32—C42—O42	−1.3 (2)
O31—C31—C41—O41	−2.6 (2)	C52—C32—C42—O42	117.17 (18)
C51—C31—C41—O41	−122.64 (18)	C22—C32—C42—O42	−119.87 (17)
C21—C31—C41—O41	114.22 (17)	O32—C32—C42—O52	179.80 (13)
O31—C31—C41—O51	178.02 (13)	C52—C32—C42—O52	−61.77 (17)
C51—C31—C41—O51	57.93 (18)	C22—C32—C42—O52	61.19 (16)
C21—C31—C41—O51	−65.20 (16)	O32—C32—C52—C62	68.54 (18)
O31—C31—C51—C61	−64.5 (2)	C42—C32—C52—C62	−49.98 (19)
C41—C31—C51—C61	55.4 (2)	C22—C32—C52—C62	−169.64 (15)
C21—C31—C51—C61	174.30 (16)	C12—O12—C72—C82	−88.6 (2)
C11—O11—C7A1—C8A1	−165.5 (3)	C42—O52—C9A2—C10A2	95.3 (5)
C7B1—O11—C7A1—C8A1	73 (2)	C9B2—O52—C9A2—C10A2	39.3 (12)
C11—O11—C7B1—C8B1	−101.3 (9)	C42—O52—C9B2—C10B2	152.0 (5)
C7A1—O11—C7B1—C8B1	−31.9 (14)	C9A2—O52—C9B2—C10B2	−75.6 (14)
C41—O51—C91—C101	80.6 (2)	O62—S12—C112—C162	−13.71 (18)
O61—S11—C111—C121	−161.28 (14)	O72—S12—C112—C162	−144.77 (17)
O71—S11—C111—C121	−28.25 (16)	N12—S12—C112—C162	101.13 (17)
N11—S11—C111—C121	85.03 (15)	O62—S12—C112—C122	166.24 (15)
O61—S11—C111—C161	23.77 (17)	O72—S12—C112—C122	35.18 (18)
O71—S11—C111—C161	156.80 (15)	N12—S12—C112—C122	−78.92 (16)
N11—S11—C111—C161	−89.92 (16)	C162—C112—C122—C132	2.3 (3)
C161—C111—C121—C131	0.0 (3)	S12—C112—C122—C132	−177.69 (16)
S11—C111—C121—C131	−174.93 (14)	C112—C122—C132—C142	0.2 (3)
C111—C121—C131—C141	0.3 (3)	C122—C132—C142—C152	−2.2 (3)

C121—C131—C141—C151	−0.1 (3)	C122—C132—C142—C172	178.7 (2)
C121—C131—C141—C171	179.41 (18)	C132—C142—C152—C162	1.9 (4)
C131—C141—C151—C161	−0.3 (3)	C172—C142—C152—C162	−179.0 (2)
C171—C141—C151—C161	−179.8 (2)	C122—C112—C162—C152	−2.6 (3)
C141—C151—C161—C111	0.5 (3)	S12—C112—C162—C152	177.35 (18)
C121—C111—C161—C151	−0.4 (3)	C142—C152—C162—C112	0.5 (4)
S11—C111—C161—C151	174.53 (15)	S11—N11—H11—C21	140.2 (12)
O62—S12—N12—C22	49.44 (15)	S12—N12—H12—C22	−143.3 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11—H11···O32	0.84 (2)	2.23 (2)	3.0426 (18)	162 (2)
O31—H31···O22	0.80 (2)	2.10 (2)	2.7747 (17)	142 (2)
N12—H12···O31	0.86 (2)	2.19 (2)	3.019 (2)	161 (2)
O32—H32···O21	0.81 (2)	2.15 (2)	2.8321 (17)	142 (2)