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(4a*R**,10b*R**)-8,10-Dimethoxy-5-[(4-nitrophenyl)-sulfonyl]-3,4,4a,5,6,10b-hexahydrophenanthridine

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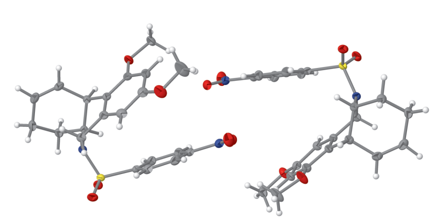
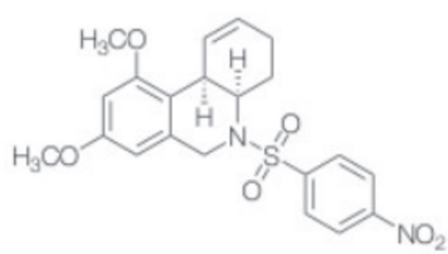
The title compound, $C_{21}H_{22}N_2O_6S$, which was obtained during a study directed to the synthesis of the anti-cancer natural product, pancratistatin, crystallizes with two independent molecules in the asymmetric unit, related by an approximate inversion center near (1/4, 1/2, 1/4) in space group $P2_1/c$. They have similar but not identical shapes. The crystal structure confirms the expected molecular structure of the compound. In the extended structure, C—H···O interactions connect the molecules into a two-dimensional network lying perpendicular to the *b* axis.

3D view



Chemical scheme



Structure description

The title compound, $C_{21}H_{22}N_2O_6S$, was prepared from a substituted aziridine as a model compound in a project directed toward the synthesis of the anti-cancer natural product, pancratistatin (McClachlan *et al.*, 2005). The full details of this chemistry will be published in due course. The title compound crystallizes with two independent molecules in the asymmetric unit, *A* and *B*, as seen in Fig. 1. (The atom numbering in molecule *B* follows that in molecule *A*, with the addition of 20 to each atom's number. The a,b numbering follows IUPAC practice.) The crystal structure confirms the expected molecular structure of the title compound, with identical chirality at C4a and C10*b* (both *R*) in molecule *A* and C24*a* and C30*b* (both *S*) in molecule *B* in the arbitrarily chosen asymmetric unit. As the compound crystallizes in the centrosymmetric space group $P2_1/c$, the unit cell contains equal numbers of chiral molecules and their enantiomers, *i.e.*, the compound is racemic. In addition, the two independent molecules are related by an approximate inversion center near (1/4, 1/2, 1/4), as can be seen in Fig. 1. Inverting molecule *B* again with the crystallographic inversion center at (1/2, 1/2, 1/2) relates this molecule to molecule *A* by an approximate translation (1/2, 0, 1/2) along the *ac* diagonal,

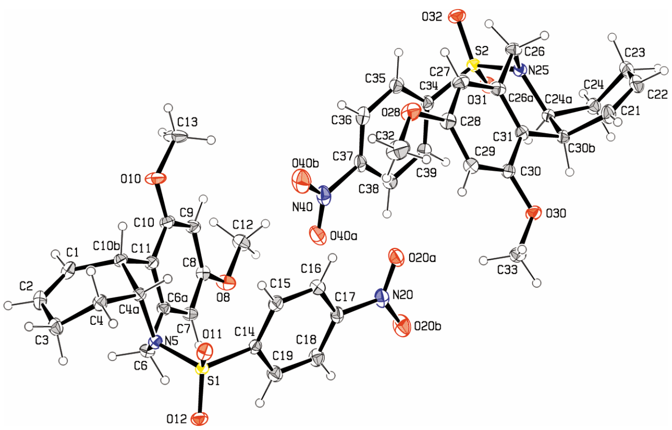


Figure 1
The asymmetric unit of the title compound, with displacement ellipsoids drawn at the 50% probability level.

as can be seen in projection in Fig. 2. Carolyn Brock has pointed out that approximate symmetry relations often exist between independent molecules in structures with $Z' > 1$ (Brock, 2022, 2024), although most of her analyses have focused on non-centrosymmetric space groups.

The two independent molecules have similar, but not identical shapes, as can be seen from the superposition of an inverted molecule *B* onto molecule *A* in Fig. 3. The r.m.s. deviation between non-hydrogen atoms in the superposed structures is 0.43 Å, with a maximum deviation of 1.29 Å for atoms O20*B* and O40*B*. Of the fused three-ring phenanthridine system, the six-membered inner ring containing nitrogen atom N5/N25 is held in a boat shape, with ends C6/C10*b* (*A*) and C26/C30*b* (*B*). The bridge hydrogen atoms H4a and H10*b* are on the same side of the molecule, which pushes ring C1–C4/C4a/C11*b* to lie approximately at right angles to the general plane of the other two fused rings. A search of the CSD Database (August 2025 version; Groom *et al.*, 2016) using the atoms of the fused three-ring system with the double bond between C1 and C2 but without hydrogen atoms, gave 30 hits. Of these, four hits and three structures have only H atoms at C4a and C10*b*: refcodes CAVRAT (von Wangelin *et al.*, 2025), IHUVOY01 (Liu *et al.*, 2014) and REKBEP (Crich & Krishnamurthy, 2006). In all three cases, the H atoms at the equivalent positions to our atoms C4a and C10*b* have the same chirality, leading to a general shape of the three-ringed system similar to the present case.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O31[i]	0.95	2.62	3.5424 (17)	164
C12—H12*B*···O32[ii]	0.98	2.55	3.2682 (18)	130
C12—H12*B*···O40*A*	0.98	2.49	3.2696 (19)	137
C15—H15···O28[iii]	0.95	2.45	3.2953 (18)	148
C24*A*—H24*C*···O8[i]	1.00	2.62	3.5134 (17)	149
C32—H32*A*···O40*B*[iii]	0.98	2.59	3.443 (2)	145
C33—H33*B*···O20*A*	0.98	2.52	3.4825 (19)	168
C39—H39···O20*B*[iv]	0.95	2.65	3.603 (2)	178
C35—H35···O8[i]	0.95	2.56	3.1495 (18)	120

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+2$; (iii) $-x+2, -y+1, -z+2$; (iv) $x, y, z+1$.

A list of potential C—H ··· O hydrogen bonds is given in Table 1. The interactions C12—H12*B*···O40*A* and C33—H33*B*···O20*A* link the two molecules in the asymmetric unit together. Three of the contacts link pairs of molecules related by an inversion center at (1/2, 1/2, 1/2), as can be seen in Fig. 2. The remaining C—H···O contacts link these groups of four molecules into a two-dimensional network lying perpendicular to the *b* axis. The closest intermolecular H···H contacts are H7···H24*C*($1-x$, $1-y$, $1-z$) = 2.13 Å and H22···H31*B*($x, \frac{3}{2}-y, \frac{1}{2}-z$) = 2.30 Å. All other intermolecular H···H contacts are 2.36 Å or greater.

Synthesis and crystallization

To a cool (0 °C) solution of **1** (0.1087 g; 0.39 mmol) in dry CH_2Cl_2 (2 ml) was added solid 4-nitrobenzenesulfonyl

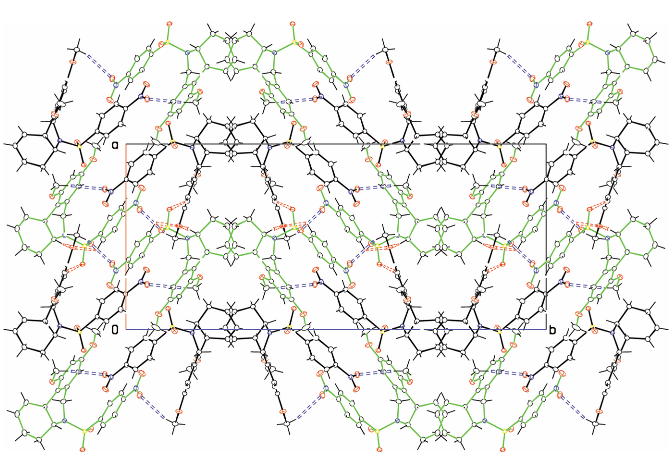


Figure 2
Packing diagram for the title compound. Molecule *A* is coloured black, and molecule *B* green. Blue dashed lines indicate C—H···O interactions between molecules *A* and *B*, while red dashed lines show interactions with the pair of molecules at ($1-x$, $1-y$, $1-z$).

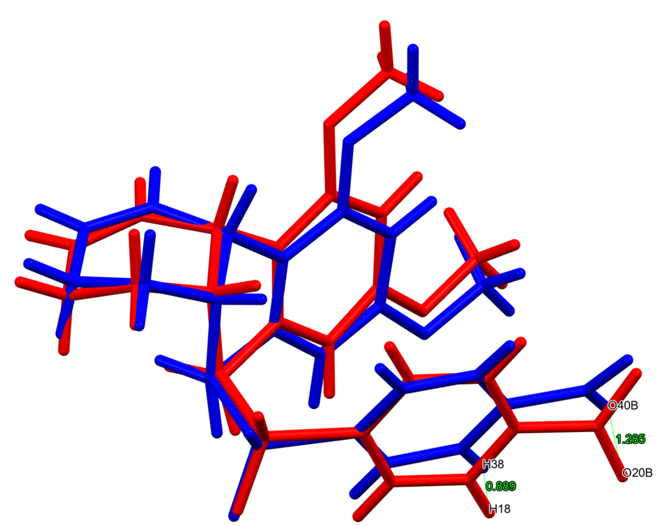


Figure 3
Overlay plot of molecules *A* and *B*, with *A* in red and *B* in blue. The two atom pairs furthest apart are shown.

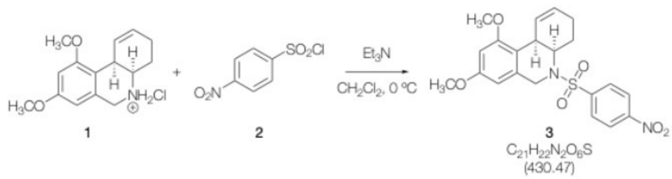


Figure 4
Reaction scheme.

chloride (**2**; 0.1049 g; 0.47 mmol; 1.2 eq) followed by the addition of neat triethylamine (0.13 ml; 0.098 g; 0.96 mmol; 2.5 eq) (see reaction scheme in Fig. 4). The reaction was stirred at this temperature for 30 minutes, whereupon it was poured into ether and washed with water. The organic layer was then washed successively with 1*M* HCl, saturated $NaHCO_3$, water and brine. The ether layer was dried over $MgSO_4$, filtered and concentrated *in vacuo* to give the crude sulfonamide as a yellow glass that crystallized on standing. This was chromatographed on SiO_2, eluting with EtOAc:hex/2:5 from which a purified sample of the title compound, **3**, crystallized upon standing.

^{1}H NMR (400 MHz, $CDCl_3$): *d* 8.05–8.07 (*d*, *J* = 8.7 Hz, 2H), *d* 7.76–7.78 (*d*, *J* = 8.7 Hz, 2H), *d* 6.20 (*s*, 1H), 6.02 (*s*, 1H), *d* 5.81–5.83 (*m*, 1H), *d* 5.47–5.49 (*m*, 1H), *d* 4.54–4.58 (*d*, *J* = 16.3 Hz, 1H), *d* 4.35–4.39 (*d*, *J* = 16.3 Hz, 1H), *d* 4.05–4.08 (*m*, 1H), 3.83–3.85 (*m*, 1H), d 3.70 (*s*, 3H), d 3.69 (*s*, 3H), d 2.23–2.33 (*m*, 2H), *d* 2.12–2.16 (*m*, 1H), *d* 1.48–1.86 (*m*, 1H).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{22}N_2O_6S$
M_r	430.46
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	130
a, b, c (Å)	14.0490 (4), 30.0167 (9), 10.0866 (3)
β (°)	109.468 (1)
V (Å^3)	4010.4 (2)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.80
Crystal size (mm)	0.31 × 0.22 × 0.17
Data collection	
Diffractometer	Bruker D8 with PHOTON III detector
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.659, 0.754
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	97099, 8165, 8126
R_{int}	0.039
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.084, 1.13
No. of reflections	8165
No. of parameters	545
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.41

Computer programs: *APEX4* and *SAINT* (Bruker, 2022), SHELXT2019 (Sheldrick 2015*a*), *SHELXL2019* (Sheldrick 2015*b*), *ORTEP* III (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

Acknowledgements

We are grateful to Carolyn Brock and Sean Parkin for helpful discussions. Continuing support from the Department of Chemistry and Biochemistry at Fordham University is acknowledged and appreciated. The X-ray Diffractometer purchase was funded by the grant detailed below.

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full crystallographic data

IUCrData (2025). **10**, x251115 [https://doi.org/10.1107/S2414314625011150]

(4a*R**,10b*R**)-8,10-Dimethoxy-5-[(4-nitrophenyl)sulfonyl]-3,4,4a,5,6,10b-hexahydrophenanthridine

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Crystal data

$C_{21}H_{22}N_2O_6S$
M_r = 430.46
Monoclinic, $P2_1/c$
a = 14.0490 (4) Å
b = 30.0167 (9) Å
c = 10.0866 (3) Å
β = 109.468 (1)°
V = 4010.4 (2) Å^3
Z = 8
F(000) = 1808
D_x = 1.426 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9717 reflections
θ = 4.5–74.4°
μ = 1.80 mm^{-1}
T = 130 K
Block, yellow
0.31 × 0.22 × 0.17 mm

Data collection

Bruker D8 with PHOTON III detector diffractometer
Radiation source: microfocus
φ and ω shutterless scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.659, T_{max} = 0.754
97099 measured reflections
8165 independent reflections
8126 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 74.5°, θ_{min} = 3.3°
h = −17→17
k = −37→37
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.084
S = 1.13
8165 reflections
545 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.026P)^2 + 2.560P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.94870 (11)	0.25816 (5)	0.67438 (16)	0.0243 (3)
H1	0.897712	0.241645	0.695120	0.029*
C2	1.00916 (12)	0.23624 (5)	0.62052 (16)	0.0266 (3)
H2	0.997449	0.205367	0.601121	0.032*
C3	1.09543 (11)	0.25806 (5)	0.58880 (16)	0.0257 (3)
H3A	1.076224	0.263381	0.486357	0.031*
H3B	1.154739	0.237997	0.617181	0.031*
C4	1.12317 (10)	0.30226 (5)	0.66715 (15)	0.0210 (3)
H4A	1.171831	0.318403	0.632801	0.025*
H4B	1.156292	0.296356	0.768738	0.025*
C4A	1.02997 (10)	0.33137 (4)	0.64615 (14)	0.0173 (3)
H4A1	1.052052	0.359811	0.699126	0.017*
N5	0.98193 (8)	0.34236 (4)	0.49316 (12)	0.0171 (2)
C6	0.87796 (10)	0.32601 (5)	0.42045 (14)	0.0190 (3)
H6A	0.879456	0.293432	0.406054	0.023*
H6B	0.850527	0.340349	0.326998	0.023*
C6A	0.81067 (10)	0.33626 (4)	0.50524 (14)	0.0180 (3)
C7	0.71397 (10)	0.35287 (5)	0.44442 (14)	0.0196 (3)
H7	0.688478	0.359075	0.346507	0.024*
C8	0.65462 (10)	0.36037 (5)	0.52819 (14)	0.0196 (3)
C9	0.69327 (10)	0.35412 (5)	0.67320 (14)	0.0206 (3)
H9	0.653384	0.360452	0.730664	0.025*
C10	0.79211 (11)	0.33830 (5)	0.73238 (14)	0.0203 (3)
C11	0.85123 (10)	0.32831 (4)	0.64914 (14)	0.0183 (3)
C10B	0.95513 (10)	0.30779 (5)	0.70530 (14)	0.0191 (3)
H10B	0.980329	0.311662	0.809736	0.019*
O8	0.55768 (7)	0.37374 (4)	0.45705 (11)	0.0260 (2)
C12	0.49169 (11)	0.38288 (5)	0.53539 (16)	0.0254 (3)
H12A	0.424665	0.390797	0.470561	0.038*
H12B	0.518809	0.407713	0.600019	0.038*
H12C	0.486406	0.356372	0.589244	0.038*
O10	0.83736 (8)	0.33101 (4)	0.87362 (10)	0.0290 (2)
C13	0.78436 (13)	0.34577 (7)	0.96395 (16)	0.0362 (4)
H13A	0.827498	0.342182	1.062181	0.054*
H13B	0.722835	0.328024	0.946464	0.054*
H13C	0.766327	0.377243	0.945277	0.054*
S1	1.01283 (2)	0.38887 (2)	0.43588 (3)	0.01768 (8)
O11	1.11285 (7)	0.39955 (3)	0.52662 (11)	0.0229 (2)
O12	0.99192 (8)	0.38435 (3)	0.28724 (10)	0.0245 (2)
C14	0.93163 (10)	0.43182 (4)	0.45622 (14)	0.0185 (3)
C15	0.95430 (11)	0.45349 (5)	0.58486 (15)	0.0231 (3)
H15	1.012007	0.445080	0.661661	0.028*
C16	0.89186 (11)	0.48751 (5)	0.60004 (15)	0.0241 (3)
H16	0.905763	0.502634	0.687191	0.029*
C17	0.80891 (10)	0.49892 (4)	0.48542 (15)	0.0208 (3)

C18	0.78519 (11)	0.47749 (5)	0.35725 (16)	0.0251 (3)
H18	0.727413	0.486006	0.280708	0.030*
C19	0.84732 (11)	0.44333 (5)	0.34248 (15)	0.0243 (3)
H19	0.832448	0.427964	0.255593	0.029*
N20	0.74292 (9)	0.53544 (4)	0.50023 (14)	0.0251 (3)
O20A	0.75675 (9)	0.55033 (3)	0.61827 (12)	0.0300 (2)
O20B	0.67753 (9)	0.54883 (4)	0.39379 (13)	0.0374 (3)
C21	0.60556 (12)	0.73759 (5)	0.93903 (17)	0.0269 (3)
H21	0.668102	0.751315	0.946693	0.032*
C22	0.54434 (13)	0.75894 (5)	0.99282 (17)	0.0299 (3)
H22	0.566007	0.786538	1.039182	0.036*
C23	0.44237 (12)	0.74146 (5)	0.98373 (17)	0.0293 (3)
H23A	0.393530	0.766398	0.964646	0.035*
H23B	0.446074	0.727901	1.074789	0.035*
C24	0.40587 (11)	0.70674 (5)	0.86733 (16)	0.0231 (3)
H24A	0.388528	0.721626	0.774700	0.028*
H24B	0.344091	0.692226	0.873083	0.028*
C24A	0.48673 (10)	0.67140 (4)	0.87960 (14)	0.0174 (3)
H24C	0.459678	0.649885	0.800205	0.017*
N25	0.50776 (8)	0.64619 (4)	1.01483 (12)	0.0173 (2)
C26	0.61178 (10)	0.64899 (5)	1.11877 (14)	0.0209 (3)
H26A	0.619707	0.626634	1.193858	0.025*
H26B	0.622562	0.678886	1.162734	0.025*
C26A	0.68946 (10)	0.64069 (5)	1.04828 (14)	0.0192 (3)
C27	0.77174 (10)	0.61279 (5)	1.10455 (14)	0.0221 (3)
H27	0.782848	0.598560	1.192553	0.026*
C28	0.83793 (10)	0.60600 (5)	1.02962 (15)	0.0222 (3)
C29	0.82250 (10)	0.62638 (5)	0.89996 (15)	0.0208 (3)
H29	0.867858	0.621453	0.849551	0.025*
C30	0.73888 (10)	0.65418 (4)	0.84593 (14)	0.0184 (3)
C31	0.67214 (10)	0.66196 (4)	0.91935 (14)	0.0183 (3)
C30B	0.58264 (10)	0.69282 (4)	0.86619 (14)	0.0186 (3)
H30B	0.570271	0.697974	0.763855	0.019*
O28	0.91723 (8)	0.57787 (4)	1.09176 (11)	0.0317 (3)
C32	0.98958 (14)	0.57149 (8)	1.0218 (2)	0.0452 (5)
H32A	1.043726	0.551930	1.078436	0.068*
H32B	1.018101	0.600350	1.009288	0.068*
H32C	0.956463	0.557827	0.929609	0.068*
O30	0.71697 (7)	0.67612 (3)	0.72038 (10)	0.0224 (2)
C33	0.77642 (11)	0.66600 (5)	0.63390 (16)	0.0252 (3)
H33A	0.748508	0.681441	0.543576	0.038*
H33B	0.775494	0.633786	0.617792	0.038*
H33C	0.846073	0.675835	0.680948	0.038*
S2	0.45126 (2)	0.59815 (2)	1.00168 (3)	0.01761 (8)
O31	0.35200 (7)	0.60336 (3)	0.90064 (11)	0.0226 (2)
O32	0.46291 (8)	0.58351 (3)	1.14117 (11)	0.0254 (2)
C34	0.51642 (10)	0.56000 (4)	0.92854 (15)	0.0190 (3)
C35	0.48500 (11)	0.55444 (5)	0.78342 (15)	0.0227 (3)

H35	0.426771	0.569550	0.724723	0.027*
C36	0.53954 (11)	0.52659 (5)	0.72492 (16)	0.0248 (3)
H36	0.519075	0.521986	0.626198	0.030*
C37	0.62415 (11)	0.50589 (4)	0.81450 (16)	0.0229 (3)
C38	0.65638 (11)	0.51090 (5)	0.95883 (16)	0.0254 (3)
H38	0.715213	0.496044	1.016930	0.031*
C39	0.60097 (11)	0.53809 (5)	1.01700 (15)	0.0233 (3)
H39	0.620510	0.541720	1.116052	0.028*
N40	0.68215 (10)	0.47617 (4)	0.75286 (15)	0.0290 (3)
O40A	0.64651 (9)	0.46745 (4)	0.62715 (13)	0.0337 (3)
O40B	0.76304 (9)	0.46191 (4)	0.83064 (15)	0.0428 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0233 (7)	0.0205 (7)	0.0290 (7)	0.0005 (5)	0.0088 (6)	0.0078 (6)
C2	0.0283 (7)	0.0170 (7)	0.0323 (8)	0.0015 (6)	0.0071 (6)	0.0013 (6)
C3	0.0263 (7)	0.0218 (7)	0.0311 (8)	0.0069 (6)	0.0123 (6)	−0.0003 (6)
C4	0.0174 (6)	0.0216 (7)	0.0235 (7)	0.0028 (5)	0.0061 (5)	0.0032 (5)
C4A	0.0177 (6)	0.0171 (6)	0.0160 (6)	0.0016 (5)	0.0042 (5)	0.0007 (5)
N5	0.0160 (5)	0.0176 (5)	0.0179 (5)	0.0006 (4)	0.0059 (4)	0.0014 (4)
C6	0.0179 (6)	0.0222 (7)	0.0169 (6)	−0.0010 (5)	0.0058 (5)	−0.0021 (5)
C6A	0.0190 (6)	0.0177 (6)	0.0179 (6)	−0.0017 (5)	0.0069 (5)	−0.0016 (5)
C7	0.0184 (6)	0.0230 (7)	0.0160 (6)	−0.0007 (5)	0.0039 (5)	−0.0008 (5)
C8	0.0164 (6)	0.0191 (6)	0.0218 (7)	−0.0004 (5)	0.0044 (5)	−0.0004 (5)
C9	0.0203 (6)	0.0235 (7)	0.0204 (7)	0.0019 (5)	0.0102 (5)	0.0003 (5)
C10	0.0220 (7)	0.0226 (7)	0.0171 (6)	0.0023 (5)	0.0075 (5)	0.0029 (5)
C11	0.0184 (6)	0.0187 (6)	0.0184 (6)	0.0012 (5)	0.0067 (5)	0.0017 (5)
C10B	0.0194 (6)	0.0216 (7)	0.0173 (6)	0.0037 (5)	0.0073 (5)	0.0034 (5)
O8	0.0165 (5)	0.0394 (6)	0.0214 (5)	0.0058 (4)	0.0055 (4)	−0.0007 (4)
C12	0.0186 (7)	0.0313 (8)	0.0279 (7)	0.0013 (6)	0.0097 (6)	−0.0033 (6)
O10	0.0264 (5)	0.0467 (7)	0.0166 (5)	0.0136 (5)	0.0110 (4)	0.0073 (4)
C13	0.0307 (8)	0.0630 (12)	0.0194 (7)	0.0129 (8)	0.0143 (6)	0.0048 (7)
S1	0.01737 (15)	0.01847 (16)	0.01969 (16)	0.00300 (12)	0.00948 (12)	0.00345 (12)
O11	0.0169 (5)	0.0228 (5)	0.0302 (5)	0.0004 (4)	0.0097 (4)	0.0040 (4)
O12	0.0286 (5)	0.0286 (5)	0.0207 (5)	0.0063 (4)	0.0140 (4)	0.0048 (4)
C14	0.0185 (6)	0.0165 (6)	0.0220 (6)	0.0011 (5)	0.0088 (5)	0.0033 (5)
C15	0.0233 (7)	0.0223 (7)	0.0220 (7)	0.0029 (5)	0.0055 (6)	0.0032 (5)
C16	0.0287 (7)	0.0224 (7)	0.0227 (7)	0.0009 (6)	0.0104 (6)	−0.0015 (5)
C17	0.0204 (6)	0.0164 (6)	0.0291 (7)	0.0014 (5)	0.0128 (6)	0.0022 (5)
C18	0.0207 (7)	0.0243 (7)	0.0271 (7)	0.0049 (6)	0.0036 (6)	0.0014 (6)
C19	0.0244 (7)	0.0239 (7)	0.0225 (7)	0.0036 (6)	0.0051 (6)	−0.0012 (6)
N20	0.0241 (6)	0.0187 (6)	0.0364 (7)	0.0005 (5)	0.0153 (5)	−0.0001 (5)
O20A	0.0377 (6)	0.0215 (5)	0.0384 (6)	0.0003 (4)	0.0231 (5)	−0.0030 (4)
O20B	0.0280 (6)	0.0360 (6)	0.0432 (7)	0.0148 (5)	0.0051 (5)	−0.0010 (5)
C21	0.0292 (8)	0.0174 (7)	0.0353 (8)	−0.0056 (6)	0.0125 (6)	−0.0020 (6)
C22	0.0403 (9)	0.0184 (7)	0.0326 (8)	−0.0034 (6)	0.0145 (7)	−0.0057 (6)
C23	0.0371 (8)	0.0224 (7)	0.0349 (8)	0.0049 (6)	0.0207 (7)	−0.0026 (6)

C24	0.0222 (7)	0.0218 (7)	0.0276 (7)	0.0041 (5)	0.0114 (6)	0.0024 (6)
C24A	0.0187 (6)	0.0171 (6)	0.0172 (6)	0.0002 (5)	0.0070 (5)	−0.0002 (5)
N25	0.0175 (5)	0.0177 (5)	0.0174 (5)	−0.0017 (4)	0.0067 (4)	−0.0007 (4)
C26	0.0204 (7)	0.0247 (7)	0.0166 (6)	−0.0036 (5)	0.0048 (5)	−0.0027 (5)
C26A	0.0177 (6)	0.0210 (6)	0.0178 (6)	−0.0058 (5)	0.0047 (5)	−0.0040 (5)
C27	0.0198 (6)	0.0266 (7)	0.0171 (6)	−0.0031 (5)	0.0024 (5)	0.0008 (5)
C28	0.0158 (6)	0.0249 (7)	0.0225 (7)	0.0001 (5)	0.0018 (5)	0.0004 (5)
C29	0.0170 (6)	0.0226 (7)	0.0229 (7)	−0.0005 (5)	0.0068 (5)	−0.0014 (5)
C30	0.0192 (6)	0.0171 (6)	0.0192 (6)	−0.0024 (5)	0.0069 (5)	−0.0003 (5)
C31	0.0171 (6)	0.0169 (6)	0.0203 (6)	−0.0030 (5)	0.0057 (5)	−0.0021 (5)
C30B	0.0210 (6)	0.0171 (6)	0.0201 (6)	0.0001 (5)	0.0101 (5)	−0.0002 (5)
O28	0.0222 (5)	0.0424 (7)	0.0285 (6)	0.0114 (5)	0.0060 (4)	0.0094 (5)
C32	0.0332 (9)	0.0629 (13)	0.0429 (10)	0.0258 (9)	0.0172 (8)	0.0180 (9)
O30	0.0238 (5)	0.0248 (5)	0.0230 (5)	0.0064 (4)	0.0135 (4)	0.0061 (4)
C33	0.0266 (7)	0.0287 (7)	0.0255 (7)	0.0066 (6)	0.0156 (6)	0.0047 (6)
S2	0.01831 (16)	0.01753 (15)	0.01911 (16)	−0.00212 (11)	0.00907 (12)	−0.00057 (11)
O31	0.0167 (5)	0.0251 (5)	0.0266 (5)	−0.0023 (4)	0.0079 (4)	−0.0032 (4)
O32	0.0316 (5)	0.0266 (5)	0.0220 (5)	−0.0050 (4)	0.0142 (4)	0.0021 (4)
C34	0.0210 (6)	0.0142 (6)	0.0240 (7)	−0.0025 (5)	0.0102 (5)	−0.0002 (5)
C35	0.0247 (7)	0.0195 (7)	0.0237 (7)	0.0011 (5)	0.0078 (6)	0.0008 (5)
C36	0.0300 (7)	0.0207 (7)	0.0251 (7)	−0.0006 (6)	0.0111 (6)	−0.0016 (6)
C37	0.0249 (7)	0.0139 (6)	0.0340 (8)	−0.0019 (5)	0.0153 (6)	−0.0013 (5)
C38	0.0231 (7)	0.0191 (7)	0.0323 (8)	0.0015 (5)	0.0069 (6)	0.0029 (6)
C39	0.0254 (7)	0.0195 (7)	0.0236 (7)	−0.0014 (5)	0.0060 (6)	0.0014 (5)
N40	0.0299 (7)	0.0187 (6)	0.0445 (8)	−0.0010 (5)	0.0205 (6)	−0.0008 (5)
O40A	0.0411 (6)	0.0250 (5)	0.0432 (7)	−0.0047 (5)	0.0249 (5)	−0.0094 (5)
O40B	0.0332 (6)	0.0399 (7)	0.0579 (8)	0.0137 (5)	0.0190 (6)	0.0017 (6)

Geometric parameters (Å, º)

C1—C2	1.326 (2)	C21—C22	1.325 (2)
C1—C10B	1.518 (2)	C21—C30B	1.5138 (19)
C1—H1	0.9500	C21—H21	0.9500
C2—C3	1.503 (2)	C22—C23	1.499 (2)
C2—H2	0.9500	C22—H22	0.9500
C3—C4	1.527 (2)	C23—C24	1.525 (2)
C3—H3A	0.9900	C23—H23A	0.9900
C3—H3B	0.9900	C23—H23B	0.9900
C4—C4A	1.5291 (18)	C24—C24A	1.5289 (18)
C4—H4A	0.9900	C24—H24A	0.9900
C4—H4B	0.9900	C24—H24B	0.9900
C4A—N5	1.5004 (16)	C24A—N25	1.5005 (17)
C4A—C10B	1.5430 (18)	C24A—C30B	1.5392 (18)
C4A—H4A1	1.0000	C24A—H24C	1.0000
N5—C6	1.4826 (16)	N25—C26	1.4901 (17)
N5—S1	1.6244 (11)	N25—S2	1.6300 (11)
C6—C6A	1.5028 (18)	C26—C26A	1.5086 (19)
C6—H6A	0.9900	C26—H26A	0.9900

C6—H6B	0.9900	C26—H26B	0.9900
C6A—C7	1.3838 (19)	C26A—C27	1.387 (2)
C6A—C11	1.3918 (19)	C26A—C31	1.3953 (19)
C7—C8	1.3891 (19)	C27—C28	1.395 (2)
C7—H7	0.9500	C27—H27	0.9500
C8—O8	1.3710 (16)	C28—O28	1.3719 (17)
C8—C9	1.3929 (19)	C28—C29	1.394 (2)
C9—C10	1.3992 (19)	C29—C30	1.3953 (19)
C9—H9	0.9500	C29—H29	0.9500
C10—O10	1.3704 (16)	C30—O30	1.3684 (16)
C10—C11	1.3962 (19)	C30—C31	1.3946 (19)
C11—C10B	1.5098 (18)	C31—C30B	1.5090 (19)
C10B—H10B	1.0000	C30B—H30B	1.0000
O8—C12	1.4308 (17)	O28—C32	1.431 (2)
C12—H12A	0.9800	C32—H32A	0.9800
C12—H12B	0.9800	C32—H32B	0.9800
C12—H12C	0.9800	C32—H32C	0.9800
O10—C13	1.4258 (18)	O30—C33	1.4269 (16)
C13—H13A	0.9800	C33—H33A	0.9800
C13—H13B	0.9800	C33—H33B	0.9800
C13—H13C	0.9800	C33—H33C	0.9800
S1—O11	1.4345 (10)	S2—O32	1.4305 (10)
S1—O12	1.4349 (10)	S2—O31	1.4353 (10)
S1—C14	1.7782 (14)	S2—C34	1.7732 (14)
C14—C19	1.3903 (19)	C34—C39	1.390 (2)
C14—C15	1.390 (2)	C34—C35	1.391 (2)
C15—C16	1.388 (2)	C35—C36	1.391 (2)
C15—H15	0.9500	C35—H35	0.9500
C16—C17	1.383 (2)	C36—C37	1.378 (2)
C16—H16	0.9500	C36—H36	0.9500
C17—C18	1.382 (2)	C37—C38	1.381 (2)
C17—N20	1.4752 (18)	C37—N40	1.4778 (19)
C18—C19	1.386 (2)	C38—C39	1.386 (2)
C18—H18	0.9500	C38—H38	0.9500
C19—H19	0.9500	C39—H39	0.9500
N20—O20A	1.2251 (17)	N40—O40A	1.2263 (18)
N20—O20B	1.2250 (17)	N40—O40B	1.2230 (19)
C2—C1—C10B	124.67 (13)	C22—C21—C30B	124.47 (14)
C2—C1—H1	117.7	C22—C21—H21	117.8
C10B—C1—H1	117.7	C30B—C21—H21	117.8
C1—C2—C3	122.90 (13)	C21—C22—C23	122.88 (14)
C1—C2—H2	118.6	C21—C22—H22	118.6
C3—C2—H2	118.6	C23—C22—H22	118.6
C2—C3—C4	110.70 (12)	C22—C23—C24	110.82 (12)
C2—C3—H3A	109.5	C22—C23—H23A	109.5
C4—C3—H3A	109.5	C24—C23—H23A	109.5
C2—C3—H3B	109.5	C22—C23—H23B	109.5

C4—C3—H3B	109.5	C24—C23—H23B	109.5
H3A—C3—H3B	108.1	H23A—C23—H23B	108.1
C3—C4—C4A	111.46 (11)	C23—C24—C24A	111.20 (12)
C3—C4—H4A	109.3	C23—C24—H24A	109.4
C4A—C4—H4A	109.3	C24A—C24—H24A	109.4
C3—C4—H4B	109.3	C23—C24—H24B	109.4
C4A—C4—H4B	109.3	C24A—C24—H24B	109.4
H4A—C4—H4B	108.0	H24A—C24—H24B	108.0
N5—C4A—C4	109.82 (11)	N25—C24A—C24	109.84 (11)
N5—C4A—C10B	111.57 (10)	N25—C24A—C30B	112.19 (11)
C4—C4A—C10B	110.28 (11)	C24—C24A—C30B	110.59 (11)
N5—C4A—H4A1	108.4	N25—C24A—H24C	108.0
C4—C4A—H4A1	108.4	C24—C24A—H24C	108.0
C10B—C4A—H4A1	108.4	C30B—C24A—H24C	108.0
C6—N5—C4A	117.86 (10)	C26—N25—C24A	117.45 (10)
C6—N5—S1	116.39 (9)	C26—N25—S2	116.35 (9)
C4A—N5—S1	118.22 (9)	C24A—N25—S2	115.41 (9)
N5—C6—C6A	110.71 (11)	N25—C26—C26A	110.67 (11)
N5—C6—H6A	109.5	N25—C26—H26A	109.5
C6A—C6—H6A	109.5	C26A—C26—H26A	109.5
N5—C6—H6B	109.5	N25—C26—H26B	109.5
C6A—C6—H6B	109.5	C26A—C26—H26B	109.5
H6A—C6—H6B	108.1	H26A—C26—H26B	108.1
C7—C6A—C11	121.63 (12)	C27—C26A—C31	121.37 (13)
C7—C6A—C6	122.15 (12)	C27—C26A—C26	122.83 (12)
C11—C6A—C6	116.22 (12)	C31—C26A—C26	115.78 (12)
C6A—C7—C8	119.23 (12)	C26A—C27—C28	118.80 (13)
C6A—C7—H7	120.4	C26A—C27—H27	120.6
C8—C7—H7	120.4	C28—C27—H27	120.6
O8—C8—C9	124.10 (12)	O28—C28—C29	123.20 (13)
O8—C8—C7	114.96 (12)	O28—C28—C27	115.40 (13)
C9—C8—C7	120.93 (12)	C29—C28—C27	121.40 (13)
C8—C9—C10	118.54 (12)	C30—C29—C28	118.45 (13)
C8—C9—H9	120.7	C30—C29—H29	120.8
C10—C9—H9	120.7	C28—C29—H29	120.8
O10—C10—C11	115.34 (12)	O30—C30—C31	115.30 (12)
O10—C10—C9	123.24 (12)	O30—C30—C29	123.35 (12)
C11—C10—C9	121.41 (12)	C31—C30—C29	121.35 (12)
C6A—C11—C10	118.12 (12)	C26A—C31—C30	118.62 (12)
C6A—C11—C10B	118.02 (12)	C26A—C31—C30B	118.55 (12)
C10—C11—C10B	123.82 (12)	C30—C31—C30B	122.83 (12)
C11—C10B—C1	109.83 (11)	C31—C30B—C21	110.80 (12)
C11—C10B—C4A	111.47 (11)	C31—C30B—C24A	111.26 (11)
C1—C10B—C4A	111.85 (11)	C21—C30B—C24A	112.27 (11)
C11—C10B—H10B	107.8	C31—C30B—H30B	107.4
C1—C10B—H10B	107.8	C21—C30B—H30B	107.4
C4A—C10B—H10B	107.8	C24A—C30B—H30B	107.4
C8—O8—C12	118.72 (11)	C28—O28—C32	117.34 (12)

O8—C12—H12A	109.5	O28—C32—H32A	109.5
O8—C12—H12B	109.5	O28—C32—H32B	109.5
H12A—C12—H12B	109.5	H32A—C32—H32B	109.5
O8—C12—H12C	109.5	O28—C32—H32C	109.5
H12A—C12—H12C	109.5	H32A—C32—H32C	109.5
H12B—C12—H12C	109.5	H32B—C32—H32C	109.5
C10—O10—C13	117.04 (11)	C30—O30—C33	117.80 (11)
O10—C13—H13A	109.5	O30—C33—H33A	109.5
O10—C13—H13B	109.5	O30—C33—H33B	109.5
H13A—C13—H13B	109.5	H33A—C33—H33B	109.5
O10—C13—H13C	109.5	O30—C33—H33C	109.5
H13A—C13—H13C	109.5	H33A—C33—H33C	109.5
H13B—C13—H13C	109.5	H33B—C33—H33C	109.5
O11—S1—O12	120.24 (6)	O32—S2—O31	119.84 (6)
O11—S1—N5	106.63 (6)	O32—S2—N25	107.39 (6)
O12—S1—N5	107.72 (6)	O31—S2—N25	107.04 (6)
O11—S1—C14	107.10 (6)	O32—S2—C34	107.76 (6)
O12—S1—C14	105.86 (6)	O31—S2—C34	106.79 (6)
N5—S1—C14	108.93 (6)	N25—S2—C34	107.48 (6)
C19—C14—C15	121.41 (13)	C39—C34—C35	121.49 (13)
C19—C14—S1	119.20 (11)	C39—C34—S2	119.18 (11)
C15—C14—S1	119.39 (10)	C35—C34—S2	119.24 (11)
C14—C15—C16	119.39 (13)	C36—C35—C34	119.47 (13)
C14—C15—H15	120.3	C36—C35—H35	120.3
C16—C15—H15	120.3	C34—C35—H35	120.3
C17—C16—C15	118.51 (13)	C37—C36—C35	118.00 (14)
C17—C16—H16	120.7	C37—C36—H36	121.0
C15—C16—H16	120.7	C35—C36—H36	121.0
C18—C17—C16	122.69 (13)	C38—C37—C36	123.37 (13)
C18—C17—N20	118.49 (13)	C38—C37—N40	118.44 (13)
C16—C17—N20	118.82 (13)	C36—C37—N40	118.19 (13)
C17—C18—C19	118.73 (13)	C37—C38—C39	118.51 (13)
C17—C18—H18	120.6	C37—C38—H38	120.7
C19—C18—H18	120.6	C39—C38—H38	120.7
C14—C19—C18	119.27 (13)	C38—C39—C34	119.15 (13)
C14—C19—H19	120.4	C38—C39—H39	120.4
C18—C19—H19	120.4	C34—C39—H39	120.4
O20A—N20—O20B	124.18 (13)	O40A—N40—O40B	124.09 (14)
O20A—N20—C17	117.91 (12)	O40A—N40—C37	118.13 (13)
O20B—N20—C17	117.92 (12)	O40B—N40—C37	117.78 (14)

C10B—C1—C2—C3	2.7 (2)	C30B—C21—C22—C23	−1.9 (3)
C1—C2—C3—C4	17.9 (2)	C21—C22—C23—C24	−19.2 (2)
C2—C3—C4—C4A	−49.57 (16)	C22—C23—C24—C24A	50.05 (17)
C3—C4—C4A—N5	−61.70 (14)	C23—C24—C24A—N25	63.46 (15)
C3—C4—C4A—C10B	61.65 (15)	C23—C24—C24A—C30B	−60.90 (15)
C4—C4A—N5—C6	117.03 (12)	C24—C24A—N25—C26	−117.81 (12)
C10B—C4A—N5—C6	−5.56 (15)	C30B—C24A—N25—C26	5.62 (16)

C4—C4A—N5—S1	−94.30 (12)	C24—C24A—N25—S2	99.01 (11)
C10B—C4A—N5—S1	143.11 (9)	C30B—C24A—N25—S2	−137.56 (9)
C4A—N5—C6—C6A	48.04 (15)	C24A—N25—C26—C26A	−48.18 (15)
S1—N5—C6—C6A	−101.19 (11)	S2—N25—C26—C26A	94.66 (12)
N5—C6—C6A—C7	136.21 (13)	N25—C26—C26A—C27	−134.50 (13)
N5—C6—C6A—C11	−43.49 (16)	N25—C26—C26A—C31	43.72 (16)
C11—C6A—C7—C8	−2.2 (2)	C31—C26A—C27—C28	−0.2 (2)
C6—C6A—C7—C8	178.09 (12)	C26—C26A—C27—C28	177.94 (13)
C6A—C7—C8—O8	−175.47 (12)	C26A—C27—C28—O28	−179.76 (13)
C6A—C7—C8—C9	4.1 (2)	C26A—C27—C28—C29	−0.4 (2)
O8—C8—C9—C10	176.93 (13)	O28—C28—C29—C30	179.55 (13)
C7—C8—C9—C10	−2.6 (2)	C27—C28—C29—C30	0.3 (2)
C8—C9—C10—O10	179.97 (13)	C28—C29—C30—O30	179.45 (13)
C8—C9—C10—C11	−0.8 (2)	C28—C29—C30—C31	0.5 (2)
C7—C6A—C11—C10	−1.1 (2)	C27—C26A—C31—C30	0.9 (2)
C6—C6A—C11—C10	178.61 (12)	C26—C26A—C31—C30	−177.36 (12)
C7—C6A—C11—C10B	176.69 (12)	C27—C26A—C31—C30B	−178.41 (12)
C6—C6A—C11—C10B	−3.61 (18)	C26—C26A—C31—C30B	3.34 (18)
O10—C10—C11—C6A	−178.09 (12)	O30—C30—C31—C26A	179.91 (12)
C9—C10—C11—C6A	2.6 (2)	C29—C30—C31—C26A	−1.0 (2)
O10—C10—C11—C10B	4.3 (2)	O30—C30—C31—C30B	−0.82 (19)
C9—C10—C11—C10B	−175.01 (13)	C29—C30—C31—C30B	178.22 (12)
C6A—C11—C10B—C1	−77.42 (15)	C26A—C31—C30B—C21	78.86 (15)
C10—C11—C10B—C1	100.23 (15)	C30—C31—C30B—C21	−100.41 (15)
C6A—C11—C10B—C4A	47.13 (16)	C26A—C31—C30B—C24A	−46.79 (16)
C10—C11—C10B—C4A	−135.22 (14)	C30—C31—C30B—C24A	133.94 (13)
C2—C1—C10B—C11	132.95 (15)	C22—C21—C30B—C31	−133.25 (16)
C2—C1—C10B—C4A	8.6 (2)	C22—C21—C30B—C24A	−8.2 (2)
N5—C4A—C10B—C11	−40.59 (15)	N25—C24A—C30B—C31	40.34 (15)
C4—C4A—C10B—C11	−162.91 (11)	C24—C24A—C30B—C31	163.35 (11)
N5—C4A—C10B—C1	82.81 (13)	N25—C24A—C30B—C21	−84.49 (14)
C4—C4A—C10B—C1	−39.51 (15)	C24—C24A—C30B—C21	38.52 (16)
C9—C8—O8—C12	1.4 (2)	C29—C28—O28—C32	3.4 (2)
C7—C8—O8—C12	−179.07 (12)	C27—C28—O28—C32	−177.25 (15)
C11—C10—O10—C13	172.66 (14)	C31—C30—O30—C33	−173.75 (12)
C9—C10—O10—C13	−8.1 (2)	C29—C30—O30—C33	7.23 (19)
C6—N5—S1—O11	176.22 (9)	C26—N25—S2—O32	48.08 (11)
C4A—N5—S1—O11	27.10 (11)	C24A—N25—S2—O32	−168.32 (9)
C6—N5—S1—O12	−53.44 (11)	C26—N25—S2—O31	177.97 (9)
C4A—N5—S1—O12	157.44 (9)	C24A—N25—S2—O31	−38.44 (10)
C6—N5—S1—C14	60.96 (11)	C26—N25—S2—C34	−67.62 (11)
C4A—N5—S1—C14	−88.17 (10)	C24A—N25—S2—C34	75.97 (10)
O11—S1—C14—C19	148.52 (11)	O32—S2—C34—C39	−30.21 (13)
O12—S1—C14—C19	19.08 (13)	O31—S2—C34—C39	−160.18 (11)
N5—S1—C14—C19	−96.51 (12)	N25—S2—C34—C39	85.25 (12)
O11—S1—C14—C15	−30.81 (13)	O32—S2—C34—C35	153.16 (11)
O12—S1—C14—C15	−160.25 (11)	O31—S2—C34—C35	23.19 (13)
N5—S1—C14—C15	84.16 (12)	N25—S2—C34—C35	−91.38 (12)

C19—C14—C15—C16	−0.4 (2)	C39—C34—C35—C36	−0.4 (2)
S1—C14—C15—C16	178.94 (11)	S2—C34—C35—C36	176.14 (11)
C14—C15—C16—C17	−0.4 (2)	C34—C35—C36—C37	−0.8 (2)
C15—C16—C17—C18	0.8 (2)	C35—C36—C37—C38	1.0 (2)
C15—C16—C17—N20	−179.22 (13)	C35—C36—C37—N40	179.83 (13)
C16—C17—C18—C19	−0.4 (2)	C36—C37—C38—C39	0.1 (2)
N20—C17—C18—C19	179.58 (13)	N40—C37—C38—C39	−178.79 (13)
C15—C14—C19—C18	0.7 (2)	C37—C38—C39—C34	−1.3 (2)
S1—C14—C19—C18	−178.57 (11)	C35—C34—C39—C38	1.5 (2)
C17—C18—C19—C14	−0.4 (2)	S2—C34—C39—C38	−175.10 (11)
C18—C17—N20—O20A	170.76 (13)	C38—C37—N40—O40A	171.06 (13)
C16—C17—N20—O20A	−9.26 (19)	C36—C37—N40—O40A	−7.84 (19)
C18—C17—N20—O20B	−8.95 (19)	C38—C37—N40—O40B	−9.2 (2)
C16—C17—N20—O20B	171.02 (13)	C36—C37—N40—O40B	171.93 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O31^{i}	0.95	2.62	3.5424 (17)	164
C12—H12*B*···O32^{ii}	0.98	2.55	3.2682 (18)	130
C12—H12*B*···O40*A*	0.98	2.49	3.2696 (19)	137
C15—H15···O28^{iii}	0.95	2.45	3.2953 (18)	148
C24*A*—H24*C*···O8^{i}	1.00	2.62	3.5134 (17)	149
C32—H32*A*···O40*B*^{iii}	0.98	2.59	3.443 (2)	145
C33—H33*B*···O20*A*	0.98	2.52	3.4825 (19)	168
C39—H39···O20*B*^{iv}	0.95	2.65	3.603 (2)	178
C35—H35···O8^{i}	0.95	2.56	3.1495 (18)	120

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