IUCrData

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N,*N*,*N*-Triethylethanaminium 5,11,17,23-tetra-*tert*-butyl-25-[(ethoxycarbonyl)methoxy]-26,28-dihydroxy-27-oxido-2,8,14,20-tetrathiacalix[4]arene: a molecular salt

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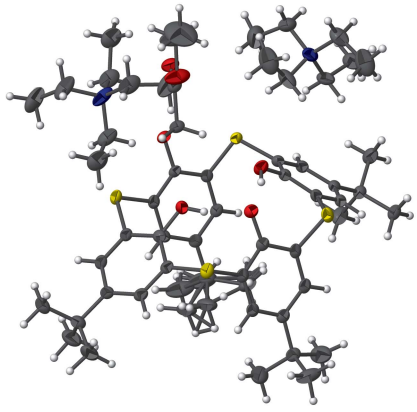
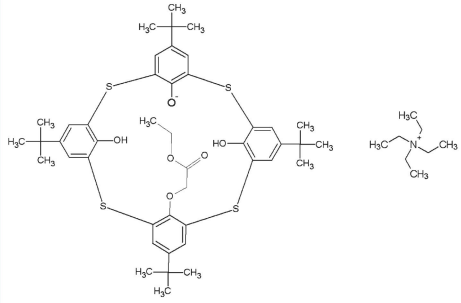
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecular salt, $C_8H_{20}N^+\cdot C_{44}H_{53}O_6S_4^-$, the conformation of the anionic tetrathiacalix[4]arene, which is cone-shaped, is primarily determined by intramolecular O—H···O hydrogen bonds. There are also short intramolecular C— H···O contacts present. The guest species do not sit within the bowl of the calixarene. One of the *t*-butyl groups in the anion is disordered over two sets of sites with refined occupancies of 0.706 (6) and 0.294 (6). Atoms of both cations are equally disordered over centers of symmetry. In the crystal, extensive O—H···O and C—H···O hydrogen bonds and weak O—H···S interactions link the thiacalixarene anions and tetraethylammonium cations, forming a three-dimensional network.

3D view



Chemical scheme



Structure description

Calixarenes (Gutsche, 1989) have been used extensively as molecular platforms to build up supramolecular structures. The design of this kind of structure consists of functionalizing the upper and lower rims of the calixarenes with ligands able to bind to metal cations or other active functional groups. Their numerous applications include catalysis (Homden & Redshaw, 2008) and metal recognition (Arora *et al.*, 2007). Since its discovery in 1997, *p*-*tert*-butylthiacalixarene, which is a calixarene analogue with additional features due to the presence of the bridging sulfur atoms in the skeleton structure,

has attracted a great deal of research beyond that on the classical calixarenes. This includes work on a wide range of applications in supramolecular chemistry (Iki & Miyano, 2001). Based on these findings and as an extension of our work on related compounds, we report here the synthesis and crystal structure of the title thiacalixarene salt.

The calixarene unit (Fig. 1) displays a cone conformation. Its bond lengths and bond angles are comparable to those in the inclusion complex 25-benzoylmethoxy-5,11,17,23-tetra-*tert*-butyl-26,27,28-trihydroxy-2,8,14,20-tetrathiacalix[4]-arene–tetraethylammonium chloride (1/1) (Akkurt *et al.*, 2015) and the molecular salt *N*,*N*,*N*-triethyl-3-ethanaminium-5,11,17,23-tetra-*tert*-butyl-25-cyanomethoxy-26,28-dihydroxy-27-oxido-2,8,14,20-tetrathiacalix[4]arene (Omran *et al.*, 2016). The conformation of the anionic calix[4]arene anion is primarily determined by the intramolecular O—H···O hydrogen bonds and to a lesser extent by short C—H···O contacts (Fig. 1 and Table 1). In the crystal, anions and cations are linked by C—H···O hydrogen bonds, forming a three-dimensional network.

Synthesis and crystallization

A mixture of *p*-*tert*-butyl thiacalix[4]arene (TCA) (1 g, 1.38 mmol), anhydrous K_2CO_3 (5.0 g), tetraethylammonium bromide (TEAB; 0.5 g) and ethyl bromoacetate (0.15 ml, 1.38 mmol) in 50 ml benzene was heated under reflux at 373 K for 2 d. The mixture was filtered to remove any impurities and non-reacted material. The filtrate was evaporated to almost dryness. The viscous residue was treated with 50 ml methanol and left overnight. The colourless crystals that formed were filtered off and dried under vacuum (yield *ca* 90%).

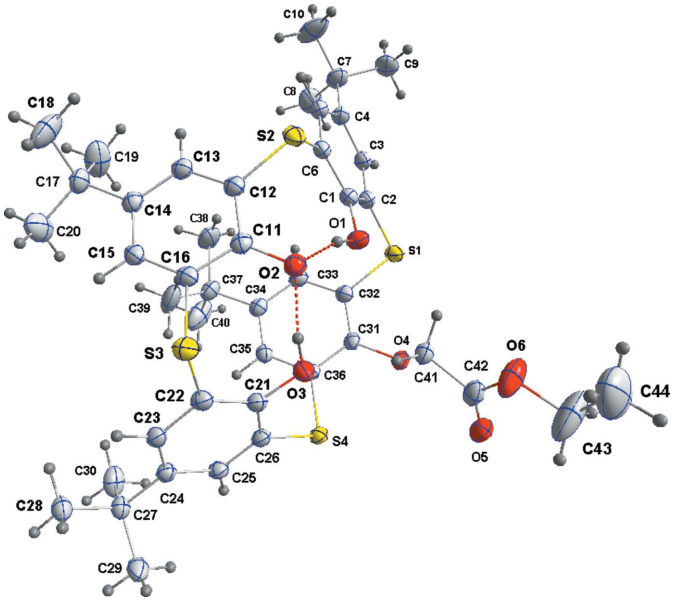


Figure 1
The anion of the title salt with labeling scheme and 50% probability ellipsoids. Intramolecular hydrogen bonds are shown as dashed lines. Only the major occupancy component of the disordered *t*-butyl group is shown and, for clarity, the two fully disordered cations are omitted.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O2	0.87	1.75	2.607 (3)	166
O3—H3*A*···O2	0.87	1.69	2.539 (3)	166
C3—H3···O5^{ii}	0.95	2.57	3.347 (4)	139
C41—H41*A*···O3	0.99	2.48	3.444 (4)	165
C52—H52*B*···O4^{i}	0.96	2.60	3.544 (16)	169
C57—H57*A*···O2^{iii}	0.97	2.30	3.158 (7)	147

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_8H_{20}N^+\cdot C_{44}H_{53}O_6S_4^-$
M_r	936.35
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, *b*, *c* (Å)	9.9806 (4), 15.6499 (6), 17.5330 (7)
α, β, γ (°)	87.413 (2), 83.429 (2), 81.713 (2)
V (Å^3)	2691.03 (18)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.98
Crystal size (mm)	0.22 × 0.12 × 0.07
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.71, 0.87
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	46349, 10841, 9347
R_{int}	0.048
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.069, 0.188, 1.11
No. of reflections	10841
No. of parameters	654
No. of restraints	153
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.06, −0.53

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. One *t*-butyl group is rotationally disordered over two resolved sites with an occupancy ratio 0.706 (6):0.294 (6). The two components were refined subject to restraints that their geometries be approximately the same. Both cations are equally disordered over centers of symmetry and were refined subject to restraints that their geometries be regular.

Acknowledgements

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References

Akkurt, M., Jasinski, J. P., Mohamed, S. K., Omran, O. A. & Albayati, M. R. (2015). *Acta Cryst.* E**71**, o830–o831.

Arora, V., Chawla, H. M. & Singh, S. P. (2007). *ARKIVOC*, **(ii)**, 172–200.

Brandenburg, K. & Putz, H. (2012). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.

Bruker (2016). *APEX3*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Gutsche, C. D. (1989). *Calixarenes Revisited*. In *Monograph in Supramolecular Chemistry*, edited by J. F. Stoddart. Cambridge: The Royal Society of Chemistry.

Homden, D. M. & Redshaw, C. (2008). *Chem. Rev.* **108**, 5086–5130.

Iki, N. & Miyano, S. (2001). *J. Inclusion Phenom. Macrocyclic Chem.* **41**, 99–105.

Omran, O. A., Mague, J. T., Mohamed, S. K., Akkurt, M. & Mohamed, A. F. (2016). *IUCrData*, **1**, x160115.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2016). **1**, x161465 [doi:10.1107/S2414314616014656]

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Crystal data

$C_8H_{20}N^+\cdot C_{44}H_{53}O_6S_4^-$
M_r = 936.35
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 9.9806 (4) Å
b = 15.6499 (6) Å
c = 17.5330 (7) Å
α = 87.413 (2)°
β = 83.429 (2)°
γ = 81.713 (2)°
V = 2691.03 (18) Å^3
Z = 2
$F(000)$ = 1008
D_x = 1.156 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9537 reflections
θ = 2.5–74.5°
μ = 1.98 mm^{-1}
T = 150 K
Column, colourless
0.22 × 0.12 × 0.07 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.71, T_{max} = 0.87
46349 measured reflections
10841 independent reflections
9347 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 74.7°, θ_{min} = 2.9°
h = −12→12
k = −19→19
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.188
S = 1.11
10841 reflections
654 parameters
153 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0698P)^2 + 5.6956P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 2.06 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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)
S1	0.46809 (8)	0.49576 (5)	0.38104 (5)	0.0289 (2)	
S2	0.13554 (7)	0.31004 (5)	0.24231 (5)	0.0275 (2)	
S3	0.52535 (8)	0.02517 (5)	0.22563 (5)	0.0286 (2)	
S4	0.84948 (8)	0.20761 (5)	0.37261 (4)	0.0258 (2)	
O1	0.3530 (2)	0.33889 (14)	0.34716 (13)	0.0291 (7)	
O2	0.3563 (2)	0.18145 (14)	0.30363 (12)	0.0273 (6)	
O3	0.5936 (2)	0.14732 (15)	0.34589 (13)	0.0309 (7)	
O4	0.6659 (2)	0.35546 (14)	0.44602 (12)	0.0261 (6)	
O5	0.6979 (3)	0.28423 (19)	0.58736 (15)	0.0443 (9)	
O6	0.4813 (4)	0.2546 (2)	0.59910 (16)	0.0620 (11)	
C1	0.2972 (3)	0.4091 (2)	0.30901 (17)	0.0243 (8)	
C2	0.3371 (3)	0.4894 (2)	0.32156 (17)	0.0249 (8)	
C3	0.2747 (3)	0.5643 (2)	0.28872 (18)	0.0270 (9)	
C4	0.1715 (3)	0.5645 (2)	0.24076 (18)	0.0279 (9)	
C5	0.1373 (3)	0.4840 (2)	0.22570 (18)	0.0275 (9)	
C6	0.1982 (3)	0.4072 (2)	0.25863 (17)	0.0240 (8)	
C7	0.1082 (4)	0.6498 (2)	0.2051 (2)	0.0363 (11)	
C8	0.2193 (5)	0.6896 (3)	0.1552 (3)	0.0538 (14)	
C9	0.0468 (4)	0.7118 (2)	0.2694 (2)	0.0421 (11)	
C10	−0.0038 (5)	0.6369 (3)	0.1564 (3)	0.0588 (16)	
C11	0.3580 (3)	0.1824 (2)	0.22850 (18)	0.0242 (8)	
C12	0.2732 (3)	0.2460 (2)	0.18884 (18)	0.0252 (9)	
C13	0.2868 (3)	0.2526 (2)	0.10933 (18)	0.0262 (9)	
C14	0.3810 (3)	0.1971 (2)	0.06355 (18)	0.0256 (8)	
C15	0.4551 (3)	0.1294 (2)	0.10176 (18)	0.0263 (9)	
C16	0.4433 (3)	0.12080 (19)	0.18184 (18)	0.0246 (8)	
C17	0.3929 (3)	0.2070 (2)	−0.02452 (19)	0.0305 (9)	
C18	0.2708 (5)	0.1757 (4)	−0.0540 (2)	0.0567 (18)	
C19	0.3916 (6)	0.3020 (3)	−0.0494 (3)	0.0589 (16)	
C20	0.5233 (5)	0.1563 (3)	−0.0624 (2)	0.0569 (16)	
C21	0.6987 (3)	0.10936 (19)	0.29917 (17)	0.0245 (8)	
C22	0.6868 (3)	0.05206 (19)	0.24193 (18)	0.0253 (8)	
C23	0.8029 (3)	0.01268 (19)	0.19769 (18)	0.0250 (8)	
C24	0.9336 (3)	0.02840 (19)	0.20733 (17)	0.0235 (8)	
C25	0.9440 (3)	0.08845 (19)	0.26252 (17)	0.0244 (8)	

C26	0.8306 (3)	0.12798 (19)	0.30730 (17)	0.0245 (8)	
C27	1.0618 (3)	−0.0117 (2)	0.15774 (18)	0.0273 (9)	
C28	1.0304 (3)	−0.0785 (2)	0.10379 (19)	0.0317 (10)	
C29	1.1681 (4)	−0.0550 (3)	0.2085 (2)	0.0377 (11)	
C30	1.1207 (4)	0.0601 (3)	0.1081 (2)	0.0406 (11)	
C31	0.6762 (3)	0.35961 (19)	0.36644 (16)	0.0220 (8)	
C32	0.5989 (3)	0.42567 (19)	0.32802 (18)	0.0246 (8)	
C33	0.6177 (3)	0.4328 (2)	0.24818 (18)	0.0270 (9)	
C34	0.7089 (3)	0.3731 (2)	0.20490 (18)	0.0260 (9)	
C35	0.7833 (3)	0.3065 (2)	0.24414 (17)	0.0245 (8)	
C36	0.7663 (3)	0.29866 (19)	0.32440 (17)	0.0226 (8)	
C37	0.7281 (4)	0.3785 (2)	0.11688 (19)	0.0339 (10)	
C38	0.6134 (8)	0.4411 (5)	0.0832 (4)	0.059 (2)	0.706 (6)
C39	0.7155 (9)	0.2896 (4)	0.0858 (3)	0.059 (2)	0.706 (6)
C40	0.8640 (8)	0.4062 (7)	0.0899 (4)	0.069 (3)	0.706 (6)
C41	0.5647 (3)	0.3054 (2)	0.47958 (17)	0.0288 (9)	
C42	0.5938 (4)	0.2804 (2)	0.56065 (19)	0.0344 (10)	
C43	0.4916 (8)	0.2275 (5)	0.6789 (3)	0.093 (3)	
C44	0.3632 (9)	0.1984 (6)	0.7084 (4)	0.127 (4)	
C38A	0.5941 (13)	0.3871 (11)	0.0869 (9)	0.059 (2)	0.294 (6)
C39A	0.8170 (17)	0.2982 (9)	0.0817 (8)	0.059 (2)	0.294 (6)
C40A	0.7998 (19)	0.4590 (10)	0.0951 (10)	0.069 (3)	0.294 (6)
N1	1.00000	0.50000	0.50000	0.0450 (14)	
C45	0.9800 (6)	0.5207 (5)	0.4162 (2)	0.048 (2)	0.500
C46	0.8365 (9)	0.5479 (12)	0.3991 (5)	0.058 (2)	0.500
C47	0.9322 (7)	0.4206 (3)	0.5234 (4)	0.053 (3)	0.500
C48	1.0034 (17)	0.3371 (4)	0.4915 (10)	0.083 (4)	0.500
C49	1.1519 (3)	0.4855 (5)	0.5063 (3)	0.048 (2)	0.500
C50	1.1933 (9)	0.4517 (12)	0.5826 (5)	0.058 (2)	0.500
C51	0.9333 (7)	0.5744 (3)	0.5499 (4)	0.062 (3)	0.500
C52	0.9833 (16)	0.6592 (4)	0.5308 (9)	0.073 (4)	0.500
N2	0.8401 (4)	−0.0345 (2)	0.5115 (2)	0.0351 (17)	0.500
C53	0.7118 (6)	0.0254 (4)	0.4961 (4)	0.051 (3)	0.500
C54	0.6053 (8)	0.0420 (6)	0.5630 (6)	0.074 (3)	0.500
C55	0.9329 (6)	−0.0409 (4)	0.4366 (3)	0.040 (2)	0.500
C56	1.0600 (10)	−0.1045 (8)	0.4360 (6)	0.050 (4)	0.500
C57	0.8002 (7)	−0.1210 (4)	0.5410 (4)	0.0491 (17)	0.500
C58	0.7307 (10)	−0.1667 (5)	0.4870 (6)	0.074 (3)	0.500
C59	0.9115 (8)	0.0013 (5)	0.5724 (4)	0.055 (3)	0.500
C60	0.9523 (19)	0.0889 (7)	0.5552 (9)	0.076 (7)	0.500
H5	0.07020	0.48130	0.19190	0.0330*	
H8A	0.28730	0.70300	0.18730	0.0810*	
H8B	0.17920	0.74280	0.13000	0.0810*	
H8C	0.26310	0.64870	0.11620	0.0810*	
H1A	0.34260	0.28990	0.32870	0.0440*	
H3	0.30270	0.61780	0.29900	0.0320*	
H3A	0.51350	0.15040	0.33010	0.0460*	
H10A	−0.04270	0.69290	0.13530	0.0880*	

H10B	−0.07530	0.61080	0.18830	0.0880*	
H10C	0.03450	0.59860	0.11420	0.0880*	
H13	0.22960	0.29690	0.08510	0.0310*	
H15	0.51570	0.08770	0.07240	0.0320*	
H18A	0.27480	0.18590	−0.10980	0.0850*	
H18B	0.18630	0.20730	−0.02920	0.0850*	
H18C	0.27280	0.11380	−0.04210	0.0850*	
H19A	0.46800	0.32420	−0.03030	0.0880*	
H19B	0.30570	0.33540	−0.02830	0.0880*	
H19C	0.40020	0.30720	−0.10560	0.0880*	
H20A	0.53020	0.16800	−0.11800	0.0860*	
H9A	0.11820	0.72160	0.30070	0.0630*	
H9B	−0.02490	0.68640	0.30180	0.0630*	
H9C	0.00790	0.76690	0.24680	0.0630*	
H25	1.03130	0.10240	0.26940	0.0290*	
H28A	1.11480	−0.10300	0.07350	0.0470*	
H28B	0.96570	−0.05060	0.06920	0.0470*	
H28C	0.99070	−0.12470	0.13400	0.0470*	
H29A	1.19610	−0.01140	0.23940	0.0570*	
H29B	1.24750	−0.08290	0.17610	0.0570*	
H29C	1.12890	−0.09860	0.24260	0.0570*	
H30A	1.14820	0.10160	0.14140	0.0610*	
H30B	1.05150	0.08960	0.07700	0.0610*	
H30C	1.20020	0.03490	0.07430	0.0610*	
H33	0.56730	0.47940	0.22270	0.0320*	
H35	0.84700	0.26550	0.21580	0.0290*	
H38A	0.52500	0.42260	0.10100	0.0880*	0.706 (6)
H38B	0.61460	0.49970	0.10030	0.0880*	0.706 (6)
H38C	0.62780	0.44050	0.02700	0.0880*	0.706 (6)
H39A	0.62580	0.27360	0.10450	0.0880*	0.706 (6)
H39B	0.72570	0.29270	0.02950	0.0880*	0.706 (6)
H39C	0.78680	0.24610	0.10370	0.0880*	0.706 (6)
H40A	0.87600	0.40970	0.03360	0.1040*	0.706 (6)
H40B	0.86810	0.46300	0.11010	0.1040*	0.706 (6)
H40C	0.93650	0.36410	0.10830	0.1040*	0.706 (6)
H41A	0.56750	0.25290	0.44970	0.0350*	
H41B	0.47310	0.33950	0.47950	0.0350*	
H43A	0.56850	0.18040	0.68250	0.1120*	
H43B	0.50740	0.27650	0.70890	0.1120*	
H44A	0.28850	0.24580	0.70400	0.1900*	
H44B	0.36590	0.18010	0.76250	0.1900*	
H44C	0.34870	0.14960	0.67870	0.1900*	
H20B	0.52170	0.09440	−0.05200	0.0860*	
H20C	0.60200	0.17380	−0.04170	0.0860*	
H23	0.79220	−0.02630	0.15960	0.0300*	
H38D	0.60700	0.39060	0.03060	0.0880*	0.294 (6)
H38E	0.54920	0.33680	0.10380	0.0880*	0.294 (6)
H38F	0.53740	0.43970	0.10630	0.0880*	0.294 (6)

H39D	0.90660	0.29120	0.10080	0.0880*	0.294 (6)
H39E	0.77290	0.24690	0.09620	0.0880*	0.294 (6)
H39F	0.82810	0.30540	0.02560	0.0880*	0.294 (6)
H40D	0.88810	0.45150	0.11570	0.1040*	0.294 (6)
H40E	0.81370	0.46600	0.03900	0.1040*	0.294 (6)
H40F	0.74290	0.51040	0.11670	0.1040*	0.294 (6)
H45A	1.01600	0.47230	0.38470	0.0580*	0.500
H45B	1.02740	0.56820	0.39830	0.0580*	0.500
H46A	0.82420	0.56210	0.34630	0.0860*	0.500
H46B	0.78920	0.50010	0.41610	0.0860*	0.500
H46C	0.80070	0.59690	0.42990	0.0860*	0.500
H47A	0.83640	0.43410	0.51920	0.0640*	0.500
H47B	0.94360	0.40660	0.57640	0.0640*	0.500
H48A	0.95740	0.28890	0.50910	0.1240*	0.500
H48B	0.99060	0.35040	0.43860	0.1240*	0.500
H48C	1.09890	0.32270	0.49640	0.1240*	0.500
H49A	1.19400	0.53680	0.49630	0.0570*	0.500
H49B	1.19760	0.44030	0.47350	0.0570*	0.500
H50A	1.28310	0.43780	0.59830	0.0860*	0.500
H50B	1.14340	0.49790	0.61280	0.0860*	0.500
H50C	1.14700	0.40180	0.59010	0.0860*	0.500
H51A	0.95850	0.56610	0.60120	0.0740*	0.500
H51B	0.83710	0.57410	0.55070	0.0740*	0.500
H52A	0.93880	0.70840	0.55920	0.1090*	0.500
H52B	1.08020	0.65650	0.52970	0.1090*	0.500
H52C	0.95880	0.66460	0.47930	0.1090*	0.500
H53A	0.66910	0.00120	0.45660	0.0610*	0.500
H53B	0.73840	0.08010	0.47620	0.0610*	0.500
H54A	0.54380	0.09500	0.55290	0.1110*	0.500
H54B	0.64960	0.04870	0.60900	0.1110*	0.500
H54C	0.55310	−0.00670	0.57110	0.1110*	0.500
H55A	0.94820	0.01600	0.41840	0.0480*	0.500
H55B	0.88740	−0.06510	0.39350	0.0480*	0.500
H56A	1.11310	−0.10620	0.38670	0.0760*	0.500
H56B	1.10740	−0.08000	0.47240	0.0760*	0.500
H56C	1.04600	−0.16200	0.45290	0.0760*	0.500
H57A	0.74430	−0.11430	0.59000	0.0590*	0.500
H57B	0.88410	−0.15790	0.54970	0.0590*	0.500
H58A	0.64570	−0.13040	0.47680	0.1110*	0.500
H58B	0.71010	−0.22180	0.51090	0.1110*	0.500
H58C	0.78920	−0.17740	0.43860	0.1110*	0.500
H59A	0.99100	−0.03740	0.57900	0.0660*	0.500
H59B	0.85210	−0.00080	0.61940	0.0660*	0.500
H60A	0.99490	0.10120	0.59900	0.1140*	0.500
H60B	1.01480	0.09210	0.50960	0.1140*	0.500
H60C	0.87240	0.13030	0.55080	0.1140*	0.500

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0270 (4)	0.0264 (4)	0.0338 (4)	0.0025 (3)	−0.0098 (3)	−0.0108 (3)
S2	0.0183 (3)	0.0311 (4)	0.0337 (4)	−0.0034 (3)	−0.0026 (3)	−0.0076 (3)
S3	0.0261 (4)	0.0219 (4)	0.0398 (4)	−0.0045 (3)	−0.0103 (3)	−0.0027 (3)
S4	0.0283 (4)	0.0246 (4)	0.0256 (4)	0.0011 (3)	−0.0120 (3)	−0.0050 (3)
O1	0.0325 (12)	0.0235 (11)	0.0329 (12)	−0.0009 (9)	−0.0131 (9)	−0.0028 (9)
O2	0.0257 (11)	0.0308 (11)	0.0260 (11)	−0.0056 (9)	−0.0031 (8)	−0.0020 (9)
O3	0.0237 (11)	0.0381 (13)	0.0315 (12)	0.0001 (9)	−0.0073 (9)	−0.0104 (10)
O4	0.0282 (11)	0.0304 (11)	0.0211 (10)	−0.0054 (9)	−0.0057 (8)	−0.0046 (9)
O5	0.0498 (16)	0.0520 (16)	0.0312 (13)	0.0028 (12)	−0.0157 (12)	−0.0062 (11)
O6	0.074 (2)	0.088 (2)	0.0310 (14)	−0.0394 (19)	−0.0065 (14)	0.0145 (15)
C1	0.0211 (14)	0.0274 (15)	0.0228 (14)	0.0013 (11)	−0.0012 (11)	−0.0021 (12)
C2	0.0238 (14)	0.0259 (15)	0.0246 (14)	0.0004 (11)	−0.0039 (11)	−0.0052 (12)
C3	0.0275 (15)	0.0260 (15)	0.0267 (15)	−0.0002 (12)	−0.0018 (12)	−0.0065 (12)
C4	0.0292 (16)	0.0295 (16)	0.0235 (15)	0.0019 (12)	−0.0035 (12)	−0.0020 (12)
C5	0.0235 (14)	0.0348 (17)	0.0232 (14)	0.0015 (12)	−0.0032 (11)	−0.0056 (13)
C6	0.0191 (13)	0.0296 (15)	0.0222 (14)	−0.0001 (11)	−0.0003 (11)	−0.0062 (12)
C7	0.0416 (19)	0.0319 (18)	0.0344 (18)	0.0027 (14)	−0.0114 (15)	0.0031 (14)
C8	0.063 (3)	0.047 (2)	0.045 (2)	0.003 (2)	0.001 (2)	0.0159 (19)
C9	0.046 (2)	0.0301 (18)	0.046 (2)	0.0096 (15)	−0.0074 (17)	0.0021 (16)
C10	0.076 (3)	0.040 (2)	0.064 (3)	0.006 (2)	−0.044 (3)	0.007 (2)
C11	0.0203 (14)	0.0272 (15)	0.0272 (15)	−0.0084 (11)	−0.0044 (11)	−0.0035 (12)
C12	0.0224 (14)	0.0245 (15)	0.0301 (16)	−0.0046 (11)	−0.0056 (12)	−0.0051 (12)
C13	0.0249 (15)	0.0241 (15)	0.0312 (16)	−0.0052 (11)	−0.0070 (12)	−0.0037 (12)
C14	0.0237 (14)	0.0275 (15)	0.0278 (15)	−0.0081 (12)	−0.0046 (12)	−0.0043 (12)
C15	0.0223 (14)	0.0257 (15)	0.0324 (16)	−0.0039 (11)	−0.0054 (12)	−0.0082 (13)
C16	0.0203 (13)	0.0218 (14)	0.0331 (16)	−0.0037 (11)	−0.0063 (12)	−0.0061 (12)
C17	0.0335 (17)	0.0340 (17)	0.0250 (15)	−0.0091 (13)	−0.0007 (13)	−0.0026 (13)
C18	0.059 (3)	0.092 (4)	0.0280 (19)	−0.037 (3)	−0.0103 (18)	0.002 (2)
C19	0.095 (4)	0.041 (2)	0.039 (2)	−0.012 (2)	0.001 (2)	0.0055 (18)
C20	0.053 (3)	0.073 (3)	0.037 (2)	0.008 (2)	0.0066 (19)	−0.001 (2)
C21	0.0250 (15)	0.0229 (14)	0.0255 (15)	−0.0002 (11)	−0.0068 (12)	−0.0009 (12)
C22	0.0274 (15)	0.0202 (14)	0.0298 (15)	−0.0035 (11)	−0.0096 (12)	−0.0003 (12)
C23	0.0302 (15)	0.0195 (14)	0.0266 (15)	−0.0029 (11)	−0.0086 (12)	−0.0014 (12)
C24	0.0272 (15)	0.0204 (14)	0.0235 (14)	−0.0029 (11)	−0.0068 (12)	0.0007 (11)
C25	0.0252 (14)	0.0230 (14)	0.0264 (15)	−0.0037 (11)	−0.0088 (12)	0.0006 (12)
C26	0.0259 (15)	0.0241 (15)	0.0245 (14)	−0.0012 (11)	−0.0099 (12)	−0.0009 (12)
C27	0.0291 (16)	0.0280 (16)	0.0254 (15)	−0.0050 (12)	−0.0035 (12)	−0.0041 (12)
C28	0.0325 (17)	0.0319 (17)	0.0310 (16)	−0.0039 (13)	−0.0025 (13)	−0.0097 (14)
C29	0.0294 (17)	0.045 (2)	0.0373 (19)	0.0058 (14)	−0.0070 (14)	−0.0130 (16)
C30	0.048 (2)	0.041 (2)	0.0344 (18)	−0.0198 (17)	0.0075 (16)	−0.0053 (16)
C31	0.0215 (13)	0.0255 (14)	0.0206 (14)	−0.0057 (11)	−0.0050 (11)	−0.0046 (11)
C32	0.0230 (14)	0.0223 (14)	0.0295 (15)	−0.0031 (11)	−0.0060 (12)	−0.0053 (12)
C33	0.0284 (15)	0.0237 (15)	0.0298 (16)	−0.0031 (12)	−0.0088 (12)	0.0015 (12)
C34	0.0262 (15)	0.0275 (15)	0.0258 (15)	−0.0083 (12)	−0.0038 (12)	−0.0005 (12)
C35	0.0225 (14)	0.0275 (15)	0.0238 (14)	−0.0044 (11)	−0.0014 (11)	−0.0048 (12)

C36	0.0190 (13)	0.0237 (14)	0.0260 (15)	−0.0030 (11)	−0.0059 (11)	−0.0031 (12)
C37	0.0381 (18)	0.0396 (19)	0.0251 (16)	−0.0082 (15)	−0.0059 (13)	0.0025 (14)
C38	0.077 (4)	0.062 (4)	0.032 (2)	0.016 (4)	−0.018 (2)	0.006 (3)
C39	0.098 (5)	0.050 (3)	0.031 (2)	−0.008 (3)	−0.023 (3)	−0.007 (2)
C40	0.062 (4)	0.118 (6)	0.035 (3)	−0.042 (4)	−0.003 (3)	0.013 (4)
C41	0.0308 (16)	0.0349 (17)	0.0216 (15)	−0.0069 (13)	−0.0037 (12)	−0.0011 (13)
C42	0.046 (2)	0.0327 (18)	0.0254 (16)	−0.0061 (15)	−0.0055 (14)	−0.0037 (13)
C43	0.120 (5)	0.136 (6)	0.037 (3)	−0.064 (5)	−0.020 (3)	0.026 (3)
C44	0.137 (7)	0.149 (8)	0.073 (4)	0.001 (6)	0.037 (5)	0.043 (5)
C38A	0.077 (4)	0.062 (4)	0.032 (2)	0.016 (4)	−0.018 (2)	0.006 (3)
C39A	0.098 (5)	0.050 (3)	0.031 (2)	−0.008 (3)	−0.023 (3)	−0.007 (2)
C40A	0.062 (4)	0.118 (6)	0.035 (3)	−0.042 (4)	−0.003 (3)	0.013 (4)
N1	0.037 (2)	0.074 (3)	0.029 (2)	−0.029 (2)	0.0085 (17)	−0.020 (2)
C45	0.044 (4)	0.069 (5)	0.034 (3)	−0.013 (3)	0.000 (3)	−0.016 (3)
C46	0.050 (4)	0.069 (3)	0.061 (4)	−0.020 (3)	−0.017 (3)	−0.012 (4)
C47	0.047 (4)	0.076 (5)	0.045 (4)	−0.035 (4)	−0.002 (3)	−0.008 (4)
C48	0.093 (7)	0.092 (7)	0.073 (7)	−0.039 (5)	−0.005 (5)	−0.034 (5)
C49	0.038 (4)	0.066 (4)	0.043 (4)	−0.023 (3)	0.000 (3)	−0.008 (3)
C50	0.050 (4)	0.069 (3)	0.061 (4)	−0.020 (3)	−0.017 (3)	−0.012 (4)
C51	0.053 (4)	0.084 (5)	0.051 (4)	−0.021 (4)	0.011 (3)	−0.036 (4)
C52	0.074 (6)	0.080 (6)	0.074 (7)	−0.030 (5)	−0.008 (5)	−0.040 (5)
N2	0.042 (3)	0.032 (3)	0.029 (3)	−0.002 (2)	−0.001 (2)	0.008 (2)
C53	0.048 (5)	0.038 (4)	0.059 (5)	0.006 (3)	0.005 (4)	0.014 (4)
C54	0.050 (4)	0.054 (4)	0.114 (7)	−0.003 (3)	0.002 (4)	−0.003 (4)
C55	0.043 (4)	0.046 (4)	0.027 (3)	0.004 (3)	−0.002 (3)	0.009 (3)
C56	0.047 (7)	0.060 (7)	0.036 (6)	0.008 (5)	0.007 (5)	0.006 (5)
C57	0.045 (3)	0.042 (3)	0.058 (3)	−0.008 (3)	0.000 (3)	0.015 (3)
C58	0.050 (4)	0.054 (4)	0.114 (7)	−0.003 (3)	0.002 (4)	−0.003 (4)
C59	0.081 (7)	0.051 (5)	0.032 (4)	−0.001 (4)	−0.018 (4)	−0.001 (4)
C60	0.100 (14)	0.050 (8)	0.082 (12)	−0.011 (7)	−0.025 (10)	−0.015 (7)

Geometric parameters (Å, º)

S1—C2	1.779 (3)	C19—H19A	0.9800
S1—C32	1.781 (3)	C19—H19B	0.9800
S2—C6	1.772 (3)	C20—H20B	0.9800
S2—C12	1.779 (3)	C20—H20C	0.9800
S3—C16	1.785 (3)	C20—H20A	0.9800
S3—C22	1.780 (3)	C23—H23	0.9500
S4—C26	1.774 (3)	C25—H25	0.9500
S4—C36	1.773 (3)	C28—H28A	0.9800
O1—C1	1.344 (4)	C28—H28C	0.9800
O2—C11	1.315 (4)	C28—H28B	0.9800
O3—C21	1.339 (4)	C29—H29B	0.9800
O4—C31	1.387 (3)	C29—H29A	0.9800
O4—C41	1.425 (4)	C29—H29C	0.9800
O5—C42	1.198 (5)	C30—H30B	0.9800
O6—C42	1.346 (5)	C30—H30A	0.9800

O6—C43	1.454 (6)	C30—H30C	0.9800
O1—H1A	0.8700	C33—H33	0.9500
O3—H3A	0.8700	C35—H35	0.9500
N1—C45^{i}	1.520 (4)	C38—H38C	0.9800
N1—C47^{i}	1.518 (6)	C38—H38B	0.9800
N1—C51	1.516 (6)	C38—H38A	0.9800
N1—C51^{i}	1.516 (6)	C38A—H38E	0.9800
N1—C45	1.520 (4)	C38A—H38D	0.9800
N1—C49^{i}	1.516 (3)	C38A—H38F	0.9800
N1—C47	1.518 (6)	C39—H39C	0.9800
N1—C49	1.516 (3)	C39—H39A	0.9800
N2—C57	1.518 (7)	C39—H39B	0.9800
N2—C59	1.518 (8)	C39A—H39F	0.9800
N2—C53	1.517 (7)	C39A—H39D	0.9800
N2—C55	1.516 (7)	C39A—H39E	0.9800
C1—C2	1.406 (4)	C40—H40C	0.9800
C1—C6	1.403 (4)	C40—H40B	0.9800
C2—C3	1.380 (4)	C40—H40A	0.9800
C3—C4	1.402 (4)	C40A—H40F	0.9800
C4—C5	1.396 (4)	C40A—H40D	0.9800
C4—C7	1.531 (5)	C40A—H40E	0.9800
C5—C6	1.398 (4)	C41—H41B	0.9900
C7—C9	1.535 (5)	C41—H41A	0.9900
C7—C8	1.520 (6)	C43—H43A	0.9900
C7—C10	1.523 (6)	C43—H43B	0.9900
C11—C12	1.421 (4)	C44—H44A	0.9800
C11—C16	1.414 (4)	C44—H44B	0.9800
C12—C13	1.386 (4)	C44—H44C	0.9800
C13—C14	1.392 (4)	C45—C46	1.494 (12)
C14—C15	1.394 (4)	C47—C48	1.494 (11)
C14—C17	1.538 (5)	C49—C50	1.497 (12)
C15—C16	1.398 (4)	C51—C52	1.495 (11)
C17—C20	1.522 (6)	C45—H45A	0.9600
C17—C18	1.527 (6)	C45—H45B	0.9600
C17—C19	1.529 (6)	C46—H46B	0.9600
C21—C22	1.402 (4)	C46—H46C	0.9600
C21—C26	1.413 (4)	C46—H46A	0.9600
C22—C23	1.399 (4)	C47—H47A	0.9600
C23—C24	1.392 (4)	C47—H47B	0.9600
C24—C25	1.401 (4)	C48—H48C	0.9600
C24—C27	1.533 (4)	C48—H48A	0.9600
C25—C26	1.385 (4)	C48—H48B	0.9600
C27—C28	1.529 (4)	C49—H49B	0.9600
C27—C30	1.533 (5)	C49—H49A	0.9600
C27—C29	1.527 (5)	C50—H50A	0.9600
C31—C32	1.394 (4)	C50—H50B	0.9600
C31—C36	1.388 (4)	C50—H50C	0.9600
C32—C33	1.393 (4)	C51—H51A	0.9600

C33—C34	1.392 (4)	C51—H51B	0.9600
C34—C37	1.533 (5)	C52—H52B	0.9600
C34—C35	1.393 (4)	C52—H52C	0.9600
C35—C36	1.400 (4)	C52—H52A	0.9600
C37—C40	1.502 (9)	C53—C54	1.495 (12)
C37—C39A	1.540 (15)	C55—C56	1.495 (13)
C37—C40A	1.549 (17)	C57—C58	1.498 (12)
C37—C39	1.544 (7)	C59—C60	1.494 (15)
C37—C38	1.549 (9)	C53—H53A	0.9700
C37—C38A	1.478 (14)	C53—H53B	0.9700
C41—C42	1.506 (4)	C54—H54A	0.9800
C43—C44	1.453 (12)	C54—H54B	0.9800
C3—H3	0.9500	C54—H54C	0.9800
C5—H5	0.9500	C55—H55A	0.9600
C8—H8B	0.9800	C55—H55B	1.0400
C8—H8C	0.9800	C56—H56A	0.9600
C8—H8A	0.9800	C56—H56B	0.9600
C9—H9C	0.9800	C56—H56C	0.9600
C9—H9A	0.9800	C57—H57A	0.9700
C9—H9B	0.9800	C57—H57B	0.9700
C10—H10B	0.9800	C58—H58A	0.9800
C10—H10A	0.9800	C58—H58B	0.9800
C10—H10C	0.9800	C58—H58C	0.9800
C13—H13	0.9500	C59—H59A	0.9400
C15—H15	0.9500	C59—H59B	0.9600
C18—H18B	0.9800	C60—H60A	0.9600
C18—H18A	0.9800	C60—H60B	0.9600
C18—H18C	0.9800	C60—H60C	0.9600
C19—H19C	0.9800		

C2—S1—C32	97.27 (15)	H20A—C20—H20C	109.00
C6—S2—C12	105.11 (14)	C22—C23—H23	119.00
C16—S3—C22	104.12 (14)	C24—C23—H23	119.00
C26—S4—C36	98.04 (14)	C24—C25—H25	119.00
C31—O4—C41	113.2 (2)	C26—C25—H25	119.00
C42—O6—C43	115.8 (4)	C27—C28—H28A	109.00
C1—O1—H1A	115.00	C27—C28—H28B	109.00
C21—O3—H3A	116.00	C27—C28—H28C	110.00
C47—N1—C49	112.9 (4)	H28B—C28—H28C	109.00
C47—N1—C51	109.2 (3)	H28A—C28—H28B	109.00
C47—N1—C47^{i}	180.00	H28A—C28—H28C	109.00
C47—N1—C49^{i}	67.1 (4)	C27—C29—H29C	110.00
C45^{i}—N1—C47	73.0 (4)	H29A—C29—H29B	110.00
C45—N1—C51^{i}	69.4 (4)	C27—C29—H29B	109.00
C45^{i}—N1—C49	72.3 (3)	H29A—C29—H29C	109.00
C47^{i}—N1—C49	67.1 (4)	C27—C29—H29A	109.00
C49—N1—C49^{i}	180.00	H29B—C29—H29C	109.00
C49—N1—C51^{i}	70.7 (4)	C27—C30—H30B	109.00

C45^{i}—N1—C51	69.4 (4)	H30A—C30—H30B	110.00
C47—N1—C51^{i}	70.8 (3)	C27—C30—H30C	109.00
C49—N1—C51	109.3 (4)	H30B—C30—H30C	109.00
C51—N1—C51^{i}	180.00	H30A—C30—H30C	109.00
C45^{i}—N1—C47^{i}	107.0 (4)	C27—C30—H30A	109.00
C45^{i}—N1—C49^{i}	107.7 (3)	C32—C33—H33	119.00
C45^{i}—N1—C51^{i}	110.7 (4)	C34—C33—H33	119.00
C47^{i}—N1—C49^{i}	112.9 (4)	C36—C35—H35	119.00
C47^{i}—N1—C51^{i}	109.2 (3)	C34—C35—H35	119.00
C49^{i}—N1—C51^{i}	109.3 (4)	H38B—C38—H38C	110.00
C49^{i}—N1—C51	70.7 (4)	C37—C38—H38A	109.00
C45—N1—C49^{i}	72.3 (3)	H38A—C38—H38C	109.00
C45—N1—C47^{i}	73.0 (4)	C37—C38—H38B	110.00
C45—N1—C47	107.0 (4)	H38A—C38—H38B	109.00
C45—N1—C49	107.7 (3)	C37—C38—H38C	109.00
C45—N1—C51	110.7 (4)	H38D—C38A—H38F	109.00
C47^{i}—N1—C51	70.8 (3)	H38E—C38A—H38F	109.00
C45—N1—C45^{i}	180.00	C37—C38A—H38D	109.00
C53—N2—C57	108.4 (4)	C37—C38A—H38E	109.00
C53—N2—C59	110.9 (4)	H38D—C38A—H38E	110.00
C53—N2—C55	107.0 (4)	C37—C38A—H38F	110.00
C55—N2—C57	112.9 (4)	H39A—C39—H39C	109.00
C55—N2—C59	109.4 (4)	H39B—C39—H39C	110.00
C57—N2—C59	108.2 (4)	H39A—C39—H39B	109.00
O1—C1—C6	123.6 (3)	C37—C39—H39A	109.00
C2—C1—C6	117.9 (3)	C37—C39—H39B	109.00
O1—C1—C2	118.5 (3)	C37—C39—H39C	109.00
C1—C2—C3	120.7 (3)	H39D—C39A—H39F	109.00
S1—C2—C1	120.2 (2)	H39E—C39A—H39F	109.00
S1—C2—C3	119.1 (2)	C37—C39A—H39E	109.00
C2—C3—C4	122.5 (3)	C37—C39A—H39F	109.00
C3—C4—C5	116.4 (3)	H39D—C39A—H39E	110.00
C5—C4—C7	123.8 (3)	C37—C39A—H39D	109.00
C3—C4—C7	119.8 (3)	H40A—C40—H40C	110.00
C4—C5—C6	122.3 (3)	H40A—C40—H40B	109.00
S2—C6—C1	121.3 (2)	C37—C40—H40C	110.00
C1—C6—C5	120.2 (3)	C37—C40—H40A	109.00
S2—C6—C5	118.2 (2)	H40B—C40—H40C	109.00
C4—C7—C8	108.8 (3)	C37—C40—H40B	109.00
C4—C7—C9	109.2 (3)	C37—C40A—H40F	109.00
C8—C7—C9	109.1 (3)	H40D—C40A—H40F	110.00
C8—C7—C10	109.3 (3)	C37—C40A—H40D	109.00
C9—C7—C10	108.6 (3)	H40E—C40A—H40F	109.00
C4—C7—C10	111.9 (3)	H40D—C40A—H40E	109.00
O2—C11—C16	122.7 (3)	C37—C40A—H40E	109.00
C12—C11—C16	115.6 (3)	C42—C41—H41A	110.00
O2—C11—C12	121.8 (3)	O4—C41—H41A	110.00
S2—C12—C11	118.8 (2)	O4—C41—H41B	110.00

S2—C12—C13	119.6 (2)	H41A—C41—H41B	108.00
C11—C12—C13	121.3 (3)	C42—C41—H41B	110.00
C12—C13—C14	122.7 (3)	O6—C43—H43A	110.00
C13—C14—C17	120.9 (3)	H43A—C43—H43B	108.00
C15—C14—C17	122.6 (3)	C44—C43—H43B	110.00
C13—C14—C15	116.3 (3)	O6—C43—H43B	110.00
C14—C15—C16	122.2 (3)	C44—C43—H43A	111.00
S3—C16—C11	119.3 (2)	C43—C44—H44A	110.00
S3—C16—C15	119.1 (2)	H44A—C44—H44B	109.00
C11—C16—C15	121.3 (3)	C43—C44—H44B	109.00
C14—C17—C19	110.3 (3)	C43—C44—H44C	109.00
C18—C17—C20	109.0 (3)	H44A—C44—H44C	110.00
C18—C17—C19	107.7 (4)	H44B—C44—H44C	109.00
C14—C17—C18	109.4 (3)	N1—C45—C46	116.1 (5)
C19—C17—C20	108.0 (3)	N1—C47—C48	116.1 (7)
C14—C17—C20	112.2 (3)	N1—C49—C50	115.8 (5)
O3—C21—C22	124.2 (3)	N1—C51—C52	115.8 (7)
C22—C21—C26	117.3 (3)	N1—C45—H45A	111.00
O3—C21—C26	118.5 (3)	H45A—C45—H45B	108.00
C21—C22—C23	120.4 (3)	C46—C45—H45B	105.00
S3—C22—C23	118.5 (2)	N1—C45—H45B	109.00
S3—C22—C21	121.2 (2)	C46—C45—H45A	107.00
C22—C23—C24	122.6 (3)	C45—C46—H46A	116.00
C25—C24—C27	119.8 (3)	H46A—C46—H46B	109.00
C23—C24—C27	123.4 (3)	C45—C46—H46B	105.00
C23—C24—C25	116.7 (3)	C45—C46—H46C	107.00
C24—C25—C26	121.8 (3)	H46A—C46—H46C	109.00
S4—C26—C25	119.6 (2)	H46B—C46—H46C	109.00
S4—C26—C21	119.1 (2)	N1—C47—H47B	108.00
C21—C26—C25	121.2 (3)	N1—C47—H47A	109.00
C24—C27—C29	110.4 (3)	C48—C47—H47A	117.00
C24—C27—C30	108.7 (3)	C48—C47—H47B	97.00
C29—C27—C30	109.3 (3)	H47A—C47—H47B	108.00
C28—C27—C29	108.9 (3)	H48A—C48—H48B	109.00
C24—C27—C28	111.9 (2)	H48A—C48—H48C	109.00
C28—C27—C30	107.7 (3)	H48B—C48—H48C	110.00
O4—C31—C32	120.6 (3)	C47—C48—H48A	113.00
O4—C31—C36	119.9 (3)	C47—C48—H48B	97.00
C32—C31—C36	119.5 (3)	C47—C48—H48C	118.00
S1—C32—C33	120.3 (2)	C50—C49—H49A	105.00
C31—C32—C33	120.0 (3)	N1—C49—H49A	113.00
S1—C32—C31	119.6 (2)	N1—C49—H49B	111.00
C32—C33—C34	121.4 (3)	C50—C49—H49B	101.00
C35—C34—C37	120.0 (3)	H49A—C49—H49B	110.00
C33—C34—C37	122.2 (3)	C49—C50—H50B	97.00
C33—C34—C35	117.8 (3)	C49—C50—H50A	129.00
C34—C35—C36	121.5 (3)	H50A—C50—H50B	109.00
C31—C36—C35	119.7 (3)	H50A—C50—H50C	109.00

S4—C36—C31	119.5 (2)	C49—C50—H50C	101.00
S4—C36—C35	120.7 (2)	H50B—C50—H50C	109.00
C34—C37—C38A	109.8 (7)	C52—C51—H51A	98.00
C38A—C37—C40A	111.3 (10)	C52—C51—H51B	116.00
C34—C37—C40	109.6 (4)	N1—C51—H51A	111.00
C39A—C37—C40A	109.2 (9)	N1—C51—H51B	105.00
C38A—C37—C39A	108.0 (9)	H51A—C51—H51B	110.00
C34—C37—C39	108.8 (3)	H52B—C52—H52C	109.00
C38—C37—C40	109.9 (5)	C51—C52—H52A	118.00
C34—C37—C39A	112.6 (6)	C51—C52—H52B	114.00
C38—C37—C39	104.4 (5)	C51—C52—H52C	96.00
C34—C37—C40A	106.0 (7)	H52A—C52—H52B	109.00
C39—C37—C40	111.6 (5)	H52A—C52—H52C	109.00
C34—C37—C38	112.5 (4)	N2—C53—C54	116.3 (6)
O4—C41—C42	108.1 (3)	N2—C55—C56	116.3 (6)
O6—C42—C41	108.4 (3)	N2—C57—C58	115.4 (6)
O5—C42—O6	125.3 (3)	N2—C59—C60	116.0 (8)
O5—C42—C41	126.3 (3)	N2—C53—H53A	109.00
O6—C43—C44	107.0 (6)	N2—C53—H53B	108.00
C4—C3—H3	119.00	C54—C53—H53A	107.00
C2—C3—H3	119.00	C54—C53—H53B	109.00
C4—C5—H5	119.00	H53A—C53—H53B	108.00
C6—C5—H5	119.00	C53—C54—H54A	110.00
C7—C8—H8C	109.00	C53—C54—H54B	109.00
H8A—C8—H8B	109.00	C53—C54—H54C	110.00
C7—C8—H8B	110.00	H54A—C54—H54B	109.00
C7—C8—H8A	109.00	H54A—C54—H54C	109.00
H8B—C8—H8C	109.00	H54B—C54—H54C	109.00
H8A—C8—H8C	109.00	N2—C55—H55A	109.00
H9A—C9—H9C	109.00	N2—C55—H55B	112.00
H9B—C9—H9C	109.00	C56—C55—H55A	114.00
C7—C9—H9A	109.00	C56—C55—H55B	100.00
C7—C9—H9B	109.00	H55A—C55—H55B	105.00
H9A—C9—H9B	109.00	C55—C56—H56A	112.00
C7—C9—H9C	109.00	C55—C56—H56B	101.00
C7—C10—H10A	109.00	C55—C56—H56C	115.00
C7—C10—H10B	109.00	H56A—C56—H56B	109.00
H10B—C10—H10C	109.00	H56A—C56—H56C	110.00
H10A—C10—H10C	109.00	H56B—C56—H56C	109.00
C7—C10—H10C	109.00	N2—C57—H57A	110.00
H10A—C10—H10B	109.00	N2—C57—H57B	106.00
C14—C13—H13	119.00	C58—C57—H57A	110.00
C12—C13—H13	119.00	C58—C57—H57B	107.00
C14—C15—H15	119.00	H57A—C57—H57B	108.00
C16—C15—H15	119.00	C57—C58—H58A	109.00
H18B—C18—H18C	109.00	C57—C58—H58B	109.00
C17—C18—H18B	110.00	C57—C58—H58C	110.00
C17—C18—H18A	109.00	H58A—C58—H58B	109.00

H18A—C18—H18C	109.00	H58A—C58—H58C	109.00
C17—C18—H18C	109.00	H58B—C58—H58C	110.00
H18A—C18—H18B	109.00	N2—C59—H59A	108.00
C17—C19—H19A	110.00	N2—C59—H59B	106.00
C17—C19—H19B	109.00	C60—C59—H59A	108.00
C17—C19—H19C	109.00	C60—C59—H59B	112.00
H19A—C19—H19B	110.00	H59A—C59—H59B	107.00
H19A—C19—H19C	109.00	C59—C60—H60A	105.00
H19B—C19—H19C	110.00	C59—C60—H60B	114.00
C17—C20—H20C	110.00	C59—C60—H60C	109.00
H20A—C20—H20B	109.00	H60A—C60—H60B	110.00
C17—C20—H20B	110.00	H60A—C60—H60C	110.00
C17—C20—H20A	109.00	H60B—C60—H60C	109.00
H20B—C20—H20C	109.00		

C32—S1—C2—C1	58.5 (3)	C7—C4—C5—C6	179.3 (3)
C32—S1—C2—C3	−122.2 (3)	C3—C4—C7—C8	60.4 (4)
C2—S1—C32—C31	−131.5 (3)	C3—C4—C7—C9	−58.5 (4)
C2—S1—C32—C33	44.0 (3)	C3—C4—C7—C10	−178.8 (3)
C12—S2—C6—C1	−70.3 (3)	C4—C5—C6—C1	0.2 (5)
C12—S2—C6—C5	115.7 (3)	C4—C5—C6—S2	174.3 (2)
C6—S2—C12—C11	97.0 (3)	O2—C11—C16—S3	13.7 (4)
C6—S2—C12—C13	−89.8 (3)	C16—C11—C12—C13	−7.6 (4)
C22—S3—C16—C11	−92.9 (3)	O2—C11—C12—S2	−14.5 (4)
C22—S3—C16—C15	92.8 (3)	O2—C11—C12—C13	172.4 (3)
C16—S3—C22—C21	72.0 (3)	C16—C11—C12—S2	165.4 (2)
C16—S3—C22—C23	−109.9 (3)	C12—C11—C16—C15	7.9 (4)
C36—S4—C26—C21	−66.2 (3)	O2—C11—C16—C15	−172.2 (3)
C36—S4—C26—C25	110.6 (3)	C12—C11—C16—S3	−166.3 (2)
C26—S4—C36—C31	136.8 (3)	S2—C12—C13—C14	−171.6 (2)
C26—S4—C36—C35	−38.7 (3)	C11—C12—C13—C14	1.4 (5)
C41—O4—C31—C32	90.6 (3)	C12—C13—C14—C17	−179.8 (3)
C41—O4—C31—C36	−90.8 (3)	C12—C13—C14—C15	4.8 (5)
C31—O4—C41—C42	161.1 (2)	C13—C14—C15—C16	−4.5 (5)
C43—O6—C42—O5	−1.7 (6)	C17—C14—C15—C16	−179.8 (3)
C43—O6—C42—C41	179.7 (4)	C15—C14—C17—C19	−140.0 (4)
C42—O6—C43—C44	−177.2 (5)	C15—C14—C17—C20	−19.5 (4)
C49^{i}—N1—C45—C46	7.3 (9)	C13—C14—C17—C20	165.4 (3)
C51^{i}—N1—C45—C46	126.7 (10)	C13—C14—C17—C18	−73.5 (4)
C45—N1—C47—C48	72.4 (9)	C13—C14—C17—C19	44.9 (4)
C49—N1—C47—C48	−46.0 (9)	C15—C14—C17—C18	101.6 (4)
C51—N1—C47—C48	−167.8 (9)	C14—C15—C16—S3	172.2 (2)
C45^{i}—N1—C47—C48	−107.6 (9)	C14—C15—C16—C11	−2.0 (5)
C49^{i}—N1—C47—C48	134.0 (9)	C26—C21—C22—C23	2.8 (4)
C51^{i}—N1—C47—C48	12.2 (9)	O3—C21—C26—C25	177.7 (3)
C45—N1—C49—C50	−171.5 (9)	C22—C21—C26—S4	174.2 (2)
C47—N1—C49—C50	−53.6 (10)	O3—C21—C26—S4	−5.6 (4)
C51—N1—C49—C50	68.3 (9)	O3—C21—C22—S3	0.7 (4)

C45^{i}—N1—C49—C50	8.5 (9)	O3—C21—C22—C23	−177.5 (3)
C47^{i}—N1—C49—C50	126.5 (10)	C26—C21—C22—S3	−179.1 (2)
C51^{i}—N1—C49—C50	−111.7 (9)	C22—C21—C26—C25	−2.5 (4)
C45—N1—C51—C52	−59.0 (9)	S3—C22—C23—C24	−178.7 (2)
C47—N1—C51—C52	−176.5 (8)	C21—C22—C23—C24	−0.6 (5)
C49—N1—C51—C52	59.5 (8)	C22—C23—C24—C27	−177.9 (3)
C45^{i}—N1—C51—C52	121.0 (9)	C22—C23—C24—C25	−2.0 (4)
C47^{i}—N1—C51—C52	3.5 (8)	C23—C24—C25—C26	2.3 (4)
C49^{i}—N1—C51—C52	−120.5 (8)	C27—C24—C25—C26	178.4 (3)
C47—N1—C45—C46	65.6 (10)	C25—C24—C27—C30	−63.8 (4)
C49—N1—C45—C46	−172.7 (9)	C25—C24—C27—C29	56.0 (4)
C51—N1—C45—C46	−53.3 (10)	C23—C24—C27—C28	−6.8 (4)
C47^{i}—N1—C45—C46	−114.4 (10)	C23—C24—C27—C29	−128.2 (3)
C57—N2—C55—C56	−54.4 (8)	C23—C24—C27—C30	112.0 (3)
C59—N2—C55—C56	66.2 (7)	C25—C24—C27—C28	177.4 (3)
C53—N2—C57—C58	60.9 (7)	C24—C25—C26—S4	−176.7 (2)
C55—N2—C53—C54	−179.4 (6)	C24—C25—C26—C21	0.0 (5)
C57—N2—C53—C54	58.6 (7)	O4—C31—C32—C33	175.2 (3)
C59—N2—C53—C54	−60.1 (7)	O4—C31—C32—S1	−9.3 (4)
C53—N2—C55—C56	−173.6 (6)	C32—C31—C36—C35	3.0 (4)
C57—N2—C59—C60	−177.0 (9)	O4—C31—C36—S4	8.9 (4)
C55—N2—C59—C60	59.7 (10)	C36—C31—C32—S1	172.1 (2)
C55—N2—C57—C58	−57.5 (7)	C36—C31—C32—C33	−3.4 (5)
C59—N2—C57—C58	−178.7 (6)	O4—C31—C36—C35	−175.6 (3)
C53—N2—C59—C60	−58.2 (10)	C32—C31—C36—S4	−172.5 (2)
C6—C1—C2—S1	−176.9 (2)	S1—C32—C33—C34	−172.9 (2)
C6—C1—C2—C3	3.7 (4)	C31—C32—C33—C34	2.6 (5)
O1—C1—C6—S2	1.1 (4)	C32—C33—C34—C35	−1.2 (5)
O1—C1—C2—C3	−174.6 (3)	C32—C33—C34—C37	178.3 (3)
O1—C1—C2—S1	4.7 (4)	C33—C34—C37—C38	−14.1 (5)
C2—C1—C6—S2	−177.1 (2)	C33—C34—C37—C39	−129.2 (5)
C2—C1—C6—C5	−3.3 (4)	C33—C34—C37—C40	108.4 (5)
O1—C1—C6—C5	175.0 (3)	C33—C34—C35—C36	0.8 (5)
C1—C2—C3—C4	−1.1 (5)	C37—C34—C35—C36	−178.7 (3)
S1—C2—C3—C4	179.5 (2)	C35—C34—C37—C39	50.3 (5)
C2—C3—C4—C7	−179.0 (3)	C35—C34—C37—C40	−72.0 (5)
C2—C3—C4—C5	−1.9 (5)	C35—C34—C37—C38	165.4 (4)
C5—C4—C7—C8	−116.4 (4)	C34—C35—C36—C31	−1.8 (5)
C5—C4—C7—C9	124.7 (3)	C34—C35—C36—S4	173.8 (2)
C5—C4—C7—C10	4.4 (5)	O4—C41—C42—O6	163.3 (3)
C3—C4—C5—C6	2.4 (5)	O4—C41—C42—O5	−15.3 (4)

Symmetry code: (i) −*x*+2, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···S2	0.87	2.67	3.093 (2)	111

O1—H1*A*···O2	0.87	1.75	2.607 (3)	166
O3—H3*A*···S3	0.87	2.72	3.104 (2)	108
O3—H3*A*···O2	0.87	1.69	2.539 (3)	166
C3—H3···O5^{ii}	0.95	2.57	3.347 (4)	139
C41—H41*A*···O3	0.99	2.48	3.444 (4)	165
C52—H52*B*···O4^{i}	0.96	2.60	3.544 (16)	169
C57—H57*A*···O2^{iii}	0.97	2.30	3.158 (7)	147

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