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

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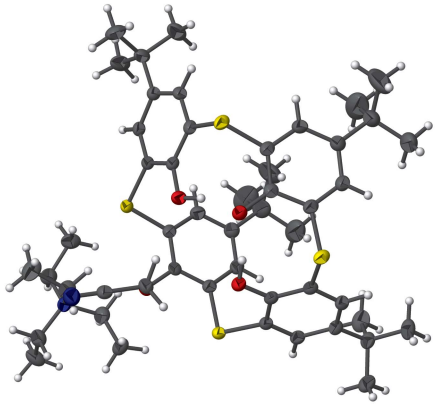
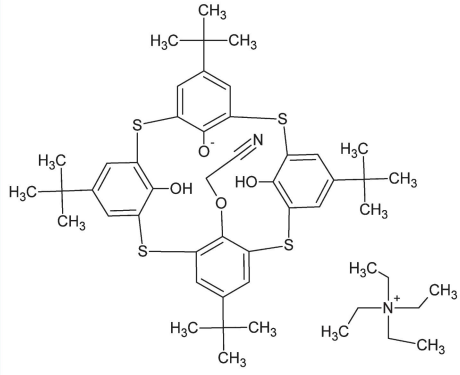
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecular salt, $C_8H_{20}N^+\cdot C_{42}H_{48}NO_4S_4^-$, 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 intramolecular C—H···O short contacts present. In the crystal, the anions (*A*) and cations (*C*) are linked by C—H···O and C—H···S hydrogen bonds, forming –*A*–*C*–*A*–*C*– chains along [001]. The chains are linked *via* C—H···N_{cyano} hydrogen bonds, forming ribbons along [001].

3D view



Chemical scheme



Structure description

Thiacalixarene compounds are of great interest in both fundamental and applied chemistry. They have a wide range of applications within catalysis, molecular recognition, and ion-separation techniques (Asfari *et al.*, 2001; Lhoták, 2004; Morohashi *et al.*, 2006; Beer & Gale, 2001). Thiacalixarenes have been used as artificial receptors for different chemical species, such as ions and materials. They are also widely used for different applications in biological, medical, environmental and chemical sciences, such as sensor devices (Marenco *et al.*, 2001; Kim *et al.*, 2001) and for optical sensing (Leyton *et al.*, 2004, 2005; Haugland, 2005; Martínez-Máñez & Sancenón, 2003; Stibor, 2005; Martinez-Manez & Sancenon, 2003; Matthews & Beer, 2005; Kim *et al.*, 2004; Budka *et al.*, 2002; Métivier *et*

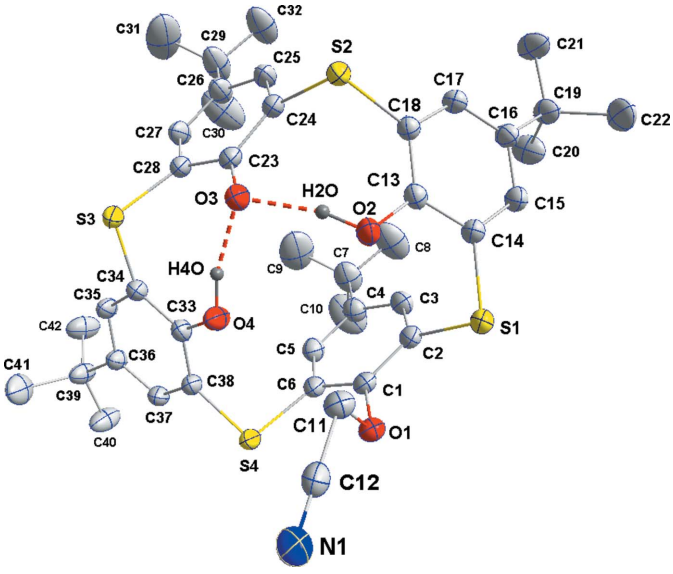


Figure 1
A view of the molecular structure of the title molecular salt, with the atom labelling and 50% probability ellipsoids. H atoms attached to carbon have been omitted for clarity. The intramolecular O—H···O hydrogen bonds are shown as dashed lines (see Table 1).

al., 2004). In this context and following on our on-going study we report herein on the synthesis and crystal structure of the title compound.

The calixarene unit (Fig. 1) displays a cone conformation. Its bond lengths and bond angles are comparable with those of 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). 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).

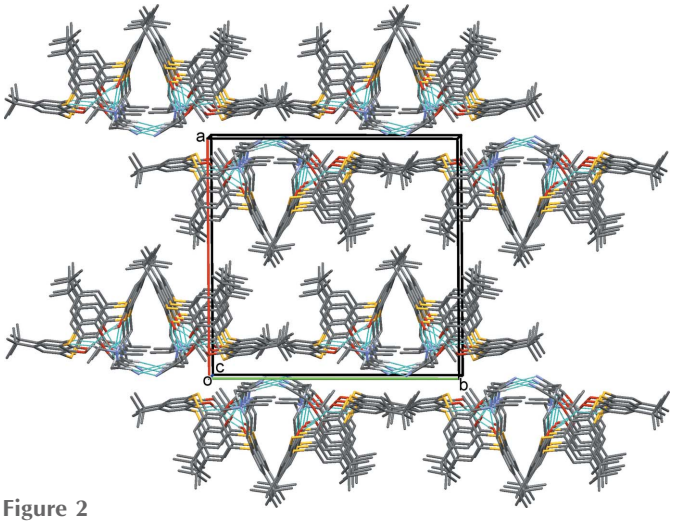


Figure 2
A view along the *c*-axis of the crystal packing of the title molecular salt. The hydrogen bonds are shown as dashed lines (see Table 1), and for clarity only those H atoms involved in hydrogen bonding have been included.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*O*···O3	0.92 (3)	1.66 (3)	2.5649 (19)	165 (3)
O4—H4*O*···O3	0.92 (3)	1.61 (3)	2.503 (2)	164 (3)
C11—H11*A*···O4	0.99	2.22	3.187 (3)	165
C46—H46*A*···O3^{i}	0.98	2.54	3.311 (3)	135
C49—H49*B*···S4	0.99	2.80	3.714 (3)	154
C43—H43*A*···S2^{i}	0.99	2.85	3.773 (2)	156
C45—H45*B*···N1^{ii}	0.99	2.39	3.328 (3)	158

Symmetry codes: (i) $x, y, z-1$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_8H_{20}N^+\cdot C_{42}H_{48}NO_4S_4^-$
M_r	889.30
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, *b*, *c* (Å)	20.7072 (8), 20.4462 (8), 12.8292 (5)
β (°)	107.294 (1)
V (Å^3)	5186.1 (4)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.00
Crystal size (mm)	0.29 × 0.24 × 0.16
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2015)
T_{min}, T_{max}	0.67, 0.73
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	115328, 10201, 9168
R_{int}	0.041
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.136, 1.02
No. of reflections	10201
No. of parameters	565
No. of restraints	48
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.96, −0.46

Computer programs: *APEX2* (Bruker, 2015), *SAINT* (Bruker, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012), *Mercury* (Macrae *et al.*, 2008), *SHELXTL* (Sheldrick, 2008).

In the crystal, (Fig. 2 and Table 1), –anion–cation–anion–cation– chains are formed, *via* C—H···O and C—H···S hydrogen bonds, which are linked by C—H—N_{nitro} hydrogen bonds forming ribbons along the *c*-axis direction.

Synthesis and crystallization

A mixture of thiocalixarene (TCA) (1 g, 1.38 mmol), anhydrous K_2CO_3 (5.0 g), tetraethylammonium bromide (TEAB; 0.5 g) and chloroacetonitrile (1 ml, 1.38 mmol) in 50 ml benzene was heated under reflux at 373 K for 3 d. The mixture was filtered off to remove any impurities and non-reacted

material. The filtrate was evaporated to almost dryness. The viscous residue was treated with 40 ml methanol and left overnight. The colourless crystals that formed were filtered off and dried under vacuum (yield *ca* 90%).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The *t*-butyl groups containing atoms C7 and C29 appear to be slightly disordered but resolved. Alternate locations for the constituent atoms could not be adequately defined so these atoms were refined with suitable ISOR instructions. A total potential solvent-accessible void of 423 Å^3 was detected by checkcif (Spek, 2009), but no unusual residual electron density was found in the final difference Fourier map.

Acknowledgements

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full crystallographic data

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_N_,_N_,_N_-Triethylethanaminium 5,11,17,23-tetra-*tert*-butyl-25-cyanomethoxy-26,28-dihydroxy-27-oxido-2,8,14,20-tetrathiacalix[4]arene

Crystal data

$C_8H_{20}N^+·C_{42}H_{48}NO_4S_4^-$
M_r = 889.30
Monoclinic, $P2_1/c$
a = 20.7072 (8) Å
b = 20.4462 (8) Å
c = 12.8292 (5) Å
β = 107.294 (1)°
V = 5186.1 (4) Å^3
Z = 4
$F(000)$ = 1912
D_x = 1.139 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9932 reflections
θ = 4.2–72.0°
μ = 2.00 mm^{-1}
T = 150 K
Block, colourless
0.29 × 0.24 × 0.16 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, 2015)
T_{min} = 0.67, T_{max} = 0.73
115328 measured reflections
10201 independent reflections
9168 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 72.2°, θ_{min} = 2.2°
h = −25→25
k = −23→25
l = −15→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.136
S = 1.02
10201 reflections
565 parameters
48 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0755P)^2 + 4.1001P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Special details

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. H-atoms were placed in calculated positions (C—H = 0.95 − 0.98 Å) and included as riding contributions with isotropic displacement parameters 1.2 − 1.5 times those of the attached carbon atoms. The *t*-butyl groups containing C7 and C29 appear to be slightly disordered but resolved, alternate locations for the constituent atoms could not be adequately defined so these atoms were refined with suitable ISOR instructions.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.92074 (2)	0.55962 (2)	0.51446 (4)	0.02830 (12)
S2	0.85736 (2)	0.56088 (2)	0.90306 (4)	0.02764 (12)
S3	0.70271 (2)	0.33988 (2)	0.77354 (4)	0.02817 (12)
S4	0.76405 (2)	0.34104 (2)	0.38248 (4)	0.02978 (12)
O1	0.89209 (7)	0.42093 (6)	0.44118 (11)	0.0282 (3)
O2	0.89646 (7)	0.50112 (6)	0.70932 (11)	0.0297 (3)
O3	0.82306 (6)	0.42861 (6)	0.79166 (11)	0.0270 (3)
O4	0.78968 (7)	0.36465 (7)	0.61744 (12)	0.0303 (3)
H4O	0.7955 (14)	0.3843 (14)	0.684 (2)	0.052 (8)*
N1	0.98779 (10)	0.28926 (9)	0.51873 (16)	0.0403 (4)
C1	0.83418 (9)	0.45740 (9)	0.43337 (15)	0.0255 (4)
C2	0.83926 (10)	0.52374 (9)	0.45829 (15)	0.0267 (4)
C3	0.78090 (10)	0.56030 (9)	0.44667 (17)	0.0310 (4)
H3	0.7848	0.6058	0.4619	0.037*
C4	0.71706 (11)	0.53196 (10)	0.41335 (18)	0.0349 (4)
C5	0.71296 (10)	0.46517 (10)	0.38938 (16)	0.0319 (4)
H5	0.6698	0.4449	0.3651	0.038*
C6	0.77060 (10)	0.42773 (9)	0.40027 (15)	0.0270 (4)
C7	0.65254 (13)	0.57064 (13)	0.4061 (3)	0.0544 (7)
C8	0.66527 (17)	0.64193 (16)	0.4329 (4)	0.0856 (11)
H8A	0.6221	0.6643	0.4241	0.128*
H8B	0.6880	0.6615	0.3836	0.128*
H8C	0.6940	0.6465	0.5086	0.128*
C9	0.61375 (19)	0.5382 (2)	0.4743 (4)	0.0938 (13)
H9A	0.6055	0.4923	0.4525	0.141*
H9B	0.5704	0.5607	0.4632	0.141*
H9C	0.6401	0.5406	0.5515	0.141*
C10	0.60555 (18)	0.5678 (2)	0.2853 (4)	0.0939 (13)
H10A	0.5946	0.5221	0.2642	0.141*
H10B	0.6289	0.5875	0.2369	0.141*
H10C	0.5637	0.5919	0.2793	0.141*
C11	0.92217 (10)	0.39347 (10)	0.54718 (16)	0.0305 (4)

H11A	0.8868	0.3816	0.5815	0.037*
H11B	0.9534	0.4253	0.5949	0.037*
C12	0.95920 (10)	0.33505 (9)	0.53114 (17)	0.0303 (4)
C13	0.88864 (9)	0.56624 (9)	0.70798 (15)	0.0253 (4)
C14	0.90143 (9)	0.60232 (9)	0.62221 (15)	0.0262 (4)
C15	0.89394 (10)	0.66985 (9)	0.61706 (16)	0.0280 (4)
H15	0.9037	0.6929	0.5592	0.034*
C16	0.87241 (10)	0.70510 (9)	0.69451 (15)	0.0276 (4)
C17	0.86019 (9)	0.66912 (9)	0.77870 (15)	0.0271 (4)
H17	0.8457	0.6915	0.8327	0.033*
C18	0.86846 (9)	0.60133 (9)	0.78691 (15)	0.0251 (4)
C19	0.85799 (11)	0.77855 (9)	0.67815 (17)	0.0333 (4)
C20	0.79788 (14)	0.78781 (12)	0.5746 (2)	0.0494 (6)
H20A	0.8085	0.7678	0.5122	0.074*
H20B	0.7892	0.8346	0.5608	0.074*
H20C	0.7576	0.7669	0.5848	0.074*
C21	0.83961 (14)	0.80920 (11)	0.7743 (2)	0.0441 (5)
H21A	0.7987	0.7883	0.7820	0.066*
H21B	0.8314	0.8561	0.7610	0.066*
H21C	0.8770	0.8028	0.8414	0.066*
C22	0.91987 (13)	0.81420 (11)	0.6641 (2)	0.0460 (6)
H22A	0.9574	0.8107	0.7316	0.069*
H22B	0.9088	0.8604	0.6478	0.069*
H22C	0.9330	0.7943	0.6039	0.069*
C23	0.77192 (9)	0.45778 (9)	0.81276 (14)	0.0249 (4)
C24	0.77682 (10)	0.52198 (9)	0.85585 (15)	0.0269 (4)
C25	0.72103 (11)	0.55341 (10)	0.87230 (17)	0.0335 (4)
H25	0.7262	0.5968	0.8998	0.040*
C26	0.65797 (11)	0.52373 (11)	0.85000 (19)	0.0389 (5)
C27	0.65382 (10)	0.45883 (10)	0.81410 (17)	0.0334 (4)
H27	0.6120	0.4363	0.8011	0.040*
C28	0.70869 (10)	0.42597 (9)	0.79669 (15)	0.0267 (4)
C29	0.59569 (14)	0.55869 (13)	0.8647 (3)	0.0608 (8)
C30	0.53932 (18)	0.5610 (2)	0.7480 (4)	0.1010 (15)
H30A	0.5279	0.5164	0.7211	0.151*
H30B	0.5569	0.5853	0.6963	0.151*
H30C	0.4987	0.5829	0.7551	0.151*
C31	0.5663 (2)	0.5227 (2)	0.9389 (4)	0.1002 (13)
H31A	0.5997	0.5198	1.0113	0.150*
H31B	0.5537	0.4786	0.9103	0.150*
H31C	0.5261	0.5458	0.9447	0.150*
C32	0.60961 (15)	0.62952 (14)	0.8985 (3)	0.0668 (8)
H32A	0.5679	0.6501	0.9035	0.100*
H32B	0.6258	0.6526	0.8442	0.100*
H32C	0.6442	0.6316	0.9698	0.100*
C33	0.72790 (9)	0.34001 (8)	0.57209 (15)	0.0251 (4)
C34	0.68142 (9)	0.32748 (9)	0.63031 (15)	0.0253 (4)
C35	0.62000 (10)	0.29772 (9)	0.57874 (16)	0.0282 (4)

H35	0.5897	0.2893	0.6200	0.034*
C36	0.60085 (9)	0.27960 (9)	0.46909 (15)	0.0272 (4)
C37	0.64562 (9)	0.29534 (9)	0.41049 (15)	0.0267 (4)
H37	0.6334	0.2857	0.3347	0.032*
C38	0.70778 (10)	0.32484 (9)	0.46019 (15)	0.0261 (4)
C39	0.53485 (10)	0.24160 (11)	0.42033 (17)	0.0355 (5)
C40	0.51721 (12)	0.23662 (14)	0.29580 (19)	0.0484 (6)
H40A	0.5517	0.2106	0.2765	0.073*
H40B	0.5157	0.2806	0.2646	0.073*
H40C	0.4730	0.2156	0.2666	0.073*
C41	0.54450 (13)	0.17207 (12)	0.4682 (2)	0.0499 (6)
H41A	0.5030	0.1468	0.4375	0.075*
H41B	0.5546	0.1744	0.5477	0.075*
H41C	0.5821	0.1508	0.4498	0.075*
C42	0.47587 (11)	0.27431 (15)	0.4489 (2)	0.0521 (6)
H42A	0.4705	0.3192	0.4209	0.078*
H42B	0.4851	0.2751	0.5284	0.078*
H42C	0.4342	0.2496	0.4158	0.078*
N2	0.88722 (8)	0.36897 (8)	0.12749 (13)	0.0283 (3)
C43	0.87371 (12)	0.44158 (11)	0.1339 (2)	0.0408 (5)
H43A	0.8639	0.4603	0.0596	0.049*
H43B	0.8326	0.4470	0.1574	0.049*
C44	0.93046 (12)	0.48059 (11)	0.2101 (2)	0.0426 (5)
H44A	0.9425	0.4613	0.2832	0.064*
H44B	0.9157	0.5259	0.2134	0.064*
H44C	0.9700	0.4799	0.1830	0.064*
C45	0.95338 (11)	0.35790 (12)	0.09947 (19)	0.0403 (5)
H45A	0.9913	0.3738	0.1612	0.048*
H45B	0.9596	0.3103	0.0927	0.048*
C46	0.95788 (12)	0.39044 (14)	−0.00313 (19)	0.0461 (6)
H46A	0.9208	0.3750	−0.0653	0.069*
H46B	1.0013	0.3796	−0.0149	0.069*
H46C	0.9545	0.4379	0.0039	0.069*
C47	0.82960 (11)	0.33850 (12)	0.03894 (18)	0.0395 (5)
H47A	0.8401	0.2919	0.0311	0.047*
H47B	0.8260	0.3605	−0.0313	0.047*
C48	0.76091 (12)	0.34328 (13)	0.06242 (19)	0.0447 (5)
H48A	0.7645	0.3229	0.1331	0.067*
H48B	0.7263	0.3206	0.0048	0.067*
H48C	0.7483	0.3894	0.0643	0.067*
C49	0.89485 (13)	0.33790 (11)	0.23751 (18)	0.0402 (5)
H49A	0.9374	0.3541	0.2895	0.048*
H49B	0.8571	0.3530	0.2639	0.048*
C50	0.89602 (15)	0.26399 (12)	0.2399 (2)	0.0493 (6)
H50A	0.8524	0.2471	0.1947	0.074*
H50B	0.9044	0.2488	0.3152	0.074*
H50C	0.9321	0.2481	0.2113	0.074*
H2O	0.8739 (15)	0.4783 (15)	0.750 (3)	0.062 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0305 (2)	0.0269 (2)	0.0324 (2)	−0.00680 (17)	0.01683 (19)	−0.00495 (17)
S2	0.0334 (2)	0.0271 (2)	0.0221 (2)	−0.00818 (17)	0.00771 (18)	−0.00116 (16)
S3	0.0384 (3)	0.0251 (2)	0.0231 (2)	−0.00878 (18)	0.01242 (19)	−0.00128 (16)
S4	0.0361 (3)	0.0277 (2)	0.0325 (3)	−0.00817 (18)	0.0209 (2)	−0.00831 (18)
O1	0.0305 (7)	0.0281 (7)	0.0308 (7)	0.0006 (5)	0.0166 (6)	−0.0016 (5)
O2	0.0352 (7)	0.0219 (6)	0.0367 (7)	−0.0030 (5)	0.0177 (6)	−0.0004 (5)
O3	0.0279 (6)	0.0257 (6)	0.0279 (7)	−0.0025 (5)	0.0090 (5)	−0.0014 (5)
O4	0.0290 (7)	0.0351 (7)	0.0292 (7)	−0.0081 (6)	0.0122 (6)	−0.0079 (6)
N1	0.0464 (10)	0.0317 (9)	0.0475 (11)	0.0030 (8)	0.0211 (9)	0.0029 (8)
C1	0.0290 (9)	0.0273 (9)	0.0240 (9)	−0.0007 (7)	0.0136 (7)	−0.0005 (7)
C2	0.0308 (9)	0.0268 (9)	0.0252 (9)	−0.0042 (7)	0.0124 (7)	0.0001 (7)
C3	0.0347 (10)	0.0251 (9)	0.0339 (10)	0.0004 (8)	0.0116 (8)	0.0006 (8)
C4	0.0336 (10)	0.0328 (10)	0.0381 (11)	0.0017 (8)	0.0105 (8)	0.0013 (8)
C5	0.0287 (9)	0.0335 (10)	0.0334 (10)	−0.0042 (8)	0.0090 (8)	−0.0021 (8)
C6	0.0320 (10)	0.0275 (9)	0.0247 (9)	−0.0050 (7)	0.0132 (7)	−0.0028 (7)
C7	0.0373 (12)	0.0430 (13)	0.0825 (19)	0.0086 (10)	0.0171 (12)	0.0006 (12)
C8	0.0545 (16)	0.0566 (17)	0.141 (3)	0.0122 (14)	0.0225 (18)	−0.0166 (18)
C9	0.064 (2)	0.083 (2)	0.154 (4)	0.0144 (18)	0.063 (2)	−0.001 (2)
C10	0.0577 (19)	0.078 (2)	0.119 (3)	0.0164 (17)	−0.016 (2)	−0.001 (2)
C11	0.0315 (10)	0.0320 (10)	0.0308 (10)	0.0012 (8)	0.0135 (8)	−0.0016 (8)
C12	0.0310 (10)	0.0293 (10)	0.0338 (10)	−0.0050 (8)	0.0146 (8)	0.0002 (8)
C13	0.0240 (9)	0.0226 (9)	0.0291 (9)	−0.0034 (7)	0.0078 (7)	−0.0010 (7)
C14	0.0274 (9)	0.0257 (9)	0.0282 (9)	−0.0044 (7)	0.0123 (7)	−0.0031 (7)
C15	0.0320 (9)	0.0260 (9)	0.0275 (9)	−0.0041 (7)	0.0108 (8)	0.0013 (7)
C16	0.0317 (9)	0.0243 (9)	0.0264 (9)	−0.0019 (7)	0.0079 (7)	−0.0010 (7)
C17	0.0293 (9)	0.0267 (9)	0.0262 (9)	−0.0025 (7)	0.0095 (7)	−0.0034 (7)
C18	0.0257 (9)	0.0257 (9)	0.0238 (9)	−0.0046 (7)	0.0072 (7)	−0.0003 (7)
C19	0.0436 (11)	0.0240 (9)	0.0335 (10)	0.0013 (8)	0.0131 (9)	0.0014 (8)
C20	0.0614 (15)	0.0366 (12)	0.0434 (13)	0.0106 (11)	0.0050 (11)	0.0068 (10)
C21	0.0645 (15)	0.0278 (10)	0.0443 (13)	0.0070 (10)	0.0227 (11)	−0.0007 (9)
C22	0.0589 (14)	0.0264 (10)	0.0573 (15)	−0.0073 (10)	0.0242 (12)	−0.0002 (10)
C23	0.0300 (9)	0.0260 (9)	0.0198 (8)	−0.0022 (7)	0.0091 (7)	0.0012 (7)
C24	0.0332 (10)	0.0266 (9)	0.0228 (9)	−0.0064 (7)	0.0109 (7)	−0.0008 (7)
C25	0.0412 (11)	0.0281 (10)	0.0365 (11)	−0.0068 (8)	0.0195 (9)	−0.0067 (8)
C26	0.0403 (11)	0.0352 (11)	0.0489 (13)	−0.0061 (9)	0.0250 (10)	−0.0079 (9)
C27	0.0336 (10)	0.0345 (10)	0.0371 (11)	−0.0098 (8)	0.0181 (9)	−0.0060 (8)
C28	0.0342 (10)	0.0260 (9)	0.0220 (9)	−0.0065 (7)	0.0115 (7)	−0.0017 (7)
C29	0.0520 (15)	0.0441 (14)	0.103 (2)	−0.0077 (11)	0.0478 (15)	−0.0189 (14)
C30	0.0491 (18)	0.090 (3)	0.151 (4)	0.0132 (17)	0.009 (2)	−0.035 (3)
C31	0.112 (2)	0.083 (2)	0.145 (3)	0.0097 (19)	0.100 (2)	0.002 (2)
C32	0.0532 (15)	0.0460 (15)	0.111 (3)	0.0008 (12)	0.0392 (17)	−0.0199 (16)
C33	0.0278 (9)	0.0204 (8)	0.0287 (9)	−0.0030 (7)	0.0106 (7)	−0.0026 (7)
C34	0.0316 (9)	0.0217 (8)	0.0246 (9)	−0.0028 (7)	0.0114 (7)	−0.0021 (7)
C35	0.0303 (9)	0.0284 (9)	0.0305 (10)	−0.0053 (7)	0.0162 (8)	−0.0036 (7)
C36	0.0276 (9)	0.0271 (9)	0.0284 (9)	−0.0032 (7)	0.0109 (7)	−0.0044 (7)

C37	0.0308 (9)	0.0249 (9)	0.0263 (9)	−0.0018 (7)	0.0112 (7)	−0.0043 (7)
C38	0.0309 (9)	0.0231 (8)	0.0287 (9)	−0.0030 (7)	0.0154 (8)	−0.0031 (7)
C39	0.0294 (10)	0.0453 (12)	0.0348 (11)	−0.0095 (9)	0.0143 (8)	−0.0103 (9)
C40	0.0376 (12)	0.0724 (17)	0.0357 (12)	−0.0192 (11)	0.0117 (9)	−0.0160 (11)
C41	0.0478 (13)	0.0445 (13)	0.0587 (15)	−0.0224 (11)	0.0180 (12)	−0.0075 (11)
C42	0.0309 (11)	0.0752 (18)	0.0513 (14)	−0.0042 (11)	0.0139 (10)	−0.0177 (13)
N2	0.0310 (8)	0.0276 (8)	0.0254 (8)	0.0002 (6)	0.0072 (6)	−0.0012 (6)
C43	0.0431 (12)	0.0325 (11)	0.0473 (13)	0.0034 (9)	0.0141 (10)	0.0017 (9)
C44	0.0473 (13)	0.0294 (10)	0.0496 (13)	−0.0043 (9)	0.0120 (10)	−0.0030 (9)
C45	0.0372 (11)	0.0441 (12)	0.0396 (12)	0.0050 (9)	0.0113 (9)	−0.0030 (10)
C46	0.0360 (11)	0.0661 (16)	0.0398 (12)	0.0060 (11)	0.0168 (10)	0.0058 (11)
C47	0.0403 (11)	0.0457 (12)	0.0301 (11)	−0.0053 (9)	0.0070 (9)	−0.0037 (9)
C48	0.0371 (12)	0.0571 (15)	0.0372 (12)	−0.0116 (10)	0.0069 (9)	−0.0014 (10)
C49	0.0500 (13)	0.0397 (12)	0.0291 (11)	−0.0045 (10)	0.0093 (9)	0.0000 (9)
C50	0.0692 (16)	0.0362 (12)	0.0372 (12)	−0.0037 (11)	0.0079 (11)	0.0060 (10)

Geometric parameters (Å, º)

S1—C14	1.7781 (19)	C26—C27	1.399 (3)
S1—C2	1.7836 (19)	C26—C29	1.534 (3)
S2—C18	1.7780 (19)	C27—C28	1.394 (3)
S2—C24	1.7832 (19)	C27—H27	0.9500
S3—C34	1.7759 (19)	C29—C31	1.470 (5)
S3—C28	1.7832 (19)	C29—C32	1.515 (4)
S4—C38	1.7753 (18)	C29—C30	1.603 (6)
S4—C6	1.7870 (19)	C30—H30A	0.9800
O1—C1	1.390 (2)	C30—H30B	0.9800
O1—C11	1.431 (2)	C30—H30C	0.9800
O2—C13	1.341 (2)	C31—H31A	0.9800
O2—H2O	0.93 (3)	C31—H31B	0.9800
O3—C23	1.312 (2)	C31—H31C	0.9800
O4—C33	1.336 (2)	C32—H32A	0.9800
O4—H4O	0.91 (3)	C32—H32B	0.9800
N1—C12	1.144 (3)	C32—H32C	0.9800
C1—C2	1.390 (3)	C33—C38	1.405 (3)
C1—C6	1.396 (3)	C33—C34	1.406 (3)
C2—C3	1.391 (3)	C34—C35	1.388 (3)
C3—C4	1.389 (3)	C35—C36	1.393 (3)
C3—H3	0.9500	C35—H35	0.9500
C4—C5	1.397 (3)	C36—C37	1.394 (3)
C4—C7	1.532 (3)	C36—C39	1.534 (3)
C5—C6	1.390 (3)	C37—C38	1.393 (3)
C5—H5	0.9500	C37—H37	0.9500
C7—C8	1.503 (4)	C39—C42	1.530 (3)
C7—C9	1.506 (5)	C39—C40	1.533 (3)
C7—C10	1.567 (5)	C39—C41	1.538 (3)
C8—H8A	0.9800	C40—H40A	0.9800
C8—H8B	0.9800	C40—H40B	0.9800

C8—H8C	0.9800	C40—H40C	0.9800
C9—H9A	0.9800	C41—H41A	0.9800
C9—H9B	0.9800	C41—H41B	0.9800
C9—H9C	0.9800	C41—H41C	0.9800
C10—H10A	0.9800	C42—H42A	0.9800
C10—H10B	0.9800	C42—H42B	0.9800
C10—H10C	0.9800	C42—H42C	0.9800
C11—C12	1.467 (3)	N2—C49	1.513 (3)
C11—H11A	0.9900	N2—C47	1.515 (3)
C11—H11B	0.9900	N2—C43	1.517 (3)
C13—C18	1.402 (3)	N2—C45	1.533 (3)
C13—C14	1.414 (3)	C43—C44	1.513 (3)
C14—C15	1.389 (3)	C43—H43A	0.9900
C15—C16	1.403 (3)	C43—H43B	0.9900
C15—H15	0.9500	C44—H44A	0.9800
C16—C17	1.391 (3)	C44—H44B	0.9800
C16—C19	1.533 (3)	C44—H44C	0.9800
C17—C18	1.397 (3)	C45—C46	1.502 (3)
C17—H17	0.9500	C45—H45A	0.9900
C19—C21	1.529 (3)	C45—H45B	0.9900
C19—C22	1.531 (3)	C46—H46A	0.9800
C19—C20	1.538 (3)	C46—H46B	0.9800
C20—H20A	0.9800	C46—H46C	0.9800
C20—H20B	0.9800	C47—C48	1.542 (3)
C20—H20C	0.9800	C47—H47A	0.9900
C21—H21A	0.9800	C47—H47B	0.9900
C21—H21B	0.9800	C48—H48A	0.9800
C21—H21C	0.9800	C48—H48B	0.9800
C22—H22A	0.9800	C48—H48C	0.9800
C22—H22B	0.9800	C49—C50	1.511 (3)
C22—H22C	0.9800	C49—H49A	0.9900
C23—C24	1.416 (3)	C49—H49B	0.9900
C23—C28	1.421 (3)	C50—H50A	0.9800
C24—C25	1.392 (3)	C50—H50B	0.9800
C25—C26	1.390 (3)	C50—H50C	0.9800
C25—H25	0.9500		

C14—S1—C2	96.41 (9)	C32—C29—C26	112.7 (2)
C18—S2—C24	105.29 (8)	C31—C29—C30	107.1 (3)
C34—S3—C28	107.27 (8)	C32—C29—C30	105.2 (3)
C38—S4—C6	98.68 (8)	C26—C29—C30	107.7 (3)
C1—O1—C11	113.65 (14)	C29—C30—H30A	109.5
C13—O2—H2O	115.3 (19)	C29—C30—H30B	109.5
C33—O4—H4O	114.5 (18)	H30A—C30—H30B	109.5
O1—C1—C2	120.13 (16)	C29—C30—H30C	109.5
O1—C1—C6	120.27 (16)	H30A—C30—H30C	109.5
C2—C1—C6	119.60 (17)	H30B—C30—H30C	109.5
C1—C2—C3	119.71 (17)	C29—C31—H31A	109.5

C1—C2—S1	119.47 (15)	C29—C31—H31B	109.5
C3—C2—S1	120.65 (15)	H31A—C31—H31B	109.5
C4—C3—C2	121.73 (18)	C29—C31—H31C	109.5
C4—C3—H3	119.1	H31A—C31—H31C	109.5
C2—C3—H3	119.1	H31B—C31—H31C	109.5
C3—C4—C5	117.74 (19)	C29—C32—H32A	109.5
C3—C4—C7	122.44 (19)	C29—C32—H32B	109.5
C5—C4—C7	119.78 (19)	H32A—C32—H32B	109.5
C6—C5—C4	121.49 (18)	C29—C32—H32C	109.5
C6—C5—H5	119.3	H32A—C32—H32C	109.5
C4—C5—H5	119.3	H32B—C32—H32C	109.5
C5—C6—C1	119.69 (17)	O4—C33—C38	118.85 (16)
C5—C6—S4	120.22 (14)	O4—C33—C34	123.72 (17)
C1—C6—S4	119.91 (15)	C38—C33—C34	117.42 (16)
C8—C7—C9	112.4 (3)	C35—C34—C33	120.12 (17)
C8—C7—C4	113.4 (2)	C35—C34—S3	117.80 (14)
C9—C7—C4	110.1 (2)	C33—C34—S3	121.67 (14)
C8—C7—C10	106.2 (3)	C34—C35—C36	122.92 (17)
C9—C7—C10	106.0 (3)	C34—C35—H35	118.5
C4—C7—C10	108.3 (2)	C36—C35—H35	118.5
C7—C8—H8A	109.5	C35—C36—C37	116.60 (17)
C7—C8—H8B	109.5	C35—C36—C39	119.86 (17)
H8A—C8—H8B	109.5	C37—C36—C39	123.48 (17)
C7—C8—H8C	109.5	C38—C37—C36	121.71 (17)
H8A—C8—H8C	109.5	C38—C37—H37	119.1
H8B—C8—H8C	109.5	C36—C37—H37	119.1
C7—C9—H9A	109.5	C37—C38—C33	121.08 (16)
C7—C9—H9B	109.5	C37—C38—S4	119.69 (14)
H9A—C9—H9B	109.5	C33—C38—S4	119.19 (14)
C7—C9—H9C	109.5	C42—C39—C40	108.6 (2)
H9A—C9—H9C	109.5	C42—C39—C36	111.02 (18)
H9B—C9—H9C	109.5	C40—C39—C36	111.47 (17)
C7—C10—H10A	109.5	C42—C39—C41	109.1 (2)
C7—C10—H10B	109.5	C40—C39—C41	108.5 (2)
H10A—C10—H10B	109.5	C36—C39—C41	108.12 (18)
C7—C10—H10C	109.5	C39—C40—H40A	109.5
H10A—C10—H10C	109.5	C39—C40—H40B	109.5
H10B—C10—H10C	109.5	H40A—C40—H40B	109.5
O1—C11—C12	106.51 (15)	C39—C40—H40C	109.5
O1—C11—H11A	110.4	H40A—C40—H40C	109.5
C12—C11—H11A	110.4	H40B—C40—H40C	109.5
O1—C11—H11B	110.4	C39—C41—H41A	109.5
C12—C11—H11B	110.4	C39—C41—H41B	109.5
H11A—C11—H11B	108.6	H41A—C41—H41B	109.5
N1—C12—C11	179.6 (2)	C39—C41—H41C	109.5
O2—C13—C18	124.03 (17)	H41A—C41—H41C	109.5
O2—C13—C14	118.58 (16)	H41B—C41—H41C	109.5
C18—C13—C14	117.39 (17)	C39—C42—H42A	109.5

C15—C14—C13	120.78 (17)	C39—C42—H42B	109.5
C15—C14—S1	119.93 (14)	H42A—C42—H42B	109.5
C13—C14—S1	119.10 (14)	C39—C42—H42C	109.5
C14—C15—C16	122.11 (17)	H42A—C42—H42C	109.5
C14—C15—H15	118.9	H42B—C42—H42C	109.5
C16—C15—H15	118.9	C49—N2—C47	111.56 (16)
C17—C16—C15	116.60 (17)	C49—N2—C43	109.31 (16)
C17—C16—C19	123.46 (17)	C47—N2—C43	109.02 (16)
C15—C16—C19	119.74 (17)	C49—N2—C45	107.70 (16)
C16—C17—C18	122.47 (17)	C47—N2—C45	108.83 (16)
C16—C17—H17	118.8	C43—N2—C45	110.42 (16)
C18—C17—H17	118.8	C44—C43—N2	115.48 (18)
C17—C18—C13	120.63 (17)	C44—C43—H43A	108.4
C17—C18—S2	118.77 (14)	N2—C43—H43A	108.4
C13—C18—S2	120.51 (14)	C44—C43—H43B	108.4
C21—C19—C22	108.52 (18)	N2—C43—H43B	108.4
C21—C19—C16	112.08 (17)	H43A—C43—H43B	107.5
C22—C19—C16	110.29 (17)	C43—C44—H44A	109.5
C21—C19—C20	108.33 (19)	C43—C44—H44B	109.5
C22—C19—C20	109.30 (19)	H44A—C44—H44B	109.5
C16—C19—C20	108.26 (17)	C43—C44—H44C	109.5
C19—C20—H20A	109.5	H44A—C44—H44C	109.5
C19—C20—H20B	109.5	H44B—C44—H44C	109.5
H20A—C20—H20B	109.5	C46—C45—N2	115.63 (18)
C19—C20—H20C	109.5	C46—C45—H45A	108.4
H20A—C20—H20C	109.5	N2—C45—H45A	108.4
H20B—C20—H20C	109.5	C46—C45—H45B	108.4
C19—C21—H21A	109.5	N2—C45—H45B	108.4
C19—C21—H21B	109.5	H45A—C45—H45B	107.4
H21A—C21—H21B	109.5	C45—C46—H46A	109.5
C19—C21—H21C	109.5	C45—C46—H46B	109.5
H21A—C21—H21C	109.5	H46A—C46—H46B	109.5
H21B—C21—H21C	109.5	C45—C46—H46C	109.5
C19—C22—H22A	109.5	H46A—C46—H46C	109.5
C19—C22—H22B	109.5	H46B—C46—H46C	109.5
H22A—C22—H22B	109.5	N2—C47—C48	113.19 (18)
C19—C22—H22C	109.5	N2—C47—H47A	108.9
H22A—C22—H22C	109.5	C48—C47—H47A	108.9
H22B—C22—H22C	109.5	N2—C47—H47B	108.9
O3—C23—C24	122.24 (16)	C48—C47—H47B	108.9
O3—C23—C28	121.83 (16)	H47A—C47—H47B	107.8
C24—C23—C28	115.91 (17)	C47—C48—H48A	109.5
C25—C24—C23	121.38 (17)	C47—C48—H48B	109.5
C25—C24—S2	118.51 (14)	H48A—C48—H48B	109.5
C23—C24—S2	119.81 (14)	C47—C48—H48C	109.5
C26—C25—C24	122.58 (18)	H48A—C48—H48C	109.5
C26—C25—H25	118.7	H48B—C48—H48C	109.5
C24—C25—H25	118.7	C50—C49—N2	115.82 (18)

C25—C26—C27	116.35 (19)	C50—C49—H49A	108.3
C25—C26—C29	122.9 (2)	N2—C49—H49A	108.3
C27—C26—C29	120.7 (2)	C50—C49—H49B	108.3
C28—C27—C26	122.46 (18)	N2—C49—H49B	108.3
C28—C27—H27	118.8	H49A—C49—H49B	107.4
C26—C27—H27	118.8	C49—C50—H50A	109.5
C27—C28—C23	121.06 (17)	C49—C50—H50B	109.5
C27—C28—S3	118.86 (14)	H50A—C50—H50B	109.5
C23—C28—S3	119.43 (14)	C49—C50—H50C	109.5
C31—C29—C32	111.9 (3)	H50A—C50—H50C	109.5
C31—C29—C26	111.8 (3)	H50B—C50—H50C	109.5

C11—O1—C1—C2	88.6 (2)	C18—S2—C24—C23	88.97 (16)
C11—O1—C1—C6	−91.5 (2)	C23—C24—C25—C26	1.4 (3)
O1—C1—C2—C3	177.82 (16)	S2—C24—C25—C26	−172.31 (17)
C6—C1—C2—C3	−2.0 (3)	C24—C25—C26—C27	2.7 (3)
O1—C1—C2—S1	−6.8 (2)	C24—C25—C26—C29	−178.2 (2)
C6—C1—C2—S1	173.30 (14)	C25—C26—C27—C28	−2.7 (3)
C14—S1—C2—C1	−132.43 (15)	C29—C26—C27—C28	178.1 (2)
C14—S1—C2—C3	42.87 (17)	C26—C27—C28—C23	−1.3 (3)
C1—C2—C3—C4	1.8 (3)	C26—C27—C28—S3	169.47 (17)
S1—C2—C3—C4	−173.54 (16)	O3—C23—C28—C27	−176.61 (17)
C2—C3—C4—C5	−1.3 (3)	C24—C23—C28—C27	5.2 (3)
C2—C3—C4—C7	176.6 (2)	O3—C23—C28—S3	12.7 (2)
C3—C4—C5—C6	1.2 (3)	C24—C23—C28—S3	−165.54 (13)
C7—C4—C5—C6	−176.8 (2)	C34—S3—C28—C27	98.80 (17)
C4—C5—C6—C1	−1.5 (3)	C34—S3—C28—C23	−90.29 (16)
C4—C5—C6—S4	173.55 (16)	C25—C26—C29—C31	−123.3 (3)
O1—C1—C6—C5	−177.91 (17)	C27—C26—C29—C31	55.9 (4)
C2—C1—C6—C5	2.0 (3)	C25—C26—C29—C32	3.8 (4)
O1—C1—C6—S4	7.0 (2)	C27—C26—C29—C32	−177.1 (3)
C2—C1—C6—S4	−173.17 (14)	C25—C26—C29—C30	119.4 (3)
C38—S4—C6—C5	−44.99 (18)	C27—C26—C29—C30	−61.5 (3)
C38—S4—C6—C1	130.11 (16)	O4—C33—C34—C35	−175.62 (17)
C3—C4—C7—C8	2.9 (4)	C38—C33—C34—C35	3.7 (3)
C5—C4—C7—C8	−179.3 (3)	O4—C33—C34—S3	−3.2 (3)
C3—C4—C7—C9	−124.0 (3)	C38—C33—C34—S3	176.13 (14)
C5—C4—C7—C9	53.8 (4)	C28—S3—C34—C35	−116.91 (16)
C3—C4—C7—C10	120.4 (3)	C28—S3—C34—C33	70.45 (17)
C5—C4—C7—C10	−61.7 (3)	C33—C34—C35—C36	−0.7 (3)
C1—O1—C11—C12	153.88 (15)	S3—C34—C35—C36	−173.45 (15)
O2—C13—C14—C15	179.88 (17)	C34—C35—C36—C37	−2.6 (3)
C18—C13—C14—C15	−0.2 (3)	C34—C35—C36—C39	174.73 (18)
O2—C13—C14—S1	4.9 (2)	C35—C36—C37—C38	3.0 (3)
C18—C13—C14—S1	−175.16 (13)	C39—C36—C37—C38	−174.29 (18)
C2—S1—C14—C15	−107.23 (16)	C36—C37—C38—C33	0.0 (3)
C2—S1—C14—C13	67.80 (16)	C36—C37—C38—S4	177.71 (15)
C13—C14—C15—C16	−1.2 (3)	O4—C33—C38—C37	175.99 (17)

S1—C14—C15—C16	173.77 (15)	C34—C33—C38—C37	−3.3 (3)
C14—C15—C16—C17	1.3 (3)	O4—C33—C38—S4	−1.8 (2)
C14—C15—C16—C19	−173.68 (18)	C34—C33—C38—S4	178.92 (14)
C15—C16—C17—C18	−0.2 (3)	C6—S4—C38—C37	120.67 (16)
C19—C16—C17—C18	174.62 (18)	C6—S4—C38—C33	−61.55 (16)
C16—C17—C18—C13	−1.1 (3)	C35—C36—C39—C42	49.2 (3)
C16—C17—C18—S2	175.52 (15)	C37—C36—C39—C42	−133.6 (2)
O2—C13—C18—C17	−178.77 (17)	C35—C36—C39—C40	170.4 (2)
C14—C13—C18—C17	1.3 (3)	C37—C36—C39—C40	−12.4 (3)
O2—C13—C18—S2	4.6 (3)	C35—C36—C39—C41	−70.4 (2)
C14—C13—C18—S2	−175.31 (13)	C37—C36—C39—C41	106.8 (2)
C24—S2—C18—C17	104.29 (16)	C49—N2—C43—C44	64.3 (2)
C24—S2—C18—C13	−79.04 (16)	C47—N2—C43—C44	−173.51 (19)
C17—C16—C19—C21	9.1 (3)	C45—N2—C43—C44	−54.0 (2)
C15—C16—C19—C21	−176.29 (19)	C49—N2—C45—C46	−174.9 (2)
C17—C16—C19—C22	130.1 (2)	C47—N2—C45—C46	64.0 (2)
C15—C16—C19—C22	−55.3 (2)	C43—N2—C45—C46	−55.7 (2)
C17—C16—C19—C20	−110.4 (2)	C49—N2—C47—C48	58.0 (2)
C15—C16—C19—C20	64.3 (2)	C43—N2—C47—C48	−62.9 (2)
O3—C23—C24—C25	176.56 (17)	C45—N2—C47—C48	176.64 (19)
C28—C23—C24—C25	−5.2 (3)	C47—N2—C49—C50	48.8 (3)
O3—C23—C24—S2	−9.8 (2)	C43—N2—C49—C50	169.4 (2)
C28—C23—C24—S2	168.39 (13)	C45—N2—C49—C50	−70.6 (2)
C18—S2—C24—C25	−97.21 (16)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*O*···O3	0.92 (3)	1.66 (3)	2.5649 (19)	165 (3)
O4—H4*O*···O3	0.92 (3)	1.61 (3)	2.503 (2)	164 (3)
C11—H11*A*···O4	0.99	2.22	3.187 (3)	165
C46—H46*A*···O3^{i}	0.98	2.54	3.311 (3)	135
C49—H49*B*···S4	0.99	2.80	3.714 (3)	154
C43—H43*A*···S2^{i}	0.99	2.85	3.773 (2)	156
C45—H45*B*···N1^{ii}	0.99	2.39	3.328 (3)	158

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