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Bis(15-crown-5-κ^5O)barium tetrakis(isothiocynato-κN)zinc(II)

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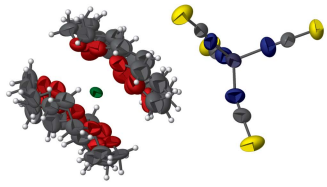
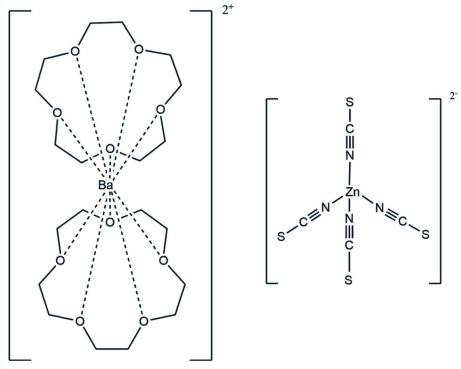
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[Ba(C_{10}H_{20}O_5)_2][Zn(NCS)_4]$, the 15-crown-5 molecules are disordered over two positions with site occupancies of 0.706 (4) and 0.294 (4). The Ba^{2+} ions are sandwiched between the 15-crown-5 rings and Zn^{2+} ions are surrounded by four N atoms from the thiocyanate ligands in a distorted tetrahedral geometry. The crystal studied was refined as an inversion twin.

3D view



Chemical scheme



Structure description

Complexes of 15-crown-5 ether can exhibit biological activities and have been used in the electronics industry. As a result of their selective coordination to specific metal ions, they are frequently used in phase-transfer catalysis (Alasundkar *et al.*, 2011) for toxic metal sequestration. They are also used in battery electrolytes (Ligon *et al.*, 2004) and in electronic and optical devices (Yen *et al.*, 2008).

The geometric parameters of the title molecule (Fig. 1) agree well with those reported for similar structures (Cao *et al.*, 2010; Vafaee *et al.*, 2012; Amini & Ng, 2012). In the title compound, the Ba^{2+} ions are sandwiched between two 15-crown-5 rings, with the Ba ion coordinated to all ten oxygen atoms of the crown ligands. The Zn^{2+} ions are coordinated by four N atoms from the thiocyanate ligands in a distorted tetrahedral geometry. The two 15-crown-5 molecules are disordered over two positions with a shared site occupancy ratio of 0.706 (4) to 0.294 (4). In the crystal, a C—H···S interaction (Table 1) is observed.

Synthesis and crystallization

Zinc(II) dichloride (0.25 mmol, 136.15 g) and ammonium thiocyanate (1 mmol, 76.12 mg) were dissolved in deionized water. An aqueous solution (5 ml) of barium(II) chloride (0.25 mmol, 52.07 mg) was added dropwise and the mixture was stirred for an additional

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

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17A···S3^{i}	0.97	2.70	3.62 (3)	159

Symmetry code: (i) $-x, -y, z-\frac{1}{2}$.

3 h and then added dropwise to a 1,2-dichloroethane solution (10 ml) of 15-crown-5 (0.5 mmol, 134.16 mg). The transparent clear solution was filtered and then held at room temperature for 7–10 days. Transparent colourless crystals were obtained in a yield of 98% (16.42 mmol), m.p. 186.7°C.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The two 15-crown-5 rings are disordered over two positions. The site occupancy factors of the disordered O and C atoms, shared between the two molecules, refined to 0.706 (4) for the major component during anisotropic refinement. The C—O and C—C bond distances were restrained to target values of 1.38 (1) and 1.53 (1) Å using *DFIX* commands. Equivalent bond angles of the 15-crown-5 rings were restrained to be similar in length by restraining the 1,3 C···C and 1,4 O···O distances to be the same within an e.s.d. of 0.01 Å (SADI commands). The atoms C17, C16′, C21′, C6′ and C12′ were restrained to be at least 3.70 (1) Å from the barium ion. The components of the anisotropic displacement parameters of the disordered atoms were restrained to be equal within an effective standard deviation of 0.015 Å^2 (SIMU command; Sheldrick, 2015). The crystal studied was refined as an inversion twin.

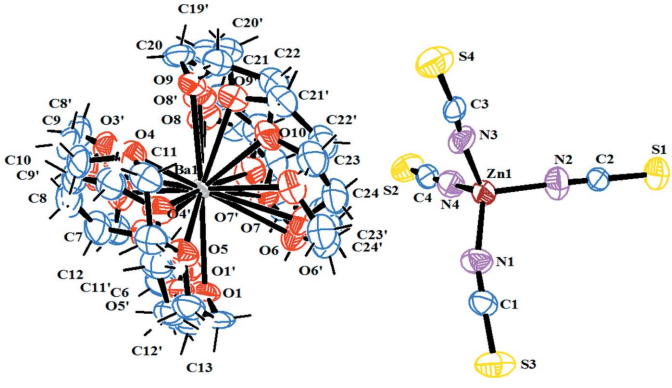

Figure 1
The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Ba(C_{10}H_{20}O_5)_2][Zn(NCS)_4]$
M_r	875.55
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	293
a, b, c (Å)	15.8990 (9), 18.3708 (9), 12.6303 (6)
V (Å^3)	3689.0 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.99
Crystal size (mm)	0.30 × 0.25 × 0.20
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.558, 0.679
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21807, 8085, 5766
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.659
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.106, 1.01
No. of reflections	8085
No. of parameters	669
No. of restraints	1611
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.79, −0.51
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.47 (5)

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

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full crystallographic data

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Crystal data

$[Ba(C_{10}H_{20}O_5)_2][Zn(NCS)_4]$
M_r = 875.55
Orthorhombic, $Pna2_1$
a = 15.8990 (9) Å
b = 18.3708 (9) Å
c = 12.6303 (6) Å
V = 3689.0 (3) Å^3
Z = 4
F(000) = 1768
D_x = 1.576 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1622 reflections
θ = 2.2–27.9°
μ = 1.99 mm^{-1}
T = 293 K
Block, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.558, T_{max} = 0.679
21807 measured reflections
8085 independent reflections
5766 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 27.9°, θ_{min} = 2.2°
h = −20→20
k = −24→15
l = −16→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.106
S = 1.01
8085 reflections
669 parameters
1611 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 3.4899P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.47 (5)

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.

Refinement. Refined as a two-component inversion twin.
H atoms were positioned geometrically and refined using a riding model with C-H = 0.97Å and U_{iso}(H) = 1.2U_{eq}(C) for CH_2.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	−0.2080 (6)	0.0312 (5)	−0.044 (4)	0.082 (3)	
C2	−0.3149 (5)	−0.2052 (4)	−0.047 (2)	0.064 (2)	
C3	−0.0550 (12)	−0.1723 (11)	0.150 (2)	0.069 (5)	
C4	−0.0452 (13)	−0.1695 (11)	−0.253 (2)	0.087 (7)	
N1	−0.1742 (6)	−0.0216 (4)	−0.038 (3)	0.099 (5)	
N2	−0.2536 (5)	−0.1769 (5)	−0.047 (3)	0.101 (3)	
N3	−0.0818 (11)	−0.1526 (12)	0.0835 (17)	0.088 (6)	
N4	−0.0891 (12)	−0.1506 (11)	−0.1706 (16)	0.091 (5)	
S1	−0.40282 (16)	−0.24685 (17)	−0.0534 (11)	0.1158 (10)	
S2	−0.0035 (4)	−0.1979 (4)	−0.3562 (7)	0.117 (2)	
S3	−0.2589 (2)	0.10751 (16)	−0.0466 (10)	0.1284 (12)	
S4	−0.0019 (4)	−0.1958 (4)	0.2556 (7)	0.124 (3)	
Zn1	−0.14606 (6)	−0.12486 (5)	−0.0491 (4)	0.0804 (3)	
Ba1	0.29259 (2)	0.02163 (2)	−0.0497 (3)	0.04580 (12)	
O1	0.2281 (8)	0.1471 (6)	−0.1334 (9)	0.096 (3)	0.706 (4)
O2	0.3721 (9)	0.0865 (9)	−0.2225 (11)	0.129 (4)	0.706 (4)
O3	0.4672 (6)	0.0560 (7)	−0.0501 (12)	0.124 (3)	0.706 (4)
O4	0.3897 (8)	0.0546 (7)	0.1434 (10)	0.091 (3)	0.706 (4)
O5	0.2609 (8)	0.1445 (6)	0.0827 (9)	0.087 (3)	0.706 (4)
C5	0.2647 (19)	0.1848 (12)	−0.2147 (19)	0.112 (5)	0.706 (4)
H5A	0.297993	0.224538	−0.186454	0.134*	0.706 (4)
H5B	0.221433	0.205235	−0.259929	0.134*	0.706 (4)
C6	0.3215 (12)	0.1335 (13)	−0.2800 (16)	0.119 (5)	0.706 (4)
H6A	0.285932	0.104718	−0.326221	0.143*	0.706 (4)
H6B	0.357408	0.163151	−0.324713	0.143*	0.706 (4)
C7	0.4557 (10)	0.0993 (19)	−0.2328 (19)	0.128 (6)	0.706 (4)
H7A	0.463486	0.148137	−0.260320	0.154*	0.706 (4)
H7B	0.478477	0.065557	−0.284447	0.154*	0.706 (4)
C8	0.5048 (14)	0.0920 (14)	−0.1314 (13)	0.137 (5)	0.706 (4)
H8A	0.557255	0.067324	−0.147492	0.164*	0.706 (4)
H8B	0.519012	0.140510	−0.106939	0.164*	0.706 (4)
C9	0.5133 (12)	0.0486 (13)	0.0385 (12)	0.110 (5)	0.706 (4)
H9A	0.568242	0.070589	0.028730	0.132*	0.706 (4)
H9B	0.521061	−0.002555	0.054776	0.132*	0.706 (4)
C10	0.4674 (9)	0.0857 (12)	0.1271 (16)	0.097 (5)	0.706 (4)
H10A	0.500408	0.082211	0.191479	0.116*	0.706 (4)
H10B	0.460424	0.136860	0.110266	0.116*	0.706 (4)
C11	0.3441 (10)	0.0921 (9)	0.2191 (13)	0.091 (4)	0.706 (4)
H11A	0.381159	0.105081	0.277062	0.109*	0.706 (4)
H11B	0.300652	0.060394	0.247056	0.109*	0.706 (4)
C12	0.3035 (14)	0.1603 (9)	0.1766 (13)	0.088 (4)	0.706 (4)

H12A	0.264374	0.179606	0.228376	0.105*	0.706 (4)
H12B	0.346239	0.196895	0.163330	0.105*	0.706 (4)
C13	0.2237 (15)	0.2051 (10)	0.0409 (13)	0.098 (5)	0.706 (4)
H13A	0.265737	0.242789	0.031791	0.118*	0.706 (4)
H13B	0.181607	0.223042	0.089970	0.118*	0.706 (4)
C14	0.1822 (9)	0.1893 (7)	−0.0656 (11)	0.096 (4)	0.706 (4)
H14A	0.128790	0.165311	−0.052605	0.115*	0.706 (4)
H14B	0.170227	0.235284	−0.100136	0.115*	0.706 (4)
O1′	0.2852 (17)	0.1042 (16)	−0.2459 (19)	0.108 (5)	0.294 (4)
O2′	0.4359 (15)	0.048 (2)	−0.175 (2)	0.129 (5)	0.294 (4)
O3′	0.4532 (13)	0.0353 (16)	0.042 (2)	0.105 (5)	0.294 (4)
O4′	0.3183 (16)	0.1095 (13)	0.1288 (19)	0.091 (5)	0.294 (4)
O5′	0.2611 (14)	0.1729 (9)	−0.055 (2)	0.094 (4)	0.294 (4)
C5′	0.345 (2)	0.078 (2)	−0.317 (3)	0.120 (7)	0.294 (4)
H5′1	0.341929	0.106007	−0.382375	0.144*	0.294 (4)
H5′2	0.332772	0.027639	−0.333960	0.144*	0.294 (4)
C6′	0.433 (3)	0.084 (4)	−0.270 (4)	0.127 (6)	0.294 (4)
H6′1	0.473624	0.063676	−0.318559	0.152*	0.294 (4)
H6′2	0.446782	0.135067	−0.258931	0.152*	0.294 (4)
C7′	0.516 (2)	0.031 (4)	−0.144 (3)	0.129 (6)	0.294 (4)
H7′1	0.553344	0.071039	−0.159630	0.154*	0.294 (4)
H7′2	0.535568	−0.011560	−0.182984	0.154*	0.294 (4)
C8′	0.517 (2)	0.015 (2)	−0.026 (2)	0.119 (6)	0.294 (4)
H8′1	0.522976	−0.037641	−0.018326	0.143*	0.294 (4)
H8′2	0.568412	0.035981	0.002033	0.143*	0.294 (4)
C9′	0.470 (3)	0.101 (2)	0.090 (4)	0.104 (5)	0.294 (4)
H9′1	0.468443	0.140982	0.039086	0.125*	0.294 (4)
H9′2	0.524554	0.101062	0.124646	0.125*	0.294 (4)
C10′	0.3984 (17)	0.108 (2)	0.171 (3)	0.099 (5)	0.294 (4)
H10C	0.402030	0.066506	0.218588	0.119*	0.294 (4)
H10D	0.407008	0.151391	0.211957	0.119*	0.294 (4)
C11′	0.287 (3)	0.1798 (19)	0.122 (4)	0.096 (6)	0.294 (4)
H11C	0.333565	0.210583	0.144738	0.115*	0.294 (4)
H11D	0.245233	0.183067	0.176965	0.115*	0.294 (4)
C12′	0.249 (4)	0.220 (2)	0.027 (2)	0.099 (6)	0.294 (4)
H12C	0.189662	0.229092	0.038435	0.118*	0.294 (4)
H12D	0.277536	0.265725	0.014665	0.118*	0.294 (4)
C13′	0.230 (4)	0.198 (3)	−0.150 (2)	0.096 (6)	0.294 (4)
H13C	0.224218	0.250272	−0.145439	0.115*	0.294 (4)
H13D	0.175008	0.177254	−0.160880	0.115*	0.294 (4)
C14′	0.285 (5)	0.1798 (17)	−0.246 (5)	0.105 (6)	0.294 (4)
H14C	0.260919	0.198955	−0.310578	0.126*	0.294 (4)
H14D	0.341725	0.198944	−0.237613	0.126*	0.294 (4)
O6	0.1178 (5)	0.0147 (5)	−0.0427 (17)	0.101 (3)	0.706 (4)
O7	0.2053 (10)	−0.0369 (11)	−0.2151 (16)	0.110 (5)	0.706 (4)
O8	0.3521 (10)	−0.1071 (8)	−0.1523 (13)	0.112 (4)	0.706 (4)
O9	0.3616 (9)	−0.0934 (7)	0.0655 (13)	0.102 (4)	0.706 (4)
O10	0.2058 (9)	−0.0489 (10)	0.1197 (16)	0.106 (4)	0.706 (4)

C15	0.0744 (15)	−0.0076 (18)	−0.1349 (17)	0.113 (5)	0.706 (4)
H15A	0.026463	0.024294	−0.145259	0.136*	0.706 (4)
H15B	0.052925	−0.056429	−0.123661	0.136*	0.706 (4)
C16	0.1272 (11)	−0.0073 (11)	−0.2348 (19)	0.111 (5)	0.706 (4)
H16A	0.099027	−0.035209	−0.289449	0.133*	0.706 (4)
H16B	0.133572	0.042291	−0.259979	0.133*	0.706 (4)
C17	0.2204 (13)	−0.1008 (13)	−0.264 (2)	0.121 (5)	0.706 (4)
H17A	0.217919	−0.093518	−0.340257	0.145*	0.706 (4)
H17B	0.176820	−0.135368	−0.245224	0.145*	0.706 (4)
C18	0.3054 (14)	−0.1324 (12)	−0.2354 (17)	0.111 (5)	0.706 (4)
H18A	0.296871	−0.184020	−0.223281	0.134*	0.706 (4)
H18B	0.340495	−0.128307	−0.297995	0.134*	0.706 (4)
C19	0.3847 (18)	−0.1645 (10)	−0.0933 (16)	0.114 (5)	0.706 (4)
H19A	0.433213	−0.184605	−0.129651	0.137*	0.706 (4)
H19B	0.342714	−0.202631	−0.087598	0.137*	0.706 (4)
C20	0.4100 (12)	−0.1406 (11)	0.0148 (14)	0.114 (5)	0.706 (4)
H20A	0.414748	−0.183750	0.058637	0.137*	0.706 (4)
H20B	0.465856	−0.119568	0.009594	0.137*	0.706 (4)
C21	0.3240 (11)	−0.1136 (14)	0.1556 (15)	0.113 (5)	0.706 (4)
H21A	0.337074	−0.078537	0.210625	0.136*	0.706 (4)
H21B	0.345844	−0.160520	0.177624	0.136*	0.706 (4)
C22	0.2298 (11)	−0.1187 (10)	0.143 (2)	0.106 (5)	0.706 (4)
H22A	0.215022	−0.151628	0.085718	0.127*	0.706 (4)
H22B	0.203438	−0.135525	0.207668	0.127*	0.706 (4)
C23	0.1238 (12)	−0.0334 (14)	0.144 (2)	0.133 (5)	0.706 (4)
H23A	0.121589	0.008468	0.191018	0.159*	0.706 (4)
H23B	0.098804	−0.074488	0.180941	0.159*	0.706 (4)
C24	0.0751 (18)	−0.018 (2)	0.0440 (19)	0.125 (5)	0.706 (4)
H24A	0.051250	−0.063211	0.019500	0.150*	0.706 (4)
H24B	0.028491	0.013875	0.062654	0.150*	0.706 (4)
O6′	0.1244 (14)	0.0199 (15)	−0.138 (2)	0.109 (5)	0.294 (4)
O7′	0.2470 (17)	−0.0667 (16)	−0.224 (2)	0.119 (6)	0.294 (4)
O8′	0.3612 (16)	−0.1139 (11)	−0.0725 (19)	0.114 (5)	0.294 (4)
O9′	0.2826 (15)	−0.0828 (13)	0.118 (2)	0.108 (5)	0.294 (4)
O10′	0.1431 (15)	−0.0005 (17)	0.076 (2)	0.124 (5)	0.294 (4)
C15′	0.104 (3)	−0.042 (2)	−0.197 (3)	0.106 (6)	0.294 (4)
H15C	0.049672	−0.036101	−0.230905	0.127*	0.294 (4)
H15D	0.101849	−0.084698	−0.151533	0.127*	0.294 (4)
C16′	0.174 (2)	−0.0488 (18)	−0.279 (2)	0.117 (6)	0.294 (4)
H16C	0.160910	−0.086338	−0.330078	0.140*	0.294 (4)
H16D	0.181830	−0.003061	−0.316198	0.140*	0.294 (4)
C17′	0.265 (3)	−0.1401 (17)	−0.234 (5)	0.111 (6)	0.294 (4)
H17C	0.274509	−0.153408	−0.306814	0.134*	0.294 (4)
H17D	0.219577	−0.169705	−0.205205	0.134*	0.294 (4)
C18′	0.345 (3)	−0.148 (2)	−0.168 (3)	0.108 (6)	0.294 (4)
H18C	0.350646	−0.199875	−0.154140	0.130*	0.294 (4)
H18D	0.390715	−0.135004	−0.214482	0.130*	0.294 (4)
C19′	0.372 (4)	−0.163 (2)	0.009 (2)	0.111 (6)	0.294 (4)

H19C	0.431275	−0.165348	0.025578	0.133*	0.294 (4)
H19D	0.355533	−0.210851	−0.017237	0.133*	0.294 (4)
C20′	0.324 (3)	−0.148 (2)	0.111 (4)	0.105 (6)	0.294 (4)
H20C	0.282350	−0.186836	0.119675	0.126*	0.294 (4)
H20D	0.362816	−0.151909	0.169262	0.126*	0.294 (4)
C21′	0.2027 (19)	−0.091 (3)	0.163 (4)	0.118 (6)	0.294 (4)
H21C	0.201569	−0.062424	0.227027	0.141*	0.294 (4)
H21D	0.197671	−0.141760	0.183974	0.141*	0.294 (4)
C22′	0.123 (3)	−0.0722 (17)	0.100 (5)	0.121 (6)	0.294 (4)
H22C	0.116527	−0.101875	0.037079	0.145*	0.294 (4)
H22D	0.072384	−0.075852	0.143282	0.145*	0.294 (4)
C23′	0.073 (2)	0.042 (2)	0.063 (3)	0.128 (6)	0.294 (4)
H23C	0.082273	0.092269	0.081008	0.154*	0.294 (4)
H23D	0.024533	0.022989	0.102010	0.154*	0.294 (4)
C24′	0.066 (2)	0.028 (2)	−0.056 (3)	0.121 (6)	0.294 (4)
H24C	0.031867	−0.014969	−0.060824	0.146*	0.294 (4)
H24D	0.030886	0.067897	−0.080071	0.146*	0.294 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.095 (6)	0.066 (5)	0.085 (9)	0.002 (4)	0.012 (13)	−0.001 (14)
C2	0.061 (4)	0.076 (5)	0.055 (5)	0.002 (4)	0.005 (15)	0.015 (13)
C3	0.050 (9)	0.057 (12)	0.098 (15)	0.007 (7)	0.016 (9)	−0.014 (10)
C4	0.072 (12)	0.063 (13)	0.124 (19)	−0.011 (9)	−0.015 (12)	−0.005 (11)
N1	0.113 (6)	0.066 (5)	0.118 (14)	0.015 (4)	0.007 (12)	−0.008 (9)
N2	0.077 (5)	0.109 (6)	0.116 (7)	−0.020 (4)	0.006 (19)	−0.015 (18)
N3	0.064 (9)	0.080 (12)	0.118 (14)	0.004 (7)	−0.029 (9)	−0.017 (10)
N4	0.097 (12)	0.077 (11)	0.100 (12)	−0.002 (9)	−0.001 (9)	−0.013 (9)
S1	0.0708 (14)	0.123 (2)	0.153 (3)	−0.0241 (14)	−0.014 (6)	0.009 (6)
S2	0.122 (5)	0.127 (6)	0.102 (5)	0.037 (5)	−0.004 (4)	−0.015 (4)
S3	0.164 (3)	0.0907 (19)	0.131 (3)	0.0455 (19)	0.007 (8)	0.014 (6)
S4	0.118 (5)	0.138 (7)	0.117 (6)	0.041 (6)	0.009 (5)	0.018 (5)
Zn1	0.0705 (5)	0.0603 (5)	0.1104 (8)	−0.0022 (4)	0.008 (2)	0.000 (2)
Ba1	0.0530 (2)	0.03330 (18)	0.0511 (2)	−0.00542 (14)	−0.0009 (7)	0.0001 (6)
O1	0.127 (8)	0.051 (6)	0.110 (8)	0.000 (5)	−0.045 (7)	0.025 (6)
O2	0.125 (9)	0.161 (10)	0.102 (8)	−0.042 (8)	0.003 (7)	0.080 (8)
O3	0.088 (6)	0.168 (8)	0.116 (7)	−0.039 (5)	−0.020 (9)	0.030 (9)
O4	0.100 (7)	0.092 (7)	0.080 (7)	−0.016 (6)	−0.026 (6)	−0.002 (6)
O5	0.111 (7)	0.057 (6)	0.092 (7)	−0.005 (5)	−0.007 (6)	−0.023 (5)
C5	0.132 (11)	0.092 (9)	0.111 (11)	−0.009 (9)	−0.035 (9)	0.040 (9)
C6	0.142 (10)	0.128 (10)	0.087 (9)	−0.017 (9)	−0.009 (9)	0.065 (9)
C7	0.114 (10)	0.160 (11)	0.111 (10)	−0.039 (10)	0.011 (10)	0.051 (10)
C8	0.101 (9)	0.173 (11)	0.137 (10)	−0.043 (9)	0.008 (9)	0.035 (10)
C9	0.073 (8)	0.141 (10)	0.116 (9)	−0.027 (8)	−0.047 (9)	0.029 (9)
C10	0.089 (8)	0.115 (9)	0.086 (9)	−0.036 (8)	−0.044 (8)	0.011 (8)
C11	0.128 (10)	0.078 (9)	0.067 (8)	−0.013 (8)	−0.011 (8)	−0.002 (7)
C12	0.115 (9)	0.076 (8)	0.072 (8)	0.000 (8)	−0.011 (8)	−0.018 (7)

C13	0.118 (10)	0.057 (8)	0.120 (9)	0.010 (7)	0.007 (8)	−0.008 (8)
C14	0.120 (8)	0.052 (6)	0.116 (10)	0.024 (6)	−0.031 (9)	0.025 (8)
O1′	0.123 (10)	0.098 (10)	0.103 (10)	−0.021 (9)	−0.023 (9)	0.046 (9)
O2′	0.108 (10)	0.160 (11)	0.118 (10)	−0.036 (10)	0.006 (10)	0.042 (10)
O3′	0.081 (9)	0.129 (10)	0.105 (9)	−0.028 (9)	−0.034 (9)	0.026 (9)
O4′	0.120 (10)	0.069 (9)	0.083 (9)	−0.002 (9)	−0.029 (9)	−0.014 (8)
O5′	0.115 (9)	0.061 (7)	0.104 (9)	0.017 (7)	−0.019 (10)	0.006 (9)
C5′	0.137 (13)	0.134 (13)	0.088 (12)	−0.027 (12)	−0.001 (12)	0.063 (12)
C6′	0.128 (12)	0.148 (12)	0.105 (11)	−0.026 (11)	0.010 (11)	0.051 (11)
C7′	0.099 (11)	0.163 (12)	0.124 (11)	−0.041 (11)	−0.001 (11)	0.030 (12)
C8′	0.086 (10)	0.153 (12)	0.117 (11)	−0.032 (10)	−0.026 (11)	0.026 (11)
C9′	0.089 (9)	0.126 (10)	0.096 (10)	−0.029 (9)	−0.036 (10)	0.010 (10)
C10′	0.114 (10)	0.096 (10)	0.087 (10)	−0.017 (9)	−0.027 (9)	−0.005 (9)
C11′	0.124 (11)	0.066 (10)	0.097 (11)	−0.005 (10)	−0.008 (10)	−0.021 (10)
C12′	0.123 (11)	0.058 (10)	0.115 (11)	0.004 (10)	−0.013 (10)	−0.005 (10)
C13′	0.119 (11)	0.060 (10)	0.110 (11)	0.012 (10)	−0.030 (11)	0.028 (11)
C14′	0.129 (12)	0.082 (10)	0.103 (11)	−0.007 (10)	−0.028 (11)	0.050 (10)
O6	0.053 (4)	0.100 (5)	0.149 (8)	−0.004 (4)	−0.024 (9)	0.007 (9)
O7	0.109 (9)	0.108 (9)	0.113 (8)	0.001 (7)	−0.065 (7)	−0.023 (7)
O8	0.140 (9)	0.073 (7)	0.123 (8)	0.028 (7)	−0.049 (8)	−0.064 (7)
O9	0.100 (7)	0.062 (7)	0.143 (9)	−0.012 (6)	−0.034 (7)	0.021 (7)
O10	0.094 (8)	0.094 (8)	0.131 (9)	−0.015 (7)	0.031 (8)	0.033 (8)
C15	0.074 (8)	0.118 (10)	0.146 (10)	−0.007 (8)	−0.066 (9)	−0.005 (9)
C16	0.107 (9)	0.105 (10)	0.121 (10)	−0.010 (8)	−0.078 (8)	−0.006 (9)
C17	0.141 (11)	0.121 (11)	0.101 (9)	−0.007 (9)	−0.052 (9)	−0.060 (9)
C18	0.140 (11)	0.087 (9)	0.107 (9)	0.012 (9)	−0.029 (10)	−0.075 (8)
C19	0.130 (10)	0.059 (8)	0.154 (10)	0.032 (7)	−0.021 (9)	−0.025 (8)
C20	0.120 (10)	0.062 (9)	0.161 (10)	0.024 (8)	−0.044 (9)	0.004 (8)
C21	0.113 (9)	0.091 (10)	0.136 (11)	−0.011 (8)	−0.025 (9)	0.034 (9)
C22	0.109 (9)	0.081 (9)	0.128 (10)	−0.009 (8)	0.005 (9)	0.014 (9)
C23	0.117 (9)	0.128 (10)	0.154 (11)	−0.018 (9)	0.031 (10)	0.019 (10)
C24	0.089 (9)	0.126 (10)	0.161 (10)	−0.018 (9)	0.027 (10)	0.010 (10)
O6′	0.087 (9)	0.104 (10)	0.137 (10)	0.000 (9)	−0.044 (10)	−0.004 (10)
O7′	0.136 (12)	0.104 (11)	0.117 (11)	−0.003 (10)	−0.044 (11)	−0.051 (10)
O8′	0.133 (9)	0.057 (8)	0.150 (10)	0.022 (8)	−0.026 (10)	−0.018 (10)
O9′	0.109 (10)	0.079 (10)	0.137 (10)	−0.007 (9)	−0.008 (10)	0.020 (9)
O10′	0.102 (9)	0.119 (10)	0.150 (11)	−0.022 (9)	0.011 (10)	0.020 (10)
C15′	0.089 (11)	0.107 (12)	0.122 (11)	−0.010 (10)	−0.067 (10)	−0.017 (11)
C16′	0.119 (12)	0.116 (12)	0.115 (11)	−0.002 (10)	−0.057 (10)	−0.034 (11)
C17′	0.140 (12)	0.082 (11)	0.112 (11)	0.007 (11)	−0.031 (11)	−0.064 (10)
C18′	0.136 (11)	0.064 (10)	0.126 (11)	0.026 (10)	−0.033 (11)	−0.053 (11)
C19′	0.118 (11)	0.059 (10)	0.156 (11)	0.015 (10)	−0.038 (11)	0.002 (11)
C20′	0.109 (10)	0.065 (10)	0.141 (11)	0.001 (9)	−0.024 (10)	0.016 (10)
C21′	0.115 (10)	0.100 (11)	0.138 (11)	−0.012 (10)	0.008 (10)	0.018 (10)
C22′	0.108 (10)	0.110 (11)	0.144 (11)	−0.021 (10)	0.024 (10)	0.014 (10)
C23′	0.099 (10)	0.126 (11)	0.159 (12)	−0.015 (10)	0.014 (11)	0.013 (12)
C24′	0.086 (10)	0.121 (10)	0.157 (11)	−0.003 (10)	−0.019 (12)	0.005 (12)

Geometric parameters (Å, º)

C1—N1	1.112 (12)	C10′—H10C	0.97
C1—S3	1.619 (10)	C10′—H10D	0.97
C2—N2	1.105 (10)	C11′—C12′	1.529 (14)
C2—S1	1.595 (9)	C11′—H11C	0.97
C3—N3	1.00 (3)	C11′—H11D	0.97
C3—S4	1.64 (3)	C12′—H12C	0.97
C4—N4	1.30 (3)	C12′—H12D	0.97
C4—S2	1.55 (3)	C13′—C14′	1.530 (14)
N1—Zn1	1.955 (9)	C13′—H13C	0.97
N2—Zn1	1.959 (8)	C13′—H13D	0.97
N3—Zn1	2.03 (2)	C14′—H14C	0.97
N4—Zn1	1.84 (2)	C14′—H14D	0.97
Ba1—O7	2.729 (14)	O6—C15	1.415 (12)
Ba1—O8′	2.734 (18)	O6—C24	1.419 (12)
Ba1—O1	2.736 (10)	O7—C17	1.350 (12)
Ba1—O6	2.783 (8)	O7—C16	1.379 (11)
Ba1—O2	2.790 (11)	O8—C18	1.367 (11)
Ba1—O9	2.791 (14)	O8—C19	1.391 (12)
Ba1—O4′	2.80 (2)	O9—C20	1.324 (11)
Ba1—O3′	2.82 (2)	O9—C21	1.338 (12)
Ba1—O2′	2.82 (2)	O10—C23	1.369 (12)
Ba1—O5′	2.825 (15)	O10—C22	1.370 (12)
Ba1—O7′	2.83 (2)	C15—C16	1.515 (13)
Ba1—O3	2.847 (8)	C15—H15A	0.97
O1—C14	1.366 (11)	C15—H15B	0.97
O1—C5	1.368 (12)	C16—H16A	0.97
O2—C7	1.356 (12)	C16—H16B	0.97
O2—C6	1.386 (12)	C17—C18	1.515 (12)
O3—C9	1.344 (11)	C17—H17A	0.97
O3—C8	1.360 (11)	C17—H17B	0.97
O4—C10	1.377 (12)	C18—H18A	0.97
O4—C11	1.385 (12)	C18—H18B	0.97
O5—C13	1.367 (12)	C19—C20	1.490 (12)
O5—C12	1.396 (11)	C19—H19A	0.97
C5—C6	1.543 (13)	C19—H19B	0.97
C5—H5A	0.97	C20—H20A	0.97
C5—H5B	0.97	C20—H20B	0.97
C6—H6A	0.97	C21—C22	1.510 (13)
C6—H6B	0.97	C21—H21A	0.97
C7—C8	1.507 (13)	C21—H21B	0.97
C7—H7A	0.97	C22—H22A	0.97
C7—H7B	0.97	C22—H22B	0.97
C8—H8A	0.97	C23—C24	1.513 (13)
C8—H8B	0.97	C23—H23A	0.97
C9—C10	1.500 (13)	C23—H23B	0.97
C9—H9A	0.97	C24—H24A	0.97

C9—H9B	0.97	C24—H24B	0.97
C10—H10A	0.97	O6′—C15′	1.396 (14)
C10—H10B	0.97	O6′—C24′	1.396 (14)
C11—C12	1.508 (12)	O7′—C17′	1.382 (14)
C11—H11A	0.97	O7′—C16′	1.387 (13)
C11—H11B	0.97	O8′—C19′	1.377 (14)
C12—H12A	0.97	O8′—C18′	1.383 (13)
C12—H12B	0.97	O9′—C20′	1.374 (14)
C13—C14	1.526 (12)	O9′—C21′	1.398 (13)
C13—H13A	0.97	O10′—C23′	1.369 (14)
C13—H13B	0.97	O10′—C22′	1.390 (14)
C14—H14A	0.97	C15′—C16′	1.535 (14)
C14—H14B	0.97	C15′—H15C	0.97
O1′—C14′	1.389 (14)	C15′—H15D	0.97
O1′—C5′	1.393 (14)	C16′—H16C	0.97
O2′—C7′	1.368 (14)	C16′—H16D	0.97
O2′—C6′	1.370 (14)	C17′—C18′	1.525 (14)
O3′—C8′	1.381 (13)	C17′—H17C	0.97
O3′—C9′	1.382 (14)	C17′—H17D	0.97
O4′—C10′	1.378 (14)	C18′—H18C	0.97
O4′—C11′	1.384 (14)	C18′—H18D	0.97
O5′—C12′	1.364 (13)	C19′—C20′	1.524 (14)
O5′—C13′	1.369 (13)	C19′—H19C	0.97
C5′—C6′	1.526 (14)	C19′—H19D	0.97
C5′—H5′1	0.97	C20′—H20C	0.97
C5′—H5′2	0.97	C20′—H20D	0.97
C6′—H6′1	0.97	C21′—C22′	1.536 (14)
C6′—H6′2	0.97	C21′—H21C	0.97
C7′—C8′	1.527 (14)	C21′—H21D	0.97
C7′—H7′1	0.97	C22′—H22C	0.97
C7′—H7′2	0.97	C22′—H22D	0.97
C8′—H8′1	0.97	C23′—C24′	1.528 (14)
C8′—H8′2	0.97	C23′—H23C	0.97
C9′—C10′	1.533 (14)	C23′—H23D	0.97
C9′—H9′1	0.97	C24′—H24C	0.97
C9′—H9′2	0.97	C24′—H24D	0.97

N1—C1—S3	177 (4)	C12′—C11′—H11C	104.8
N2—C2—S1	178 (3)	O4′—C11′—H11D	104.8
N3—C3—S4	172 (2)	C12′—C11′—H11D	104.8
N4—C4—S2	172.1 (19)	H11C—C11′—H11D	105.8
C1—N1—Zn1	162.2 (19)	O5′—C12′—C11′	104 (3)
C2—N2—Zn1	178 (2)	O5′—C12′—H12C	111.0
C3—N3—Zn1	172 (2)	C11′—C12′—H12C	111.0
C4—N4—Zn1	176.7 (18)	O5′—C12′—H12D	111.0
N4—Zn1—N1	115.0 (11)	C11′—C12′—H12D	111.0
N4—Zn1—N2	108.5 (11)	H12C—C12′—H12D	109.0
N1—Zn1—N2	105.8 (4)	O5′—C13′—C14′	115 (4)

N4—Zn1—N3	112.1 (4)	O5′—C13′—H13C	108.6
N1—Zn1—N3	107.4 (10)	C14′—C13′—H13C	108.6
N2—Zn1—N3	107.7 (11)	O5′—C13′—H13D	108.6
O7—Ba1—O1	81.1 (5)	C14′—C13′—H13D	108.6
O7—Ba1—O6	59.9 (4)	H13C—C13′—H13D	107.6
O1—Ba1—O6	71.1 (4)	O1′—C14′—C13′	102 (3)
O7—Ba1—O2	78.4 (6)	O1′—C14′—H14C	111.3
O1—Ba1—O2	60.5 (3)	C13′—C14′—H14C	111.3
O6—Ba1—O2	119.8 (5)	O1′—C14′—H14D	111.3
O7—Ba1—O9	107.5 (5)	C13′—C14′—H14D	111.3
O1—Ba1—O9	170.8 (4)	H14C—C14′—H14D	109.2
O6—Ba1—O9	110.0 (4)	C15—O6—C24	106.3 (8)
O2—Ba1—O9	123.6 (4)	C15—O6—Ba1	118.3 (13)
O8′—Ba1—O4′	123.4 (7)	C24—O6—Ba1	121.4 (15)
O8′—Ba1—O3′	76.3 (8)	C17—O7—C16	114.9 (11)
O4′—Ba1—O3′	59.0 (5)	C17—O7—Ba1	127.2 (10)
O8′—Ba1—O2′	76.9 (10)	C16—O7—Ba1	116.1 (10)
O4′—Ba1—O2′	103.7 (10)	C18—O8—C19	110.8 (10)
O3′—Ba1—O2′	58.9 (5)	C18—O8—Ba1	116.7 (10)
O8′—Ba1—O5′	164.6 (8)	C19—O8—Ba1	120.5 (11)
O4′—Ba1—O5′	58.6 (5)	C20—O9—C21	119.3 (12)
O3′—Ba1—O5′	94.8 (8)	C20—O9—Ba1	118.2 (12)
O2′—Ba1—O5′	87.8 (10)	C21—O9—Ba1	118.5 (12)
O8′—Ba1—O7′	59.8 (5)	C23—O10—C22	114.2 (11)
O4′—Ba1—O7′	173.5 (8)	C23—O10—Ba1	122.4 (12)
O3′—Ba1—O7′	127.2 (7)	C22—O10—Ba1	116.7 (14)
O2′—Ba1—O7′	82.3 (11)	O6—C15—C16	114.4 (19)
O5′—Ba1—O7′	120.0 (8)	O6—C15—H15A	108.6
O7—Ba1—O3	125.6 (6)	C16—C15—H15A	108.6
O1—Ba1—O3	100.3 (4)	O6—C15—H15B	108.7
O6—Ba1—O3	169.7 (3)	C16—C15—H15B	108.7
O2—Ba1—O3	57.5 (3)	H15A—C15—H15B	107.6
O9—Ba1—O3	77.6 (4)	O7—C16—C15	110 (2)
C14—O1—C5	114.3 (10)	O7—C16—H16A	109.6
C14—O1—Ba1	115.8 (7)	C15—C16—H16A	109.6
C5—O1—Ba1	123.8 (12)	O7—C16—H16B	109.6
C7—O2—C6	114.2 (11)	C15—C16—H16B	109.6
C7—O2—Ba1	126.4 (11)	H16A—C16—H16B	108.1
C6—O2—Ba1	114.4 (11)	O7—C17—C18	112.4 (15)
C9—O3—C8	115.9 (10)	O7—C17—H17A	109.1
C9—O3—Ba1	120.5 (11)	C18—C17—H17A	109.1
C8—O3—Ba1	122.5 (11)	O7—C17—H17B	109.1
C10—O4—C11	111.5 (10)	C18—C17—H17B	109.1
C10—O4—Ba1	115.6 (10)	H17A—C17—H17B	107.9
C11—O4—Ba1	113.5 (10)	O8—C18—C17	122.6 (16)
C13—O5—C12	111.6 (10)	O8—C18—H18A	106.7
C13—O5—Ba1	119.6 (9)	C17—C18—H18A	106.7
C12—O5—Ba1	125.2 (9)	O8—C18—H18B	106.7

O1—C5—C6	110.0 (16)	C17—C18—H18B	106.7
O1—C5—H5A	109.7	H18A—C18—H18B	106.6
C6—C5—H5A	109.7	O8—C19—C20	111.6 (16)
O1—C5—H5B	109.7	O8—C19—H19A	109.3
C6—C5—H5B	109.7	C20—C19—H19A	109.3
H5A—C5—H5B	108.2	O8—C19—H19B	109.3
O2—C6—C5	116 (2)	C20—C19—H19B	109.3
O2—C6—H6A	108.3	H19A—C19—H19B	108.0
C5—C6—H6A	108.3	O9—C20—C19	119 (2)
O2—C6—H6B	108.3	O9—C20—H20A	107.7
C5—C6—H6B	108.3	C19—C20—H20A	107.7
H6A—C6—H6B	107.4	O9—C20—H20B	107.7
O2—C7—C8	114 (2)	C19—C20—H20B	107.7
O2—C7—H7A	108.7	H20A—C20—H20B	107.1
C8—C7—H7A	108.7	O9—C21—C22	111.7 (19)
O2—C7—H7B	108.7	O9—C21—H21A	109.3
C8—C7—H7B	108.7	C22—C21—H21A	109.3
H7A—C7—H7B	107.6	O9—C21—H21B	109.3
O3—C8—C7	117.2 (18)	C22—C21—H21B	109.3
O3—C8—H8A	108.0	H21A—C21—H21B	107.9
C7—C8—H8A	108.0	O10—C22—C21	103.9 (17)
O3—C8—H8B	108.0	O10—C22—H22A	111.0
C7—C8—H8B	108.0	C21—C22—H22A	111.0
H8A—C8—H8B	107.2	O10—C22—H22B	111.0
O3—C9—C10	108.1 (17)	C21—C22—H22B	111.0
O3—C9—H9A	110.1	H22A—C22—H22B	109.0
C10—C9—H9A	110.1	O10—C23—C24	110 (2)
O3—C9—H9B	110.1	O10—C23—H23A	109.7
C10—C9—H9B	110.1	C24—C23—H23A	109.7
H9A—C9—H9B	108.4	O10—C23—H23B	109.7
O4—C10—C9	111.1 (16)	C24—C23—H23B	109.7
O4—C10—H10A	109.4	H23A—C23—H23B	108.2
C9—C10—H10A	109.4	O6—C24—C23	119 (2)
O4—C10—H10B	109.4	O6—C24—H24A	107.6
C9—C10—H10B	109.4	C23—C24—H24A	107.6
H10A—C10—H10B	108.0	O6—C24—H24B	107.6
O4—C11—C12	113.1 (15)	C23—C24—H24B	107.6
O4—C11—H11A	109.0	H24A—C24—H24B	107.0
C12—C11—H11A	109.0	C15′—O6′—C24′	109.4 (13)
O4—C11—H11B	109.0	C15′—O6′—Ba1	115 (2)
C12—C11—H11B	109.0	C24′—O6′—Ba1	109 (2)
H11A—C11—H11B	107.8	C17′—O7′—C16′	111.0 (13)
O5—C12—C11	109.7 (14)	C17′—O7′—Ba1	125 (2)
O5—C12—H12A	109.7	C16′—O7′—Ba1	117.8 (12)
C11—C12—H12A	109.7	C19′—O8′—C18′	111.8 (14)
O5—C12—H12B	109.7	C19′—O8′—Ba1	125 (2)
C11—C12—H12B	109.7	C18′—O8′—Ba1	115.5 (19)
H12A—C12—H12B	108.2	C20′—O9′—C21′	111.2 (14)

O5—C13—C14	111.9 (13)	C20′—O9′—Ba1	121 (2)
O5—C13—H13A	109.2	C21′—O9′—Ba1	115.0 (14)
C14—C13—H13A	109.2	C23′—O10′—C22′	111.7 (14)
O5—C13—H13B	109.2	C23′—O10′—Ba1	122 (2)
C14—C13—H13B	109.2	C22′—O10′—Ba1	116 (3)
H13A—C13—H13B	107.9	O6′—C15′—C16′	105 (2)
O1—C14—C13	115.4 (14)	O6′—C15′—H15C	110.8
O1—C14—H14A	108.4	C16′—C15′—H15C	110.8
C13—C14—H14A	108.4	O6′—C15′—H15D	110.8
O1—C14—H14B	108.4	C16′—C15′—H15D	110.8
C13—C14—H14B	108.4	H15C—C15′—H15D	108.9
H14A—C14—H14B	107.5	O7′—C16′—C15′	107 (3)
C14′—O1′—C5′	110.1 (14)	O7′—C16′—H16C	110.4
C14′—O1′—Ba1	121 (3)	C15′—C16′—H16C	110.4
C5′—O1′—Ba1	110 (2)	O7′—C16′—H16D	110.4
C7′—O2′—C6′	113.4 (14)	C15′—C16′—H16D	110.4
C7′—O2′—Ba1	123.4 (19)	H16C—C16′—H16D	108.6
C6′—O2′—Ba1	123 (2)	O7′—C17′—C18′	103 (3)
C8′—O3′—C9′	111.6 (14)	O7′—C17′—H17C	111.3
C8′—O3′—Ba1	113 (2)	C18′—C17′—H17C	111.3
C9′—O3′—Ba1	116 (2)	O7′—C17′—H17D	111.2
C10′—O4′—C11′	112.1 (14)	C18′—C17′—H17D	111.2
C10′—O4′—Ba1	115 (2)	H17C—C17′—H17D	109.2
C11′—O4′—Ba1	116 (2)	O8′—C18′—C17′	126 (4)
C12′—O5′—C13′	113.9 (14)	O8′—C18′—H18C	105.8
C12′—O5′—Ba1	129 (2)	C17′—C18′—H18C	105.8
C13′—O5′—Ba1	114 (2)	O8′—C18′—H18D	105.8
O1′—C5′—C6′	110 (4)	C17′—C18′—H18D	105.8
O1′—C5′—H5′1	109.6	H18C—C18′—H18D	106.2
C6′—C5′—H5′1	109.6	O8′—C19′—C20′	117 (4)
O1′—C5′—H5′2	109.6	O8′—C19′—H19C	108.1
C6′—C5′—H5′2	109.6	C20′—C19′—H19C	108.1
H5′1—C5′—H5′2	108.1	O8′—C19′—H19D	108.1
O2′—C6′—C5′	110 (4)	C20′—C19′—H19D	108.1
O2′—C6′—H6′1	109.7	H19C—C19′—H19D	107.3
C5′—C6′—H6′1	109.7	O9′—C20′—C19′	117 (4)
O2′—C6′—H6′2	109.7	O9′—C20′—H20C	108.0
C5′—C6′—H6′2	109.7	C19′—C20′—H20C	108.0
H6′1—C6′—H6′2	108.2	O9′—C20′—H20D	108.1
O2′—C7′—C8′	110 (3)	C19′—C20′—H20D	108.1
O2′—C7′—H7′1	109.7	H20C—C20′—H20D	107.3
C8′—C7′—H7′1	109.7	O9′—C21′—C22′	121 (3)
O2′—C7′—H7′2	109.7	O9′—C21′—H21C	107.0
C8′—C7′—H7′2	109.7	C22′—C21′—H21C	107.0
H7′1—C7′—H7′2	108.2	O9′—C21′—H21D	107.0
O3′—C8′—C7′	123 (4)	C22′—C21′—H21D	107.0
O3′—C8′—H8′1	106.5	H21C—C21′—H21D	106.7
C7′—C8′—H8′1	106.5	O10′—C22′—C21′	98 (2)

O3′—C8′—H8′2	106.5	O10′—C22′—H22C	112.2
C7′—C8′—H8′2	106.5	C21′—C22′—H22C	112.2
H8′1—C8′—H8′2	106.5	O10′—C22′—H22D	112.2
O3′—C9′—C10′	102 (3)	C21′—C22′—H22D	112.2
O3′—C9′—H9′1	111.4	H22C—C22′—H22D	109.8
C10′—C9′—H9′1	111.4	O10′—C23′—C24′	95 (3)
O3′—C9′—H9′2	111.4	O10′—C23′—H23C	112.8
C10′—C9′—H9′2	111.4	C24′—C23′—H23C	112.8
H9′1—C9′—H9′2	109.2	O10′—C23′—H23D	112.8
O4′—C10′—C9′	116 (3)	C24′—C23′—H23D	112.8
O4′—C10′—H10C	108.3	H23C—C23′—H23D	110.2
C9′—C10′—H10C	108.3	O6′—C24′—C23′	135 (4)
O4′—C10′—H10D	108.3	O6′—C24′—H24C	103.4
C9′—C10′—H10D	108.3	C23′—C24′—H24C	103.4
H10C—C10′—H10D	107.4	O6′—C24′—H24D	103.4
O4′—C11′—C12′	130 (4)	C23′—C24′—H24D	103.4
O4′—C11′—H11C	104.8	H24C—C24′—H24D	105.2

C14—O1—C5—C6	174.7 (18)	C24—O6—C15—C16	−155 (3)
Ba1—O1—C5—C6	23 (3)	Ba1—O6—C15—C16	−14 (3)
C7—O2—C6—C5	−114 (3)	C17—O7—C16—C15	113 (3)
Ba1—O2—C6—C5	42 (2)	Ba1—O7—C16—C15	−53 (2)
O1—C5—C6—O2	−44 (3)	O6—C15—C16—O7	44 (3)
C6—O2—C7—C8	140 (3)	C16—O7—C17—C18	−177 (2)
Ba1—O2—C7—C8	−14 (4)	Ba1—O7—C17—C18	−13 (4)
C9—O3—C8—C7	178 (2)	C19—O8—C18—C17	135 (3)
Ba1—O3—C8—C7	−13 (3)	Ba1—O8—C18—C17	−8 (3)
O2—C7—C8—O3	17 (4)	O7—C17—C18—O8	13 (4)
C8—O3—C9—C10	119 (2)	C18—O8—C19—C20	−161 (2)
Ba1—O3—C9—C10	−49 (2)	Ba1—O8—C19—C20	−19 (3)
C11—O4—C10—C9	−175.1 (14)	C21—O9—C20—C19	117 (2)
Ba1—O4—C10—C9	−43.5 (19)	Ba1—O9—C20—C19	−41 (2)
O3—C9—C10—O4	61 (2)	O8—C19—C20—O9	40 (3)
C10—O4—C11—C12	79 (2)	C20—O9—C21—C22	−112 (2)
Ba1—O4—C11—C12	−53.3 (17)	Ba1—O9—C21—C22	45 (2)
C13—O5—C12—C11	−179.5 (18)	C23—O10—C22—C21	−156 (2)
Ba1—O5—C12—C11	−21 (2)	Ba1—O10—C22—C21	52 (2)
O4—C11—C12—O5	49 (2)	O9—C21—C22—O10	−63 (3)
C12—O5—C13—C14	176.0 (19)	C22—O10—C23—C24	−115 (3)
Ba1—O5—C13—C14	16 (3)	Ba1—O10—C23—C24	36 (3)
C5—O1—C14—C13	−104 (2)	C15—O6—C24—C23	153 (3)
Ba1—O1—C14—C13	49.4 (17)	Ba1—O6—C24—C23	14 (4)
O5—C13—C14—O1	−43 (3)	O10—C23—C24—O6	−31 (4)
C14′—O1′—C5′—C6′	77 (6)	C24′—O6′—C15′—C16′	−176 (3)
Ba1—O1′—C5′—C6′	−59 (4)	Ba1—O6′—C15′—C16′	−53 (4)
C7′—O2′—C6′—C5′	161 (5)	C17′—O7′—C16′—C15′	102 (5)
Ba1—O2′—C6′—C5′	−24 (8)	Ba1—O7′—C16′—C15′	−52 (3)
O1′—C5′—C6′—O2′	56 (7)	O6′—C15′—C16′—O7′	68 (4)

C6′—O2′—C7′—C8′	161 (5)	C16′—O7′—C17′—C18′	−179 (4)
Ba1—O2′—C7′—C8′	−14 (7)	Ba1—O7′—C17′—C18′	−28 (6)
C9′—O3′—C8′—C7′	−94 (5)	C19′—O8′—C18′—C17′	118 (6)
Ba1—O3′—C8′—C7′	38 (5)	Ba1—O8′—C18′—C17′	−32 (6)
O2′—C7′—C8′—O3′	−17 (7)	O7′—C17′—C18′—O8′	40 (7)
C8′—O3′—C9′—C10′	−173 (3)	C18′—O8′—C19′—C20′	−132 (5)
Ba1—O3′—C9′—C10′	57 (4)	Ba1—O8′—C19′—C20′	15 (7)
C11′—O4′—C10′—C9′	−99 (5)	C21′—O9′—C20′—C19′	138 (5)
Ba1—O4′—C10′—C9′	37 (4)	Ba1—O9′—C20′—C19′	−2 (6)
O3′—C9′—C10′—O4′	−62 (5)	O8′—C19′—C20′—O9′	−8 (8)
C10′—O4′—C11′—C12′	128 (5)	C20′—O9′—C21′—C22′	−118 (5)
Ba1—O4′—C11′—C12′	−7 (7)	Ba1—O9′—C21′—C22′	24 (5)
C13′—O5′—C12′—C11′	180 (4)	C23′—O10′—C22′—C21′	−152 (3)
Ba1—O5′—C12′—C11′	20 (6)	Ba1—O10′—C22′—C21′	61 (4)
O4′—C11′—C12′—O5′	−7 (7)	O9′—C21′—C22′—O10′	−56 (5)
C12′—O5′—C13′—C14′	142 (4)	C22′—O10′—C23′—C24′	−91 (4)
Ba1—O5′—C13′—C14′	−56 (5)	Ba1—O10′—C23′—C24′	53 (3)
C5′—O1′—C14′—C13′	−169 (4)	C15′—O6′—C24′—C23′	130 (5)
Ba1—O1′—C14′—C13′	−38 (6)	Ba1—O6′—C24′—C23′	4 (5)
O5′—C13′—C14′—O1′	61 (6)	O10′—C23′—C24′—O6′	−36 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17*A*···S3^{i}	0.97	2.70	3.62 (3)	159

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