

# Crystal structure of a copper–mefenamate complex solvated with diglyme and water

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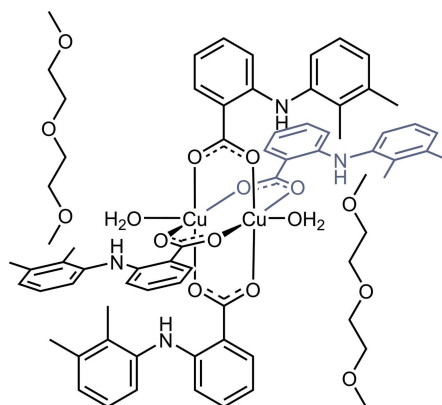
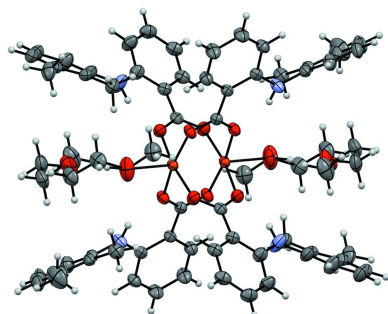
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In the copper–mefenamate complex tetrakis[ $\mu$ -2-(2,3-dimethylanilino)benzoato- $\kappa^2 O:O'$ ]bis[aquacopper(II)]–1-methoxy-2-(2-methoxyethoxy)ethane (1/2),  $[\text{Cu}_2(\text{C}_{15}\text{H}_{14}\text{NO}_2)_4(\text{H}_2\text{O})_2] \cdot 2\text{C}_6\text{H}_{14}\text{O}_3$ , the asymmetric unit comprises a  $\text{Cu}^{\text{II}}$  cation coordinated to two mefenamate ligands solvated with a water molecule and a diglyme molecule. The complex adopts a paddlewheel motif and is compared to structural analogues crystallized with dimethylformamide and dimethyl sulfoxide.

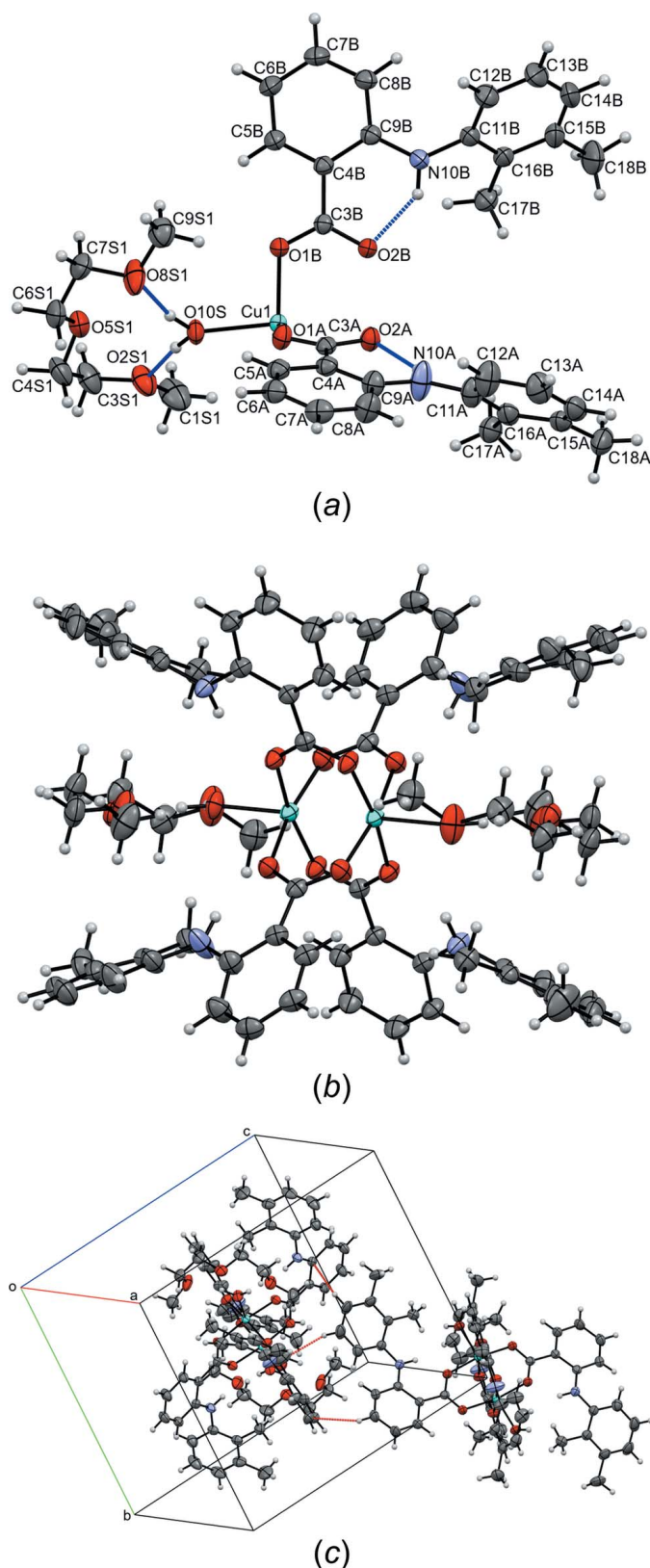
## 1. Chemical context

Mefenamic acid is a non-steroidal anti-inflammatory drug (NSAID) that is synthesized through reaction of 2-chlorobenzoic acid and 2,3-dimethylaniline in the presence of a copper catalyst (Trinus *et al.*, 1977). Subsequently, pharmacopoeia specifications for mefenamic acid specify a maximum limit of 10 ppm for the quantity of copper present in the final drug product (British Pharmacopoeia, 2017). In exploring strategies to ensure removal of copper from the crude reaction mixture, a new copper–mefenamate complex was isolated. The crystal structure of a copper–mefenamate complex solvated with water and diglyme is reported.



## 2. Structural commentary

The complex  $[\text{Cu}_2(\text{mefenamate})_4(\text{H}_2\text{O})_2] \cdot 2(\text{diglyme})$  crystallizes in the space group  $P2_1/n$ , with a  $\{\text{Cu}_2(\text{RCO}_2)_4(\text{H}_2\text{O})_2\}$



**Figure 1**  
Views of  $[\text{Cu}_2(\text{mefenamate})_4(\text{H}_2\text{O})_2] \cdot 2(\text{diglyme})$  as an ORTEP representation with ellipsoids set to 50% probability: (a) asymmetric unit with hydrogen bonds highlighted (dashed blue lines), (b) a single paddlewheel unit of the complex, and (c) neighbouring units with edge-to-face interactions highlighted (dashed red lines).

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{N10A}-\text{H10D} \cdots \text{O2A}$	0.86 (3)	1.86 (3)	2.604 (2)	143 (2)
$\text{N10B}-\text{H10C} \cdots \text{O2B}$	0.89 (2)	1.87 (2)	2.6065 (18)	139 (2)

paddlewheel motif that is typical for coordination of four carboxylate groups to two  $\text{Cu}^{\text{II}}$  cations (Chong *et al.*, 2022). Within the asymmetric unit (Fig. 1a), the planes of the 2,3-dimethylphenyls from the two mefenamate molecules are  $42.61 (1)^\circ$  apart. A water molecule occupies each of the apical positions of the paddlewheel motif, which is hydrogen bonded to a diglyme molecule (Fig. 1a). The diglyme molecule is oriented such that it fits between the 2,3-dimethylphenyl units of the two mefenamate molecules in the asymmetric unit and is hydrogen bonded to the coordinated water *via* the diglyme outer oxygen positions (Fig. 1a). A distorted square-pyramidal geometry is adopted by each  $\text{Cu}^{\text{II}}$  cation in the paddlewheel motif (Fig. 1b), with equatorial  $\text{Cu}-\text{O}$  distances of 1.968 (1), 1.961 (1), 1.954 (1), and 1.969 (1)  $\text{\AA}$  between  $\text{Cu}^{\text{II}}$  and the carboxylate moieties. The axial  $\text{Cu}-\text{O}$  distance, between the copper(II) cation and water molecule, is 2.108 (1)  $\text{\AA}$ . The distance between the two  $\text{Cu}^{\text{II}}$  cations is 2.6126 (4)  $\text{\AA}$ . There is an intramolecular bond between the amine and carboxylate groups of the mefenamate, with  $\text{O} \cdots \text{H}$  distances of 1.86 (3) and 1.87 (2)  $\text{\AA}$  for mefenamate units *A* and *B*, respectively (Table 1).

### 3. Supramolecular features

There are no obvious interactions, such as  $\pi-\pi$  stacking, between neighbouring paddlewheel units within the packed structure. The paddlewheel units interact through edge-to-face interactions of the phenyl groups of the mefenamate ligands (Fig. 1c). In the global packing of the structure, the paddlewheel units are arranged as 2D sheets along the crystallographic *ab* plane, with symmetry-equivalent sheets repeating throughout the crystallographic *c* axis at a distance corresponding to *c*. A second 2D arrangement is intercalated halfway between the symmetry-equivalent sheets.

### 4. Database survey

There are three other similar copper–mefenamate paddlewheel structures in the CSD (version 5.43, November 2021; Groom *et al.*, 2016), with different solvents occupying the apical positions. Two entries, MPANCU10 (Yatsimirskii *et al.*, 1979) and MPANCU20 (Mys'kiv *et al.*, 1982), are with *N,N*-dimethylformamide (DMF) and one entry, SUTPIG (Facchin *et al.*, 1998), has dimethyl sulfoxide (DMSO) occupying the apical position. The DMF analogue also crystallizes in a monoclinic space group (Table 2). The cell volume of  $[\text{Cu}_2(\text{mefenamate})_4(\text{H}_2\text{O})_2] \cdot 2(\text{diglyme})$  [ $3538.64 (12) \text{\AA}^3$ ] is larger than the DMF analogue ( $3026.535 \text{\AA}^3$ ), to accommodate the larger diglyme molecule. The axial  $\text{Cu}-\text{O}$  distance in  $[\text{Cu}_2(\text{mefenamate})_4(\text{H}_2\text{O})_2] \cdot 2(\text{diglyme})$  is shorter than those

Table 2

Comparison of selected geometries (Å, °).

Coordinates are unavailable for entry MPANCU10. There are two values per structure, corresponding to the two mefenamate units in the asymmetric unit as denoted *A* and *B* in our atom-numbering scheme.

	This work		MPANCU20		SUTPIG	
Space group	<i>P</i> 21/ <i>n</i>		<i>P</i> 21/ <i>c</i>		$\bar{P}1$	
O1—C3—C4—C9	171.1 (2)	179.7 (1)	170.98	179.70	153 (1)	180 (1)
C4—C9—N10—C11	174.3 (2)	171.2 (2)	−166.40	171.56	171 (1)	172 (1)
C9—N10—C11—C16	144.7 (2)	−124.9 (2)	−155.25	−109.34	−107 (2)	135 (2)
Cu—O <sub>mefenamate</sub>	1.961 (1)	1.954 (1)	1.9737	1.9605	1.972 (7)	1.949 (7)
Cu—O <sub>solvent</sub>	2.108 (1)		2.1561		2.17 (1)	
Cu···Cu	2.6126 (4)		2.6120		2.627 (3)	

in structures MPANCU20 and SUTPIG (Table 2). This may be attributed to the higher polarity of water (1.000) compared to DMF and DMSO (0.386 and 0.444, respectively; Reichardt & Welton, 2011). In the DMSO analogue, the 2,3-dimethylphenyls from the two mefenamate molecules within the asymmetric unit are almost coplanar, the planes are 9.06° apart, and the methyl groups of the DMSO point away from the 2,3-dimethylphenyls. For the DMF analogue, the two 2,3-dimethylphenyls are oriented such that they can accommodate one of the methyl groups from the DMF, therefore the planes are 70.22° apart.

Three polymorphic forms are known for mefenamic acid, with significant differences between the forms in the C9—N10—C11—C16 torsion angle  $\tau_3$  (Fig. 1*a*; SeethaLekshmi & Guru Row, 2012). The larger torsion angle  $\tau_3$  observed with the copper complex (Table 2) is more consistent with those of the form I polymorph of −119.99° (XYANAC; McConnell & Company, 1976) and −120.1 (1)° (XYANAC06; Mague & Ouzidan, 2017). The increased torsional angle can be explained by the location of the dimethylphenyl group with respect to the diglyme group. The phenyl group needs to rotate to ensure a more planar packing arrangement with the diglyme molecule. In comparison to other polymorphs, the metastable form II suffers from significant disorder around the dimethylphenyl ring system, however the torsion angle  $\tau_3$  is 68 (2)° for XYANAC04 (SeethaLekshmi & Guru Row, 2012), 74.5 (3)° for XYANAC05 (Yang *et al.*, 2012) and −90 (2)° for XYANAC07 (Abbas *et al.*, 2017). The latter of these data collections is at high pressure and the disorder is not modelled, possibly because of the lack of data present due to the diamond anvil cell. The thermal parameters indicate that some disorder may still be present even at these higher pressures. For metastable form III, the reported torsion angle  $\tau_3$  is −80.8 (2)° (XYANAC03; SeethaLekshmi & Guru Row, 2012).

## 5. Synthesis and crystallization

Chemicals were purchased from commercial suppliers and used as received without further purification. Deionized water was obtained from an in-house Milli-Q (Millipore) purification system. A solution was prepared comprising mefenamic acid (25.0 g), diglyme (281.6 g), water (74.7 g) and copper (II) acetate (7.3 g). An aliquot (4 mL) of this solution was removed and mefenamic acid (0.4 g) added to generate a

slurry. The mixture was filtered and the filtrate stored in the dark at room temperature for two weeks, after which large green block-shaped crystals of the complex had formed.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The diglyme moiety was found to be disordered over two positions. Initial isotropic refinement of the diglyme allowed the residual electron density to be observed. Using the functionality in *OLEX2*, the atoms were moved to ensure that they overlapped the electron density in a

Table 3  
Experimental details.

Crystal data	
Chemical formula	[Cu <sub>2</sub> (C <sub>15</sub> H <sub>14</sub> NO <sub>2</sub> ) <sub>4</sub> (H <sub>2</sub> O) <sub>2</sub> ] <sub>2</sub> ·2C <sub>6</sub> H <sub>14</sub> O <sub>3</sub>
<i>M<sub>r</sub></i>	1392.54
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>n</i>
Temperature (K)	105
<i>a</i> , <i>b</i> , <i>c</i> (Å)	15.5420 (3), 14.0010 (3), 16.3217 (3)
$\beta$ (°)	94.791 (1)
<i>V</i> (Å <sup>3</sup> )	3539.25 (12)
<i>Z</i>	2
Radiation type	Cu <i>K</i> $\alpha$
$\mu$ (mm <sup>−1</sup> )	1.30
Crystal size (mm)	0.2 × 0.15 × 0.1
Data collection	
Diffractionmeter	Bruker Photon100 CMOS
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2016)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.781, 0.881
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	209288, 6424, 5989
<i>R<sub>int</sub></i> ( $\sin \theta/\lambda$ ) <sub>max</sub> (Å <sup>−1</sup> )	0.039 0.603
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.033, 0.089, 1.06
No. of reflections	6424
No. of parameters	477
No. of restraints	410
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>−3</sup> )	0.28, −0.40

Computer programs: *APEX3* and *SAINTE* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

zigzag bonding pattern usually observed for alkyl chains. Distance restraints were applied to ensure the molecular integrity. Using the SPLIT function, the alkyl chain was duplicated and rotated to align with the remaining electron density. This model was refined isotropically before applying EADP restraints to the atoms and refining anisotropically. This provided a stable refined structure. The water hydrogen atoms were added from the difference map and refined with ideal DFIX restraints in place. C-bound hydrogen atoms were placed geometrically and a riding model applied [ $C-H = 0.95-0.99 \text{ \AA}$ ;  $U_{iso}(H) = 1.2-1.5U_{eq}(C)$ ]. All data underpinning this publication are openly available from the University of Strathclyde KnowledgeBase at <https://doi.org/10.15129/39f97ad1-8173-4999-b0b6-41c6ae923fe6>.

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## supporting information

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## Crystal structure of a copper–mefenamate complex solvated with diglyme and water

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### Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINTE* (Bruker, 2016); data reduction: *SAINTE* (Bruker, 2016); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

Tetrakis[ $\mu$ -2-(2,3-dimethylanilino)benzoato- $\kappa^2$ O:O']bis[aquacopper(II)]-1-methoxy-2-(2-methoxyethoxy)ethane (1/2)

### Crystal data

[Cu<sub>2</sub>(C<sub>15</sub>H<sub>14</sub>NO<sub>2</sub>)<sub>4</sub>(H<sub>2</sub>O)<sub>2</sub>]<sub>2</sub>·2C<sub>6</sub>H<sub>14</sub>O<sub>3</sub>  
*M<sub>r</sub>* = 1392.54  
 Monoclinic, *P2<sub>1</sub>/n*  
*a* = 15.5420 (3) Å  
*b* = 14.0010 (3) Å  
*c* = 16.3217 (3) Å  
 $\beta$  = 94.791 (1)°  
*V* = 3539.25 (12) Å<sup>3</sup>  
*Z* = 2

*F*(000) = 1468  
*D<sub>x</sub>* = 1.307 Mg m<sup>-3</sup>  
 Cu *K* $\alpha$  radiation,  $\lambda$  = 1.54178 Å  
 Cell parameters from 9398 reflections  
 $\theta$  = 4.9–68.2°  
 $\mu$  = 1.30 mm<sup>-1</sup>  
*T* = 105 K  
 Block, clear green  
 0.2 × 0.15 × 0.1 mm

### Data collection

Bruker Photon100 CMOS  
 diffractometer  
 Radiation source: Incoatec microfocus Cu  
 source  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2016)  
*T<sub>min</sub>* = 0.781, *T<sub>max</sub>* = 0.881

209288 measured reflections  
 6424 independent reflections  
 5989 reflections with *I* > 2 $\sigma$ (*I*)  
*R<sub>int</sub>* = 0.039  
 $\theta_{\max}$  = 68.3°,  $\theta_{\min}$  = 4.9°  
*h* = -18→18  
*k* = -16→16  
*l* = -19→19

### Refinement

Refinement on *F*<sup>2</sup>  
 Least-squares matrix: full  
*R*[*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.033  
*wR*(*F*<sup>2</sup>) = 0.089  
*S* = 1.06  
 6424 reflections  
 477 parameters

410 restraints  
 Primary atom site location: dual  
 Hydrogen site location: mixed  
 H atoms treated by a mixture of independent  
 and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 2.0003P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.28 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.40 \text{ e } \text{\AA}^{-3}$$

### Special details

**Experimental.** The X-ray intensities were collected on a Bruker D8 Venture diffractometer using a Photon 100 Detector. The data were reduced using APEX3 and absorption correction applied using SADABS (Bruker, 2016). The crystal structure was solved and refined using SHELXT and SHELXL via the Olex2 refinement package (Dolomanov *et al.*, 2009). Non-hydrogen atom positions were refined anisotropically.

**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.** RIGU restraint applied. Diglyme disorder modelled using DFIX and SADI restraints. The ADPs for both diglyme parts were constrained using EADP constraint.

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Cu1	0.54253 (2)	0.42405 (2)	0.48032 (2)	0.02442 (8)	
O1B	0.51049 (8)	0.45091 (8)	0.36430 (7)	0.0329 (3)	
O2B	0.43845 (8)	0.58088 (8)	0.39902 (7)	0.0326 (3)	
O1A	0.43605 (8)	0.35049 (8)	0.48736 (7)	0.0351 (3)	
O2A	0.36511 (7)	0.48032 (8)	0.52427 (7)	0.0331 (3)	
O10S	0.62229 (8)	0.30515 (9)	0.46326 (8)	0.0376 (3)	
N10B	0.37240 (10)	0.69540 (10)	0.28457 (9)	0.0362 (3)	
O2S1	0.7835 (9)	0.2813 (9)	0.5321 (12)	0.0540 (12)	0.666 (3)
C3B	0.46922 (10)	0.52671 (11)	0.34617 (9)	0.0265 (3)	
C9B	0.41162 (10)	0.63824 (11)	0.22997 (9)	0.0285 (3)	
C3A	0.37072 (10)	0.39031 (11)	0.51303 (9)	0.0284 (3)	
C4A	0.29745 (11)	0.32888 (12)	0.53288 (10)	0.0308 (3)	
C4B	0.45728 (10)	0.55460 (11)	0.25802 (9)	0.0269 (3)	
O5S1	0.73581 (16)	0.15001 (18)	0.40989 (17)	0.0438 (6)	0.666 (3)
C11B	0.33426 (11)	0.78619 (12)	0.27016 (10)	0.0312 (3)	
C8B	0.40932 (11)	0.65984 (13)	0.14555 (10)	0.0345 (4)	
H8B	0.3794	0.7152	0.1250	0.041*	
C5B	0.49629 (11)	0.49735 (13)	0.20199 (10)	0.0348 (4)	
H5B	0.5262	0.4414	0.2212	0.042*	
C5A	0.30263 (12)	0.23152 (12)	0.51507 (10)	0.0349 (4)	
H5A	0.3501	0.2088	0.4875	0.042*	
N10A	0.21962 (12)	0.45875 (13)	0.59054 (14)	0.0588 (5)	
C16A	0.17474 (12)	0.58519 (13)	0.67658 (11)	0.0367 (4)	
O8S1	0.5611 (3)	0.1715 (4)	0.3438 (5)	0.0604 (14)	0.666 (3)
C16B	0.36286 (11)	0.86224 (12)	0.32109 (10)	0.0322 (3)	
C15A	0.10932 (12)	0.64349 (13)	0.70386 (11)	0.0388 (4)	
C6B	0.49276 (13)	0.51950 (15)	0.11960 (11)	0.0447 (4)	
H6B	0.5192	0.4792	0.0821	0.054*	
C7B	0.44963 (13)	0.60229 (15)	0.09242 (11)	0.0429 (4)	
H7B	0.4481	0.6193	0.0360	0.052*	
C17A	0.26827 (12)	0.60465 (15)	0.70369 (12)	0.0441 (4)	

H17A	0.2948	0.6400	0.6605	0.066*	
H17B	0.2987	0.5440	0.7139	0.066*	
H17C	0.2720	0.6426	0.7543	0.066*	
C6A	0.24089 (12)	0.16743 (13)	0.53636 (11)	0.0400 (4)	
H6A	0.2446	0.1018	0.5222	0.048*	
C9A	0.22586 (11)	0.36315 (13)	0.57261 (12)	0.0395 (4)	
C17B	0.43678 (13)	0.85116 (14)	0.38602 (11)	0.0418 (4)	
H17D	0.4145	0.8498	0.4404	0.063*	
H17E	0.4766	0.9051	0.3830	0.063*	
H17F	0.4674	0.7914	0.3770	0.063*	
C11A	0.15206 (12)	0.50948 (14)	0.62317 (13)	0.0453 (4)	
C12B	0.26720 (12)	0.79882 (15)	0.20959 (12)	0.0439 (4)	
H12B	0.2476	0.7465	0.1760	0.053*	
C14A	0.02351 (12)	0.62150 (15)	0.68039 (12)	0.0447 (4)	
H14A	-0.0210	0.6595	0.7002	0.054*	
C18A	0.13044 (14)	0.72995 (17)	0.75676 (13)	0.0536 (5)	
H18A	0.1576	0.7096	0.8103	0.080*	
H18B	0.0773	0.7651	0.7647	0.080*	
H18C	0.1703	0.7714	0.7297	0.080*	
C15B	0.32210 (14)	0.95162 (14)	0.30921 (12)	0.0453 (4)	
C14B	0.25653 (16)	0.96269 (16)	0.24775 (13)	0.0561 (6)	
H14B	0.2299	1.0234	0.2395	0.067*	
C7A	0.17319 (12)	0.20059 (14)	0.57892 (11)	0.0422 (4)	
H7A	0.1319	0.1567	0.5964	0.051*	
C8A	0.16519 (13)	0.29586 (15)	0.59604 (13)	0.0473 (5)	
H8A	0.1177	0.3170	0.6243	0.057*	
C13B	0.22881 (14)	0.88734 (18)	0.19800 (13)	0.0561 (6)	
H13B	0.1835	0.8962	0.1559	0.067*	
C6S1	0.6846 (5)	0.0737 (6)	0.3762 (5)	0.0517 (16)	0.666 (3)
H6SA	0.6530	0.0435	0.4196	0.062*	0.666 (3)
H6SB	0.7220	0.0247	0.3535	0.062*	0.666 (3)
C13A	0.00184 (13)	0.54565 (16)	0.62903 (15)	0.0534 (5)	
H13A	-0.0572	0.5313	0.6143	0.064*	
C12A	0.06577 (13)	0.49027 (16)	0.59881 (16)	0.0569 (6)	
H12A	0.0509	0.4395	0.5617	0.068*	
C3S1	0.8407 (4)	0.2105 (3)	0.5096 (3)	0.0564 (12)	0.666 (3)
H3SA	0.8808	0.1936	0.5577	0.068*	0.666 (3)
H3SB	0.8753	0.2356	0.4661	0.068*	0.666 (3)
C7S1	0.6224 (2)	0.1110 (2)	0.3099 (2)	0.0487 (8)	0.666 (3)
H7SA	0.6538	0.1472	0.2697	0.058*	0.666 (3)
H7SB	0.5922	0.0570	0.2808	0.058*	0.666 (3)
C18B	0.3508 (2)	1.03494 (17)	0.36428 (18)	0.0787 (8)	
H18D	0.3400	1.0200	0.4212	0.118*	
H18E	0.3182	1.0922	0.3463	0.118*	
H18F	0.4126	1.0464	0.3609	0.118*	
C1S1	0.8212 (6)	0.3611 (4)	0.5730 (4)	0.0698 (15)	0.666 (3)
H1SA	0.8572	0.3952	0.5361	0.105*	0.666 (3)
H1SB	0.8571	0.3400	0.6219	0.105*	0.666 (3)

H1SC	0.7758	0.4037	0.5896	0.105*	0.666 (3)
C4S1	0.7934 (3)	0.1233 (3)	0.4788 (3)	0.0558 (10)	0.666 (3)
H4SA	0.8347	0.0746	0.4623	0.067*	0.666 (3)
H4SB	0.7605	0.0959	0.5226	0.067*	0.666 (3)
H10C	0.3857 (14)	0.6801 (16)	0.3367 (15)	0.049 (6)*	
H10D	0.2643 (16)	0.4898 (18)	0.5786 (15)	0.057 (7)*	
H10A	0.6808 (5)	0.2953 (16)	0.4844 (13)	0.064 (7)*	
H10B	0.6103 (14)	0.2545 (13)	0.4247 (13)	0.085 (9)*	
C9S2	0.4948 (9)	0.2144 (16)	0.3063 (12)	0.0550 (15)	0.31 (3)
H9SD	0.4759	0.1747	0.2586	0.082*	0.31 (3)
H9SE	0.4922	0.2819	0.2903	0.082*	0.31 (3)
H9SF	0.4568	0.2033	0.3503	0.082*	0.31 (3)
O2S2	0.795 (2)	0.274 (2)	0.536 (2)	0.0540 (12)	0.334 (3)
C3S2	0.8316 (8)	0.1859 (8)	0.5313 (7)	0.0564 (12)	0.334 (3)
H3SC	0.8115	0.1445	0.5750	0.068*	0.334 (3)
H3SD	0.8951	0.1922	0.5410	0.068*	0.334 (3)
C1S2	0.8244 (13)	0.3376 (10)	0.5961 (9)	0.0698 (15)	0.334 (3)
H1SD	0.7960	0.3995	0.5862	0.105*	0.334 (3)
H1SE	0.8870	0.3454	0.5949	0.105*	0.334 (3)
H1SF	0.8116	0.3132	0.6500	0.105*	0.334 (3)
C4S2	0.8103 (7)	0.1404 (7)	0.4509 (6)	0.0558 (10)	0.334 (3)
H4SC	0.8281	0.1827	0.4068	0.067*	0.334 (3)
H4SD	0.8426	0.0796	0.4483	0.067*	0.334 (3)
O5S2	0.7218 (4)	0.1224 (4)	0.4386 (3)	0.0438 (6)	0.334 (3)
C6S2	0.6944 (11)	0.0843 (14)	0.3610 (11)	0.0517 (16)	0.334 (3)
H6SC	0.7120	0.0165	0.3589	0.062*	0.334 (3)
H6SD	0.7230	0.1193	0.3180	0.062*	0.334 (3)
C7S2	0.6002 (5)	0.0912 (5)	0.3437 (5)	0.0487 (8)	0.334 (3)
H7SC	0.5813	0.0560	0.2927	0.058*	0.334 (3)
H7SD	0.5705	0.0637	0.3896	0.058*	0.334 (3)
O8S2	0.5806 (7)	0.1903 (9)	0.3344 (11)	0.0604 (14)	0.334 (3)
C9S1	0.5085 (5)	0.2183 (6)	0.2840 (7)	0.0550 (15)	0.69 (3)
H9SA	0.5442	0.2550	0.2486	0.082*	0.69 (3)
H9SB	0.4697	0.2617	0.3103	0.082*	0.69 (3)
H9SC	0.4743	0.1713	0.2508	0.082*	0.69 (3)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.03002 (14)	0.02114 (13)	0.02236 (13)	0.00405 (8)	0.00367 (9)	-0.00087 (8)
O1B	0.0443 (6)	0.0296 (6)	0.0245 (5)	0.0110 (5)	0.0006 (5)	-0.0010 (4)
O2B	0.0447 (7)	0.0288 (6)	0.0245 (5)	0.0108 (5)	0.0040 (5)	0.0000 (4)
O1A	0.0371 (6)	0.0271 (6)	0.0420 (6)	0.0001 (5)	0.0089 (5)	-0.0062 (5)
O2A	0.0346 (6)	0.0259 (6)	0.0394 (6)	-0.0001 (5)	0.0078 (5)	-0.0027 (5)
O10S	0.0403 (7)	0.0311 (6)	0.0403 (7)	0.0141 (5)	-0.0020 (5)	-0.0086 (5)
N10B	0.0532 (9)	0.0289 (7)	0.0262 (7)	0.0110 (6)	0.0012 (6)	0.0013 (6)
O2S1	0.045 (4)	0.046 (2)	0.066 (2)	0.0094 (16)	-0.020 (2)	-0.0047 (19)
C3B	0.0281 (7)	0.0246 (7)	0.0268 (7)	-0.0014 (6)	0.0016 (6)	-0.0018 (6)



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C9B	0.0307 (8)	0.0270 (8)	0.0273 (7)	-0.0023 (6)	-0.0005 (6)	-0.0005 (6)
C3A	0.0351 (8)	0.0281 (8)	0.0213 (7)	0.0004 (6)	-0.0015 (6)	-0.0016 (6)
C4A	0.0350 (8)	0.0298 (8)	0.0272 (8)	-0.0032 (6)	0.0004 (6)	-0.0011 (6)
C4B	0.0295 (7)	0.0265 (7)	0.0243 (7)	-0.0008 (6)	0.0000 (6)	-0.0008 (6)
O5S1	0.0477 (11)	0.0355 (14)	0.0483 (16)	0.0125 (10)	0.0050 (10)	-0.0008 (10)
C11B	0.0338 (8)	0.0309 (8)	0.0296 (8)	0.0056 (6)	0.0063 (6)	0.0038 (6)
C8B	0.0415 (9)	0.0342 (9)	0.0269 (8)	0.0021 (7)	-0.0024 (7)	0.0022 (7)
C5B	0.0409 (9)	0.0349 (9)	0.0281 (8)	0.0064 (7)	0.0003 (7)	-0.0022 (7)
C5A	0.0436 (9)	0.0321 (8)	0.0284 (8)	-0.0026 (7)	0.0001 (7)	-0.0021 (7)
N10A	0.0418 (9)	0.0365 (9)	0.1029 (16)	-0.0080 (7)	0.0353 (10)	-0.0175 (9)
C16A	0.0372 (9)	0.0356 (9)	0.0390 (9)	0.0052 (7)	0.0128 (7)	0.0097 (7)
O8S1	0.057 (2)	0.045 (2)	0.075 (2)	0.0121 (18)	-0.018 (2)	-0.0332 (19)
C16B	0.0368 (8)	0.0312 (8)	0.0297 (8)	0.0053 (7)	0.0099 (7)	0.0026 (6)
C15A	0.0424 (9)	0.0416 (10)	0.0337 (9)	0.0107 (8)	0.0103 (7)	0.0103 (7)
C6B	0.0567 (11)	0.0521 (11)	0.0254 (8)	0.0160 (9)	0.0036 (8)	-0.0046 (8)
C7B	0.0528 (11)	0.0512 (11)	0.0243 (8)	0.0080 (9)	0.0001 (7)	0.0024 (7)
C17A	0.0387 (9)	0.0484 (11)	0.0462 (11)	0.0061 (8)	0.0093 (8)	-0.0007 (9)
C6A	0.0521 (10)	0.0306 (9)	0.0364 (9)	-0.0079 (8)	-0.0010 (8)	-0.0018 (7)
C9A	0.0370 (9)	0.0341 (9)	0.0478 (10)	-0.0039 (7)	0.0062 (8)	-0.0050 (8)
C17B	0.0481 (10)	0.0396 (10)	0.0371 (9)	0.0009 (8)	-0.0005 (8)	-0.0044 (8)
C11A	0.0384 (9)	0.0359 (9)	0.0645 (12)	-0.0005 (8)	0.0205 (9)	-0.0007 (9)
C12B	0.0419 (10)	0.0491 (11)	0.0396 (10)	0.0082 (8)	-0.0038 (8)	-0.0009 (8)
C14A	0.0396 (10)	0.0490 (11)	0.0474 (10)	0.0120 (8)	0.0141 (8)	0.0103 (9)
C18A	0.0523 (12)	0.0632 (13)	0.0456 (11)	0.0199 (10)	0.0059 (9)	-0.0103 (10)
C15B	0.0596 (12)	0.0338 (9)	0.0444 (10)	0.0148 (8)	0.0160 (9)	0.0014 (8)
C14B	0.0713 (14)	0.0515 (12)	0.0467 (11)	0.0362 (11)	0.0115 (10)	0.0074 (9)
C7A	0.0441 (10)	0.0414 (10)	0.0403 (10)	-0.0143 (8)	-0.0004 (8)	0.0007 (8)
C8A	0.0400 (10)	0.0432 (10)	0.0604 (12)	-0.0096 (8)	0.0142 (9)	-0.0069 (9)
C13B	0.0518 (12)	0.0723 (14)	0.0433 (11)	0.0313 (11)	-0.0020 (9)	0.0054 (10)
C6S1	0.071 (2)	0.033 (2)	0.051 (3)	0.0145 (16)	0.006 (2)	-0.009 (2)
C13A	0.0347 (10)	0.0564 (13)	0.0707 (14)	-0.0004 (9)	0.0128 (9)	0.0044 (11)
C12A	0.0415 (10)	0.0480 (12)	0.0837 (16)	-0.0075 (9)	0.0195 (10)	-0.0120 (11)
C3S1	0.0391 (17)	0.053 (3)	0.075 (3)	0.0136 (18)	-0.0069 (19)	0.0068 (19)
C7S1	0.067 (2)	0.0370 (16)	0.042 (2)	0.0056 (13)	0.0058 (14)	-0.0119 (14)
C18B	0.123 (2)	0.0385 (12)	0.0743 (17)	0.0224 (14)	0.0046 (16)	-0.0143 (11)
C1S1	0.0702 (18)	0.057 (3)	0.076 (4)	0.001 (3)	-0.032 (3)	-0.005 (2)
C4S1	0.058 (2)	0.041 (2)	0.067 (3)	0.0176 (15)	-0.0042 (19)	0.0105 (18)
C9S2	0.057 (2)	0.0484 (16)	0.059 (4)	0.0007 (19)	-0.001 (2)	-0.009 (3)
O2S2	0.045 (4)	0.046 (2)	0.066 (2)	0.0094 (16)	-0.020 (2)	-0.0047 (19)
C3S2	0.0391 (17)	0.053 (3)	0.075 (3)	0.0136 (18)	-0.0069 (19)	0.0068 (19)
C1S2	0.0702 (18)	0.057 (3)	0.076 (4)	0.001 (3)	-0.032 (3)	-0.005 (2)
C4S2	0.058 (2)	0.041 (2)	0.067 (3)	0.0176 (15)	-0.0042 (19)	0.0105 (18)
O5S2	0.0477 (11)	0.0355 (14)	0.0483 (16)	0.0125 (10)	0.0050 (10)	-0.0008 (10)
C6S2	0.071 (2)	0.033 (2)	0.051 (3)	0.0145 (16)	0.006 (2)	-0.009 (2)
C7S2	0.067 (2)	0.0370 (16)	0.042 (2)	0.0056 (13)	0.0058 (14)	-0.0119 (14)
O8S2	0.057 (2)	0.045 (2)	0.075 (2)	0.0121 (18)	-0.018 (2)	-0.0332 (19)
C9S1	0.057 (2)	0.0484 (16)	0.059 (4)	0.0007 (19)	-0.001 (2)	-0.009 (3)

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*Geometric parameters (Å, °)*

Cu1—Cu1 <sup>i</sup>	2.6126 (4)	C11A—C12A	1.393 (3)
Cu1—O1B	1.9539 (11)	C12B—H12B	0.9500
Cu1—O2B <sup>i</sup>	1.9682 (11)	C12B—C13B	1.382 (3)
Cu1—O1A	1.9608 (12)	C14A—H14A	0.9500
Cu1—O2A <sup>i</sup>	1.9689 (11)	C14A—C13A	1.377 (3)
Cu1—O10S	2.1078 (11)	C18A—H18A	0.9800
O1B—C3B	1.2624 (19)	C18A—H18B	0.9800
O2B—Cu1 <sup>i</sup>	1.9682 (11)	C18A—H18C	0.9800
O2B—C3B	1.2715 (19)	C15B—C14B	1.378 (3)
O1A—C3A	1.260 (2)	C15B—C18B	1.517 (3)
O2A—Cu1 <sup>i</sup>	1.9690 (11)	C14B—H14B	0.9500
O2A—C3A	1.278 (2)	C14B—C13B	1.378 (3)
O10S—H10A	0.956 (3)	C7A—H7A	0.9500
O10S—H10B	0.956 (3)	C7A—C8A	1.371 (3)
N10B—C9B	1.377 (2)	C8A—H8A	0.9500
N10B—C11B	1.414 (2)	C13B—H13B	0.9500
N10B—H10C	0.88 (2)	C6S1—H6SA	0.9900
O2S1—C3S1	1.401 (10)	C6S1—H6SB	0.9900
O2S1—C1S1	1.404 (10)	C6S1—C7S1	1.484 (8)
C3B—C4B	1.487 (2)	C13A—H13A	0.9500
C9B—C4B	1.425 (2)	C13A—C12A	1.383 (3)
C9B—C8B	1.408 (2)	C12A—H12A	0.9500
C3A—C4A	1.484 (2)	C3S1—H3SA	0.9900
C4A—C5A	1.397 (2)	C3S1—H3SB	0.9900
C4A—C9A	1.418 (2)	C3S1—C4S1	1.490 (7)
C4B—C5B	1.392 (2)	C7S1—H7SA	0.9900
O5S1—C6S1	1.416 (8)	C7S1—H7SB	0.9900
O5S1—C4S1	1.428 (5)	C18B—H18D	0.9800
C11B—C16B	1.400 (2)	C18B—H18E	0.9800
C11B—C12B	1.387 (2)	C18B—H18F	0.9800
C8B—H8B	0.9500	C1S1—H1SA	0.9800
C8B—C7B	1.373 (3)	C1S1—H1SB	0.9800
C5B—H5B	0.9500	C1S1—H1SC	0.9800
C5B—C6B	1.377 (2)	C4S1—H4SA	0.9900
C5A—H5A	0.9500	C4S1—H4SB	0.9900
C5A—C6A	1.379 (3)	C9S2—H9SD	0.9800
N10A—C9A	1.375 (2)	C9S2—H9SE	0.9800
N10A—C11A	1.409 (2)	C9S2—H9SF	0.9800
N10A—H10D	0.86 (2)	C9S2—O8S2	1.414 (14)
C16A—C15A	1.405 (2)	O2S2—C3S2	1.369 (19)
C16A—C17A	1.509 (3)	O2S2—C1S2	1.37 (2)
C16A—C11A	1.399 (3)	C3S2—H3SC	0.9900
O8S1—C7S1	1.421 (7)	C3S2—H3SD	0.9900
O8S1—C9S1	1.383 (8)	C3S2—C4S2	1.471 (15)
C16B—C17B	1.505 (2)	C1S2—H1SD	0.9800
C16B—C15B	1.409 (2)	C1S2—H1SE	0.9800

C15A—C14A	1.391 (3)	C1S2—H1SF	0.9800
C15A—C18A	1.507 (3)	C4S2—H4SC	0.9900
C6B—H6B	0.9500	C4S2—H4SD	0.9900
C6B—C7B	1.393 (3)	C4S2—O5S2	1.397 (12)
C7B—H7B	0.9500	O5S2—C6S2	1.407 (17)
C17A—H17A	0.9800	C6S2—H6SC	0.9900
C17A—H17B	0.9800	C6S2—H6SD	0.9900
C17A—H17C	0.9800	C6S2—C7S2	1.471 (17)
C6A—H6A	0.9500	C7S2—H7SC	0.9900
C6A—C7A	1.388 (3)	C7S2—H7SD	0.9900
C9A—C8A	1.408 (3)	C7S2—O8S2	1.426 (14)
C17B—H17D	0.9800	C9S1—H9SA	0.9800
C17B—H17E	0.9800	C9S1—H9SB	0.9800
C17B—H17F	0.9800	C9S1—H9SC	0.9800
O1B—Cu1—Cu1 <sup>i</sup>	89.34 (3)	H18A—C18A—H18C	109.5
O1B—Cu1—O2B <sup>i</sup>	168.92 (5)	H18B—C18A—H18C	109.5
O1B—Cu1—O1A	90.57 (5)	C16B—C15B—C18B	119.69 (19)
O1B—Cu1—O2A <sup>i</sup>	87.70 (5)	C14B—C15B—C16B	119.80 (19)
O1B—Cu1—O10S	97.42 (5)	C14B—C15B—C18B	120.51 (19)
O2B <sup>i</sup> —Cu1—Cu1 <sup>i</sup>	79.58 (3)	C15B—C14B—H14B	119.4
O2B <sup>i</sup> —Cu1—O2A <sup>i</sup>	90.74 (5)	C15B—C14B—C13B	121.24 (18)
O2B <sup>i</sup> —Cu1—O10S	93.65 (5)	C13B—C14B—H14B	119.4
O1A—Cu1—Cu1 <sup>i</sup>	88.07 (3)	C6A—C7A—H7A	119.6
O1A—Cu1—O2B <sup>i</sup>	88.85 (5)	C8A—C7A—C6A	120.85 (17)
O1A—Cu1—O2A <sup>i</sup>	168.82 (5)	C8A—C7A—H7A	119.6
O1A—Cu1—O10S	95.82 (5)	C9A—C8A—H8A	119.3
O2A <sup>i</sup> —Cu1—Cu1 <sup>i</sup>	80.87 (3)	C7A—C8A—C9A	121.44 (18)
O2A <sup>i</sup> —Cu1—O10S	95.36 (5)	C7A—C8A—H8A	119.3
O10S—Cu1—Cu1 <sup>i</sup>	172.15 (4)	C12B—C13B—H13B	120.1
C3B—O1B—Cu1	118.18 (10)	C14B—C13B—C12B	119.72 (19)
C3B—O2B—Cu1 <sup>i</sup>	128.64 (10)	C14B—C13B—H13B	120.1
C3A—O1A—Cu1	119.63 (10)	O5S1—C6S1—H6SA	109.8
C3A—O2A—Cu1 <sup>i</sup>	127.34 (10)	O5S1—C6S1—H6SB	109.8
Cu1—O10S—H10A	128.2 (12)	O5S1—C6S1—C7S1	109.2 (6)
Cu1—O10S—H10B	126.1 (13)	H6SA—C6S1—H6SB	108.3
H10A—O10S—H10B	104.9 (7)	C7S1—C6S1—H6SA	109.8
C9B—N10B—C11B	128.08 (14)	C7S1—C6S1—H6SB	109.8
C9B—N10B—H10C	113.6 (14)	C14A—C13A—H13A	119.9
C11B—N10B—H10C	116.1 (15)	C14A—C13A—C12A	120.19 (19)
C3S1—O2S1—C1S1	116.0 (10)	C12A—C13A—H13A	119.9
O1B—C3B—O2B	123.71 (14)	C11A—C12A—H12A	120.2
O1B—C3B—C4B	117.85 (13)	C13A—C12A—C11A	119.6 (2)
O2B—C3B—C4B	118.43 (13)	C13A—C12A—H12A	120.2
N10B—C9B—C4B	120.34 (14)	O2S1—C3S1—H3SA	109.4
N10B—C9B—C8B	122.13 (15)	O2S1—C3S1—H3SB	109.4
C8B—C9B—C4B	117.53 (15)	O2S1—C3S1—C4S1	111.3 (7)
O1A—C3A—O2A	123.41 (15)	H3SA—C3S1—H3SB	108.0

O1A—C3A—C4A	118.05 (14)	C4S1—C3S1—H3SA	109.4
O2A—C3A—C4A	118.53 (14)	C4S1—C3S1—H3SB	109.4
C5A—C4A—C3A	117.47 (15)	O8S1—C7S1—C6S1	110.1 (5)
C5A—C4A—C9A	119.10 (16)	O8S1—C7S1—H7SA	109.6
C9A—C4A—C3A	123.33 (15)	O8S1—C7S1—H7SB	109.6
C9B—C4B—C3B	123.03 (14)	C6S1—C7S1—H7SA	109.6
C5B—C4B—C3B	117.28 (14)	C6S1—C7S1—H7SB	109.6
C5B—C4B—C9B	119.64 (14)	H7SA—C7S1—H7SB	108.1
C6S1—O5S1—C4S1	113.8 (4)	C15B—C18B—H18D	109.5
C16B—C11B—N10B	118.49 (15)	C15B—C18B—H18E	109.5
C12B—C11B—N10B	120.86 (16)	C15B—C18B—H18F	109.5
C12B—C11B—C16B	120.58 (16)	H18D—C18B—H18E	109.5
C9B—C8B—H8B	119.5	H18D—C18B—H18F	109.5
C7B—C8B—C9B	121.08 (16)	H18E—C18B—H18F	109.5
C7B—C8B—H8B	119.5	O2S1—C1S1—H1SA	109.5
C4B—C5B—H5B	119.1	O2S1—C1S1—H1SB	109.5
C6B—C5B—C4B	121.86 (16)	O2S1—C1S1—H1SC	109.5
C6B—C5B—H5B	119.1	H1SA—C1S1—H1SB	109.5
C4A—C5A—H5A	119.0	H1SA—C1S1—H1SC	109.5
C6A—C5A—C4A	121.92 (17)	H1SB—C1S1—H1SC	109.5
C6A—C5A—H5A	119.0	O5S1—C4S1—C3S1	108.0 (4)
C9A—N10A—C11A	129.73 (17)	O5S1—C4S1—H4SA	110.1
C9A—N10A—H10D	111.9 (16)	O5S1—C4S1—H4SB	110.1
C11A—N10A—H10D	118.3 (16)	C3S1—C4S1—H4SA	110.1
C15A—C16A—C17A	120.49 (17)	C3S1—C4S1—H4SB	110.1
C11A—C16A—C15A	119.10 (17)	H4SA—C4S1—H4SB	108.4
C11A—C16A—C17A	120.41 (16)	H9SD—C9S2—H9SE	109.5
C9S1—O8S1—C7S1	112.6 (8)	H9SD—C9S2—H9SF	109.5
C11B—C16B—C17B	121.71 (15)	H9SE—C9S2—H9SF	109.5
C11B—C16B—C15B	118.49 (16)	O8S2—C9S2—H9SD	109.5
C15B—C16B—C17B	119.78 (17)	O8S2—C9S2—H9SE	109.5
C16A—C15A—C18A	121.28 (17)	O8S2—C9S2—H9SF	109.5
C14A—C15A—C16A	119.14 (18)	C3S2—O2S2—C1S2	121 (2)
C14A—C15A—C18A	119.57 (17)	O2S2—C3S2—H3SC	109.1
C5B—C6B—H6B	120.7	O2S2—C3S2—H3SD	109.1
C5B—C6B—C7B	118.52 (17)	O2S2—C3S2—C4S2	112.4 (15)
C7B—C6B—H6B	120.7	H3SC—C3S2—H3SD	107.9
C8B—C7B—C6B	121.35 (16)	C4S2—C3S2—H3SC	109.1
C8B—C7B—H7B	119.3	C4S2—C3S2—H3SD	109.1
C6B—C7B—H7B	119.3	O2S2—C1S2—H1SD	109.5
C16A—C17A—H17A	109.5	O2S2—C1S2—H1SE	109.5
C16A—C17A—H17B	109.5	O2S2—C1S2—H1SF	109.5
C16A—C17A—H17C	109.5	H1SD—C1S2—H1SE	109.5
H17A—C17A—H17B	109.5	H1SD—C1S2—H1SF	109.5
H17A—C17A—H17C	109.5	H1SE—C1S2—H1SF	109.5
H17B—C17A—H17C	109.5	C3S2—C4S2—H4SC	109.5
C5A—C6A—H6A	120.6	C3S2—C4S2—H4SD	109.5
C5A—C6A—C7A	118.74 (17)	H4SC—C4S2—H4SD	108.1

C7A—C6A—H6A	120.6	O5S2—C4S2—C3S2	110.6 (9)
N10A—C9A—C4A	119.92 (16)	O5S2—C4S2—H4SC	109.5
N10A—C9A—C8A	122.18 (17)	O5S2—C4S2—H4SD	109.5
C8A—C9A—C4A	117.82 (17)	C4S2—O5S2—C6S2	114.8 (10)
C16B—C17B—H17D	109.5	O5S2—C6S2—H6SC	109.3
C16B—C17B—H17E	109.5	O5S2—C6S2—H6SD	109.3
C16B—C17B—H17F	109.5	O5S2—C6S2—C7S2	111.7 (14)
H17D—C17B—H17E	109.5	H6SC—C6S2—H6SD	107.9
H17D—C17B—H17F	109.5	C7S2—C6S2—H6SC	109.3
H17E—C17B—H17F	109.5	C7S2—C6S2—H6SD	109.3
C16A—C11A—N10A	117.43 (17)	C6S2—C7S2—H7SC	110.4
C12A—C11A—N10A	121.68 (19)	C6S2—C7S2—H7SD	110.4
C12A—C11A—C16A	120.71 (18)	H7SC—C7S2—H7SD	108.6
C11B—C12B—H12B	119.9	O8S2—C7S2—C6S2	106.5 (10)
C13B—C12B—C11B	120.15 (19)	O8S2—C7S2—H7SC	110.4
C13B—C12B—H12B	119.9	O8S2—C7S2—H7SD	110.4
C15A—C14A—H14A	119.4	C9S2—O8S2—C7S2	117.0 (13)
C13A—C14A—C15A	121.22 (18)	O8S1—C9S1—H9SA	109.5
C13A—C14A—H14A	119.4	O8S1—C9S1—H9SB	109.5
C15A—C18A—H18A	109.5	O8S1—C9S1—H9SC	109.5
C15A—C18A—H18B	109.5	H9SA—C9S1—H9SB	109.5
C15A—C18A—H18C	109.5	H9SA—C9S1—H9SC	109.5
H18A—C18A—H18B	109.5	H9SB—C9S1—H9SC	109.5
Cu1—O1B—C3B—O2B	-8.6 (2)	C5B—C6B—C7B—C8B	-1.7 (3)
Cu1—O1B—C3B—C4B	170.41 (10)	C5A—C4A—C9A—N10A	-179.92 (18)
Cu1 <sup>i</sup> —O2B—C3B—O1B	9.2 (2)	C5A—C4A—C9A—C8A	3.2 (3)
Cu1 <sup>i</sup> —O2B—C3B—C4B	-169.80 (10)	C5A—C6A—C7A—C8A	3.2 (3)
Cu1—O1A—C3A—O2A	10.2 (2)	N10A—C9A—C8A—C7A	-178.9 (2)
Cu1—O1A—C3A—C4A	-168.37 (10)	N10A—C11A—C12A—C13A	-176.3 (2)
Cu1 <sup>i</sup> —O2A—C3A—O1A	-8.7 (2)	C16A—C15A—C14A—C13A	-2.0 (3)
Cu1 <sup>i</sup> —O2A—C3A—C4A	169.93 (10)	C16A—C11A—C12A—C13A	-1.2 (3)
O1B—C3B—C4B—C9B	179.72 (14)	C16B—C11B—C12B—C13B	1.1 (3)
O1B—C3B—C4B—C5B	-3.1 (2)	C16B—C15B—C14B—C13B	1.0 (3)
O2B—C3B—C4B—C9B	-1.2 (2)	C15A—C16A—C11A—N10A	173.66 (18)
O2B—C3B—C4B—C5B	176.01 (15)	C15A—C16A—C11A—C12A	-1.6 (3)
O1A—C3A—C4A—C5A	-5.4 (2)	C15A—C14A—C13A—C12A	-0.8 (3)
O1A—C3A—C4A—C9A	171.06 (16)	C17A—C16A—C15A—C14A	-177.50 (17)
O2A—C3A—C4A—C5A	175.93 (14)	C17A—C16A—C15A—C18A	3.5 (3)
O2A—C3A—C4A—C9A	-7.6 (2)	C17A—C16A—C11A—N10A	-5.6 (3)
N10B—C9B—C4B—C3B	-3.1 (2)	C17A—C16A—C11A—C12A	179.1 (2)
N10B—C9B—C4B—C5B	179.74 (15)	C6A—C7A—C8A—C9A	-1.2 (3)
N10B—C9B—C8B—C7B	179.34 (17)	C9A—C4A—C5A—C6A	-1.2 (3)
N10B—C11B—C16B—C17B	4.4 (2)	C9A—N10A—C11A—C16A	144.7 (2)
N10B—C11B—C16B—C15B	-177.08 (16)	C9A—N10A—C11A—C12A	-40.0 (4)
N10B—C11B—C12B—C13B	177.97 (18)	C17B—C16B—C15B—C14B	177.61 (19)
O2S1—C3S1—C4S1—O5S1	58.7 (11)	C17B—C16B—C15B—C18B	-2.4 (3)
C3B—C4B—C5B—C6B	-176.76 (17)	C11A—N10A—C9A—C4A	174.3 (2)

C9B—N10B—C11B—C16B	-124.92 (18)	C11A—N10A—C9A—C8A	-8.9 (4)
C9B—N10B—C11B—C12B	58.1 (3)	C11A—C16A—C15A—C14A	3.2 (3)
C9B—C4B—C5B—C6B	0.5 (3)	C11A—C16A—C15A—C18A	-175.80 (18)
C9B—C8B—C7B—C6B	1.3 (3)	C12B—C11B—C16B—C17B	-178.61 (17)
C3A—C4A—C5A—C6A	175.39 (15)	C12B—C11B—C16B—C15B	-0.1 (3)
C3A—C4A—C9A—N10A	3.7 (3)	C14A—C13A—C12A—C11A	2.4 (4)
C3A—C4A—C9A—C8A	-173.24 (17)	C18A—C15A—C14A—C13A	177.00 (19)
C4A—C5A—C6A—C7A	-2.0 (3)	C15B—C14B—C13B—C12B	0.0 (4)
C4A—C9A—C8A—C7A	-2.0 (3)	C6S1—O5S1—C4S1—C3S1	-178.1 (5)
C4B—C9B—C8B—C7B	0.0 (3)	C18B—C15B—C14B—C13B	-179.0 (2)
C4B—C5B—C6B—C7B	0.8 (3)	C1S1—O2S1—C3S1—C4S1	171.1 (12)
O5S1—C6S1—C7S1—O8S1	-67.3 (7)	C4S1—O5S1—C6S1—C7S1	175.2 (4)
C11B—N10B—C9B—C4B	171.23 (16)	O2S2—C3S2—C4S2—O5S2	-64 (2)
C11B—N10B—C9B—C8B	-8.1 (3)	C3S2—C4S2—O5S2—C6S2	176.1 (11)
C11B—C16B—C15B—C14B	-0.9 (3)	C1S2—O2S2—C3S2—C4S2	-163 (3)
C11B—C16B—C15B—C18B	179.1 (2)	C4S2—O5S2—C6S2—C7S2	-164.7 (10)
C11B—C12B—C13B—C14B	-1.0 (3)	O5S2—C6S2—C7S2—O8S2	68.1 (17)
C8B—C9B—C4B—C3B	176.22 (15)	C6S2—C7S2—O8S2—C9S2	171.6 (16)
C8B—C9B—C4B—C5B	-0.9 (2)	C9S1—O8S1—C7S1—C6S1	172.0 (6)

Symmetry code: (i)  $-x+1, -y+1, -z+1$ .

*Hydrogen-bond geometry* ( $\text{\AA}$ ,  $^\circ$ )

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N10A—H10D $\cdots$ O2A	0.86 (3)	1.86 (3)	2.604 (2)	143 (2)
N10B—H10C $\cdots$ O2B	0.89 (2)	1.87 (2)	2.6065 (18)	139 (2)