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# Tetra-*O*-4-methylphenylsulfonylpentaerythritol

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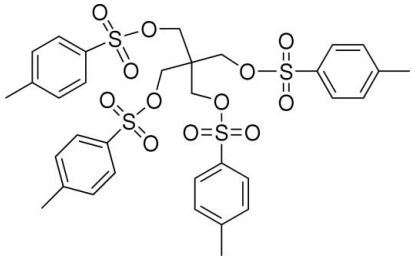
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.044; $wR$ factor = 0.120; data-to-parameter ratio = 22.6.

In the title molecule (systematic name: methanetetrayltetramethylene tetra-*p*-toluenesulfonate), $C_{33}H_{36}O_{12}S_4$, the central C atom and the S atoms exhibit distorted tetrahedral configurations. The aromatic rings in opposite arms are nearly parallel to each other, with a dihedral angle of 10.26 (8) or 3.45 (9)°. The molecules are linked into a two-dimensional network parallel to the *bc* plane by weak C—H···O hydrogen bonds, $\pi$–$\pi$ [centroid–centroid distance = 3.5806 (12) Å] and S—O···$\pi$ [O···centroid = 3.1455 (15) Å and S—O···centroid = 122.41 (7)°] intermolecular interactions. Intramolecular C—H···O hydrogen bonds are also present.

## Related literature

For bond-length data, see: Allen *et al.* (1987). For a related structure, see: Li *et al.* (2008). For general background and applications of pentaerythritol derivatives, see: Constable *et al.* (1998); Fundueanu *et al.* (1998); Jiang *et al.* (2002); Kim *et al.* (2000); Luo & Chen (2001); Mischiati *et al.* (2001); Oike *et al.* (2001).



## Experimental

### Crystal data

$C_{33}H_{36}O_{12}S_4$
$M_r$ = 752.86
Monoclinic, $P2_1/c$
$a$ = 13.2983 (2) Å
$b$ = 18.0368 (2) Å
$c$ = 15.4181 (2) Å
$\beta$ = 110.653 (1)°
$V$ = 3460.50 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.34 mm$^{-1}$
$T$ = 100.0 (1) K
0.47 × 0.41 × 0.16 mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.857, $T_{max}$ = 0.949
45048 measured reflections
10090 independent reflections
7927 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.119
$S$ = 1.04
10090 reflections
446 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.66 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.42 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C2—H2*C*···O4 | 0.97 | 2.48 | 2.849 (2) | 102 |
| C3—H3*B*···O6 | 0.97 | 2.47 | 2.905 (2) | 107 |
| C3—H3*B*···O7 | 0.97 | 2.55 | 2.876 (2) | 100 |
| C3—H3*C*···O9$^{i}$ | 0.97 | 2.46 | 3.433 (2) | 175 |
| C4—H4*A*···O4 | 0.97 | 2.55 | 2.879 (2) | 100 |
| C5—H5*B*···O12 | 0.97 | 2.44 | 2.888 (2) | 107 |
| C5—H5*C*···O7 | 0.97 | 2.49 | 2.8396 (19) | 101 |
| C7—H7*A*···O2 | 0.93 | 2.58 | 2.937 (2) | 103 |
| C8—H8*B*···O11$^{ii}$ | 0.93 | 2.52 | 3.140 (2) | 124 |
| C10—H10*A*···O6$^{i}$ | 0.93 | 2.41 | 3.257 (2) | 151 |
| C18—H18*A*···O6 | 0.93 | 2.59 | 2.932 (2) | 103 |
| C22—H22*A*···O12$^{iii}$ | 0.93 | 2.52 | 3.154 (2) | 126 |
| C25—H25*A*···O8 | 0.93 | 2.56 | 2.924 (2) | 104 |
| C28—H28*A*···O12 | 0.93 | 2.54 | 2.905 (2) | 104 |
| C29—H29*A*···O8$^{iv}$ | 0.93 | 2.42 | 3.334 (2) | 165 |
| C31—H31*A*···O12$^{iii}$ | 0.93 | 2.53 | 3.209 (2) | 130 |

Symmetry codes: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x, -y+1, -z+1$; (iii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2625).

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## References


Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–S19.

Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Constable, E. C., Housecroft, C. E., Cattalini, M. & Phillips, D. (1998). *New J. Chem.* pp. 193–200.

Fundueanu, G., Esposito, E., Mihai, D., Carpov, A., Desbrieres, J., Rinaudo, M. & Nastruzzi, C. (1998). *Int. J. Pharm.* **170**, 11–21.

Jiang, H., Lee, S. J. & Lin, W. (2002). *Org. Lett.* **4**, 2149–2152.

Kim, J., Leong, A. J., Lindoy, L. F., Kim, J., Nachbaur, J., Nezhadali, A., Rounaghi, G. & Wei, G. (2000). *J. Chem. Soc. Dalton Trans.* pp. 3453–3459.

Li, S.-X., Li, H.-M., Lu, Z.-L., Fun, H.-K. & Chantrapromma, S. (2008). *Acta Cryst.* **E64**, o1472–o1473.

Luo, F. T. & Chen, C. H. (2001). *Heterocycles*, **55**, 1663–1678.

Mischiati, C., Jeang, K.-T., Feriotto, G., Breda, L., Borgatti, M., Bianchi, N. & Gambari, R. (2001). *Antisense Nucleic Acid Drug Dev.* **11**, 209–217.

Oike, H., Hamada, M., Eguchi, S., Danda, Y. & Tezuka, Y. (2001). *Macromolecules*, **34**, 2776–2782.

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

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

# supporting information

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## Tetra-*O*-4-methylphenylsulfonylpentaerythritol

**Shu-Xian Li, Lin Zhu, Hoong-Kun Fun and Suchada Chantrapromma**

### S1. Comment

Pentaerythritol is a valuable starting point for building complex molecular and supramolecular structures due to its symmetric four-armed geometry and is widely used in macromolecular chemistry (Oike *et al.*, 2001), medicinal chemistry (Mischiati *et al.*, 2001; Fundueanu *et al.*, 1998), in the construction of dendrimers (Jiang *et al.*, 2002; Constable *et al.*, 1998) and other applications (Kim *et al.*, 2000; Luo & Chen, 2001). To explore the potential of the pentaerythritol unit in supramolecular chemistry, we report herein the synthesis and crystal structure of tetra-*O*-(4-methylphenylsulfonyl)pentaerythritol, the title compound.

In the title molecule (Fig. 1), atoms C1, S1, S2, S3 and S4 exhibit the usual distorted tetrahedral configuration. The aromatic rings in opposite arms of the molecule are nearly parallel to each other; the dihedral angles between the C6–C11 (A) and C20–C25 (B) benzene rings is 10.26 (8)° and that between the C13–C18 (C) and C27–C32 (D) benzene rings is 3.45 (9)°. The dihedral angle between the adjacent benzene rings are: A/C 49.67 (9)°, A/D 52.93 (9)°, B/C 53.20 (9)° and B/D 56.15 (9)°. The O1/O7/C1/C2/C4 plane (r.m.s. deviation 0.039 Å) forms dihedral angles of 81.59 (5)° and 84.85 (5)°, respectively, with the rings A and B. The benzene rings C and D form dihedral angles of 59.75 (5)° and 62.82 (5)°, respectively, with the O4/O10/C1/C3/C5 plane. The conformations of the four 4-methylphenylsulfonyl groups with respect to the pentaerythritol unit (C1–C5/O1/O4/O7/O10) can be indicated by torsion angles S1—O1—C2—C1 = -175.72 (10)°, S2—O4—C3—C1 = 154.00 (10)°, S3—O7—C4—C1 = -179.78 (10)° and S4—O10—C5—C1 = 154.75 (10)°. Bond lengths and angles in the title molecule are in normal ranges (Allen *et al.*, 1987) and comparable to those in a related structure (Li *et al.*, 2008).

In the crystal packing (Fig. 2), the molecules are linked into a two-dimensional network parallel to the *bc* plane by weak C—H···O hydrogen bonds (Table 1). In addition, $\pi$-$\pi$ interactions are observed between C13-C18 (centroid Cg1) and C27-C32 (centroid Cg2) benzene rings at (x, y, z) and (1+x, y, z), respectively, with centroid-centroid distance of 3.5806 (12) Å. Also, an S—O···$\pi$ intermolecular interaction is observed [O3···Cg2$^{i}$ = 3.1455 (15) Å and S1—O3···Cg2$^{i}$ = 122.41 (7)°; the symmetry code is given in Table 1].

### S2. Experimental

The title compound was synthesized by dissolving pentaerythritol (1.36 g, 10.0 mmol) in dry pyridine (80 ml) and tosyl chloride (9.5 g, 50.0 mmol) was then added. The reaction mixture was stirred for 24 h at room temperature, after which it was poured into ice-water (250 ml) containing 1 M HCl and extracted with $CH_2Cl_2$ (80 × 3 ml). The organic layer was washed with water (60 × 2 ml), dried with $MgSO_4$ and concentrated. The solid residue was recrystallized from ethanol to afford the desired compound as a white solid (6.42 g, yield: 90%). Block-shaped colourless single crystals of the title compound suitable for *X*-ray structure determination were recrystallized from ethanol by slow evaporation of the solvent in the open air at room temperature (m.p. 423 K).

### S3. Refinement

All H atoms were placed in calculated positions, with C-H = 0.93 Å, $U_{iso}$ = 1.2$U_{eq}$(C) for aromatic, C-H = 0.97 Å, $U_{iso}$ = 1.2$U_{eq}$(C) for $CH_2$ and C-H = 0.96 Å, $U_{iso}$ = 1.5$U_{eq}$(C) for $CH_3$ atoms. A rotating group model was used for the methyl groups.

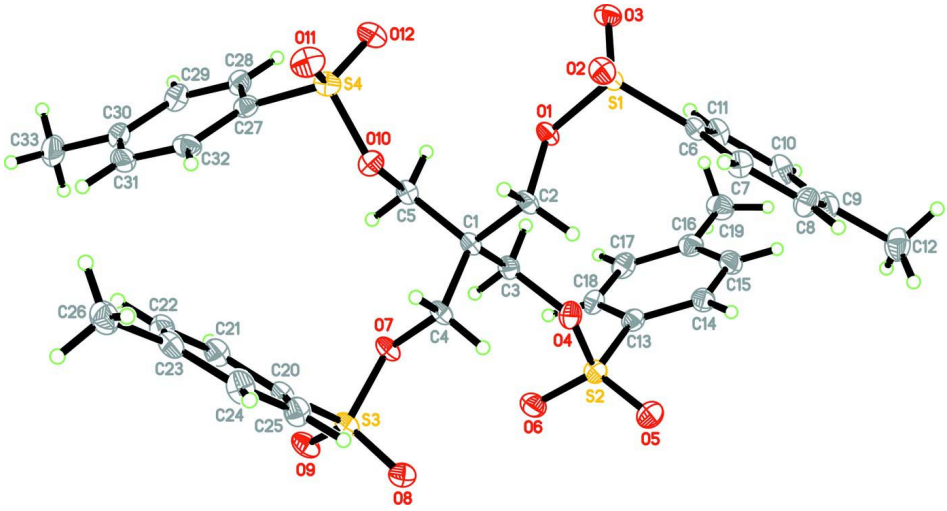


**Figure 1**

The molecular structure of the title compound, showing 40% probability displacement ellipsoids and the atomic numbering.

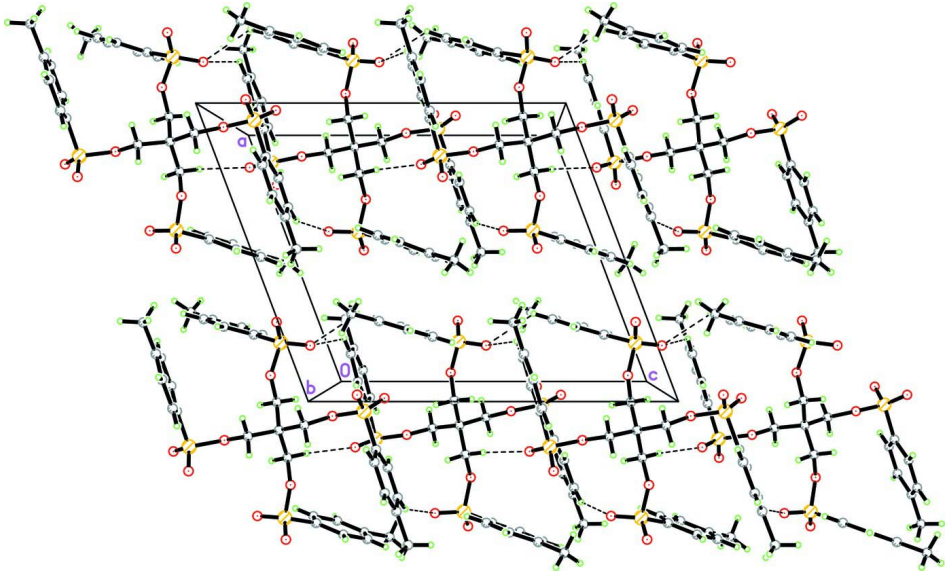


**Figure 2**

The crystal packing of the title compound, viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

**methanetetrayltetramethylene tetra-p-toluenesulfonate**

*Crystal data*

$C_{33}H_{36}O_{12}S_4$
$M_r$ = 752.86

Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

$a$ = 13.2983 (2) Å
$b$ = 18.0368 (2) Å
$c$ = 15.4181 (2) Å
$\beta$ = 110.653 (1)°
$V$ = 3460.50 (8) Å$^3$
$Z$ = 4
$F$(000) = 1576
$D_x$ = 1.445 Mg m$^{-3}$

Melting point: 423 K
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 10090 reflections
$\theta$ = 1.8–30.0°
$\mu$ = 0.34 mm$^{-1}$
$T$ = 100 K
Block, colourless
0.47 × 0.41 × 0.16 mm

*Data collection*

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.33 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.857, $T_{max}$ = 0.949

45048 measured reflections
10090 independent reflections
7927 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039
$\theta_{max}$ = 30.0°, $\theta_{min}$ = 1.8°
$h$ = −18→17
$k$ = −25→25
$l$ = −21→21

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.119
$S$ = 1.04
10090 reflections
446 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0595P)^2 + 1.2746P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.66 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.42 e Å$^{-3}$

*Special details*

**Experimental**. The low-temparture data was collected with the Oxford Cryosystem Cobra low-temperature attachment.

**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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.04280 (3) | 0.38393 (2) | 0.37155 (3) | 0.01965 (9) |
| S2 | 0.41959 (4) | 0.31806 (2) | 0.71340 (3) | 0.02583 (10) |
| S3 | 0.16570 (3) | 0.37598 (2) | 0.89436 (3) | 0.02097 (9) |
| S4 | −0.18947 (4) | 0.29379 (2) | 0.54246 (3) | 0.02429 (10) |
| O1 | 0.06272 (10) | 0.34535 (6) | 0.46843 (7) | 0.0207 (2) |
| O2 | −0.01854 (10) | 0.45006 (6) | 0.36647 (8) | 0.0249 (2) |
| O3 | 0.00233 (10) | 0.32556 (7) | 0.30634 (8) | 0.0267 (3) |

| | | | | |
|---|---|---|---|---|
| O4 | 0.30102 (10) | 0.34530 (6) | 0.65781 (9) | 0.0256 (3) |
| O5 | 0.48315 (12) | 0.38305 (7) | 0.72159 (10) | 0.0347 (3) |
| O6 | 0.41903 (11) | 0.28056 (7) | 0.79505 (9) | 0.0323 (3) |
| O7 | 0.14708 (10) | 0.33953 (6) | 0.79639 (7) | 0.0213 (2) |
| O8 | 0.24146 (10) | 0.43489 (6) | 0.90850 (8) | 0.0256 (3) |
| O9 | 0.18879 (11) | 0.31437 (6) | 0.95619 (8) | 0.0280 (3) |
| O10 | −0.07710 (10) | 0.33045 (6) | 0.60052 (8) | 0.0237 (2) |
| O11 | −0.26269 (11) | 0.35436 (7) | 0.52419 (10) | 0.0334 (3) |
| O12 | −0.17766 (11) | 0.25301 (7) | 0.46728 (8) | 0.0302 (3) |
| C1 | 0.11235 (13) | 0.34044 (8) | 0.63322 (10) | 0.0189 (3) |
| C2 | 0.08925 (14) | 0.39261 (8) | 0.55016 (11) | 0.0205 (3) |
| H2B | 0.0296 | 0.4252 | 0.5457 | 0.025* |
| H2C | 0.1518 | 0.4227 | 0.5563 | 0.025* |
| C3 | 0.21256 (13) | 0.29377 (8) | 0.64564 (12) | 0.0213 (3) |
| H3B | 0.2282 | 0.2619 | 0.6995 | 0.026* |
| H3C | 0.2015 | 0.2629 | 0.5915 | 0.026* |
| C4 | 0.12796 (14) | 0.38928 (8) | 0.71795 (11) | 0.0203 (3) |
| H4A | 0.1888 | 0.4222 | 0.7284 | 0.024* |
| H4B | 0.0643 | 0.4191 | 0.7090 | 0.024* |
| C5 | 0.01947 (13) | 0.28597 (8) | 0.61833 (11) | 0.0207 (3) |
| H5B | 0.0121 | 0.2538 | 0.5660 | 0.025* |
| H5C | 0.0322 | 0.2555 | 0.6730 | 0.025* |
| C6 | 0.17148 (13) | 0.40800 (8) | 0.37554 (10) | 0.0193 (3) |
| C7 | 0.20491 (14) | 0.48153 (9) | 0.38533 (12) | 0.0246 (3) |
| H7A | 0.1592 | 0.5190 | 0.3905 | 0.030* |
| C8 | 0.30696 (15) | 0.49811 (9) | 0.38722 (13) | 0.0284 (4) |
| H8B | 0.3296 | 0.5473 | 0.3936 | 0.034* |
| C9 | 0.37690 (14) | 0.44311 (10) | 0.37979 (12) | 0.0265 (3) |
| C10 | 0.34113 (15) | 0.36985 (9) | 0.36990 (12) | 0.0274 (4) |
| H10A | 0.3868 | 0.3324 | 0.3647 | 0.033* |
| C11 | 0.23934 (15) | 0.35158 (9) | 0.36764 (12) | 0.0249 (3) |
| H11B | 0.2165 | 0.3025 | 0.3610 | 0.030* |
| C12 | 0.48782 (16) | 0.46125 (12) | 0.38123 (15) | 0.0365 (4) |
| H12B | 0.5096 | 0.5085 | 0.4104 | 0.055* |
| H12C | 0.4874 | 0.4630 | 0.3189 | 0.055* |
| H12D | 0.5372 | 0.4238 | 0.4154 | 0.055* |
| C13 | 0.44820 (14) | 0.25381 (9) | 0.64082 (12) | 0.0250 (3) |
| C14 | 0.48460 (15) | 0.27930 (10) | 0.57213 (12) | 0.0279 (4) |
| H14A | 0.4921 | 0.3298 | 0.5641 | 0.033* |
| C15 | 0.50952 (15) | 0.22807 (10) | 0.51580 (13) | 0.0296 (4) |
| H15A | 0.5344 | 0.2447 | 0.4699 | 0.035* |
| C16 | 0.49800 (15) | 0.15206 (10) | 0.52657 (13) | 0.0290 (4) |
| C17 | 0.46100 (15) | 0.12852 (10) | 0.59613 (14) | 0.0306 (4) |
| H17A | 0.4530 | 0.0780 | 0.6042 | 0.037* |
| C18 | 0.43601 (14) | 0.17829 (9) | 0.65301 (13) | 0.0266 (3) |
| H18A | 0.4113 | 0.1617 | 0.6990 | 0.032* |
| C19 | 0.52492 (17) | 0.09697 (12) | 0.46446 (14) | 0.0370 (4) |
| H19A | 0.5668 | 0.0573 | 0.5013 | 0.056* |

| | | | | |
|---|---|---|---|---|
| H19B | 0.5654 | 0.1212 | 0.4320 | 0.056* |
| H19C | 0.4597 | 0.0773 | 0.4205 | 0.056* |
| C20 | 0.04014 (14) | 0.41323 (8) | 0.88336 (11) | 0.0211 (3) |
| C21 | −0.04285 (15) | 0.36589 (9) | 0.88235 (12) | 0.0262 (4) |
| H21A | −0.0325 | 0.3148 | 0.8863 | 0.031* |
| C22 | −0.14120 (15) | 0.39600 (10) | 0.87544 (12) | 0.0275 (4) |
| H22A | −0.1969 | 0.3646 | 0.8750 | 0.033* |
| C23 | −0.15853 (15) | 0.47227 (10) | 0.86912 (12) | 0.0257 (3) |
| C24 | −0.07485 (16) | 0.51828 (10) | 0.86920 (13) | 0.0295 (4) |
| H24A | −0.0855 | 0.5693 | 0.8647 | 0.035* |
| C25 | 0.02422 (15) | 0.48965 (9) | 0.87594 (12) | 0.0267 (4) |
| H25A | 0.0795 | 0.5211 | 0.8755 | 0.032* |
| C26 | −0.26526 (16) | 0.50341 (11) | 0.86390 (14) | 0.0345 (4) |
| H26A | −0.2727 | 0.5529 | 0.8395 | 0.052* |
| H26B | −0.2694 | 0.5043 | 0.9248 | 0.052* |
| H26C | −0.3219 | 0.4729 | 0.8240 | 0.052* |
| C27 | −0.21526 (13) | 0.23237 (9) | 0.61915 (12) | 0.0229 (3) |
| C28 | −0.21199 (14) | 0.15680 (9) | 0.60537 (12) | 0.0250 (3) |
| H28A | −0.1927 | 0.1383 | 0.5571 | 0.030* |
| C29 | −0.23782 (15) | 0.10914 (10) | 0.66464 (13) | 0.0289 (4) |
| H29A | −0.2360 | 0.0582 | 0.6556 | 0.035* |
| C30 | −0.26628 (15) | 0.13558 (11) | 0.73704 (13) | 0.0294 (4) |
| C31 | −0.26943 (15) | 0.21215 (11) | 0.74919 (13) | 0.0304 (4) |
| H31A | −0.2891 | 0.2307 | 0.7972 | 0.037* |
| C32 | −0.24395 (15) | 0.26053 (10) | 0.69117 (12) | 0.0278 (4) |
| H32A | −0.2459 | 0.3114 | 0.7000 | 0.033* |
| C33 | −0.29291 (18) | 0.08257 (13) | 0.80129 (15) | 0.0412 (5) |
| H33A | −0.3346 | 0.0421 | 0.7661 | 0.062* |
| H33B | −0.3335 | 0.1080 | 0.8328 | 0.062* |
| H33C | −0.2276 | 0.0637 | 0.8460 | 0.062* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0232 (2) | 0.02041 (17) | 0.01541 (17) | 0.00089 (14) | 0.00691 (15) | −0.00004 (13) |
| S2 | 0.0271 (2) | 0.0254 (2) | 0.0251 (2) | −0.00384 (16) | 0.00944 (17) | −0.00123 (16) |
| S3 | 0.0284 (2) | 0.01908 (17) | 0.01522 (18) | 0.00331 (14) | 0.00744 (16) | 0.00123 (13) |
| S4 | 0.0255 (2) | 0.02166 (18) | 0.0239 (2) | 0.00318 (15) | 0.00649 (17) | −0.00113 (15) |
| O1 | 0.0300 (6) | 0.0187 (5) | 0.0152 (5) | −0.0004 (4) | 0.0103 (5) | −0.0008 (4) |
| O2 | 0.0259 (6) | 0.0246 (5) | 0.0243 (6) | 0.0052 (5) | 0.0090 (5) | 0.0024 (5) |
| O3 | 0.0298 (7) | 0.0288 (6) | 0.0193 (6) | −0.0038 (5) | 0.0060 (5) | −0.0053 (5) |
| O4 | 0.0273 (6) | 0.0218 (5) | 0.0310 (6) | 0.0007 (5) | 0.0143 (5) | 0.0025 (5) |
| O5 | 0.0381 (8) | 0.0302 (6) | 0.0361 (7) | −0.0115 (5) | 0.0133 (6) | −0.0044 (5) |
| O6 | 0.0386 (8) | 0.0343 (7) | 0.0228 (6) | −0.0049 (6) | 0.0093 (6) | 0.0004 (5) |
| O7 | 0.0321 (7) | 0.0177 (5) | 0.0151 (5) | 0.0052 (4) | 0.0097 (5) | 0.0022 (4) |
| O8 | 0.0265 (6) | 0.0254 (6) | 0.0227 (6) | 0.0006 (5) | 0.0057 (5) | −0.0001 (5) |
| O9 | 0.0401 (8) | 0.0243 (6) | 0.0180 (6) | 0.0057 (5) | 0.0085 (5) | 0.0053 (4) |
| O10 | 0.0224 (6) | 0.0204 (5) | 0.0289 (6) | 0.0013 (4) | 0.0099 (5) | −0.0037 (5) |

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|---|---|---|---|---|---|---|
| O11 | 0.0310 (7) | 0.0252 (6) | 0.0390 (8) | 0.0076 (5) | 0.0063 (6) | 0.0022 (5) |
| O12 | 0.0381 (8) | 0.0297 (6) | 0.0213 (6) | 0.0014 (5) | 0.0088 (5) | −0.0021 (5) |
| C1 | 0.0248 (8) | 0.0175 (6) | 0.0161 (7) | 0.0020 (6) | 0.0091 (6) | 0.0007 (5) |
| C2 | 0.0287 (9) | 0.0184 (6) | 0.0165 (7) | 0.0010 (6) | 0.0107 (6) | −0.0016 (5) |
| C3 | 0.0241 (8) | 0.0197 (7) | 0.0225 (8) | 0.0012 (6) | 0.0110 (7) | −0.0009 (6) |
| C4 | 0.0294 (9) | 0.0172 (6) | 0.0158 (7) | 0.0033 (6) | 0.0099 (6) | 0.0020 (5) |
| C5 | 0.0245 (8) | 0.0182 (6) | 0.0212 (7) | 0.0027 (6) | 0.0103 (7) | 0.0015 (6) |
| C6 | 0.0240 (8) | 0.0199 (7) | 0.0154 (7) | 0.0012 (6) | 0.0088 (6) | 0.0012 (5) |
| C7 | 0.0283 (9) | 0.0188 (7) | 0.0278 (8) | 0.0016 (6) | 0.0112 (7) | −0.0021 (6) |
| C8 | 0.0286 (9) | 0.0227 (7) | 0.0356 (10) | −0.0018 (6) | 0.0133 (8) | −0.0006 (7) |
| C9 | 0.0257 (9) | 0.0316 (8) | 0.0244 (8) | 0.0025 (7) | 0.0115 (7) | 0.0035 (7) |
| C10 | 0.0327 (10) | 0.0254 (8) | 0.0293 (9) | 0.0092 (7) | 0.0175 (8) | 0.0048 (7) |
| C11 | 0.0348 (10) | 0.0178 (7) | 0.0263 (8) | 0.0033 (6) | 0.0159 (7) | 0.0018 (6) |
| C12 | 0.0290 (10) | 0.0412 (10) | 0.0443 (12) | 0.0038 (8) | 0.0190 (9) | 0.0072 (9) |
| C13 | 0.0197 (8) | 0.0280 (8) | 0.0260 (8) | 0.0004 (6) | 0.0066 (7) | −0.0001 (7) |
| C14 | 0.0246 (9) | 0.0318 (8) | 0.0254 (8) | 0.0006 (7) | 0.0066 (7) | 0.0050 (7) |
| C15 | 0.0270 (9) | 0.0374 (9) | 0.0237 (8) | 0.0020 (7) | 0.0083 (7) | 0.0040 (7) |
| C16 | 0.0222 (9) | 0.0348 (9) | 0.0281 (9) | 0.0030 (7) | 0.0064 (7) | −0.0026 (7) |
| C17 | 0.0265 (9) | 0.0282 (8) | 0.0381 (10) | 0.0001 (7) | 0.0125 (8) | −0.0001 (7) |
| C18 | 0.0221 (8) | 0.0274 (8) | 0.0317 (9) | −0.0013 (6) | 0.0111 (7) | 0.0012 (7) |
| C19 | 0.0365 (11) | 0.0414 (10) | 0.0337 (10) | 0.0048 (8) | 0.0130 (9) | −0.0035 (8) |
| C20 | 0.0285 (9) | 0.0197 (7) | 0.0169 (7) | 0.0023 (6) | 0.0105 (6) | 0.0002 (6) |
| C21 | 0.0354 (10) | 0.0204 (7) | 0.0254 (8) | −0.0007 (6) | 0.0140 (7) | 0.0004 (6) |
| C22 | 0.0319 (10) | 0.0280 (8) | 0.0252 (8) | −0.0043 (7) | 0.0130 (7) | −0.0007 (7) |
| C23 | 0.0311 (9) | 0.0290 (8) | 0.0191 (8) | 0.0028 (7) | 0.0116 (7) | −0.0006 (6) |
| C24 | 0.0381 (10) | 0.0216 (7) | 0.0336 (9) | 0.0063 (7) | 0.0185 (8) | 0.0012 (7) |
| C25 | 0.0331 (10) | 0.0205 (7) | 0.0295 (9) | −0.0013 (6) | 0.0149 (8) | 0.0004 (6) |
| C26 | 0.0344 (11) | 0.0411 (10) | 0.0322 (10) | 0.0068 (8) | 0.0168 (8) | −0.0009 (8) |
| C27 | 0.0178 (8) | 0.0248 (7) | 0.0242 (8) | 0.0014 (6) | 0.0051 (6) | −0.0021 (6) |
| C28 | 0.0228 (8) | 0.0244 (8) | 0.0300 (9) | 0.0010 (6) | 0.0120 (7) | −0.0043 (6) |
| C29 | 0.0254 (9) | 0.0257 (8) | 0.0373 (10) | −0.0005 (6) | 0.0133 (8) | −0.0007 (7) |
| C30 | 0.0204 (9) | 0.0401 (10) | 0.0284 (9) | −0.0018 (7) | 0.0093 (7) | 0.0017 (7) |
| C31 | 0.0254 (9) | 0.0430 (10) | 0.0236 (8) | 0.0032 (7) | 0.0097 (7) | −0.0056 (7) |
| C32 | 0.0272 (9) | 0.0296 (8) | 0.0238 (8) | 0.0034 (7) | 0.0056 (7) | −0.0064 (7) |
| C33 | 0.0358 (11) | 0.0524 (12) | 0.0406 (12) | −0.0050 (9) | 0.0198 (9) | 0.0083 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—O3 | 1.4238 (12) | C12—H12C | 0.96 |
| S1—O2 | 1.4315 (12) | C12—H12D | 0.96 |
| S1—O1 | 1.5833 (11) | C13—C14 | 1.389 (2) |
| S1—C6 | 1.7453 (17) | C13—C18 | 1.392 (2) |
| S2—O5 | 1.4244 (13) | C14—C15 | 1.386 (3) |
| S2—O6 | 1.4314 (13) | C14—H14A | 0.93 |
| S2—O4 | 1.5840 (13) | C15—C16 | 1.396 (3) |
| S2—C13 | 1.7435 (18) | C15—H15A | 0.93 |
| S3—O9 | 1.4252 (12) | C16—C17 | 1.395 (3) |
| S3—O8 | 1.4271 (13) | C16—C19 | 1.508 (3) |

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|---|---|---|---|
| S3—O7 | 1.5848 (11) | C17—C18 | 1.375 (3) |
| S3—C20 | 1.7518 (17) | C17—H17A | 0.93 |
| S4—O11 | 1.4240 (13) | C18—H18A | 0.93 |
| S4—O12 | 1.4274 (13) | C19—H19A | 0.96 |
| S4—O10 | 1.5899 (13) | C19—H19B | 0.96 |
| S4—C27 | 1.7404 (18) | C19—H19C | 0.96 |
| O1—C2 | 1.4578 (18) | C20—C21 | 1.391 (2) |
| O4—C3 | 1.458 (2) | C20—C25 | 1.393 (2) |
| O7—C4 | 1.4546 (18) | C21—C22 | 1.385 (3) |
| O10—C5 | 1.4559 (19) | C21—H21A | 0.93 |
| C1—C4 | 1.528 (2) | C22—C23 | 1.393 (2) |
| C1—C3 | 1.530 (2) | C22—H22A | 0.93 |
| C1—C2 | 1.531 (2) | C23—C24 | 1.388 (3) |
| C1—C5 | 1.531 (2) | C23—C26 | 1.502 (3) |
| C2—H2B | 0.97 | C24—C25 | 1.384 (3) |
| C2—H2C | 0.97 | C24—H24A | 0.93 |
| C3—H3B | 0.97 | C25—H25A | 0.93 |
| C3—H3C | 0.97 | C26—H26A | 0.96 |
| C4—H4A | 0.97 | C26—H26B | 0.96 |
| C4—H4B | 0.97 | C26—H26C | 0.96 |
| C5—H5B | 0.97 | C27—C28 | 1.383 (2) |
| C5—H5C | 0.97 | C27—C32 | 1.391 (2) |
| C6—C7 | 1.390 (2) | C28—C29 | 1.383 (2) |
| C6—C11 | 1.394 (2) | C28—H28A | 0.93 |
| C7—C8 | 1.380 (2) | C29—C30 | 1.384 (3) |
| C7—H7A | 0.93 | C29—H29A | 0.93 |
| C8—C9 | 1.392 (2) | C30—C31 | 1.396 (3) |
| C8—H8B | 0.93 | C30—C33 | 1.506 (3) |
| C9—C10 | 1.395 (2) | C31—C32 | 1.375 (3) |
| C9—C12 | 1.503 (3) | C31—H31A | 0.93 |
| C10—C11 | 1.382 (3) | C32—H32A | 0.93 |
| C10—H10A | 0.93 | C33—H33A | 0.96 |
| C11—H11B | 0.93 | C33—H33B | 0.96 |
| C12—H12B | 0.96 | C33—H33C | 0.96 |
| | | | |
| O3—S1—O2 | 120.75 (8) | C9—C12—H12C | 109.5 |
| O3—S1—O1 | 103.71 (7) | H12B—C12—H12C | 109.5 |
| O2—S1—O1 | 108.68 (7) | C9—C12—H12D | 109.5 |
| O3—S1—C6 | 109.30 (8) | H12B—C12—H12D | 109.5 |
| O2—S1—C6 | 109.11 (7) | H12C—C12—H12D | 109.5 |
| O1—S1—C6 | 103.91 (7) | C14—C13—C18 | 121.01 (16) |
| O5—S2—O6 | 119.85 (8) | C14—C13—S2 | 118.89 (13) |
| O5—S2—O4 | 103.83 (8) | C18—C13—S2 | 120.09 (14) |
| O6—S2—O4 | 108.03 (8) | C15—C14—C13 | 118.81 (17) |
| O5—S2—C13 | 110.30 (9) | C15—C14—H14A | 120.6 |
| O6—S2—C13 | 108.69 (8) | C13—C14—H14A | 120.6 |
| O4—S2—C13 | 105.06 (8) | C14—C15—C16 | 121.31 (17) |
| O9—S3—O8 | 120.30 (8) | C14—C15—H15A | 119.3 |

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| O9—S3—O7 | 103.79 (7) | C16—C15—H15A | 119.3 |
| O8—S3—O7 | 108.60 (7) | C17—C16—C15 | 118.28 (17) |
| O9—S3—C20 | 109.69 (8) | C17—C16—C19 | 120.99 (17) |
| O8—S3—C20 | 109.06 (7) | C15—C16—C19 | 120.73 (17) |
| O7—S3—C20 | 104.11 (7) | C18—C17—C16 | 121.45 (17) |
| O11—S4—O12 | 119.87 (8) | C18—C17—H17A | 119.3 |
| O11—S4—O10 | 103.51 (7) | C16—C17—H17A | 119.3 |
| O12—S4—O10 | 108.71 (7) | C17—C18—C13 | 119.13 (17) |
| O11—S4—C27 | 109.74 (8) | C17—C18—H18A | 120.4 |
| O12—S4—C27 | 109.16 (8) | C13—C18—H18A | 120.4 |
| O10—S4—C27 | 104.68 (7) | C16—C19—H19A | 109.5 |
| C2—O1—S1 | 117.87 (9) | C16—C19—H19B | 109.5 |
| C3—O4—S2 | 118.41 (10) | H19A—C19—H19B | 109.5 |
| C4—O7—S3 | 117.34 (9) | C16—C19—H19C | 109.5 |
| C5—O10—S4 | 117.92 (10) | H19A—C19—H19C | 109.5 |
| C4—C1—C3 | 111.13 (13) | H19B—C19—H19C | 109.5 |
| C4—C1—C2 | 106.71 (12) | C21—C20—C25 | 120.63 (16) |
| C3—C1—C2 | 110.60 (13) | C21—C20—S3 | 119.40 (12) |
| C4—C1—C5 | 110.94 (13) | C25—C20—S3 | 119.97 (13) |
| C3—C1—C5 | 106.66 (12) | C22—C21—C20 | 118.94 (15) |
| C2—C1—C5 | 110.85 (13) | C22—C21—H21A | 120.5 |
| O1—C2—C1 | 106.24 (11) | C20—C21—H21A | 120.5 |
| O1—C2—H2B | 110.5 | C21—C22—C23 | 121.42 (17) |
| C1—C2—H2B | 110.5 | C21—C22—H22A | 119.3 |
| O1—C2—H2C | 110.5 | C23—C22—H22A | 119.3 |
| C1—C2—H2C | 110.5 | C24—C23—C22 | 118.54 (17) |
| H2B—C2—H2C | 108.7 | C24—C23—C26 | 121.25 (16) |
| O4—C3—C1 | 107.03 (12) | C22—C23—C26 | 120.21 (17) |
| O4—C3—H3B | 110.3 | C25—C24—C23 | 121.23 (16) |
| C1—C3—H3B | 110.3 | C25—C24—H24A | 119.4 |
| O4—C3—H3C | 110.3 | C23—C24—H24A | 119.4 |
| C1—C3—H3C | 110.3 | C24—C25—C20 | 119.23 (17) |
| H3B—C3—H3C | 108.6 | C24—C25—H25A | 120.4 |
| O7—C4—C1 | 106.63 (11) | C20—C25—H25A | 120.4 |
| O7—C4—H4A | 110.4 | C23—C26—H26A | 109.5 |
| C1—C4—H4A | 110.4 | C23—C26—H26B | 109.5 |
| O7—C4—H4B | 110.4 | H26A—C26—H26B | 109.5 |
| C1—C4—H4B | 110.4 | C23—C26—H26C | 109.5 |
| H4A—C4—H4B | 108.6 | H26A—C26—H26C | 109.5 |
| O10—C5—C1 | 106.62 (12) | H26B—C26—H26C | 109.5 |
| O10—C5—H5B | 110.4 | C28—C27—C32 | 120.99 (16) |
| C1—C5—H5B | 110.4 | C28—C27—S4 | 119.91 (13) |
| O10—C5—H5C | 110.4 | C32—C27—S4 | 119.03 (13) |
| C1—C5—H5C | 110.4 | C27—C28—C29 | 118.85 (16) |
| H5B—C5—H5C | 108.6 | C27—C28—H28A | 120.6 |
| C7—C6—C11 | 120.93 (16) | C29—C28—H28A | 120.6 |
| C7—C6—S1 | 120.88 (13) | C28—C29—C30 | 121.41 (16) |
| C11—C6—S1 | 118.18 (12) | C28—C29—H29A | 119.3 |

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| C8—C7—C6 | 118.92 (15) | C30—C29—H29A | 119.3 |
| C8—C7—H7A | 120.5 | C29—C30—C31 | 118.61 (17) |
| C6—C7—H7A | 120.5 | C29—C30—C33 | 120.43 (18) |
| C7—C8—C9 | 121.64 (16) | C31—C30—C33 | 120.96 (18) |
| C7—C8—H8B | 119.2 | C32—C31—C30 | 120.96 (17) |
| C9—C8—H8B | 119.2 | C32—C31—H31A | 119.5 |
| C8—C9—C10 | 118.19 (16) | C30—C31—H31A | 119.5 |
| C8—C9—C12 | 121.62 (17) | C31—C32—C27 | 119.18 (16) |
| C10—C9—C12 | 120.19 (16) | C31—C32—H32A | 120.4 |
| C11—C10—C9 | 121.47 (16) | C27—C32—H32A | 120.4 |
| C11—C10—H10A | 119.3 | C30—C33—H33A | 109.5 |
| C9—C10—H10A | 119.3 | C30—C33—H33B | 109.5 |
| C10—C11—C6 | 118.85 (15) | H33A—C33—H33B | 109.5 |
| C10—C11—H11B | 120.6 | C30—C33—H33C | 109.5 |
| C6—C11—H11B | 120.6 | H33A—C33—H33C | 109.5 |
| C9—C12—H12B | 109.5 | H33B—C33—H33C | 109.5 |

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| O3—S1—O1—C2 | −170.85 (11) | O4—S2—C13—C14 | 83.71 (15) |
| O2—S1—O1—C2 | −41.20 (13) | O5—S2—C13—C18 | 151.46 (14) |
| C6—S1—O1—C2 | 74.89 (12) | O6—S2—C13—C18 | 18.19 (17) |
| O5—S2—O4—C3 | −173.46 (11) | O4—S2—C13—C18 | −97.23 (15) |
| O6—S2—O4—C3 | −45.20 (13) | C18—C13—C14—C15 | −0.4 (3) |
| C13—S2—O4—C3 | 70.68 (13) | S2—C13—C14—C15 | 178.62 (14) |
| O9—S3—O7—C4 | −176.31 (12) | C13—C14—C15—C16 | 0.4 (3) |
| O8—S3—O7—C4 | −47.20 (13) | C14—C15—C16—C17 | −0.3 (3) |
| C20—S3—O7—C4 | 68.89 (13) | C14—C15—C16—C19 | 179.71 (18) |
| O11—S4—O10—C5 | −170.33 (11) | C15—C16—C17—C18 | 0.1 (3) |
| O12—S4—O10—C5 | −41.85 (13) | C19—C16—C17—C18 | −179.86 (18) |
| C27—S4—O10—C5 | 74.70 (12) | C16—C17—C18—C13 | −0.1 (3) |
| S1—O1—C2—C1 | −175.72 (10) | C14—C13—C18—C17 | 0.3 (3) |
| C4—C1—C2—O1 | −173.83 (13) | S2—C13—C18—C17 | −178.76 (14) |
| C3—C1—C2—O1 | 65.17 (16) | O9—S3—C20—C21 | −37.17 (15) |
| C5—C1—C2—O1 | −52.92 (16) | O8—S3—C20—C21 | −170.84 (13) |
| S2—O4—C3—C1 | 154.00 (10) | O7—S3—C20—C21 | 73.38 (14) |
| C4—C1—C3—O4 | −60.20 (16) | O9—S3—C20—C25 | 142.69 (14) |
| C2—C1—C3—O4 | 58.14 (16) | O8—S3—C20—C25 | 9.02 (16) |
| C5—C1—C3—O4 | 178.76 (12) | O7—S3—C20—C25 | −106.76 (14) |
| S3—O7—C4—C1 | −179.78 (10) | C25—C20—C21—C22 | −1.1 (3) |
| C3—C1—C4—O7 | −60.81 (16) | S3—C20—C21—C22 | 178.76 (13) |
| C2—C1—C4—O7 | 178.53 (13) | C20—C21—C22—C23 | 0.3 (3) |
| C5—C1—C4—O7 | 57.68 (16) | C21—C22—C23—C24 | 0.5 (3) |
| S4—O10—C5—C1 | 154.75 (10) | C21—C22—C23—C26 | −178.59 (17) |
| C4—C1—C5—O10 | 62.45 (15) | C22—C23—C24—C25 | −0.4 (3) |
| C3—C1—C5—O10 | −176.39 (12) | C26—C23—C24—C25 | 178.66 (16) |
| C2—C1—C5—O10 | −55.93 (15) | C23—C24—C25—C20 | −0.4 (3) |
| O3—S1—C6—C7 | 142.11 (13) | C21—C20—C25—C24 | 1.2 (3) |
| O2—S1—C6—C7 | 8.11 (16) | S3—C20—C25—C24 | −178.69 (13) |
| O1—S1—C6—C7 | −107.68 (14) | O11—S4—C27—C28 | 138.81 (14) |

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|---|---|---|---|
| O3—S1—C6—C11 | −37.20 (15) | O12—S4—C27—C28 | 5.58 (17) |
| O2—S1—C6—C11 | −171.20 (12) | O10—S4—C27—C28 | −110.67 (14) |
| O1—S1—C6—C11 | 73.01 (14) | O11—S4—C27—C32 | −38.17 (16) |
| C11—C6—C7—C8 | −0.1 (2) | O12—S4—C27—C32 | −171.40 (14) |
| S1—C6—C7—C8 | −179.35 (13) | O10—S4—C27—C32 | 72.35 (15) |
| C6—C7—C8—C9 | −0.1 (3) | C32—C27—C28—C29 | 0.0 (3) |
| C7—C8—C9—C10 | 0.2 (3) | S4—C27—C28—C29 | −176.92 (14) |
| C7—C8—C9—C12 | 179.59 (17) | C27—C28—C29—C30 | −0.2 (3) |
| C8—C9—C10—C11 | −0.1 (3) | C28—C29—C30—C31 | 0.5 (3) |
| C12—C9—C10—C11 | −179.50 (17) | C28—C29—C30—C33 | −179.33 (18) |
| C9—C10—C11—C6 | 0.0 (3) | C29—C30—C31—C32 | −0.6 (3) |
| C7—C6—C11—C10 | 0.2 (2) | C33—C30—C31—C32 | 179.26 (18) |
| S1—C6—C11—C10 | 179.46 (13) | C30—C31—C32—C27 | 0.4 (3) |
| O5—S2—C13—C14 | −27.60 (17) | C28—C27—C32—C31 | −0.1 (3) |
| O6—S2—C13—C14 | −160.86 (14) | S4—C27—C32—C31 | 176.88 (14) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2—H2*C*···O4 | 0.97 | 2.48 | 2.849 (2) | 102 |
| C3—H3*B*···O6 | 0.97 | 2.47 | 2.905 (2) | 107 |
| C3—H3*B*···O7 | 0.97 | 2.55 | 2.876 (2) | 100 |
| C3—H3*C*···O9$^{i}$ | 0.97 | 2.46 | 3.433 (2) | 175 |
| C4—H4*A*···O4 | 0.97 | 2.55 | 2.879 (2) | 100 |
| C5—H5*B*···O12 | 0.97 | 2.44 | 2.888 (2) | 107 |
| C5—H5*C*···O7 | 0.97 | 2.49 | 2.8396 (19) | 101 |
| C7—H7*A*···O2 | 0.93 | 2.58 | 2.937 (2) | 103 |
| C8—H8*B*···O11$^{ii}$ | 0.93 | 2.52 | 3.140 (2) | 124 |
| C10—H10*A*···O6$^{i}$ | 0.93 | 2.41 | 3.257 (2) | 151 |
| C18—H18*A*···O6 | 0.93 | 2.59 | 2.932 (2) | 103 |
| C22—H22*A*···O12$^{iii}$ | 0.93 | 2.52 | 3.154 (2) | 126 |
| C25—H25*A*···O8 | 0.93 | 2.56 | 2.924 (2) | 104 |
| C28—H28*A*···O12 | 0.93 | 2.54 | 2.905 (2) | 104 |
| C29—H29*A*···O8$^{iv}$ | 0.93 | 2.42 | 3.334 (2) | 165 |
| C31—H31*A*···O12$^{iii}$ | 0.93 | 2.53 | 3.209 (2) | 130 |

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) −*x*, −*y*+1, −*z*+1; (iii) *x*, −*y*+1/2, *z*+1/2; (iv) −*x*, *y*−1/2, −*z*+3/2.