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5,5′,5″-Triphenyl-2,2′,2″-[2,4,6-trimethylbenzene-1,3,5-triyltris(methylidenesulfanediyl)]tris(1,3,4-oxadiazole)

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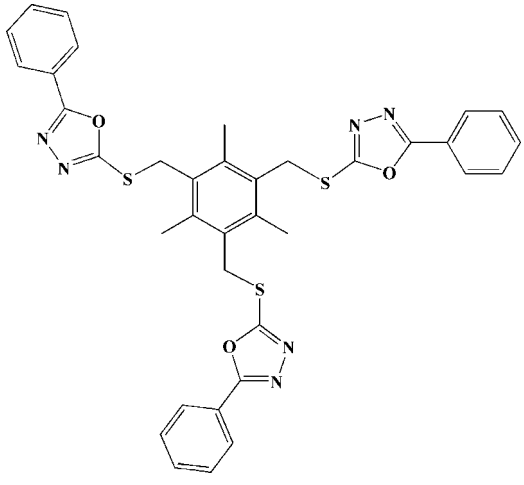
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.149; data-to-parameter ratio = 13.0.

In the title compound, $C_{36}H_{30}N_6O_3S_3$, the phenyl rings are twisted from the attached oxadiazole rings in the three arms by 1.5(2), 2.4 (2) and 25.7 (2)°. The crystal packing exhibits weak intermolecular C—H···N interactions.

Related literature

For general background to 1,3,4-oxadiazole derivatives, see Al-Talib *et al.* (1990); Wang *et al.* (2005) and to thio-based ligands with a multi-armed tripodal geometry, see: PrakashaReddy & Pedireddi (2007). For the crystal structure of an Ag complex with a related oxadiazole derivative, see: Zhang *et al.* (2007).



Experimental

Crystal data

$C_{36}H_{30}N_6O_3S_3$
M_r = 690.84
Monoclinic, $P2_1/c$
a = 19.870 (4) Å
b = 9.1305 (18) Å
c = 18.557 (4) Å
β = 107.00 (3)°
V = 3219.6 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 113 K
0.22 × 0.20 × 0.10 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 1999)
T_{min} = 0.941, T_{max} = 0.973
23119 measured reflections
5664 independent reflections
4490 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.149
S = 1.10
5664 reflections
437 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C31—H31···N5^{i}	0.95	2.55	3.338 (3)	141
C24—H24···N2^{ii}	0.95	2.57	3.394 (4)	146

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

Data collection: *CrystalClear* (Rigaku/MSC, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2772).

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supporting information

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5,5′,5′′-Triphenyl-2,2′,2′′-[2,4,6-trimethylbenzene-1,3,5-triyltris(methylidenesulfanediyl)]tris(1,3,4-oxadiazole)

Wei Wang, Yan Gao, Ming Ji, Hong-guo Yao and Hong Qiu

S1. Comment

1,3,4-Oxadiazole derivatives have wide applications in medicine, industry and coordination chemistry, so they are under intensive studies (Al-Talib *et al.*, 1990; Wang *et al.*, 2005; Zhang *et al.*, 2007). Recently, novel thio-based ligands with multi-armed tripodal geometry were synthesized, and these ligands demonstrated their significance in the supramolecular studies (PrakashaReddy & Pedireddi, 2007 and references therein). Herewith we present the title compound (I), where the 2,4,6-trimethylbenzene center contains three 5-phenyl-1,3,4-oxadiazol-2-ylsulfanylmethyl arms.

In (I) (Fig.1), two phenyloxadiazole fragments - C10—C15/C8/C9/N1/N2/O1 (A) and C20—C25/C18/C19/N3/N4/O2 (B), respectively - are situated on the one side of the central benzene ring (C1—C6), while the third phenyloxadiazole fragment - C30—C35/C28/C29/N5/N6/O3 (C) - is situated on the other side of the central benzene ring. In A and B, the oxadiazole rings are almost coplanar with the attached phenyl rings forming dihedral angles of 1.5 (2) and 2.4 (2)°, respectively. The terminal phenyl rings are roughly orthogonal to the plane of the central benzene ring with dihedral angles of 82.0 (2), 89.2 (2) and 72.4 (2)°, respectively. The crystal packing exhibits weak intermolecular C—H···N interactions (Table 1).

S2. Experimental

A suspension of 5-phenyl-1,3,4-oxadiazole-2-thiol (3.0 mmol) and 2,4,6-trimethyl-1,3,5-tribromomethyl benzene (1.0 mmol) in ethanol (10 ml) was stirred at room temperature. The reaction progress was monitored *via* TLC. The resulting precipitate was filtered off, washed with cold ethanol, dried and purified to give the target product as white solid in 80% yield. Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution in chloroform-ethanol (1:1).

S3. Refinement

All H atoms were positioned geometrically and refined as riding (C—H = 0.95–0.99 Å) and allowed to ride on their parent atoms, with U_{iso}(H) =1.2-1.5U_{eq} of the parent atom.

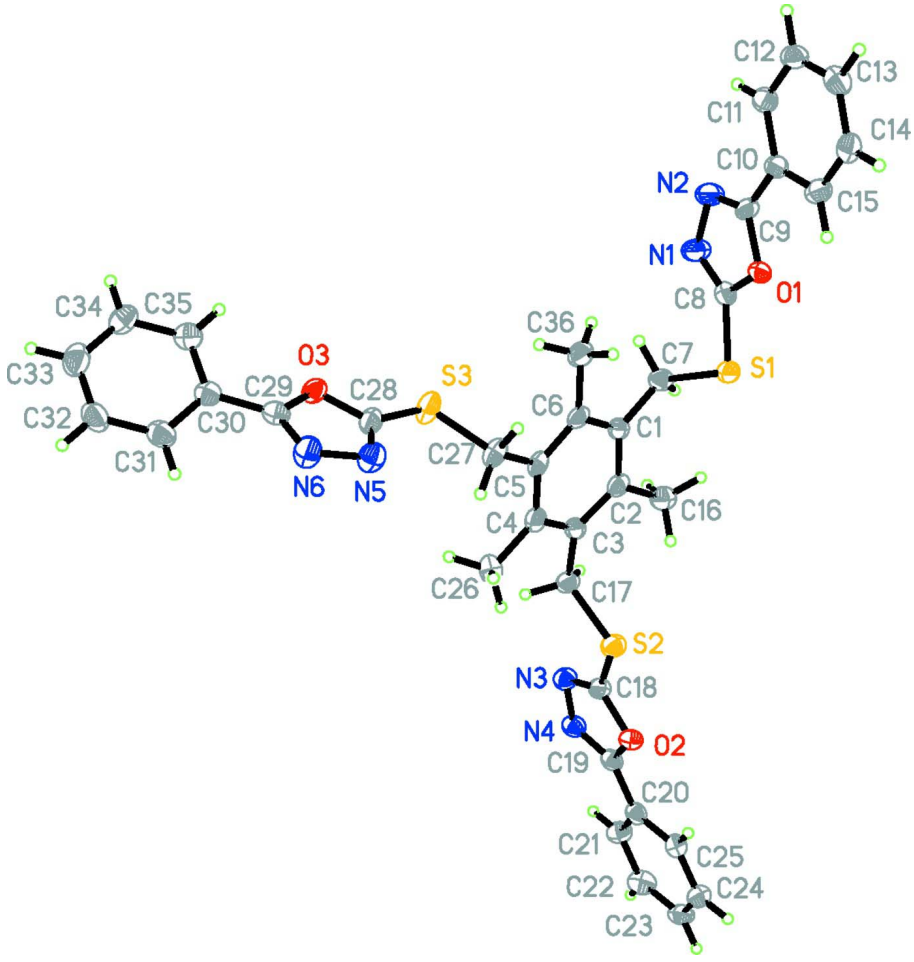

Figure 1

View of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

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c = 18.557 (4) Å
β = 107.00 (3)°
V = 3219.6 (11) Å^3
Z = 4
$F(000)$ = 1440
D_x = 1.425 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7164 reflections
θ = 2.1–27.9°
μ = 0.28 mm^{-1}
T = 113 K
Prism, colourless
0.22 × 0.20 × 0.10 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Radiation source: rotating anode
Confocal monochromator
Detector resolution: 7.31 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 1999)
T_{min} = 0.941, T_{max} = 0.973
23119 measured reflections

5664 independent reflections
4490 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -23 \rightarrow 19$
$k = -10 \rightarrow 10$
$l = -19 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.149$
$S = 1.10$
5664 reflections
437 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
$w = 1/[\sigma^2(F_o^2) + (0.0804P)^2 + 0.7757P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0130 (11)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.18609 (4)	0.29928 (8)	0.04709 (4)	0.0293 (2)
S2	0.17834 (4)	0.61632 (8)	0.36748 (4)	0.0305 (2)
S3	0.30065 (4)	0.98854 (9)	0.09276 (5)	0.0366 (3)
O1	0.24745 (9)	0.2057 (2)	−0.05257 (11)	0.0242 (5)
O2	0.12205 (9)	0.6002 (2)	0.47942 (11)	0.0260 (5)
O3	0.37150 (9)	1.2260 (2)	0.08047 (11)	0.0274 (5)
N1	0.16166 (13)	0.3621 (3)	−0.10346 (15)	0.0361 (6)
N2	0.19355 (13)	0.3179 (3)	−0.15899 (14)	0.0337 (6)
N3	0.06871 (12)	0.7678 (3)	0.39516 (14)	0.0282 (6)
N4	0.03554 (12)	0.7624 (3)	0.45304 (14)	0.0278 (6)
N5	0.43389 (12)	1.0801 (3)	0.17101 (15)	0.0350 (6)
N6	0.47315 (13)	1.2090 (3)	0.16849 (16)	0.0370 (7)
C1	0.17176 (14)	0.5716 (3)	0.10460 (16)	0.0237 (6)
C2	0.14838 (14)	0.5860 (3)	0.16842 (16)	0.0255 (6)
C3	0.17930 (14)	0.6912 (3)	0.22331 (16)	0.0249 (6)
C4	0.23874 (15)	0.7703 (3)	0.21951 (17)	0.0276 (7)
C5	0.26506 (14)	0.7483 (3)	0.15825 (17)	0.0255 (6)
C6	0.23050 (14)	0.6535 (3)	0.09961 (16)	0.0255 (6)
C7	0.13485 (14)	0.4691 (3)	0.04168 (17)	0.0279 (7)

H7A	0.1292	0.5173	−0.0075	0.033*
H7B	0.0874	0.4455	0.0456	0.033*
C8	0.19554 (14)	0.2940 (3)	−0.04264 (17)	0.0263 (7)
C9	0.24297 (14)	0.2274 (3)	−0.12660 (16)	0.0256 (6)
C10	0.29139 (14)	0.1506 (3)	−0.15903 (16)	0.0250 (6)
C11	0.28586 (15)	0.1687 (3)	−0.23545 (17)	0.0288 (7)
H11	0.2513	0.2328	−0.2656	0.035*
C12	0.33012 (15)	0.0942 (3)	−0.26695 (18)	0.0314 (7)
H12	0.3259	0.1061	−0.3190	0.038*
C13	0.38190 (15)	0.0000 (3)	−0.22227 (19)	0.0320 (7)
H13	0.4130	−0.0509	−0.2439	0.038*
C14	0.38718 (15)	−0.0176 (3)	−0.14763 (19)	0.0324 (7)
H14	0.4221	−0.0812	−0.1176	0.039*
C15	0.34215 (14)	0.0562 (3)	−0.11523 (17)	0.0300 (7)
H15	0.3460	0.0424	−0.0634	0.036*
C16	0.08921 (16)	0.4894 (4)	0.17749 (18)	0.0348 (7)
H16A	0.0438	0.5355	0.1525	0.052*
H16B	0.0940	0.4768	0.2312	0.052*
H16C	0.0916	0.3936	0.1546	0.052*
C17	0.14338 (15)	0.7269 (3)	0.28308 (16)	0.0281 (7)
H17A	0.0922	0.7089	0.2625	0.034*
H17B	0.1503	0.8319	0.2965	0.034*
C18	0.11798 (14)	0.6706 (3)	0.41349 (16)	0.0254 (6)
C19	0.06834 (13)	0.6633 (3)	0.50062 (16)	0.0245 (6)
C20	0.05478 (14)	0.6132 (3)	0.56941 (17)	0.0254 (6)
C21	−0.00131 (14)	0.6715 (3)	0.59100 (17)	0.0298 (7)
H21	−0.0313	0.7431	0.5606	0.036*
C22	−0.01283 (15)	0.6236 (4)	0.65760 (18)	0.0346 (8)
H22	−0.0506	0.6633	0.6730	0.042*
C23	0.03049 (15)	0.5184 (4)	0.70162 (18)	0.0341 (8)
H23	0.0223	0.4860	0.7470	0.041*
C24	0.08569 (16)	0.4605 (3)	0.67948 (17)	0.0327 (7)
H24	0.1150	0.3875	0.7094	0.039*
C25	0.09819 (15)	0.5085 (3)	0.61421 (17)	0.0303 (7)
H25	0.1367	0.4699	0.5998	0.036*
C26	0.27447 (18)	0.8753 (4)	0.2815 (2)	0.0409 (8)
H26A	0.3251	0.8553	0.2982	0.061*
H26B	0.2551	0.8631	0.3240	0.061*
H26C	0.2664	0.9760	0.2627	0.061*
C27	0.33018 (15)	0.8295 (3)	0.15422 (19)	0.0318 (7)
H27A	0.3600	0.7651	0.1334	0.038*
H27B	0.3580	0.8617	0.2051	0.038*
C28	0.37511 (15)	1.0980 (3)	0.11886 (17)	0.0287 (7)
C29	0.43512 (13)	1.2908 (3)	0.11594 (16)	0.0257 (7)
C30	0.44873 (14)	1.4375 (3)	0.09273 (17)	0.0274 (7)
C31	0.49555 (15)	1.5280 (4)	0.14417 (18)	0.0338 (7)
H31	0.5191	1.4929	0.1932	0.041*
C32	0.50769 (17)	1.6693 (4)	0.1237 (2)	0.0403 (8)

H32	0.5395	1.7310	0.1589	0.048*
C33	0.47366 (17)	1.7209 (4)	0.0524 (2)	0.0418 (8)
H33	0.4816	1.8183	0.0389	0.050*
C34	0.42781 (16)	1.6304 (4)	0.0003 (2)	0.0369 (8)
H34	0.4051	1.6652	−0.0491	0.044*
C35	0.41525 (15)	1.4894 (3)	0.02058 (18)	0.0315 (7)
H35	0.3837	1.4277	−0.0149	0.038*
C36	0.25732 (16)	0.6325 (3)	0.03167 (18)	0.0334 (7)
H36A	0.2810	0.7221	0.0230	0.050*
H36B	0.2176	0.6114	−0.0128	0.050*
H36C	0.2906	0.5506	0.0409	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0405 (4)	0.0254 (4)	0.0238 (4)	0.0061 (3)	0.0123 (3)	0.0017 (3)
S2	0.0366 (4)	0.0302 (5)	0.0267 (4)	0.0085 (3)	0.0127 (3)	0.0024 (3)
S3	0.0302 (4)	0.0306 (5)	0.0435 (5)	−0.0040 (3)	0.0020 (3)	0.0140 (4)
O1	0.0283 (10)	0.0238 (11)	0.0189 (11)	0.0006 (8)	0.0043 (8)	−0.0021 (8)
O2	0.0278 (10)	0.0296 (12)	0.0215 (11)	0.0002 (8)	0.0084 (8)	−0.0016 (9)
O3	0.0252 (10)	0.0298 (12)	0.0241 (11)	−0.0036 (8)	0.0022 (8)	0.0055 (9)
N1	0.0448 (15)	0.0405 (16)	0.0248 (15)	0.0129 (12)	0.0130 (12)	0.0037 (12)
N2	0.0395 (14)	0.0385 (16)	0.0229 (15)	0.0066 (12)	0.0090 (11)	0.0008 (12)
N3	0.0298 (13)	0.0302 (14)	0.0271 (14)	0.0007 (11)	0.0119 (11)	0.0008 (11)
N4	0.0277 (12)	0.0319 (14)	0.0260 (14)	−0.0018 (10)	0.0115 (11)	−0.0036 (11)
N5	0.0285 (13)	0.0358 (15)	0.0357 (16)	−0.0010 (11)	0.0016 (11)	0.0076 (12)
N6	0.0297 (13)	0.0354 (16)	0.0393 (17)	−0.0042 (11)	−0.0002 (12)	0.0057 (13)
C1	0.0279 (14)	0.0201 (15)	0.0227 (16)	0.0079 (11)	0.0067 (12)	0.0022 (12)
C2	0.0277 (14)	0.0237 (15)	0.0257 (16)	0.0065 (12)	0.0086 (12)	0.0074 (13)
C3	0.0317 (15)	0.0202 (15)	0.0232 (16)	0.0068 (12)	0.0088 (12)	0.0009 (12)
C4	0.0338 (16)	0.0207 (15)	0.0291 (17)	0.0035 (12)	0.0105 (13)	0.0036 (12)
C5	0.0276 (15)	0.0192 (15)	0.0304 (17)	0.0051 (11)	0.0092 (12)	0.0086 (12)
C6	0.0324 (15)	0.0224 (15)	0.0230 (16)	0.0095 (12)	0.0099 (12)	0.0084 (12)
C7	0.0286 (15)	0.0305 (17)	0.0233 (16)	0.0060 (12)	0.0057 (12)	0.0004 (13)
C8	0.0304 (15)	0.0214 (15)	0.0270 (17)	0.0016 (12)	0.0081 (12)	−0.0017 (12)
C9	0.0300 (15)	0.0259 (16)	0.0184 (16)	−0.0019 (12)	0.0035 (12)	0.0032 (12)
C10	0.0285 (15)	0.0249 (16)	0.0241 (16)	−0.0069 (12)	0.0114 (12)	−0.0028 (12)
C11	0.0299 (15)	0.0286 (16)	0.0252 (17)	−0.0032 (12)	0.0037 (12)	−0.0016 (13)
C12	0.0375 (16)	0.0338 (18)	0.0261 (17)	−0.0087 (13)	0.0143 (13)	−0.0032 (13)
C13	0.0282 (15)	0.0321 (18)	0.042 (2)	−0.0063 (13)	0.0195 (14)	−0.0083 (14)
C14	0.0343 (16)	0.0253 (17)	0.0368 (19)	−0.0026 (12)	0.0093 (14)	0.0030 (14)
C15	0.0319 (15)	0.0325 (17)	0.0249 (17)	−0.0028 (13)	0.0074 (12)	0.0021 (13)
C16	0.0392 (17)	0.0366 (19)	0.0297 (18)	−0.0024 (14)	0.0119 (14)	−0.0007 (14)
C17	0.0323 (15)	0.0288 (16)	0.0230 (16)	0.0051 (12)	0.0078 (12)	0.0040 (13)
C18	0.0275 (14)	0.0264 (16)	0.0219 (16)	−0.0023 (12)	0.0066 (12)	−0.0007 (12)
C19	0.0217 (14)	0.0261 (16)	0.0252 (16)	−0.0056 (11)	0.0063 (12)	−0.0053 (12)
C20	0.0246 (14)	0.0247 (16)	0.0278 (17)	−0.0064 (11)	0.0092 (12)	−0.0040 (12)
C21	0.0225 (14)	0.0382 (18)	0.0264 (17)	−0.0013 (12)	0.0037 (12)	0.0014 (14)

C22	0.0252 (15)	0.048 (2)	0.0335 (19)	−0.0034 (14)	0.0135 (13)	−0.0036 (15)
C23	0.0367 (17)	0.042 (2)	0.0220 (17)	−0.0119 (14)	0.0065 (13)	−0.0025 (14)
C24	0.0372 (17)	0.0315 (17)	0.0264 (18)	−0.0010 (13)	0.0045 (13)	0.0038 (14)
C25	0.0358 (16)	0.0246 (16)	0.0304 (18)	−0.0012 (12)	0.0095 (13)	−0.0024 (13)
C26	0.051 (2)	0.0265 (18)	0.044 (2)	−0.0055 (14)	0.0128 (16)	−0.0038 (15)
C27	0.0309 (15)	0.0277 (17)	0.0378 (19)	0.0045 (13)	0.0114 (13)	0.0111 (14)
C28	0.0322 (16)	0.0238 (16)	0.0308 (17)	0.0017 (12)	0.0104 (13)	0.0044 (13)
C29	0.0188 (13)	0.0333 (17)	0.0233 (16)	0.0011 (11)	0.0037 (11)	−0.0025 (13)
C30	0.0241 (14)	0.0329 (17)	0.0266 (17)	−0.0024 (12)	0.0096 (12)	−0.0024 (13)
C31	0.0313 (16)	0.0394 (19)	0.0308 (18)	−0.0061 (13)	0.0090 (13)	−0.0066 (14)
C32	0.0437 (18)	0.039 (2)	0.040 (2)	−0.0163 (15)	0.0159 (16)	−0.0134 (16)
C33	0.0451 (19)	0.0347 (19)	0.051 (2)	−0.0057 (15)	0.0221 (17)	0.0033 (16)
C34	0.0353 (17)	0.040 (2)	0.038 (2)	−0.0031 (14)	0.0156 (14)	0.0073 (15)
C35	0.0251 (15)	0.0378 (18)	0.0311 (18)	−0.0026 (13)	0.0077 (13)	−0.0009 (14)
C36	0.0419 (17)	0.0302 (17)	0.0327 (19)	0.0070 (13)	0.0182 (14)	0.0055 (14)

Geometric parameters (Å, º)

S1—C8	1.730 (3)	C13—C14	1.368 (4)
S1—C7	1.842 (3)	C13—H13	0.9500
S2—C18	1.736 (3)	C14—C15	1.390 (4)
S2—C17	1.822 (3)	C14—H14	0.9500
S3—C28	1.733 (3)	C15—H15	0.9500
S3—C27	1.833 (3)	C16—H16A	0.9800
O1—C8	1.364 (3)	C16—H16B	0.9800
O1—C9	1.365 (3)	C16—H16C	0.9800
O2—C18	1.364 (3)	C17—H17A	0.9900
O2—C19	1.368 (3)	C17—H17B	0.9900
O3—C28	1.360 (3)	C19—C20	1.453 (4)
O3—C29	1.376 (3)	C20—C25	1.389 (4)
N1—C8	1.292 (4)	C20—C21	1.395 (4)
N1—N2	1.417 (4)	C21—C22	1.392 (4)
N2—C9	1.290 (4)	C21—H21	0.9500
N3—C18	1.291 (4)	C22—C23	1.386 (4)
N3—N4	1.416 (3)	C22—H22	0.9500
N4—C19	1.298 (4)	C23—C24	1.384 (4)
N5—C28	1.291 (4)	C23—H23	0.9500
N5—N6	1.421 (4)	C24—C25	1.377 (4)
N6—C29	1.284 (4)	C24—H24	0.9500
C1—C2	1.399 (4)	C25—H25	0.9500
C1—C6	1.412 (4)	C26—H26A	0.9800
C1—C7	1.509 (4)	C26—H26B	0.9800
C2—C3	1.404 (4)	C26—H26C	0.9800
C2—C16	1.518 (4)	C27—H27A	0.9900
C3—C4	1.403 (4)	C27—H27B	0.9900
C3—C17	1.520 (4)	C29—C30	1.457 (4)
C4—C5	1.398 (4)	C30—C35	1.392 (4)
C4—C26	1.507 (4)	C30—C31	1.393 (4)

C5—C6	1.403 (4)	C31—C32	1.385 (5)
C5—C27	1.512 (4)	C31—H31	0.9500
C6—C36	1.518 (4)	C32—C33	1.382 (5)
C7—H7A	0.9900	C32—H32	0.9500
C7—H7B	0.9900	C33—C34	1.390 (5)
C9—C10	1.455 (4)	C33—H33	0.9500
C10—C15	1.393 (4)	C34—C35	1.384 (4)
C10—C11	1.400 (4)	C34—H34	0.9500
C11—C12	1.371 (4)	C35—H35	0.9500
C11—H11	0.9500	C36—H36A	0.9800
C12—C13	1.409 (4)	C36—H36B	0.9800
C12—H12	0.9500	C36—H36C	0.9800

C8—S1—C7	100.65 (14)	C3—C17—H17B	109.3
C18—S2—C17	96.89 (14)	S2—C17—H17B	109.3
C28—S3—C27	101.01 (14)	H17A—C17—H17B	108.0
C8—O1—C9	102.7 (2)	N3—C18—O2	113.7 (2)
C18—O2—C19	102.3 (2)	N3—C18—S2	130.3 (2)
C28—O3—C29	102.6 (2)	O2—C18—S2	116.0 (2)
C8—N1—N2	105.6 (2)	N4—C19—O2	112.1 (2)
C9—N2—N1	106.5 (2)	N4—C19—C20	129.1 (3)
C18—N3—N4	105.1 (2)	O2—C19—C20	118.7 (2)
C19—N4—N3	106.7 (2)	C25—C20—C21	119.9 (3)
C28—N5—N6	104.8 (2)	C25—C20—C19	120.0 (3)
C29—N6—N5	107.5 (2)	C21—C20—C19	120.1 (3)
C2—C1—C6	119.4 (3)	C22—C21—C20	119.2 (3)
C2—C1—C7	120.4 (3)	C22—C21—H21	120.4
C6—C1—C7	120.1 (3)	C20—C21—H21	120.4
C1—C2—C3	119.7 (3)	C23—C22—C21	120.4 (3)
C1—C2—C16	119.9 (3)	C23—C22—H22	119.8
C3—C2—C16	120.4 (3)	C21—C22—H22	119.8
C4—C3—C2	120.8 (3)	C24—C23—C22	120.0 (3)
C4—C3—C17	120.5 (3)	C24—C23—H23	120.0
C2—C3—C17	118.5 (3)	C22—C23—H23	120.0
C5—C4—C3	119.2 (3)	C25—C24—C23	120.1 (3)
C5—C4—C26	120.5 (3)	C25—C24—H24	119.9
C3—C4—C26	120.3 (3)	C23—C24—H24	119.9
C4—C5—C6	120.3 (3)	C24—C25—C20	120.3 (3)
C4—C5—C27	119.9 (3)	C24—C25—H25	119.8
C6—C5—C27	119.8 (3)	C20—C25—H25	119.8
C5—C6—C1	120.2 (3)	C4—C26—H26A	109.5
C5—C6—C36	120.7 (3)	C4—C26—H26B	109.5
C1—C6—C36	119.1 (3)	H26A—C26—H26B	109.5
C1—C7—S1	110.14 (19)	C4—C26—H26C	109.5
C1—C7—H7A	109.6	H26A—C26—H26C	109.5
S1—C7—H7A	109.6	H26B—C26—H26C	109.5
C1—C7—H7B	109.6	C5—C27—S3	107.24 (19)
S1—C7—H7B	109.6	C5—C27—H27A	110.3

H7A—C7—H7B	108.1	S3—C27—H27A	110.3
N1—C8—O1	112.8 (3)	C5—C27—H27B	110.3
N1—C8—S1	130.7 (2)	S3—C27—H27B	110.3
O1—C8—S1	116.5 (2)	H27A—C27—H27B	108.5
N2—C9—O1	112.3 (3)	N5—C28—O3	113.5 (2)
N2—C9—C10	128.4 (3)	N5—C28—S3	130.4 (2)
O1—C9—C10	119.3 (2)	O3—C28—S3	116.1 (2)
C15—C10—C11	119.5 (3)	N6—C29—O3	111.6 (3)
C15—C10—C9	120.7 (3)	N6—C29—C30	129.8 (3)
C11—C10—C9	119.8 (3)	O3—C29—C30	118.5 (2)
C12—C11—C10	120.2 (3)	C35—C30—C31	119.5 (3)
C12—C11—H11	119.9	C35—C30—C29	121.3 (3)
C10—C11—H11	119.9	C31—C30—C29	119.2 (3)
C11—C12—C13	120.1 (3)	C32—C31—C30	120.0 (3)
C11—C12—H12	120.0	C32—C31—H31	120.0
C13—C12—H12	120.0	C30—C31—H31	120.0
C14—C13—C12	119.6 (3)	C33—C32—C31	120.3 (3)
C14—C13—H13	120.2	C33—C32—H32	119.9
C12—C13—H13	120.2	C31—C32—H32	119.9
C13—C14—C15	120.8 (3)	C32—C33—C34	120.1 (3)
C13—C14—H14	119.6	C32—C33—H33	120.0
C15—C14—H14	119.6	C34—C33—H33	120.0
C14—C15—C10	119.7 (3)	C35—C34—C33	119.8 (3)
C14—C15—H15	120.1	C35—C34—H34	120.1
C10—C15—H15	120.1	C33—C34—H34	120.1
C2—C16—H16A	109.5	C34—C35—C30	120.3 (3)
C2—C16—H16B	109.5	C34—C35—H35	119.9
H16A—C16—H16B	109.5	C30—C35—H35	119.9
C2—C16—H16C	109.5	C6—C36—H36A	109.5
H16A—C16—H16C	109.5	C6—C36—H36B	109.5
H16B—C16—H16C	109.5	H36A—C36—H36B	109.5
C3—C17—S2	111.49 (19)	C6—C36—H36C	109.5
C3—C17—H17A	109.3	H36A—C36—H36C	109.5
S2—C17—H17A	109.3	H36B—C36—H36C	109.5

C8—N1—N2—C9	0.4 (3)	C9—C10—C15—C14	179.0 (3)
C18—N3—N4—C19	0.4 (3)	C4—C3—C17—S2	−91.9 (3)
C28—N5—N6—C29	−0.1 (3)	C2—C3—C17—S2	93.2 (3)
C6—C1—C2—C3	5.9 (4)	C18—S2—C17—C3	−172.6 (2)
C7—C1—C2—C3	−174.4 (2)	N4—N3—C18—O2	−0.8 (3)
C6—C1—C2—C16	−174.9 (2)	N4—N3—C18—S2	178.8 (2)
C7—C1—C2—C16	4.8 (4)	C19—O2—C18—N3	0.8 (3)
C1—C2—C3—C4	−7.5 (4)	C19—O2—C18—S2	−178.82 (18)
C16—C2—C3—C4	173.3 (3)	C17—S2—C18—N3	−5.2 (3)
C1—C2—C3—C17	167.3 (2)	C17—S2—C18—O2	174.3 (2)
C16—C2—C3—C17	−11.9 (4)	N3—N4—C19—O2	0.1 (3)
C2—C3—C4—C5	3.0 (4)	N3—N4—C19—C20	−179.1 (3)
C17—C3—C4—C5	−171.7 (3)	C18—O2—C19—N4	−0.5 (3)

C2—C3—C4—C26	−175.8 (3)	C18—O2—C19—C20	178.8 (2)
C17—C3—C4—C26	9.5 (4)	N4—C19—C20—C25	−177.6 (3)
C3—C4—C5—C6	3.0 (4)	O2—C19—C20—C25	3.2 (4)
C26—C4—C5—C6	−178.2 (3)	N4—C19—C20—C21	1.6 (5)
C3—C4—C5—C27	−178.4 (2)	O2—C19—C20—C21	−177.6 (2)
C26—C4—C5—C27	0.4 (4)	C25—C20—C21—C22	0.1 (4)
C4—C5—C6—C1	−4.5 (4)	C19—C20—C21—C22	−179.1 (3)
C27—C5—C6—C1	176.8 (2)	C20—C21—C22—C23	−0.5 (4)
C4—C5—C6—C36	178.0 (3)	C21—C22—C23—C24	0.1 (5)
C27—C5—C6—C36	−0.6 (4)	C22—C23—C24—C25	0.8 (5)
C2—C1—C6—C5	0.1 (4)	C23—C24—C25—C20	−1.2 (5)
C7—C1—C6—C5	−179.7 (2)	C21—C20—C25—C24	0.8 (4)
C2—C1—C6—C36	177.5 (2)	C19—C20—C25—C24	−180.0 (3)
C7—C1—C6—C36	−2.2 (4)	C4—C5—C27—S3	−98.1 (3)
C2—C1—C7—S1	−102.4 (3)	C6—C5—C27—S3	80.5 (3)
C6—C1—C7—S1	77.3 (3)	C28—S3—C27—C5	160.8 (2)
C8—S1—C7—C1	−125.3 (2)	N6—N5—C28—O3	1.1 (3)
N2—N1—C8—O1	−0.7 (3)	N6—N5—C28—S3	−176.8 (3)
N2—N1—C8—S1	178.4 (2)	C29—O3—C28—N5	−1.5 (3)
C9—O1—C8—N1	0.8 (3)	C29—O3—C28—S3	176.7 (2)
C9—O1—C8—S1	−178.54 (19)	C27—S3—C28—N5	−4.7 (3)
C7—S1—C8—N1	−17.2 (3)	C27—S3—C28—O3	177.5 (2)
C7—S1—C8—O1	161.9 (2)	N5—N6—C29—O3	−0.8 (3)
N1—N2—C9—O1	0.1 (3)	N5—N6—C29—C30	176.3 (3)
N1—N2—C9—C10	180.0 (3)	C28—O3—C29—N6	1.4 (3)
C8—O1—C9—N2	−0.5 (3)	C28—O3—C29—C30	−176.1 (3)
C8—O1—C9—C10	179.6 (2)	N6—C29—C30—C35	157.2 (3)
N2—C9—C10—C15	179.8 (3)	O3—C29—C30—C35	−25.9 (4)
O1—C9—C10—C15	−0.3 (4)	N6—C29—C30—C31	−23.5 (5)
N2—C9—C10—C11	−1.8 (5)	O3—C29—C30—C31	153.4 (3)
O1—C9—C10—C11	178.1 (2)	C35—C30—C31—C32	1.0 (5)
C15—C10—C11—C12	−0.1 (4)	C29—C30—C31—C32	−178.3 (3)
C9—C10—C11—C12	−178.4 (3)	C30—C31—C32—C33	−0.2 (5)
C10—C11—C12—C13	−0.6 (4)	C31—C32—C33—C34	−1.0 (5)
C11—C12—C13—C14	0.7 (4)	C32—C33—C34—C35	1.3 (5)
C12—C13—C14—C15	−0.1 (4)	C33—C34—C35—C30	−0.4 (5)
C13—C14—C15—C10	−0.6 (4)	C31—C30—C35—C34	−0.7 (4)
C11—C10—C15—C14	0.7 (4)	C29—C30—C35—C34	178.6 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C31—H31···N5^{i}	0.95	2.55	3.338 (3)	141
C24—H24···N2^{ii}	0.95	2.57	3.394 (4)	146

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