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3,6,14,17-Tetramethoxy-22,23-diphenyl-1,10,12,21-tetraazahexacyclo-[19.2.1.$0^{2,7}$.$0^{10,23}$.$0^{12,22}$.$0^{13,18}$]tetracosa-2(7),3,5,13(18),14,16-hexaene-11,24-dithione

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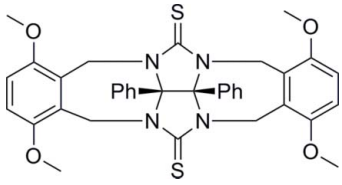
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.056; wR factor = 0.162; data-to-parameter ratio = 16.9.

The title compound, $C_{36}H_{34}N_4O_4S_2$, is a thioglycoluril derivative, which bears two phenyl substituents on its convex face and two methoxy substituted *o*-xylylenes as sidewalls of the molecular clip. There is one half-molecule in the asymmetric unit: a crystallographic twofold axis generates the complete molecule. The non-planar seven-membered rings adopt chair conformations, while the two five-membered rings exhibit envelope conformations and make a dihedral angle of 68.46 (12)°. The O atoms of the methoxy groups are coplanar with the six-membered *o*-xylylene sidewalls.

Related literature

For related structures, see: Broan *et al.* (1989); Cao *et al.* (2009); Wang *et al.* (2006); Wang & Xi (2009); Wu & Sun, (2009). For further synthetic details, see: Broan *et al.* (1989); Wu *et al.* (2002). The rigid concave shape of glycoluril makes it a versatile building block in supramolecular chemistry, see: Gao *et al.* (2009); Rowan *et al.* (1999); Hof *et al.* (2002); Kolbel & Menger (2001); Wu *et al.* (2002); Kang *et al.* (2004).



Experimental

Crystal data

$C_{36}H_{34}N_4O_4S_2$
M_r = 650.79
Monoclinic, $C2/c$
a = 17.9993 (15) Å
b = 12.5069 (11) Å
c = 16.0934 (12) Å
β = 115.961 (3)°
V = 3257.3 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 298 K
0.23 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
13570 measured reflections
3546 independent reflections
2279 reflections with $I > 2\sigma(I)$
R_{int} = 0.067

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.162
S = 0.98
3546 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

The author thanks Professor An-Xin Wu for technical assistance and Dr Meng Xiang-Gao for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2304).

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supporting information

Acta Cryst. (2010). E**66**, o1673 [doi:10.1107/S160053681002204X]

3,6,14,17-Tetramethoxy-22,23-diphenyl-1,10,12,21-tetraazahexacyclo-[19.2.1.$0^{2,7}$.$0^{10,23}$.$0^{12,22}$.$0^{13,18}$]tetracosa-2(7),3,5,13(18),14,16-hexaene-11,24-dithione

Yan Yang

S1. Comment

The rigid concave shape of glycoluril makes it a versatile building block to construct various supramolecular objects (Gao *et al.*, 2009), including molecular clips and molecular baskets (Rowan *et al.*, 1999), molecular capsules (Hof *et al.*, 2002), xerogels (Kolbel & Menger, 2001), the cucurbit[n]uril family (Wu *et al.*, 2002), and anion-binding receptors (Kang *et al.*, 2004). Based on the previous studies (Broan *et al.*, 1989; Cao *et al.*, 2009; Wang *et al.*, 2006; Wang & Xi, 2009; Wu & Sun, 2009), we report here the structure of the title thioglycoluril derivative (Fig. 1), which is a potential receptor in supramolecular chemistry.

There is one half-molecule in the asymmetric unit. The non-planar seven-membered rings adopt chair conformations, while the two five-membered rings have envelope conformation and the dihedral angle between them is 68.46°. The methoxy groups on sidewalls are coplanar with the six-membered o-xylylene sidewalls. The molecule contains three nonclassical intramolecular C—H···S, C—H···O and C—H···N hydrogen bonds, and its crystal structure is stabilized mostly by intermolecular C—H···π interactions (Table 1).

S2. Experimental

The thioglycoluril was synthesized according to a literature procedure, see : Broan *et al.*, (1989). Preparation of the title compound: A solution of thioglycoluril (326 mg, 1.00 mmol), paraformaldehyde (120 mg, 4.00 mmol) and 1,4-dimethoxybenzene (304 mg, 2.20 mmol) in TFA (5 ml) was stirred and heated at reflux for 6 h. After rotary evaporation the residue was chromatographed to yield the tile compound (521 mg, 0.80 mmol,80%). Crystals of (I) suitable for X-ray diffraction were grown by slow evaporation of a dichloromethane-methanol (1:2) solution of the title compound under 293 K.

S3. Refinement

All H atoms were positioned in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93-0.98 Å and Uĩso~(H) = 1.2U~eq~(C) or Uĩso~(H) = 1.5U~eq~(C).

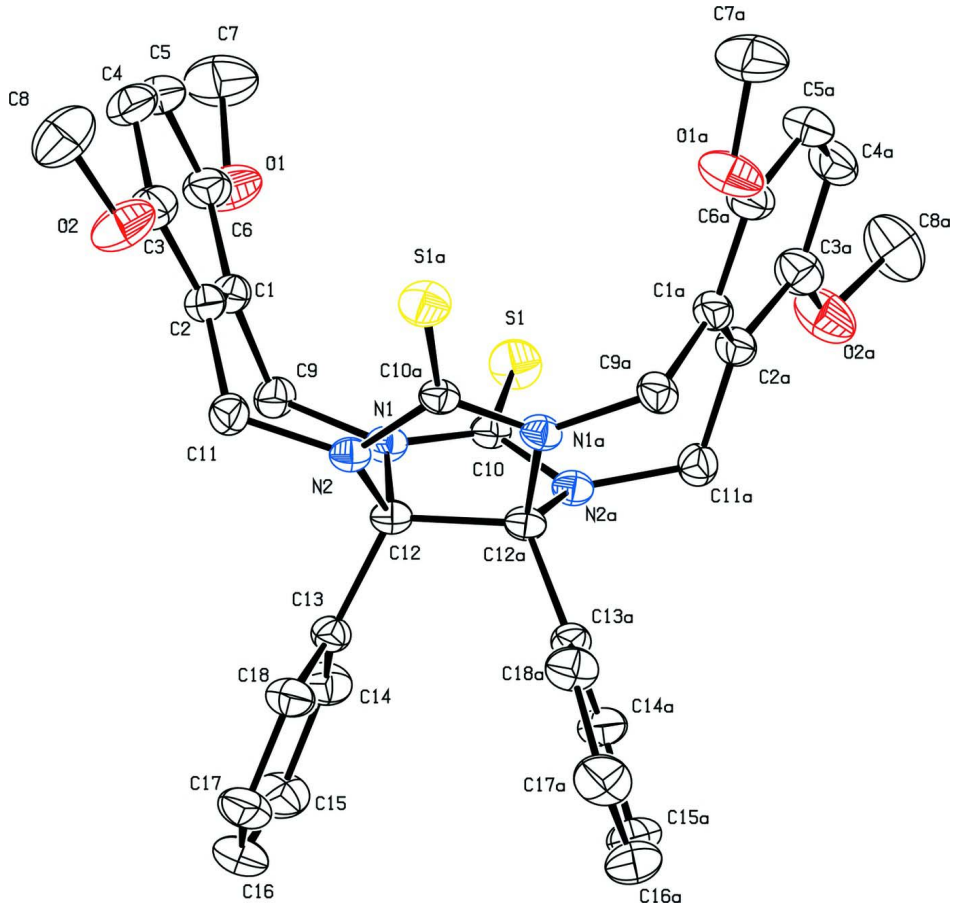

Figure 1

A view of (I), showing the atom-labelling scheme, with displacement ellipsoids drawn at the 30% probability level.

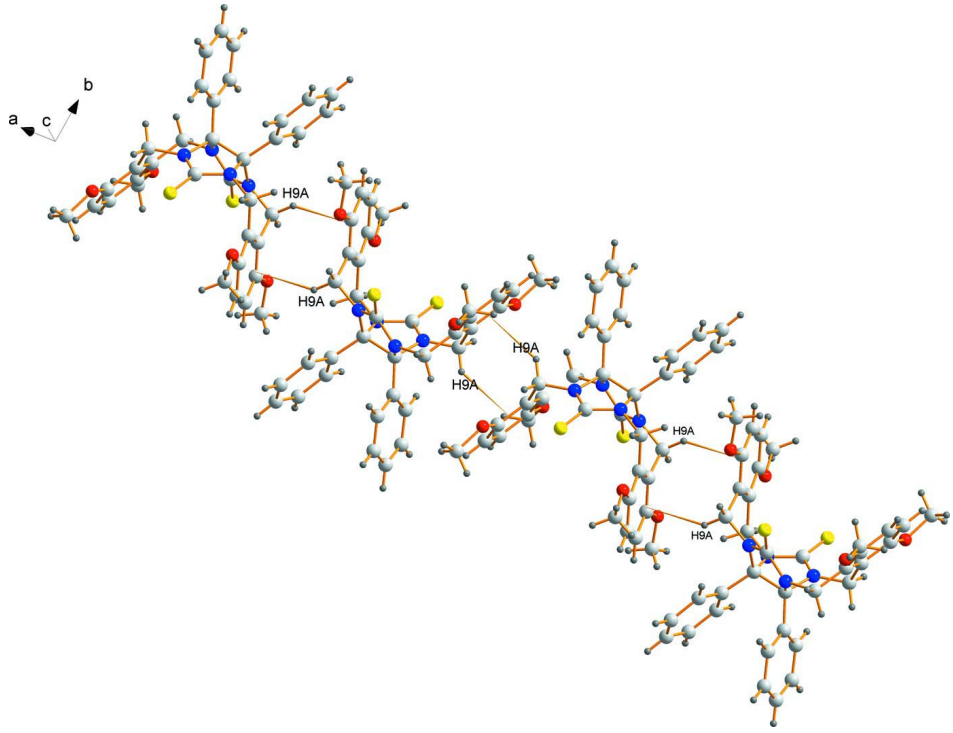

Figure 2

Packing of (I) with C—H···π interactions drawn as dashed lines showing the formation of a one-dimensional chain.

3,6,14,17-Tetramethoxy-22,23-diphenyl-1,10,12,21-tetraazahexacyclo[19.2.1.$0^{2,7}$.$0^{10,23}$.$0^{12,22}$.$0^{13,18}$]tetracosa-2(7),3,5,13 (18),14,16-hexaene-11,24-dithione

Crystal data

$C_{36}H_{34}N_4O_4S_2$
M_r = 650.79
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 17.9993 (15) Å
b = 12.5069 (11) Å
c = 16.0934 (12) Å
β = 115.961 (3)°
V = 3257.3 (5) Å^3
Z = 4

F(000) = 1368
D_x = 1.327 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 2697 reflections
θ = 2.5–21.3°
μ = 0.21 mm^{-1}
T = 298 K
Block, colorless
0.23 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
13570 measured reflections
3546 independent reflections

2279 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 27.0°, θ_{min} = 2.1°
h = −22→13
k = −15→15
l = −19→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.162$
$S = 0.98$
3546 reflections
210 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
$w = 1/[\sigma^2(F_o^2) + (0.0878P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

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. 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	0.11451 (4)	0.22118 (5)	0.14339 (5)	0.0528 (3)
N1	0.09215 (11)	0.31734 (13)	0.27979 (13)	0.0335 (5)
N2	−0.00738 (11)	0.34780 (13)	0.14082 (13)	0.0325 (4)
C13	0.07957 (13)	0.50126 (16)	0.32973 (15)	0.0343 (5)
C9	0.16813 (14)	0.27755 (17)	0.35521 (17)	0.0388 (6)
H9A	0.1970	0.3371	0.3949	0.047*
H9B	0.2036	0.2489	0.3294	0.047*
C12	0.03855 (13)	0.39284 (16)	0.29759 (15)	0.0306 (5)
C10	0.06573 (14)	0.29489 (16)	0.18917 (16)	0.0326 (5)
O2	0.06197 (14)	0.16264 (16)	0.57355 (15)	0.0713 (6)
O1	0.24132 (13)	0.08009 (14)	0.37734 (15)	0.0683 (6)
C1	0.15415 (14)	0.19204 (17)	0.41322 (17)	0.0393 (6)
C2	0.10798 (15)	0.21274 (17)	0.46227 (17)	0.0406 (6)
C6	0.19350 (16)	0.09225 (18)	0.42349 (19)	0.0477 (7)
C18	0.13789 (15)	0.53676 (19)	0.30210 (19)	0.0497 (7)
H18	0.1560	0.4916	0.2688	0.060*
C11	−0.06462 (15)	0.31850 (18)	0.04628 (16)	0.0392 (6)
H11A	−0.0343	0.3157	0.0092	0.047*
H11B	−0.1060	0.3742	0.0209	0.047*
C3	0.10368 (17)	0.1344 (2)	0.52320 (19)	0.0512 (7)
C14	0.05429 (16)	0.56979 (18)	0.37978 (18)	0.0463 (7)
H14	0.0150	0.5469	0.3988	0.056*
C4	0.14195 (17)	0.0364 (2)	0.5309 (2)	0.0578 (8)
H4	0.1379	−0.0156	0.5701	0.069*
C17	0.16966 (18)	0.6394 (2)	0.3237 (2)	0.0655 (9)

H17	0.2086	0.6631	0.3045	0.079*
C5	0.18588 (18)	0.0156 (2)	0.4811 (2)	0.0564 (8)
H5	0.2108	−0.0508	0.4863	0.068*
C15	0.0865 (2)	0.6717 (2)	0.4019 (2)	0.0638 (9)
H15	0.0693	0.7170	0.4360	0.077*
C16	0.1438 (2)	0.7055 (2)	0.3733 (2)	0.0731 (10)
H16	0.1654	0.7742	0.3878	0.088*
C7	0.2729 (2)	−0.0224 (2)	0.3750 (3)	0.0859 (11)
H7A	0.2924	−0.0550	0.4348	0.129*
H7B	0.3178	−0.0162	0.3583	0.129*
H7C	0.2301	−0.0658	0.3302	0.129*
C8	0.0599 (2)	0.0907 (3)	0.6401 (2)	0.0865 (11)
H8A	0.0241	0.0319	0.6094	0.130*
H8B	0.0396	0.1269	0.6787	0.130*
H8C	0.1146	0.0643	0.6775	0.130*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0520 (5)	0.0520 (4)	0.0612 (5)	0.0130 (3)	0.0311 (4)	−0.0081 (3)
N1	0.0300 (11)	0.0293 (9)	0.0435 (12)	0.0043 (7)	0.0181 (9)	0.0014 (8)
N2	0.0341 (11)	0.0273 (9)	0.0390 (11)	0.0020 (8)	0.0189 (9)	−0.0016 (8)
C13	0.0316 (13)	0.0300 (11)	0.0397 (13)	−0.0029 (9)	0.0141 (10)	0.0006 (9)
C9	0.0268 (13)	0.0385 (13)	0.0466 (14)	0.0035 (10)	0.0118 (11)	0.0042 (10)
C12	0.0317 (12)	0.0264 (10)	0.0391 (12)	0.0013 (9)	0.0205 (10)	0.0006 (9)
C10	0.0327 (13)	0.0270 (11)	0.0395 (14)	−0.0012 (9)	0.0170 (11)	0.0011 (9)
O2	0.0922 (16)	0.0662 (13)	0.0746 (14)	0.0174 (11)	0.0543 (13)	0.0311 (11)
O1	0.0756 (15)	0.0481 (11)	0.0968 (17)	0.0248 (10)	0.0521 (13)	0.0162 (10)
C1	0.0328 (14)	0.0343 (12)	0.0433 (14)	0.0000 (10)	0.0097 (11)	0.0030 (10)
C2	0.0390 (14)	0.0331 (12)	0.0430 (14)	−0.0015 (10)	0.0118 (12)	0.0037 (10)
C6	0.0452 (16)	0.0364 (13)	0.0582 (17)	0.0053 (11)	0.0197 (13)	0.0014 (11)
C18	0.0428 (16)	0.0428 (14)	0.0692 (19)	−0.0048 (11)	0.0300 (14)	0.0017 (12)
C11	0.0397 (14)	0.0408 (13)	0.0357 (13)	0.0020 (10)	0.0153 (11)	−0.0017 (10)
C3	0.0549 (18)	0.0474 (15)	0.0536 (17)	−0.0009 (13)	0.0259 (14)	0.0083 (12)
C14	0.0582 (17)	0.0334 (13)	0.0518 (16)	−0.0035 (11)	0.0284 (14)	−0.0037 (11)
C4	0.063 (2)	0.0437 (15)	0.0596 (18)	0.0013 (13)	0.0207 (16)	0.0190 (13)
C17	0.0486 (18)	0.0531 (17)	0.091 (2)	−0.0183 (14)	0.0267 (17)	0.0117 (16)
C5	0.065 (2)	0.0345 (14)	0.0639 (19)	0.0073 (12)	0.0226 (16)	0.0073 (13)
C15	0.090 (2)	0.0359 (14)	0.0624 (19)	−0.0065 (15)	0.0304 (17)	−0.0115 (13)
C16	0.084 (3)	0.0387 (16)	0.080 (2)	−0.0232 (16)	0.021 (2)	−0.0042 (15)
C7	0.112 (3)	0.055 (2)	0.113 (3)	0.0199 (19)	0.070 (3)	−0.0035 (18)
C8	0.099 (3)	0.095 (3)	0.076 (2)	0.009 (2)	0.048 (2)	0.036 (2)

Geometric parameters (Å, º)

S1—C10	1.652 (2)	C6—C5	1.381 (4)
N1—C10	1.351 (3)	C18—C17	1.386 (4)
N1—C9	1.462 (3)	C18—H18	0.9300

N1—C12	1.465 (3)	C11—C2^{i}	1.511 (3)
N2—C10	1.371 (3)	C11—H11A	0.9700
N2—C12^{i}	1.450 (3)	C11—H11B	0.9700
N2—C11	1.462 (3)	C3—C4	1.384 (4)
C13—C18	1.381 (3)	C14—C15	1.381 (3)
C13—C14	1.382 (3)	C14—H14	0.9300
C13—C12	1.522 (3)	C4—C5	1.375 (4)
C9—C1	1.511 (3)	C4—H4	0.9300
C9—H9A	0.9700	C17—C16	1.364 (4)
C9—H9B	0.9700	C17—H17	0.9300
C12—N2^{i}	1.450 (3)	C5—H5	0.9300
C12—C12^{i}	1.553 (4)	C15—C16	1.369 (4)
O2—C3	1.370 (3)	C15—H15	0.9300
O2—C8	1.412 (3)	C16—H16	0.9300
O1—C6	1.369 (3)	C7—H7A	0.9600
O1—C7	1.410 (3)	C7—H7B	0.9600
C1—C2	1.398 (3)	C7—H7C	0.9600
C1—C6	1.409 (3)	C8—H8A	0.9600
C2—C3	1.412 (3)	C8—H8B	0.9600
C2—C11^{i}	1.511 (3)	C8—H8C	0.9600

C10—N1—C9	125.79 (19)	N2—C11—H11A	108.6
C10—N1—C12	113.23 (17)	C2^{i}—C11—H11A	108.6
C9—N1—C12	120.91 (18)	N2—C11—H11B	108.6
C10—N2—C12^{i}	111.24 (18)	C2^{i}—C11—H11B	108.6
C10—N2—C11	122.26 (18)	H11A—C11—H11B	107.6
C12^{i}—N2—C11	120.09 (18)	O2—C3—C4	123.7 (2)
C18—C13—C14	118.6 (2)	O2—C3—C2	116.3 (2)
C18—C13—C12	120.1 (2)	C4—C3—C2	120.0 (3)
C14—C13—C12	121.1 (2)	C15—C14—C13	121.0 (3)
N1—C9—C1	113.92 (19)	C15—C14—H14	119.5
N1—C9—H9A	108.8	C13—C14—H14	119.5
C1—C9—H9A	108.8	C5—C4—C3	120.4 (2)
N1—C9—H9B	108.8	C5—C4—H4	119.8
C1—C9—H9B	108.8	C3—C4—H4	119.8
H9A—C9—H9B	107.7	C16—C17—C18	120.0 (3)
N2^{i}—C12—N1	111.61 (16)	C16—C17—H17	120.0
N2^{i}—C12—C13	112.90 (18)	C18—C17—H17	120.0
N1—C12—C13	112.20 (18)	C4—C5—C6	120.8 (2)
N2^{i}—C12—C12^{i}	103.2 (2)	C4—C5—H5	119.6
N1—C12—C12^{i}	100.82 (17)	C6—C5—H5	119.6
C13—C12—C12^{i}	115.23 (12)	C16—C15—C14	119.4 (3)
N1—C10—N2	108.02 (18)	C16—C15—H15	120.3
N1—C10—S1	126.35 (17)	C14—C15—H15	120.3
N2—C10—S1	125.57 (17)	C17—C16—C15	120.7 (3)
C3—O2—C8	119.2 (2)	C17—C16—H16	119.7
C6—O1—C7	118.2 (2)	C15—C16—H16	119.7
C2—C1—C6	119.4 (2)	O1—C7—H7A	109.5

C2—C1—C9	121.2 (2)	O1—C7—H7B	109.5
C6—C1—C9	119.2 (2)	H7A—C7—H7B	109.5
C1—C2—C3	119.4 (2)	O1—C7—H7C	109.5
C1—C2—C11^{i}	121.4 (2)	H7A—C7—H7C	109.5
C3—C2—C11^{i}	119.2 (2)	H7B—C7—H7C	109.5
O1—C6—C5	123.9 (2)	O2—C8—H8A	109.5
O1—C6—C1	116.0 (2)	O2—C8—H8B	109.5
C5—C6—C1	120.0 (3)	H8A—C8—H8B	109.5
C13—C18—C17	120.3 (3)	O2—C8—H8C	109.5
C13—C18—H18	119.8	H8A—C8—H8C	109.5
C17—C18—H18	119.8	H8B—C8—H8C	109.5
N2—C11—C2^{i}	114.50 (19)		

C10—N1—C9—C1	−106.3 (3)	C7—O1—C6—C5	11.7 (4)
C12—N1—C9—C1	77.1 (3)	C7—O1—C6—C1	−171.6 (3)
C10—N1—C12—N2^{i}	122.1 (2)	C2—C1—C6—O1	−176.5 (2)
C9—N1—C12—N2^{i}	−60.9 (2)	C9—C1—C6—O1	−1.2 (3)
C10—N1—C12—C13	−110.1 (2)	C2—C1—C6—C5	0.4 (4)
C9—N1—C12—C13	66.9 (2)	C9—C1—C6—C5	175.7 (2)
C10—N1—C12—C12^{i}	13.1 (2)	C14—C13—C18—C17	−0.5 (4)
C9—N1—C12—C12^{i}	−169.92 (18)	C12—C13—C18—C17	173.8 (2)
C18—C13—C12—N2^{i}	155.7 (2)	C10—N2—C11—C2^{i}	70.0 (3)
C14—C13—C12—N2^{i}	−30.1 (3)	C12^{i}—N2—C11—C2^{i}	−79.4 (2)
C18—C13—C12—N1	28.6 (3)	C8—O2—C3—C4	2.6 (4)
C14—C13—C12—N1	−157.3 (2)	C8—O2—C3—C2	−175.9 (3)
C18—C13—C12—C12^{i}	−86.0 (3)	C1—C2—C3—O2	175.8 (2)
C14—C13—C12—C12^{i}	88.1 (3)	C11^{i}—C2—C3—O2	−2.3 (4)
C9—N1—C10—N2	−179.57 (19)	C1—C2—C3—C4	−2.8 (4)
C12—N1—C10—N2	−2.7 (2)	C11^{i}—C2—C3—C4	179.0 (2)
C9—N1—C10—S1	−2.1 (3)	C18—C13—C14—C15	0.0 (4)
C12—N1—C10—S1	174.75 (16)	C12—C13—C14—C15	−174.3 (2)
C12^{i}—N2—C10—N1	−10.2 (2)	O2—C3—C4—C5	−177.0 (3)
C11—N2—C10—N1	−162.05 (19)	C2—C3—C4—C5	1.5 (4)
C12^{i}—N2—C10—S1	172.29 (15)	C13—C18—C17—C16	0.6 (4)
C11—N2—C10—S1	20.5 (3)	C3—C4—C5—C6	0.8 (4)
N1—C9—C1—C2	−61.3 (3)	O1—C6—C5—C4	174.9 (2)
N1—C9—C1—C6	123.5 (2)	C1—C6—C5—C4	−1.8 (4)
C6—C1—C2—C3	1.8 (4)	C13—C14—C15—C16	0.5 (4)
C9—C1—C2—C3	−173.4 (2)	C18—C17—C16—C15	−0.2 (5)
C6—C1—C2—C11^{i}	180.0 (2)	C14—C15—C16—C17	−0.4 (5)
C9—C1—C2—C11^{i}	4.8 (3)		

Symmetry code: (i) $-x, y, -z+1/2$.

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*A*···*Cg*1^{i}	0.97	2.70	3.540	145

C11—H11*A*···O2^{i}	0.97	2.26	2.757 (3)	111
C14—H14···N2^{i}	0.93	2.56	2.879 (3)	101
C18—H18···N1	0.93	2.51	2.842 (3)	102
C9—H9*B*···S1	0.97	2.73	3.189 (3)	110
C9—H9*B*···O1	0.97	2.25	2.748 (3)	111

Symmetry code: (i) $-x, y, -z+1/2$.