



Crystal structure and Hirshfeld surface analysis of 8-benzyl-1-[(4-methylphenyl)sulfonyl]-2,7,8,9-tetrahydro-1*H*-3,6:10,13-diepoxy-1,8-benzodiazacyclopentadecine ethanol hemisolvate

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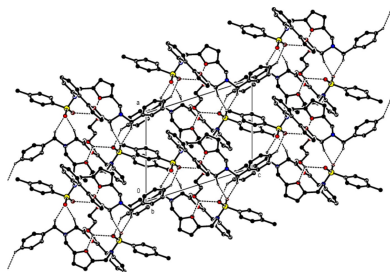
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The asymmetric unit of the title compound, $2C_{31}H_{28}N_2O_4S \cdot C_2H_6O$, contains a parent molecule and a half molecule of ethanol solvent. The main compound stabilizes its molecular conformation by forming a ring with an $R_1^2(7)$ motif with the ethanol solvent molecule. In the crystal, molecules are connected by C—H···O and O—H···O hydrogen bonds, forming a three-dimensional network. In addition, C—H··· π interactions also strengthen the molecular packing.

1. Chemical context

Intermolecular weak interactions play critical roles in maintaining supramolecular networks with diverse structures and functions, wherein multiple weak bonds can cooperate to promote both the formation and stabilization of the assemblies (Aliyeva *et al.*, 2024). *N*-Ligands bearing amino and imino moieties provide a rich coordination chemistry (Kopylovich *et al.*, 2011*a,b,c*; Mahmudov *et al.*, 2013, 2021). A number of metal complexes with *N*-ligands have been reported and characterized (Mahmoudi *et al.*, 2017*a,b*); some of them possess interesting spectroscopic, supramolecular and catalytic properties (Akbari Afkhami *et al.*, 2017; Gurbanov *et al.*, 2018, 2020). Similarly to the design of *N*-heterocycles (Abdelhamid *et al.*, 2011; Khalilov *et al.*, 2021; Safavora *et al.*, 2019), particular attention has also been paid to the decoration of the secondary coordination sphere of metal complexes (Gurbanov *et al.*, 2022*a,b*; Mahmoudi *et al.*, 2019, 2021). Depending on the attached functional groups, the chemical properties of *N*-heterocyclic ligands and their metal complexes can be improved (Aliyeva *et al.*, 2024). On the other hand, macrocyclic structures containing furan fragments have been described in the literature: furan-containing crown ethers and porphyrinoids (Märkl *et al.*, 1997), furan-containing porphyrins (Srinivasan *et al.*, 1997), cyclic oligomers of furane-containing amino acids (Chakraborty *et al.*, 2007) and anti-aromatic macrocycles in which furan blocks are interconnected through diene elements (Märkl *et al.*, 1996). Materials based on macrocycles have applications in drug discovery, can be used for the separation of isomers and metals, purification of organic solvents, chemical detection



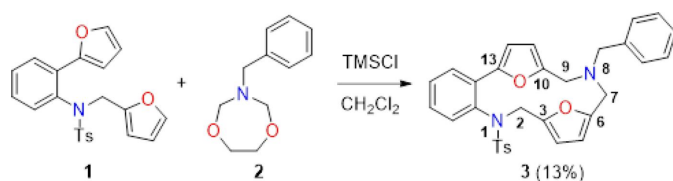
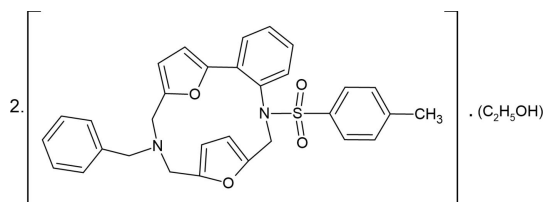


Figure 1
Synthesis of 8-benzyl-1-[(4-methylphenyl)sulfonyl]-2,7,8,9-tetrahydro-1H-3,6:10,13-diepoxy-1,8-benzodiazacyclopentadecine.

systems *etc.* Continuing our research into the chemistry of furyl-substituted sulfonamides (Guliyeva *et al.*, 2024; Mammadova *et al.*, 2023a,b; Borisova *et al.*, 2018a,b), a new approach toward the synthesis of difuryl-substituted arene-sulfonamide macrocycles has been developed. The synthetic procedure is the Mannich reaction between a difuryl-substituted toluenesulfonamide **1** and 3-benzyl-1,5,3-dioxazepane **2** under Lewis acid catalysis (Fig. 1). Trimethylsilyl chloride is the most efficient catalyst and has exhibited satisfactory results.



2. Structural commentary

The asymmetric unit of the title compound contains a parent molecule and a half molecule of the solvent ethanol. The main compound stabilizes its molecular conformation by forming a ring with an $R_1^2(7)$ motif with the ethanol solvent molecule (Fig. 2; Bernstein *et al.*, 1995). While the two furan rings (O18/C3–C6 and O19/C10–C13) in the central ring system subtend an angle of $75.50(7)^\circ$ with each other, they make dihedral angles of $50.15(7)$ and $25.58(7)^\circ$, respectively, with the benzene ring (C13A/C14–C17/C17A) in the same central ring.

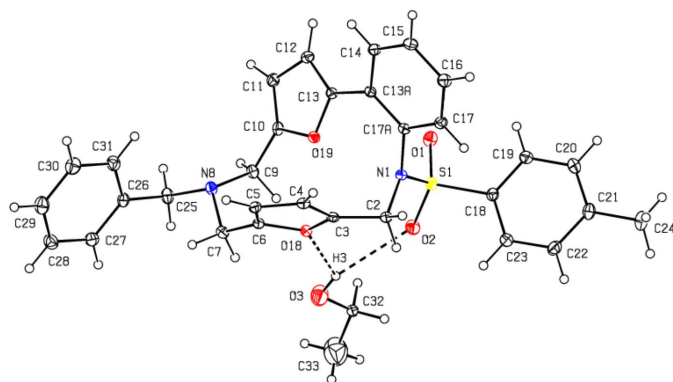


Figure 2
Molecular structure of the title compound showing the atom labelling and ellipsoids at the 30% probability level with hydrogen bonds indicated by dashed lines.

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$Cg1$, $Cg3$ and $Cg5$ are the centroids of the O18/C3–C6 furan, C13A/C14–C17/C17A benzene and C26–C31 phenyl rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C9-H9A\cdots O1^i$	0.99	2.53	3.4057 (17)	148
$C25-H25B\cdots O1^i$	0.99	2.59	3.5125 (18)	155
$O3-H3\cdots O2$	0.88 (7)	2.52 (6)	3.251 (3)	141 (6)
$O3-H3\cdots O18$	0.88 (7)	2.47 (7)	3.097 (4)	129 (5)
$C2-H2A\cdots Cg1^{ii}$	0.99	2.56	3.2916 (12)	131
$C16-H16\cdots Cg5^{iii}$	0.95	2.80	3.5220 (15)	133
$C20-H20\cdots Cg3^{iv}$	0.95	2.83	3.5707 (15)	135

Symmetry codes: (i) $-x, -y + 1, -z + 1$; (ii) $-x + 1, -y, -z + 1$; (iii) $x + 1, y, z - 1$; (iv) $-x + 1, -y + 1, -z$.

The phenyl (C26–C31) and benzene (C18–C23) rings outside the central ring make an angle of $65.91(8)^\circ$ with each other, and subtend dihedral angles of $68.95(7)$ and $48.71(7)^\circ$, respectively, with the benzene ring (C13A/C14–C17/C17A) in the central ring. The r.m.s. deviations of the planes fitted through the atoms attached to N1 and N8 are 0.0744 and 0.1889 \AA , respectively, with the distances of N1 and N8 to these planes being 0.1288 (8) and 0.3271 (10) \AA , respectively. The sums of the angles around the central atoms N1 and N8 are 356.20 and 334.96° , respectively. As can be seen, N1 is closer to the plane of neighboring atoms than N8, and the sum of the angles around it is closer to 360° . The S1 atom bonded to the N1 atom causes it to have a more planar environment. In the title compound, the N atoms are located on opposite sides of the mean plane through the thirteen-membered difuryl-containing ring. Bond length and angle values in the title compound are comparable to those in the related compounds discussed in the *Database survey* (section 4).

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, molecules are connected by $C-H\cdots O$ and $O-H\cdots O$ hydrogen bonds, forming a three-dimensional

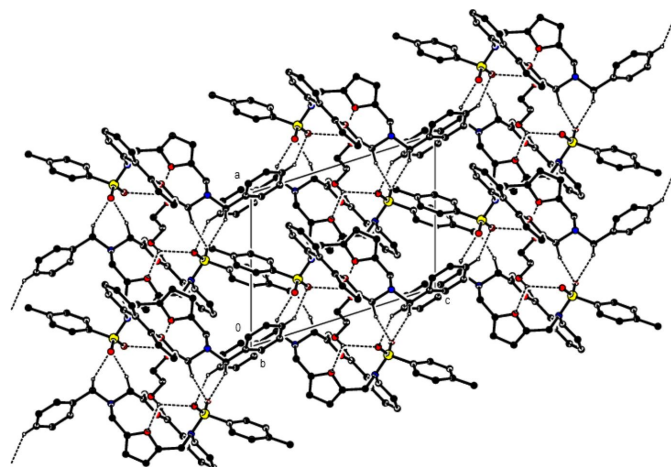


Figure 3
Crystal packing viewed along the b -axis showing $C-H\cdots O$ and $O-H\cdots O$ hydrogen bonds shown as dashed lines.

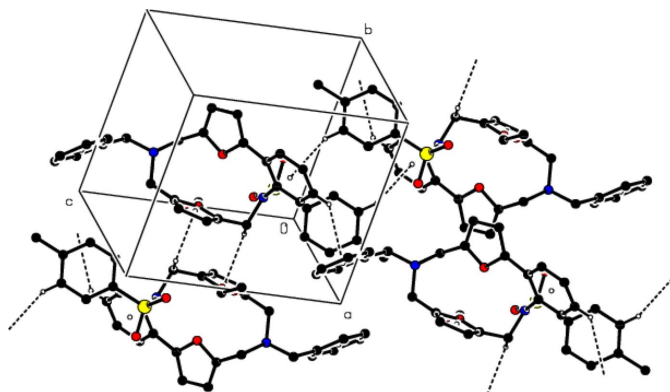


Figure 4
View of the C–H... π interactions in the crystal packing, shown as dashed lines.

network (Table 1; Fig. 3). In addition, C–H... π interactions (Table 1) also strengthen the molecular packing (Fig. 4).

Two-dimensional fingerprints and the Hirshfeld surface of the title molecule were computed using *CrystalExplorer17.5* (Spackman *et al.*, 2021). The Hirshfeld surface was mapped over d_{norm} in the range -0.1635 (red) to $+1.5099$ (blue) a.u. (Fig. 5). The overall two-dimensional fingerprint plot and those delineated into H...H, C...H/H...C and O...H/H...O contacts are illustrated in Fig. 5*a–d*, respectively. The pairs of spikes with tips at $d_e + d_i = 2.62$ Å in Fig. 5*c* and at $d_e + d_i = 2.40$ Å in Fig. 5*d* indicate weak hydrogen-bonding interactions. The most significant contributions to the Hirshfeld surface are from H...H (56.6%, Fig. 5*b*), C...H/H...C (26.6%, Fig. 5*c*) and O...H/H...O (13.9%, Fig. 5*d*) interactions, indicating that the highest contributions arise from contacts in which H atoms are involved. Except for C...C interactions (2.1%), the other contributions are less than 1.5%.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.42, update of September 2021; Groom *et al.*, 2016) found the compounds most similar to the title compound to be 7,14,16-trimethyl-17-(trifluoroacetyl)-18,19-dioxo-7,17-diazatetracyclo[11.3.1.1^{2,5}.1^{9,12}]nonadeca-2,4,9,11-tetraen-15-one (CSD refcode YEYXAF; Yıldırım *et al.*, 2023) and 1,8,12,19,24,26-hexaazapentacyclo[17.3.1.1^{3,6}.1^{8,12}.1^{14,17}]hexacos-3,5,14,16-tetraene ethyl acetate solvate dihydrate (NOYCOW; Jana *et al.*, 2019).

NOYCOW crystallizes in the monoclinic space group *I2/a* with $Z = 8$ while YEYXAF crystallizes in the orthorhombic

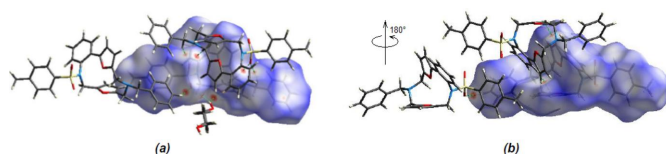


Figure 5
Front (*a*) and back (*b*) views of the three-dimensional Hirshfeld surface, showing some C–H...O and O–H...O hydrogen bonds.

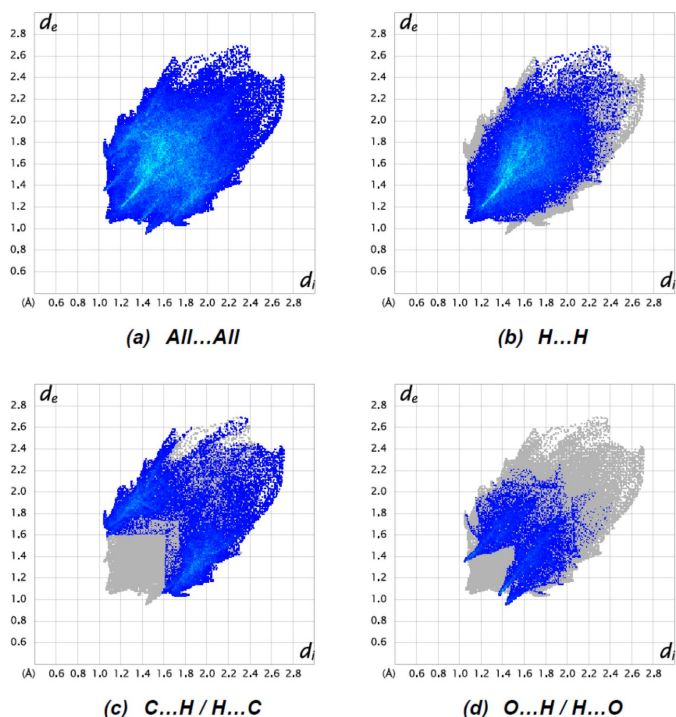


Figure 6
The two-dimensional fingerprint plots for the title molecule showing (*a*) all interactions, and delineated into (*b*) H...H, (*c*) C...H/H...C and (*d*) O...H/H...O interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

space group *Pbca* with $Z = 8$. The furan rings in YEYXAF are nearly perpendicular to the mean plane through the main twelve-membered difuryl-containing ring and their oxygen atoms are oriented towards opposite sides. In NOYCOW, the pyrrole rings are also almost perpendicular to the sixteen-membered ring, but the two pyrrolic NH atoms are oriented in the same direction.

In the title compound, the N atoms are located on either side of the mean plane through the thirteen-membered difuryl-containing ring. The phenyl group of the title molecule is approximately parallel to this thirteen-membered ring, and the benzene ring attached to the S atom is also approximately parallel.

5. Synthesis and crystallization

The starting materials *N*-(2-(furan-2-yl)phenyl)-*N*-(furan-2-ylmethyl)-4-methylbenzenesulfonamide **1** (100 mg, 0.25 mmol) and 3-benzyl-1,5,3-dioxazepane **2** (52 mg, 0.27 mmol) in 5 mL of DCM were placed into a two-neck flask. The reaction mixture was purged with argon for 10 min under stirring and cooling in an ice–water bath. Chlorotrimethylsilane (TMSCl, 0.11 mL, 0.84 mmol) was added to the reaction with stirring at 273 K. After the addition, the reaction mixture was stirred for 24 h under argon. Then a saturated Na_2CO_3 solution was added to the reaction mixture to adjust the pH to ~ 7 . Then it was poured into water (20 mL) and extracted with DCM (3×10 mL). The reaction product was purified by column chromatography (SiO_2 , 20×1.1 cm,

Table 2
Experimental details.

Crystal data	
Chemical formula	$2C_{31}H_{28}N_2O_4S \cdot C_2H_6O$
M_r	1095.29
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, b, c (Å)	10.7108 (2), 11.7817 (2), 12.9233 (3)
α, β, γ (°)	73.831 (2), 67.667 (2), 67.380 (2)
V (Å ³)	1375.62 (6)
Z	1
Radiation type	Cu $K\alpha$
μ (mm ⁻¹)	1.39
Crystal size (mm)	0.28 × 0.25 × 0.21
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2021)
T_{\min}, T_{\max}	0.696, 0.759
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	41981, 5824, 5577
R_{int}	0.035
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.634
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.034, 0.088, 1.06
No. of reflections	5824
No. of parameters	375
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.36, -0.38

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXL2016/6* (Sheldrick, 2015a), *SHELXL2016/6* (Sheldrick, 2015b), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

eluent: heptane/ethyl acetate 10:1, TLC: heptane/ethyl acetate 4:1). The title compound was obtained as a colorless powder, yield 13%, 17 mg (0.032 mmol); m.p. > 523 K (with decomp.). Single crystals of the title compound were grown from EtOH. IR (KBr), ν (cm⁻¹): 1348 ($\nu_{\text{as}} \text{SO}_2$), 1162 ($\nu_{\text{s}} \text{SO}_2$). ¹H NMR (700.2 MHz, CDCl₃) (J , Hz): δ 7.47 (d , $J = 8.1$ Hz, 2H), 7.33 (d , $J = 8.1$ Hz, 1H), 7.27–7.20 (m , 7H), 7.13 (d , $J = 8.1$ Hz, 2H), 6.98 (d , $J = 7.9$ Hz, 1H), 6.30 (d , $J = 2.9$ Hz, 1H), 5.89 (d , $J = 2.9$ Hz, 1H), 5.74 (d , $J = 2.9$ Hz, 1H), 5.62 (d , $J = 2.9$ Hz, 1H), 5.15 (d , $J = 14.8$ Hz, 1H), 4.10 (d , $J = 14.8$ Hz, 1H), 3.86 (s , 2H), 3.79 (d , $J = 15.0$ Hz, 1H), 3.65 (d , $J = 15.0$ Hz, 1H), 3.57 (d , $J = 13.8$ Hz, 1H), 3.47 (d , $J = 13.8$ Hz, 1H), 2.33 (s , 3H). ¹³C{¹H} NMR (176.1 MHz, CDCl₃): δ 152.3, 152.1, 150.8, 146.4, 142.1, 138.2, 135.9, 134.9, 132.8, 128.9, 128.8, 128.3 (2C), 127.9 (2C), 127.7, 127.3 (2C), 126.7 (2C), 126.0, 114.1, 110.5, 109.6, 108.1, 107.0, 54.8, 49.7, 48.9, 48.4, 20.5. MS (ESI) m/z : [$M + H$]⁺ 525. Elemental analysis calculated (%) for C₃₁H₂₈N₂O₄S: C 70.97, H 5.38, N 5.34, S 6.11; found: C 71.11, H 5.49, N 5.59, S 5.87.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All C-bound H atoms were positioned geometrically (C–H = 0.95 and 0.99 Å) and refined using a riding model with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{C})$. The O-bound H atom of the ethanol solvent was located in difference-Fourier maps [O3–H3 = 0.88 (6) Å] and refined freely

with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The site occupation factors of the solvent atoms were fixed at 0.5.

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supporting information

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Crystal structure and Hirshfeld surface analysis of 8-benzyl-1-[(4-methylphenyl)sulfonyl]-2,7,8,9-tetrahydro-1*H*-3,6:10,13-diepoxy-1,8-benzodiazacyclopentadecine ethanol hemisolvate

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Computing details

8-Benzyl-1-[(4-methylphenyl)sulfonyl]-2,7,8,9-tetrahydro-1*H*-3,6:10,13-diepoxy-1,8-benzodiazacyclopentadecine ethanol hemisolvate

Crystal data

$2\text{C}_{31}\text{H}_{28}\text{N}_2\text{O}_4\text{S}\cdot\text{C}_2\text{H}_6\text{O}$

$M_r = 1095.29$

Triclinic, $P\bar{1}$

$a = 10.7108$ (2) Å

$b = 11.7817$ (2) Å

$c = 12.9233$ (3) Å

$\alpha = 73.831$ (2)°

$\beta = 67.667$ (2)°

$\gamma = 67.380$ (2)°

$V = 1375.62$ (6) Å³

$Z = 1$

$F(000) = 578$

$D_x = 1.322$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å

Cell parameters from 29573 reflections

$\theta = 3.7\text{--}77.3^\circ$

$\mu = 1.39$ mm⁻¹

$T = 100$ K

Prism, colourless

$0.28 \times 0.25 \times 0.21$ mm

Data collection

XtaLAB Synergy, Dualflex, HyPix
diffractometer

Radiation source: micro-focus sealed X-ray tube

φ and ω scans

Absorption correction: multi-scan
(CrysAlisPro; Rigaku OD, 2021)

$T_{\min} = 0.696$, $T_{\max} = 0.759$

41981 measured reflections

5824 independent reflections

5577 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\max} = 77.9^\circ$, $\theta_{\min} = 3.7^\circ$

$h = -13 \rightarrow 13$

$k = -14 \rightarrow 13$

$l = -16 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.088$

$S = 1.06$

5824 reflections

375 parameters

0 restraints

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0392P)^2 + 0.6403P]$

where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.36$ e Å⁻³

$\Delta\rho_{\min} = -0.38$ e Å⁻³

Extinction correction: SHELXL-2019/3
 (Sheldrick, 2015b),
 $F_c^* = k F_c [1 + 0.001 x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.0016 (2)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
S1	0.34319 (3)	0.29237 (3)	0.25323 (2)	0.01869 (9)	
O1	0.26473 (9)	0.42189 (9)	0.23711 (8)	0.0254 (2)	
O2	0.27094 (10)	0.20120 (9)	0.30881 (8)	0.0275 (2)	
N1	0.44474 (10)	0.27652 (9)	0.32641 (8)	0.0172 (2)	
C2	0.51453 (13)	0.15058 (10)	0.37966 (10)	0.0191 (2)	
H2A	0.485159	0.088176	0.364704	0.023*	
H2B	0.619013	0.129923	0.346117	0.023*	
C3	0.47475 (12)	0.14584 (10)	0.50358 (10)	0.0175 (2)	
C4	0.54024 (13)	0.15296 (11)	0.57161 (10)	0.0198 (2)	
H4	0.634721	0.154918	0.550100	0.024*	
C5	0.43909 (13)	0.15696 (11)	0.68239 (10)	0.0199 (2)	
H5	0.453219	0.162182	0.748959	0.024*	
C6	0.31931 (13)	0.15184 (10)	0.67389 (10)	0.0185 (2)	
C7	0.17501 (13)	0.15988 (11)	0.75523 (10)	0.0220 (2)	
H7A	0.131541	0.114502	0.731987	0.026*	
H7B	0.183651	0.118517	0.831302	0.026*	
N8	0.08088 (11)	0.28896 (10)	0.76194 (8)	0.0200 (2)	
C9	0.04134 (13)	0.35259 (11)	0.65683 (10)	0.0204 (2)	
H9A	-0.061979	0.397627	0.677668	0.024*	
H9B	0.060752	0.289099	0.611373	0.024*	
C10	0.11988 (12)	0.44237 (11)	0.58612 (10)	0.0189 (2)	
C11	0.09010 (13)	0.56626 (12)	0.57983 (10)	0.0223 (3)	
H11	0.006365	0.620768	0.622820	0.027*	
C12	0.20853 (13)	0.59902 (11)	0.49635 (11)	0.0221 (2)	
H12	0.219159	0.679579	0.473175	0.027*	
C13	0.30360 (12)	0.49285 (11)	0.45610 (10)	0.0173 (2)	
C13A	0.44410 (12)	0.46902 (10)	0.37101 (10)	0.0170 (2)	
C14	0.52046 (13)	0.55094 (11)	0.35073 (10)	0.0197 (2)	
H14	0.480254	0.616767	0.394083	0.024*	
C15	0.65231 (13)	0.53900 (11)	0.26973 (11)	0.0223 (2)	
H15	0.701290	0.595894	0.258244	0.027*	
C16	0.71286 (13)	0.44340 (12)	0.20519 (11)	0.0238 (3)	
H16	0.802673	0.435140	0.148619	0.029*	
C17	0.64055 (13)	0.36040 (11)	0.22444 (10)	0.0210 (2)	
H17	0.681655	0.294797	0.180736	0.025*	

C17A	0.50862 (12)	0.37150 (10)	0.30676 (10)	0.0169 (2)	
O18	0.33994 (9)	0.14221 (7)	0.56487 (7)	0.01775 (17)	
O19	0.25043 (9)	0.39580 (7)	0.51033 (7)	0.01831 (18)	
C18	0.45360 (13)	0.25328 (11)	0.11787 (10)	0.0194 (2)	
C19	0.47466 (14)	0.34721 (12)	0.02676 (11)	0.0231 (3)	
H19	0.429460	0.432036	0.036840	0.028*	
C20	0.56225 (14)	0.31628 (13)	-0.07921 (11)	0.0256 (3)	
H20	0.577191	0.380592	-0.141437	0.031*	
C21	0.62851 (13)	0.19256 (13)	-0.09572 (11)	0.0248 (3)	
C22	0.60615 (16)	0.09972 (13)	-0.00297 (12)	0.0298 (3)	
H22	0.651317	0.014844	-0.012877	0.036*	
C23	0.51916 (15)	0.12903 (12)	0.10348 (11)	0.0273 (3)	
H23	0.504526	0.064868	0.165925	0.033*	
C24	0.72086 (16)	0.15961 (15)	-0.21168 (12)	0.0332 (3)	
H24A	0.694267	0.229732	-0.269594	0.050*	
H24B	0.707489	0.086191	-0.221990	0.050*	
H24C	0.820799	0.141504	-0.218776	0.050*	
C25	-0.04484 (13)	0.29217 (13)	0.86246 (11)	0.0241 (3)	
H25A	-0.089738	0.232837	0.862308	0.029*	
H25B	-0.114917	0.376593	0.859809	0.029*	
C26	-0.00487 (12)	0.25859 (12)	0.96982 (10)	0.0207 (2)	
C27	-0.04248 (13)	0.16461 (12)	1.05579 (11)	0.0240 (3)	
H27	-0.093326	0.119180	1.046874	0.029*	
C28	-0.00605 (15)	0.13668 (13)	1.15487 (12)	0.0290 (3)	
H28	-0.033377	0.073309	1.213575	0.035*	
C29	0.06986 (15)	0.20120 (14)	1.16770 (12)	0.0318 (3)	
H29	0.095792	0.181438	1.234727	0.038*	
C30	0.10807 (15)	0.29490 (14)	1.08238 (12)	0.0306 (3)	
H30	0.159859	0.339513	1.091183	0.037*	
C31	0.07072 (14)	0.32339 (13)	0.98440 (11)	0.0258 (3)	
H31	0.096909	0.387811	0.926505	0.031*	
O3	0.1154 (3)	0.0518 (3)	0.5446 (2)	0.0509 (6)	0.5
H3	0.183 (6)	0.085 (5)	0.503 (5)	0.076*	0.5
C32	0.0470 (6)	0.0434 (4)	0.4684 (5)	0.0246 (10)	0.5
H32A	-0.011759	0.128074	0.444417	0.030*	0.5
H32B	0.121887	0.012197	0.399757	0.030*	0.5
C33	-0.0412 (13)	-0.0361 (10)	0.5180 (10)	0.093 (4)	0.5
H33A	-0.082799	-0.036983	0.462603	0.140*	0.5
H33B	0.016411	-0.120799	0.540200	0.140*	0.5
H33C	-0.117428	-0.004755	0.584925	0.140*	0.5

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01708 (14)	0.02084 (16)	0.01848 (15)	-0.00704 (11)	-0.00430 (11)	-0.00365 (11)
O1	0.0207 (4)	0.0262 (5)	0.0259 (5)	-0.0012 (4)	-0.0080 (4)	-0.0067 (4)
O2	0.0265 (5)	0.0350 (5)	0.0263 (5)	-0.0196 (4)	-0.0040 (4)	-0.0042 (4)
N1	0.0208 (5)	0.0145 (5)	0.0166 (5)	-0.0065 (4)	-0.0056 (4)	-0.0018 (4)

C2	0.0227 (6)	0.0136 (5)	0.0188 (6)	-0.0043 (4)	-0.0053 (5)	-0.0027 (4)
C3	0.0185 (5)	0.0114 (5)	0.0199 (6)	-0.0040 (4)	-0.0045 (4)	-0.0014 (4)
C4	0.0205 (6)	0.0153 (5)	0.0233 (6)	-0.0052 (4)	-0.0072 (5)	-0.0027 (4)
C5	0.0252 (6)	0.0155 (5)	0.0195 (6)	-0.0050 (4)	-0.0086 (5)	-0.0030 (4)
C6	0.0238 (6)	0.0131 (5)	0.0161 (5)	-0.0040 (4)	-0.0060 (4)	-0.0015 (4)
C7	0.0247 (6)	0.0193 (6)	0.0196 (6)	-0.0083 (5)	-0.0046 (5)	-0.0008 (4)
N8	0.0187 (5)	0.0216 (5)	0.0166 (5)	-0.0054 (4)	-0.0039 (4)	-0.0017 (4)
C9	0.0184 (5)	0.0234 (6)	0.0184 (6)	-0.0068 (5)	-0.0054 (4)	-0.0018 (5)
C10	0.0165 (5)	0.0226 (6)	0.0156 (5)	-0.0040 (4)	-0.0041 (4)	-0.0039 (4)
C11	0.0205 (6)	0.0212 (6)	0.0208 (6)	-0.0033 (5)	-0.0032 (5)	-0.0056 (5)
C12	0.0237 (6)	0.0173 (6)	0.0228 (6)	-0.0053 (5)	-0.0046 (5)	-0.0044 (5)
C13	0.0201 (6)	0.0163 (5)	0.0161 (5)	-0.0062 (4)	-0.0066 (4)	-0.0013 (4)
C13A	0.0186 (5)	0.0148 (5)	0.0160 (5)	-0.0039 (4)	-0.0067 (4)	-0.0002 (4)
C14	0.0227 (6)	0.0165 (5)	0.0205 (6)	-0.0059 (4)	-0.0077 (5)	-0.0027 (4)
C15	0.0225 (6)	0.0201 (6)	0.0262 (6)	-0.0100 (5)	-0.0078 (5)	-0.0013 (5)
C16	0.0185 (6)	0.0231 (6)	0.0264 (6)	-0.0074 (5)	-0.0021 (5)	-0.0045 (5)
C17	0.0203 (6)	0.0181 (6)	0.0222 (6)	-0.0048 (4)	-0.0039 (5)	-0.0051 (4)
C17A	0.0182 (5)	0.0147 (5)	0.0177 (5)	-0.0057 (4)	-0.0062 (4)	-0.0004 (4)
O18	0.0201 (4)	0.0168 (4)	0.0162 (4)	-0.0066 (3)	-0.0051 (3)	-0.0019 (3)
O19	0.0178 (4)	0.0160 (4)	0.0179 (4)	-0.0048 (3)	-0.0029 (3)	-0.0022 (3)
C18	0.0199 (5)	0.0222 (6)	0.0184 (6)	-0.0071 (5)	-0.0074 (4)	-0.0034 (4)
C19	0.0257 (6)	0.0201 (6)	0.0230 (6)	-0.0070 (5)	-0.0084 (5)	-0.0018 (5)
C20	0.0266 (6)	0.0291 (7)	0.0199 (6)	-0.0104 (5)	-0.0079 (5)	0.0012 (5)
C21	0.0211 (6)	0.0337 (7)	0.0203 (6)	-0.0057 (5)	-0.0086 (5)	-0.0064 (5)
C22	0.0380 (8)	0.0227 (6)	0.0261 (7)	-0.0025 (5)	-0.0115 (6)	-0.0076 (5)
C23	0.0377 (7)	0.0210 (6)	0.0216 (6)	-0.0080 (5)	-0.0100 (5)	-0.0017 (5)
C24	0.0290 (7)	0.0445 (8)	0.0224 (7)	-0.0046 (6)	-0.0076 (5)	-0.0101 (6)
C25	0.0185 (6)	0.0334 (7)	0.0197 (6)	-0.0099 (5)	-0.0034 (5)	-0.0041 (5)
C26	0.0168 (5)	0.0245 (6)	0.0181 (6)	-0.0045 (5)	-0.0029 (4)	-0.0056 (5)
C27	0.0223 (6)	0.0236 (6)	0.0253 (6)	-0.0075 (5)	-0.0054 (5)	-0.0049 (5)
C28	0.0307 (7)	0.0263 (7)	0.0251 (7)	-0.0065 (5)	-0.0094 (5)	0.0008 (5)
C29	0.0312 (7)	0.0378 (8)	0.0264 (7)	-0.0062 (6)	-0.0143 (6)	-0.0036 (6)
C30	0.0260 (7)	0.0394 (8)	0.0318 (7)	-0.0122 (6)	-0.0100 (6)	-0.0096 (6)
C31	0.0233 (6)	0.0308 (7)	0.0234 (6)	-0.0119 (5)	-0.0035 (5)	-0.0044 (5)
O3	0.0515 (15)	0.0704 (18)	0.0412 (13)	-0.0381 (14)	-0.0009 (11)	-0.0158 (12)
C32	0.032 (2)	0.0147 (16)	0.0178 (17)	-0.0037 (14)	-0.0020 (15)	-0.0027 (13)
C33	0.103 (8)	0.122 (8)	0.074 (7)	-0.060 (6)	-0.024 (6)	-0.014 (5)

Geometric parameters (Å, °)

S1—O1	1.4309 (9)	C16—H16	0.9500
S1—O2	1.4339 (9)	C17—C17A	1.3923 (16)
S1—N1	1.6246 (10)	C17—H17	0.9500
S1—C18	1.7688 (12)	C18—C19	1.3880 (17)
N1—C17A	1.4435 (14)	C18—C23	1.3900 (18)
N1—C2	1.4843 (14)	C19—C20	1.3881 (18)
C2—C3	1.4829 (16)	C19—H19	0.9500
C2—H2A	0.9900	C20—C21	1.3915 (19)

C2—H2B	0.9900	C20—H20	0.9500
C3—C4	1.3517 (17)	C21—C22	1.3942 (19)
C3—O18	1.3688 (14)	C21—C24	1.5090 (18)
C4—C5	1.4300 (17)	C22—C23	1.3867 (19)
C4—H4	0.9500	C22—H22	0.9500
C5—C6	1.3534 (17)	C23—H23	0.9500
C5—H5	0.9500	C24—H24A	0.9800
C6—O18	1.3711 (14)	C24—H24B	0.9800
C6—C7	1.4869 (17)	C24—H24C	0.9800
C7—N8	1.4712 (15)	C25—C26	1.5101 (17)
C7—H7A	0.9900	C25—H25A	0.9900
C7—H7B	0.9900	C25—H25B	0.9900
N8—C25	1.4699 (15)	C26—C27	1.3930 (18)
N8—C9	1.4875 (15)	C26—C31	1.3948 (18)
C9—C10	1.4912 (16)	C27—C28	1.3952 (19)
C9—H9A	0.9900	C27—H27	0.9500
C9—H9B	0.9900	C28—C29	1.384 (2)
C10—C11	1.3544 (18)	C28—H28	0.9500
C10—O19	1.3725 (14)	C29—C30	1.389 (2)
C11—C12	1.4235 (17)	C29—H29	0.9500
C11—H11	0.9500	C30—C31	1.3859 (19)
C12—C13	1.3609 (17)	C30—H30	0.9500
C12—H12	0.9500	C31—H31	0.9500
C13—O19	1.3690 (14)	O3—C32	1.474 (7)
C13—C13A	1.4635 (16)	O3—H3	0.88 (6)
C13A—C17A	1.4041 (16)	C32—C33	1.438 (7)
C13A—C14	1.4045 (16)	C32—H32A	0.9900
C14—C15	1.3841 (17)	C32—H32B	0.9900
C14—H14	0.9500	C33—H33A	0.9800
C15—C16	1.3911 (18)	C33—H33B	0.9800
C15—H15	0.9500	C33—H33C	0.9800
C16—C17	1.3852 (17)		
O1—S1—O2	120.65 (6)	C17A—C17—H17	119.4
O1—S1—N1	106.82 (5)	C17—C17A—C13A	120.65 (11)
O2—S1—N1	106.39 (5)	C17—C17A—N1	117.53 (10)
O1—S1—C18	107.02 (6)	C13A—C17A—N1	121.77 (10)
O2—S1—C18	107.44 (6)	C3—O18—C6	106.71 (9)
N1—S1—C18	108.00 (5)	C13—O19—C10	107.37 (9)
C17A—N1—C2	116.81 (9)	C19—C18—C23	120.47 (12)
C17A—N1—S1	119.73 (8)	C19—C18—S1	119.61 (9)
C2—N1—S1	119.66 (8)	C23—C18—S1	119.92 (10)
C3—C2—N1	110.33 (9)	C18—C19—C20	119.50 (12)
C3—C2—H2A	109.6	C18—C19—H19	120.2
N1—C2—H2A	109.6	C20—C19—H19	120.2
C3—C2—H2B	109.6	C19—C20—C21	121.04 (12)
N1—C2—H2B	109.6	C19—C20—H20	119.5
H2A—C2—H2B	108.1	C21—C20—H20	119.5

C4—C3—O18	110.28 (10)	C20—C21—C22	118.49 (12)
C4—C3—C2	133.66 (11)	C20—C21—C24	120.77 (12)
O18—C3—C2	115.88 (10)	C22—C21—C24	120.73 (13)
C3—C4—C5	106.38 (11)	C23—C22—C21	121.19 (12)
C3—C4—H4	126.8	C23—C22—H22	119.4
C5—C4—H4	126.8	C21—C22—H22	119.4
C6—C5—C4	106.62 (11)	C22—C23—C18	119.30 (12)
C6—C5—H5	126.7	C22—C23—H23	120.3
C4—C5—H5	126.7	C18—C23—H23	120.3
C5—C6—O18	109.96 (10)	C21—C24—H24A	109.5
C5—C6—C7	133.39 (11)	C21—C24—H24B	109.5
O18—C6—C7	116.59 (10)	H24A—C24—H24B	109.5
N8—C7—C6	112.77 (10)	C21—C24—H24C	109.5
N8—C7—H7A	109.0	H24A—C24—H24C	109.5
C6—C7—H7A	109.0	H24B—C24—H24C	109.5
N8—C7—H7B	109.0	N8—C25—C26	110.98 (10)
C6—C7—H7B	109.0	N8—C25—H25A	109.4
H7A—C7—H7B	107.8	C26—C25—H25A	109.4
C25—N8—C7	109.86 (10)	N8—C25—H25B	109.4
C25—N8—C9	111.95 (9)	C26—C25—H25B	109.4
C7—N8—C9	113.15 (9)	H25A—C25—H25B	108.0
N8—C9—C10	113.10 (10)	C27—C26—C31	118.74 (12)
N8—C9—H9A	109.0	C27—C26—C25	121.66 (11)
C10—C9—H9A	109.0	C31—C26—C25	119.59 (11)
N8—C9—H9B	109.0	C26—C27—C28	120.51 (12)
C10—C9—H9B	109.0	C26—C27—H27	119.7
H9A—C9—H9B	107.8	C28—C27—H27	119.7
C11—C10—O19	109.65 (10)	C29—C28—C27	120.05 (13)
C11—C10—C9	133.17 (11)	C29—C28—H28	120.0
O19—C10—C9	117.17 (10)	C27—C28—H28	120.0
C10—C11—C12	106.75 (11)	C28—C29—C30	119.86 (13)
C10—C11—H11	126.6	C28—C29—H29	120.1
C12—C11—H11	126.6	C30—C29—H29	120.1
C13—C12—C11	106.89 (11)	C31—C30—C29	120.07 (13)
C13—C12—H12	126.6	C31—C30—H30	120.0
C11—C12—H12	126.6	C29—C30—H30	120.0
C12—C13—O19	109.34 (10)	C30—C31—C26	120.76 (13)
C12—C13—C13A	131.60 (11)	C30—C31—H31	119.6
O19—C13—C13A	119.05 (10)	C26—C31—H31	119.6
C17A—C13A—C14	117.06 (11)	C32—O3—H3	108 (4)
C17A—C13A—C13	125.36 (10)	C33—C32—O3	114.2 (4)
C14—C13A—C13	117.58 (10)	C33—C32—H32A	108.7
C15—C14—C13A	122.22 (11)	O3—C32—H32A	108.7
C15—C14—H14	118.9	C33—C32—H32B	108.7
C13A—C14—H14	118.9	O3—C32—H32B	108.7
C14—C15—C16	119.77 (11)	H32A—C32—H32B	107.6
C14—C15—H15	120.1	C32—C33—H33A	109.5
C16—C15—H15	120.1	C32—C33—H33B	109.5

C17—C16—C15	119.17 (11)	H33A—C33—H33B	109.5
C17—C16—H16	120.4	C32—C33—H33C	109.5
C15—C16—H16	120.4	H33A—C33—H33C	109.5
C16—C17—C17A	121.10 (11)	H33B—C33—H33C	109.5
C16—C17—H17	119.4		
O1—S1—N1—C17A	-36.74 (10)	C13—C13A—C17A—N1	-5.47 (18)
O2—S1—N1—C17A	-166.83 (9)	C2—N1—C17A—C17	68.97 (14)
C18—S1—N1—C17A	78.08 (10)	S1—N1—C17A—C17	-88.99 (12)
O1—S1—N1—C2	165.92 (8)	C2—N1—C17A—C13A	-108.37 (12)
O2—S1—N1—C2	35.83 (10)	S1—N1—C17A—C13A	93.67 (12)
C18—S1—N1—C2	-79.25 (9)	C4—C3—O18—C6	2.15 (12)
C17A—N1—C2—C3	79.15 (12)	C2—C3—O18—C6	-173.59 (9)
S1—N1—C2—C3	-122.87 (9)	C5—C6—O18—C3	-2.10 (12)
N1—C2—C3—C4	-99.88 (15)	C7—C6—O18—C3	175.43 (9)
N1—C2—C3—O18	74.60 (12)	C12—C13—O19—C10	-0.20 (13)
O18—C3—C4—C5	-1.38 (13)	C13A—C13—O19—C10	179.08 (10)
C2—C3—C4—C5	173.32 (12)	C11—C10—O19—C13	0.40 (13)
C3—C4—C5—C6	0.07 (13)	C9—C10—O19—C13	-179.30 (10)
C4—C5—C6—O18	1.27 (13)	O1—S1—C18—C19	14.28 (12)
C4—C5—C6—C7	-175.70 (12)	O2—S1—C18—C19	145.20 (10)
C5—C6—C7—N8	85.18 (16)	N1—S1—C18—C19	-100.41 (10)
O18—C6—C7—N8	-91.63 (12)	O1—S1—C18—C23	-166.03 (10)
C6—C7—N8—C25	-165.59 (10)	O2—S1—C18—C23	-35.11 (12)
C6—C7—N8—C9	68.49 (13)	N1—S1—C18—C23	79.28 (11)
C25—N8—C9—C10	131.45 (11)	C23—C18—C19—C20	-0.19 (19)
C7—N8—C9—C10	-103.75 (12)	S1—C18—C19—C20	179.50 (10)
N8—C9—C10—C11	-93.30 (16)	C18—C19—C20—C21	0.46 (19)
N8—C9—C10—O19	86.32 (13)	C19—C20—C21—C22	-0.6 (2)
O19—C10—C11—C12	-0.43 (14)	C19—C20—C21—C24	178.56 (12)
C9—C10—C11—C12	179.21 (13)	C20—C21—C22—C23	0.5 (2)
C10—C11—C12—C13	0.30 (14)	C24—C21—C22—C23	-178.67 (13)
C11—C12—C13—O19	-0.06 (14)	C21—C22—C23—C18	-0.2 (2)
C11—C12—C13—C13A	-179.21 (12)	C19—C18—C23—C22	0.1 (2)
C12—C13—C13A—C17A	-154.74 (13)	S1—C18—C23—C22	-179.60 (11)
O19—C13—C13A—C17A	26.17 (17)	C7—N8—C25—C26	68.38 (13)
C12—C13—C13A—C14	24.52 (19)	C9—N8—C25—C26	-165.03 (10)
O19—C13—C13A—C14	-154.57 (10)	N8—C25—C26—C27	-126.60 (12)
C17A—C13A—C14—C15	1.30 (17)	N8—C25—C26—C31	53.88 (16)
C13—C13A—C14—C15	-178.02 (11)	C31—C26—C27—C28	0.49 (19)
C13A—C14—C15—C16	0.15 (19)	C25—C26—C27—C28	-179.04 (12)
C14—C15—C16—C17	-0.92 (19)	C26—C27—C28—C29	-1.0 (2)
C15—C16—C17—C17A	0.22 (19)	C27—C28—C29—C30	0.8 (2)
C16—C17—C17A—C13A	1.28 (18)	C28—C29—C30—C31	-0.3 (2)
C16—C17—C17A—N1	-176.08 (11)	C29—C30—C31—C26	-0.2 (2)
C14—C13A—C17A—C17	-1.99 (17)	C27—C26—C31—C30	0.11 (19)
C13—C13A—C17A—C17	177.27 (11)	C25—C26—C31—C30	179.65 (12)
C14—C13A—C17A—N1	175.27 (10)		

Hydrogen-bond geometry (\AA , $^\circ$)

$Cg1$, $Cg3$ and $Cg5$ are the centroids of the O18/C3–C6 furan, C13A/C14–C17/C17A benzene and C26–C31 phenyl rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C9—H9A \cdots O1 ⁱ	0.99	2.53	3.4057 (17)	148
C25—H25B \cdots O1 ⁱ	0.99	2.59	3.5125 (18)	155
O3—H3 \cdots O2	0.88 (7)	2.52 (6)	3.251 (3)	141 (6)
O3—H3 \cdots O18	0.88 (7)	2.47 (7)	3.097 (4)	129 (5)
C2—H2A \cdots Cg1 ⁱⁱ	0.99	2.56	3.2916 (12)	131
C16—H16 \cdots Cg5 ⁱⁱⁱ	0.95	2.80	3.5220 (15)	133
C20—H20 \cdots Cg3 ^{iv}	0.95	2.83	3.5707 (15)	135

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+1, -y, -z+1$; (iii) $x+1, y, z-1$; (iv) $-x+1, -y+1, -z$.