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Crystal structure and Hirshfeld surface analysis of (*RS*)-3-hydroxy-2-{[(3a*RS*,6*RS*,7a*RS*)-2-(4-methylphenylsulfonyl)-2,3,3a,6,7,7a-hexahydro-3a,6-epoxy-1*H*-isoindol-6-yl]methyl}isoindolin-1-one

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The title compound, $C_{24}H_{24}N_2O_5S$, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. In the central ring systems of both molecules, the tetrahydrofuran rings adopt envelope conformations, the pyrrolidine rings adopt a twisted-envelope conformation and the six-membered ring is in a boat conformation. In molecules *A* and *B*, the nine-membered groups attached to the central ring system are essentially planar (r.m.s. deviations of 0.002 and 0.003 Å, respectively). They form dihedral angles of 64.97 (9) and 56.06 (10)°, respectively, with the phenyl rings. In the crystal, strong intermolecular O—H···O hydrogen bonds and weak intermolecular C—H···O contacts link the molecules, forming a three-dimensional network. In addition weak π–π stacking interactions [centroid-to centroid distance = 3.7124 (13) Å] between the pyrrolidine rings of the nine-membered groups of *A* molecules are observed. Hirshfeld surface analysis and two-dimensional fingerprint plots were used to quantify the intermolecular interactions present in the crystal, indicating that the environments of the two molecules are very similar. The most important contributions for the crystal packing are from H···H (55.8% for molecule *A* and 53.5% for molecule *B*), O···H/H···O (24.5% for molecule *A* and 26.3% for molecule *B*) and C···H/H···C (12.6% for molecule *A* and 15.7% for molecule *B*) interactions.

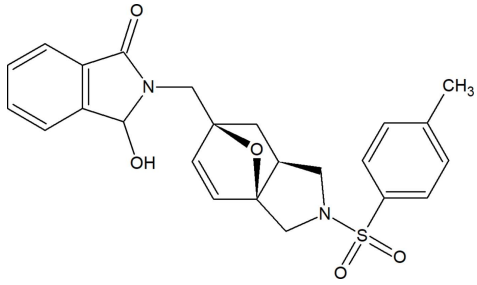
1. Chemical context

Currently, considerable attention is being paid to the development of atom- and step-economic tools in order to obtain new, practically useful materials. Tandem and domino reactions play an important role in this arsenal, since the isolation of intermediates is not required in these processes, as all reaction steps occur spontaneously (Tietze & Beifuss, 1993).

As an example of using such synthetic tools, we proposed the synthesis of compound **3**, which contains three privileged scaffolds, based on the tandem Hinsberg/IMDAF (intramolecular Diels–Alder furan; Zubkov *et al.*, 2005, 2014) reaction strategy (Demircan *et al.*, 2016; Nadirova *et al.*, 2020). Substituted sulfonamides are important because of their broad spectrum of biological activities (Anderson *et al.*, 2012) while 3-hydroxyisoindol-1-ones are well-known nitrogen-containing heterocyclic compounds with a wide range of physiological activity: agonists of muscarinic M2 receptor modulators,

antimicrobial activity *etc.* (Stiefl *et al.*, 2003; Breytenbach *et al.*, 2000).

The reaction proceeds smoothly in boiling water. Separation and subsequent crystallization of the resulting solids from ethyl acetate provides the title adduct **3** in moderate yield. The process starts with the Hinsberg *N*-sulfonylation of amine **1**, leading to the formation of the intermediate *N*-sulfonamide (**2**), which undergoes spontaneous intramolecular Diels–Alder reaction. It should be noted that the *exo*-[4 + 2] cycloaddition proceeds stereoselectively with the exclusive formation of diastereoisomer **3** (Fig. 1).



On the other hand, non-covalent interactions between molecules play an important role in the synthesis, crystal engineering, molecular recognition, and as key activating/controlling elements in the field of catalysis (Afkhami *et al.*, 2017; Asadov *et al.*, 2016; Gurbanov *et al.*, 2017, 2018; Karmakar *et al.*, 2017; Kopylovich *et al.*, 2011*a*,*b*; Ma *et al.*, 2017*a*,*b*; Maharramov *et al.*, 2018; Mahmoudi *et al.*, 2017, 2019; Mahmudov *et al.*, 2010, 2020; Mizar *et al.*, 2012; Sutradhar *et al.*, 2015). Herein, we highlight the role of weak interactions in the structural features of molecule **3**.

2. Structural commentary

As shown Fig. 2, the title compound **3** crystallizes with two independent molecules (*A* with the atom S and *B* with the atom S′) in the asymmetric unit in which the epoxyisoindole and phenyl rings are linked through an N—S—C bridge. In the central ring systems of molecules *A* and *B*, the two tetrahydrofuran rings (*A*: O3/C10–C13, O3/C10/C13/C15/C16 and *B*: O3′/C10′–C13′, O3′/C10′/C13′/C15′/C16′) adopt envelope conformations [puckering parameters (Cremer & Pople, 1975) Q = 0.508 (2), 0.600 (2) and 0.523 (2), 0.602 (2) Å, respectively], the pyrrolidine rings (*A*: N2/C13–C14/C16–C17 and *B*: N2′/C13′–C14′/C16′–C17′) adopt a twisted-envelope conformation [Q_T = 0.392 (2) Å, $\varphi(2)$ = 132.8 (4)° and Q_T = 0.408 (2) Å, $\varphi(2)$ = 310.0 (3)°, respectively] and the six-membered rings are in a boat conformation (C10–C13/C15/C16; Q_T = 0.965 (2) Å, θ = 89.90 (12)°, φ = 180.80 (15)° in molecule *A*; C10′–C13′/C15′/C16′, Q_T = 0.950 (2) Å, θ = 89.90 (12)°, φ = 0.57 (15)° in molecule *B*].

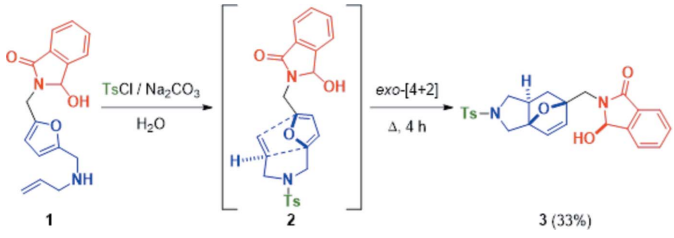


Figure 1
Synthesis of the title compound **3**.

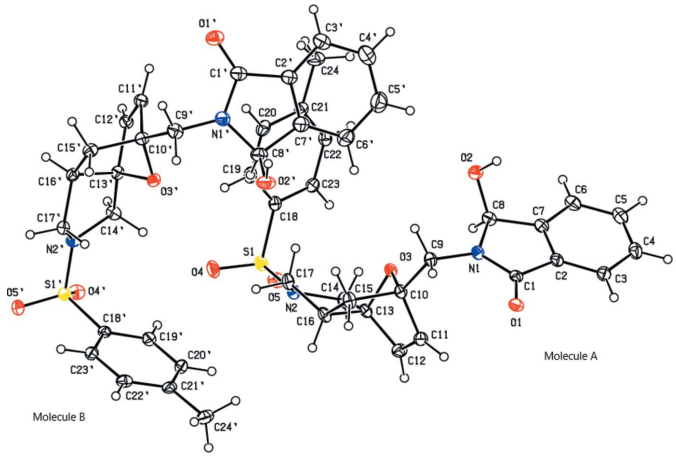


Figure 2
View of the two independent molecules, *A* and *B*, in the asymmetric unit of the title compound **3**, with displacement ellipsoids for the non-hydrogen atoms drawn at the 30% probability level.

In molecules *A* and *B*, the nine-membered groups (*A*: N1/C1–C8 and *B*: N1′/C1′–C8′) attached to the central ring system are essentially planar (r.m.s deviations of 0.002 and 0.003 Å, respectively). They form dihedral angles of 64.97 (9) and 56.06 (10)°, respectively, with the phenyl rings (*A*: C18–C23 and *B*: C18′–C23′). Fig. 3 shows the overlay of molecules *A* and *B* in the asymmetric unit (r.m.s. deviation 0.252 Å).

3. Supramolecular features

In the crystal, strong intermolecular O—H···O hydrogen bonds and weak intermolecular C—H···O contacts link the molecules, forming a three-dimensional network (Table 1, Fig. 4). In addition weak π–π stacking interactions are

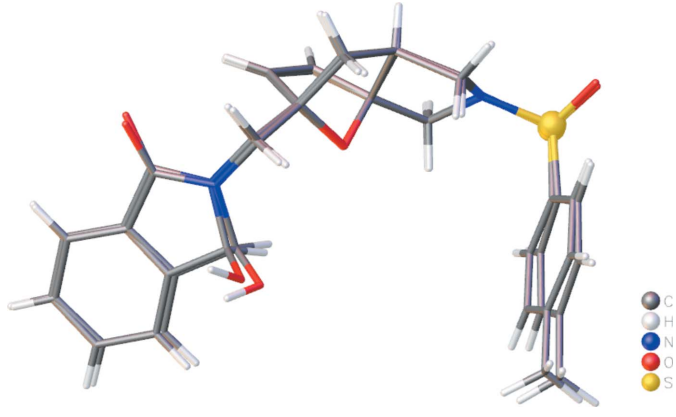


Figure 3
Overlay image of the two molecules (*A* and *B*) in the asymmetric unit of the title compound **3**.

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O5^{i}	0.95	2.47	3.333 (3)	151
C14—H14A···O5′^{ii}	0.99	2.62	3.506 (3)	149
C23—H23···O5′^{ii}	0.95	2.41	3.195 (3)	139
C14′—H14D···O4	0.99	2.58	3.482 (3)	151
C15′—H15C···O2^{iii}	0.99	2.62	3.585 (3)	165
C16′—H16′···O4′^{iv}	1.00	2.53	3.422 (3)	149
C19′—H19′···O4	0.95	2.34	3.078 (3)	134
O2—H2···O1^{v}	0.92	1.85	2.756 (2)	172
O2′—H2′···O1′^{vi}	0.90	1.95	2.840 (3)	171

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, y-1, z$; (iii) $x, y+1, z$; (iv) $-x+2, -y+2, -z+1$; (v) $-x+1, -y, -z+2$; (vi) $-x+2, -y+1, -z+2$.

observed [$Cg3\cdots Cg3(1-x, -y, 2-z)$ = 3.7124 (13) Å where $Cg3$ is the centroid of the pyrrolidine ring (N1/C1/C2/C7/C8) of the nine-membered group in molecule A, with slippage of 1.675 Å].

4. Hirshfeld surface analysis

The Hirshfeld surfaces for both independent molecules (A and B) in the asymmetric of the title compound **3** were generated using *Crystal Explorer 17* (Turner *et al.*, 2017). The d_{norm} mappings were performed in the range of −0.6446 to 1.7383 arbitrary units for the molecule A and −0.5749 to 1.6904 arbitrary units for molecule B. Bold red circles on the d_{norm} surfaces (Fig. 5*a*) indicate regions of O—H···O interactions. The C—H···O interactions also cause red spots on the Hirshfeld surfaces. The shape-index maps (Fig. 5*b*) contain red and blue triangles related to π–π interactions.

Fingerprint plots (Fig. 6) reveal that while H···H (55.8% for molecule A and 53.5% for molecule B) interactions make the greatest contributions to the surface contacts (Table 2), as would be expected for a molecule with such a predominance of H atoms, O···H/H···O (24.5% for molecule A and 26.3% for molecule B) and C···H/H···C (12.6% for molecule A and 15.7% for molecule B) contacts are also substantial. Table 3

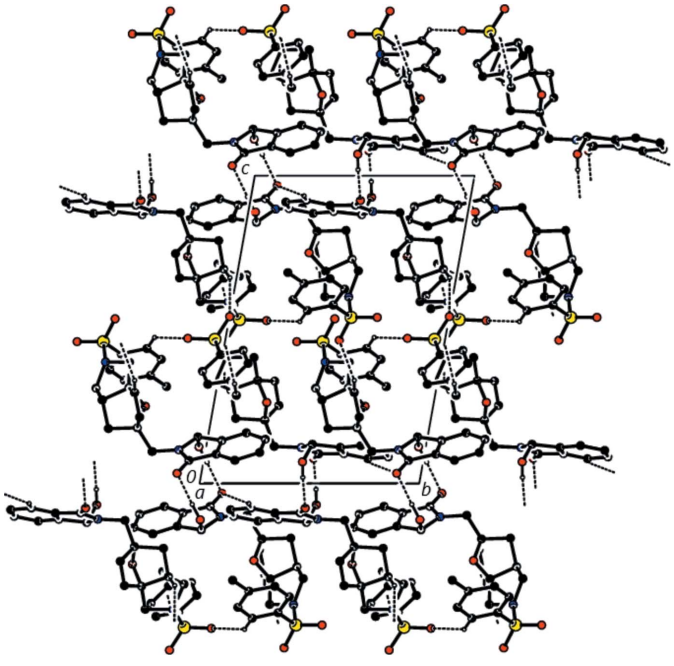


Figure 4
A view of the intermolecular C—H···O and O—H···O interactions in the crystal structure of the title compound **3**.

Table 2
Summary of short interatomic contacts (Å) in the title compound **3**.

Contact	Distance	Symmetry operation
O1···H3′	2.27	$-1+x, y, z$
H2···O1	1.85	$1-x, -y, 2-z$
O4···H19′	2.34	x, y, z
H8···H17C	2.41	$x, -1+y, z$
H12···O5	2.47	$1-x, 1-y, 1-z$
C20···O5	2.411	$2-x, 1-y, 1-z$
H11···H24B	2.43	$-1+x, y, z$
H15B···H5	2.42	$x, 1+y, z$
H22···H14C	2.23	$2-x, 1-y, 1-z$
H2′···O1′	1.95	$2-x, 1-y, 2-z$
H24F···O4′	2.40	$1-x, 2-y, 1-z$
H16′···O4′	2.53	$2-x, 2-y, 1-z$
H16′···H24F	2.41	$1+x, y, z$

Table 3
Percentage contributions of interatomic contacts to the Hirshfeld surfaces for molecules A and B of the title compound **3**.

	Molecule A	Molecule B
Contact	Percentage contribution	Percentage contribution
H···H	55.8	53.5
O···H/H···O	24.5	26.3
C···H/H···C	12.6	15.7
C···C	3.3	2.6
C···O/O···C	2.6	0.4
N···H/H···N	0.8	1.2
C···N/N···C	0.5	0.1
N···O/O···N	–	0.1
S···H/H···S	–	0.1
S···H/H···S	0.1	–

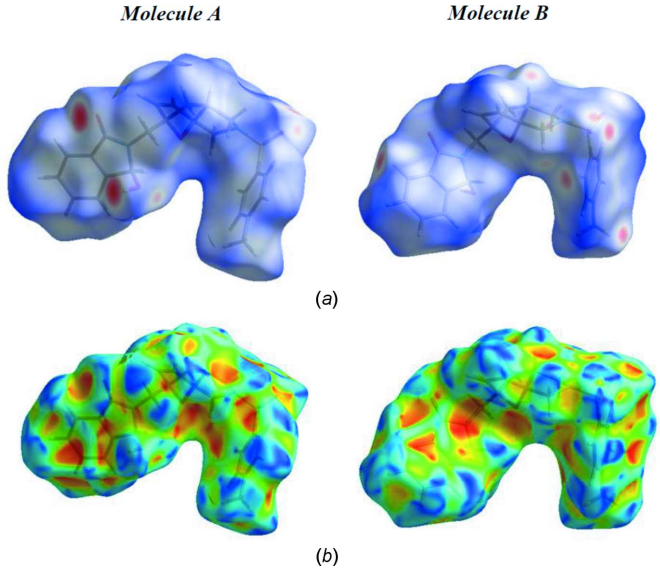


Figure 5
(*a*) View of the three-dimensional Hirshfeld surfaces for molecules A and B of the title compound **3**; (*b*) Hirshfeld surfaces plotted over shape-index.

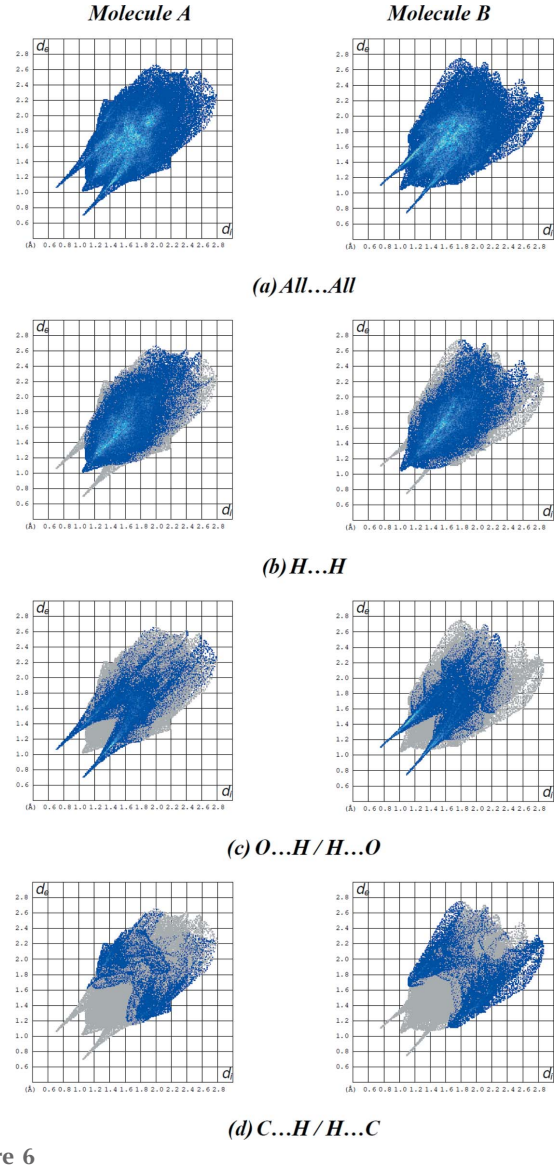


Figure 6
The two-dimensional fingerprint plots for molecules *A* and *B* of the title compound **3** showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) O···H/H···O and (*d*) C···H/H···C interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

gives the contributions of the other, less significant contacts. As shown in Table 3, the environments of the two molecules *A* and *B* are very similar. Even the packing looks pseudo-monoclinic, with a pseudo-glide plane relating the two molecules *A* and *B*.

5. Database survey

There are several examples of structures closely related to the 2-(dioxo-λ6-sulfanyl)octahydro-3a,6-epoxyisoindole skeleton of **3**. Selected examples found in the Cambridge Structural Database (CSD, version 5.40, update of August 2019; Groom *et al.*, 2016) include (3a*R*,6*S*,7a*R*)-7a-bromo-2-methylsulfonyl-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole (CSD refcode ERIVIL; Temel *et al.*, 2011), (3a*R*,6*S*,7a*R*)-7a-chloro-2-[(4-nitrophenyl)sulfonyl]-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole (AGONUH; Temel *et al.*, 2013), (3a*R*,6*S*,7a*R*)-7a-chloro-6-methyl-2-[(4-nitrophenyl)sulfonyl]-1,2,3,6,7,7a-hexahydro-3a,6-epoxyisoindole (TIJMIK; Demircan *et al.*, 2013), (3a*R*,6*S*,7a*R*)-7a-bromo-2-[(4-methylphenyl)sulfonyl]-1,2,3,6,-7,7a-hexahydro-3a,6-epoxyisoindole (UPAQEI; Koşar *et al.*, 2011), 5-chloro-7-methyl-3-[(4-methylphenyl)sulfonyl]-10-oxa-3-azatricyclo[5.2.1.01,5]dec-8-ene (YAXCIL; Temel *et al.*, 2012), *tert*-butyl 3a-chloroperhydro-2,6a-epoxyoxireno(*e*)isoindole-5-carboxylate (MIGTIG; Koşar *et al.*, 2007) and 2-(2-aminoethyl)-3a,4,7,7a-tetrahydro-1*H*-4,7-epoxyisoindole-1,3(2*H*)-dione (BILLAL; Mitchell *et al.*, 2013).

In the crystal of ERIVIL, weak intermolecular C—H···O hydrogen bonds link the molecules into $R_2^2(8)$ and $R_2^2(14)$ rings along the *b*-axis direction. In the crystal of AGONUH, C—H···O hydrogen bonds link the molecules into zigzag chains running along the *b*-axis direction. In the crystal of TIJMIK, two types of C—H···O hydrogen bonds generate $R_2^2(20)$ and $R_4^4(26)$ rings, with adjacent rings running parallel to the *ac* plane. Further C—H···O hydrogen bonds form a $C(6)$ chain, linking the molecules in the *b*-axis direction. In the crystal of UPAQEI, molecules are linked by C—H···O hydrogen bonds. In the crystal of YAXCIL, C—H···O hydrogen bonds link the molecules into a three-dimensional network. In the crystal of MIGTIG, the molecules are linked only by weak van der Waals interactions. The compound BILLAL contains two molecules in the asymmetric unit, which are hydrogen-bonded dimers. The bonds closest to linearity are between the carbonyl groups and the amine H atoms. Intermolecular hydrogen bonding involving the O atoms also occurs.

6. Synthesis and crystallization

4-Toluenesulfonyl chloride (0.61 g, 3.2 mmol) was added to 2-({5-[(allylamino)methyl]-2-furyl}methyl)-3-hydroxyisoindolin-1-one (0.79 g, 2.7 mmol) in water (10 mL) in the presence of Na_2CO_3 (0.34 g, 3.2 mmol). The resulting reaction mixture was refluxed for 4 h and then extracted with DCM (3 × 10 mL). The organic layers were dried with anhydrous $MgSO_4$. The desiccator was filtered off, the solution concentrated and the residue was recrystallized from EtOAc. The obtained precipitate was filtered off, washed with hexane (3 × 5 mL) and dried in air to give 0.4 g (33%) of (*RS*)-3-hydroxy-2-{[(3a*RS*,6*RS*,7a*RS*)-2-(4-methylphenylsulfonyl)-2,3,3a,6,7,7a-hexahydro-3a,6-epoxy-1*H*-isoindol-6-yl]methyl}isoindolin-1-one (**3**) as colourless prisms, m.p. = 468.1–469.1 K. R_f = 0.6 (EtOH–DMF, 1:2). IR (KBr), ν (cm^{-1}): 1167 (ν_s SO_2), 1340 (ν_{as} SO_2), 1679 (NCO), 3281 (OH). ^{1}H NMR (DMSO-d_6, 400 MHz, 301 K): δ = 7.74–7.43 (*m*, 8H, HAr), 6.41 (*d*, 1H, OH, *J* = 9.3), 6.37 and 6.22 (2*d*, 2H, H4, H5, *J* = 5.7), 5.68 (*d*, 1H, CH-O, *J* = 9.3), 4.20 (*d*, 1H, NCH_2A, *J* = 15.3), 3.78 (*d*, 1H, H3*A*, *J* = 12.1), 3.73 (*t*, 1H, H-1*A*, *J* = 9.5), 3.52 (*d*, 1H, NCH_2B, *J* = 15.3), 3.42 (*d*, 1H, H3*B*, *J* = 12.1), 2.79 (*t*, 1H, H-1*B*, *J* = 9.5), 2.43 (*s*, 3H, CH_3), 2.00–1.93 (*m*, 1H, H7*A*), 1.55–1.44 (*m*, 2H, H7). ^{13}C NMR (DMSO-d_6, 100.4 MHz, 301 K): δ = 166.2, 145.0, 143.4, 137.6, 135.5, 133.9, 132.0, 131.1, 129.8, 129.2, 127.2,

Table 4
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{24}N_2O_5S$
M_r	452.51
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	120
a, b, c (Å)	11.8210 (8), 11.8395 (8), 16.7336 (11)
α, β, γ (°)	77.949 (1), 79.555 (1), 77.511 (1)
V (Å^3)	2213.3 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.19
Crystal size (mm)	0.15 × 0.09 × 0.06
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.688, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29692, 13532, 8799
R_{int}	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.717
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.060, 0.147, 1.02
No. of reflections	13532
No. of parameters	581
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.41, −0.44

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

123.5, 122.4, 94.7, 92.3, 81.2, 52.8, 48.8, 44.5, 39.7, 33.8, 21.0. MS (APCI): m/z = 453 $[M + H]^+$.

7. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 4. The hydrogen atoms of the hydroxy groups were located in a difference-Fourier map and refined freely. The other hydrogen atoms were constrained to ride on their parent atoms with C—H = 0.95, 0.98, 0.99 and 1.00 Å for aromatic, methyl, methylene and methine H atoms, respectively. Isotropic displacement parameters of these atoms were constrained to $1.5U_{eq}$(C) for the methyl and to $1.2U_{eq}$(C) for all other H atoms.

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Crystal structure and Hirshfeld surface analysis of (*RS*)-3-hydroxy-2-{[(3a*RS*,6*RS*,7a*RS*)-2-(4-methylphenylsulfonyl)-2,3,3a,6,7,7a-hexahydro-3a,6-epoxy-1*H*-isoindol-6-yl]methyl}isoindolin-1-one

Dmitriy F. Mertsalov, Maryana A. Nadirova, Elena A. Sorokina, Marina A. Vinokurova, Sevim Türktekin Çelikesir, Mehmet Akkurt, Irina A. Kolesnik and Ajaya Bhattarai

Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

(*RS*)-3-Hydroxy-2-{[(3a*RS*,6*RS*,7a*RS*)-2-(4-methylphenylsulfonyl)-2,3,3a,6,7,7a-hexahydro-3a,6-epoxy-1*H*-isoindol-6-yl]methyl}isoindolin-1-one

Crystal data

$C_{24}H_{24}N_2O_5S$
M_r = 452.51
Triclinic, $P\overline{1}$
a = 11.8210 (8) Å
b = 11.8395 (8) Å
c = 16.7336 (11) Å
α = 77.949 (1)°
β = 79.555 (1)°
γ = 77.511 (1)°
V = 2213.3 (3) Å^3
Z = 4
$F(000)$ = 952
D_x = 1.358 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5394 reflections
θ = 2.3–27.2°
μ = 0.19 mm^{-1}
T = 120 K
Prism, colourless
0.15 × 0.09 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
T_{min} = 0.688, T_{max} = 0.746
29692 measured reflections
13532 independent reflections
8799 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 30.6°, θ_{min} = 1.8°
h = −16→16
k = −16→16
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.147
S = 1.02
13532 reflections

581 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0474P)^2 + 1.6525P]$
0 restraints	where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: mixed	$(\Delta/\sigma)_{max} = 0.001$
H atoms treated by a mixture of independent and constrained refinement	$\Delta\rho_{max} = 0.41$ e Å^{-3}
	$\Delta\rho_{min} = -0.44$ 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.

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

	x	y	z	U_{iso}*/U_{eq}
S1	0.74652 (5)	0.55414 (5)	0.53950 (3)	0.02594 (13)
O1	0.32628 (13)	0.11057 (14)	0.96738 (9)	0.0263 (3)
O2	0.71088 (13)	0.03280 (14)	0.88152 (10)	0.0278 (3)
H2	0.705699	−0.016702	0.931497	0.042 (8)*
O3	0.57170 (13)	0.31030 (12)	0.74923 (9)	0.0212 (3)
O4	0.75506 (15)	0.67311 (14)	0.53936 (11)	0.0353 (4)
O5	0.73338 (14)	0.51910 (15)	0.46520 (10)	0.0317 (4)
N1	0.50789 (16)	0.12179 (15)	0.89107 (10)	0.0221 (4)
N2	0.63120 (16)	0.52671 (16)	0.60548 (11)	0.0240 (4)
C1	0.41649 (19)	0.06714 (19)	0.92534 (12)	0.0216 (4)
C2	0.44704 (19)	−0.05190 (19)	0.90475 (13)	0.0235 (4)
C3	0.3823 (2)	−0.1414 (2)	0.92483 (14)	0.0280 (5)
H3	0.305319	−0.130549	0.954375	0.034*
C4	0.4354 (2)	−0.2480 (2)	0.89974 (15)	0.0334 (6)
H4	0.393844	−0.311270	0.912327	0.040*
C5	0.5482 (2)	−0.2629 (2)	0.85654 (15)	0.0339 (6)
H5	0.582760	−0.336705	0.840882	0.041*
C6	0.6117 (2)	−0.1720 (2)	0.83572 (15)	0.0310 (5)
H6	0.688286	−0.182161	0.805520	0.037*
C7	0.5589 (2)	−0.06640 (19)	0.86068 (13)	0.0242 (4)
C8	0.60631 (19)	0.04558 (19)	0.84880 (13)	0.0245 (4)
H8	0.618437	0.079526	0.788610	0.029*
C9	0.5108 (2)	0.24198 (19)	0.89628 (13)	0.0237 (4)
H9A	0.589661	0.245866	0.906416	0.028*
H9B	0.453931	0.264980	0.943998	0.028*
C10	0.48228 (19)	0.32883 (18)	0.81931 (13)	0.0217 (4)
C11	0.3729 (2)	0.3272 (2)	0.78461 (14)	0.0274 (5)
H11	0.304341	0.300502	0.814352	0.033*
C12	0.3917 (2)	0.3702 (2)	0.70465 (14)	0.0289 (5)
H12	0.340100	0.379979	0.665263	0.035*
C13	0.51173 (19)	0.40013 (19)	0.68953 (13)	0.0230 (4)
C14	0.5869 (2)	0.4180 (2)	0.60650 (13)	0.0266 (5)
H14A	0.652259	0.350464	0.601447	0.032*
H14B	0.540199	0.428583	0.561104	0.032*

C15	0.4833 (2)	0.45976 (19)	0.82203 (13)	0.0271 (5)
H15A	0.407907	0.498358	0.849741	0.032*
H15B	0.547856	0.466503	0.850003	0.032*
C16	0.5028 (2)	0.51120 (19)	0.72882 (13)	0.0262 (5)
H16	0.434974	0.573493	0.712567	0.031*
C17	0.6189 (2)	0.5493 (2)	0.69070 (14)	0.0268 (5)
H17A	0.615310	0.633446	0.691189	0.032*
H17B	0.684024	0.501509	0.719696	0.032*
C18	0.86926 (19)	0.46288 (19)	0.57944 (13)	0.0237 (4)
C19	0.9263 (2)	0.5017 (2)	0.63118 (15)	0.0295 (5)
H19	0.901762	0.579077	0.643101	0.035*
C20	1.0194 (2)	0.4264 (2)	0.66527 (14)	0.0298 (5)
H20	1.059570	0.453139	0.699867	0.036*
C21	1.0548 (2)	0.3122 (2)	0.64953 (14)	0.0268 (5)
C22	0.9972 (2)	0.2756 (2)	0.59696 (14)	0.0257 (5)
H22	1.021707	0.198304	0.584974	0.031*
C23	0.90444 (19)	0.3498 (2)	0.56163 (13)	0.0246 (4)
H23	0.865580	0.323813	0.525833	0.030*
C24	1.1564 (2)	0.2296 (2)	0.68509 (17)	0.0381 (6)
H24A	1.136052	0.151744	0.705618	0.057*
H24B	1.174711	0.259604	0.730684	0.057*
H24C	1.224817	0.223780	0.642151	0.057*
S1′	0.76670 (5)	1.04803 (5)	0.53217 (3)	0.02277 (12)
O1′	1.14505 (15)	0.50110 (16)	0.91923 (11)	0.0362 (4)
O2′	0.76049 (15)	0.54898 (17)	0.93007 (12)	0.0410 (5)
H2′	0.782753	0.534895	0.980589	0.078 (12)*
O3′	0.90933 (13)	0.76045 (13)	0.73711 (9)	0.0234 (3)
O4′	0.80016 (14)	0.99924 (15)	0.45795 (9)	0.0300 (4)
O5′	0.75650 (14)	1.17211 (14)	0.52883 (10)	0.0289 (4)
N1′	0.95957 (17)	0.56602 (18)	0.88347 (12)	0.0302 (4)
N2′	0.86625 (15)	0.98216 (16)	0.59042 (11)	0.0223 (4)
C1′	1.0534 (2)	0.4821 (2)	0.90414 (14)	0.0297 (5)
C2′	1.0214 (2)	0.3675 (2)	0.90349 (14)	0.0306 (5)
C3′	1.0859 (2)	0.2544 (2)	0.91983 (15)	0.0349 (6)
H3′	1.162486	0.240626	0.934224	0.042*
C4′	1.0340 (3)	0.1626 (3)	0.91428 (18)	0.0469 (7)
H4′	1.075607	0.084206	0.925324	0.056*
C5′	0.9228 (3)	0.1828 (3)	0.8930 (2)	0.0513 (8)
H5′	0.889731	0.118235	0.889034	0.062*
C6′	0.8584 (3)	0.2968 (3)	0.87730 (19)	0.0457 (7)
H6′	0.781783	0.310803	0.862951	0.055*
C7′	0.9096 (2)	0.3884 (2)	0.88328 (15)	0.0345 (6)
C8′	0.8596 (2)	0.5185 (2)	0.87297 (16)	0.0350 (6)
H8′	0.840457	0.547981	0.815582	0.042*
C9′	0.9530 (2)	0.6906 (2)	0.87978 (14)	0.0314 (5)
H9′A	1.003483	0.701044	0.917835	0.038*
H9′B	0.871471	0.726203	0.899287	0.038*
C10′	0.98998 (19)	0.7553 (2)	0.79436 (13)	0.0239 (4)

C11′	1.1054 (2)	0.7027 (2)	0.74680 (14)	0.0260 (5)
H11′	1.170278	0.652311	0.769535	0.031*
C12′	1.09712 (19)	0.74141 (19)	0.66761 (14)	0.0251 (5)
H12′	1.154055	0.724037	0.621769	0.030*
C13′	0.97764 (19)	0.81916 (19)	0.66568 (13)	0.0221 (4)
C14′	0.9156 (2)	0.8553 (2)	0.59063 (14)	0.0264 (5)
H14C	0.971028	0.843925	0.539741	0.032*
H14D	0.852747	0.809951	0.595442	0.032*
C15′	0.9874 (2)	0.8886 (2)	0.78895 (13)	0.0255 (5)
H15C	0.918542	0.924993	0.824380	0.031*
H15D	1.059722	0.902498	0.804252	0.031*
C16′	0.97915 (18)	0.93444 (19)	0.69668 (13)	0.0223 (4)
H16′	1.048276	0.970275	0.668076	0.027*
C17′	0.86454 (19)	1.01119 (19)	0.67252 (13)	0.0222 (4)
H17C	0.796071	0.989347	0.711767	0.027*
H17D	0.864683	1.095695	0.668901	0.027*
C18′	0.63222 (18)	1.01004 (19)	0.58149 (13)	0.0226 (4)
C19′	0.6003 (2)	0.9103 (2)	0.56757 (15)	0.0285 (5)
H19′	0.648619	0.865397	0.529054	0.034*
C20′	0.4977 (2)	0.8770 (2)	0.61023 (15)	0.0308 (5)
H20′	0.476141	0.808453	0.601103	0.037*
C21′	0.4257 (2)	0.9424 (2)	0.66633 (14)	0.0293 (5)
C22′	0.4569 (2)	1.0438 (2)	0.67779 (14)	0.0283 (5)
H22′	0.407097	1.090152	0.714863	0.034*
C23′	0.55990 (19)	1.0784 (2)	0.63577 (13)	0.0248 (4)
H23′	0.580717	1.147840	0.643989	0.030*
C24′	0.3143 (2)	0.9045 (3)	0.71372 (16)	0.0400 (6)
H24D	0.285977	0.947062	0.759935	0.060*
H24E	0.330163	0.819809	0.734947	0.060*
H24F	0.254611	0.922022	0.676926	0.060*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0286 (3)	0.0229 (3)	0.0220 (3)	−0.0052 (2)	0.0008 (2)	0.0024 (2)
O1	0.0220 (8)	0.0272 (8)	0.0249 (8)	−0.0003 (6)	−0.0020 (6)	0.0004 (6)
O2	0.0233 (8)	0.0326 (9)	0.0245 (8)	−0.0072 (7)	0.0000 (6)	0.0010 (7)
O3	0.0247 (7)	0.0199 (7)	0.0166 (7)	−0.0036 (6)	−0.0020 (6)	0.0007 (5)
O4	0.0367 (10)	0.0216 (8)	0.0409 (10)	−0.0069 (7)	0.0025 (8)	0.0042 (7)
O5	0.0322 (9)	0.0389 (10)	0.0194 (8)	−0.0058 (7)	−0.0017 (7)	0.0023 (7)
N1	0.0260 (9)	0.0207 (9)	0.0175 (8)	−0.0043 (7)	−0.0010 (7)	−0.0003 (7)
N2	0.0269 (9)	0.0236 (9)	0.0188 (9)	−0.0063 (7)	0.0026 (7)	−0.0008 (7)
C1	0.0233 (10)	0.0237 (11)	0.0159 (9)	−0.0033 (8)	−0.0067 (8)	0.0035 (8)
C2	0.0278 (11)	0.0228 (11)	0.0191 (10)	−0.0045 (9)	−0.0076 (8)	0.0015 (8)
C3	0.0327 (12)	0.0272 (12)	0.0253 (11)	−0.0083 (10)	−0.0102 (10)	0.0010 (9)
C4	0.0486 (15)	0.0247 (12)	0.0315 (12)	−0.0112 (11)	−0.0190 (11)	0.0005 (10)
C5	0.0481 (15)	0.0242 (12)	0.0308 (12)	−0.0012 (11)	−0.0153 (11)	−0.0056 (10)
C6	0.0355 (13)	0.0287 (13)	0.0266 (12)	0.0005 (10)	−0.0074 (10)	−0.0043 (9)

C7	0.0291 (11)	0.0249 (11)	0.0170 (10)	−0.0030 (9)	−0.0047 (8)	−0.0013 (8)
C8	0.0254 (11)	0.0266 (11)	0.0179 (10)	−0.0025 (9)	0.0002 (8)	−0.0013 (8)
C9	0.0294 (11)	0.0218 (11)	0.0191 (10)	−0.0056 (9)	−0.0030 (9)	−0.0012 (8)
C10	0.0252 (10)	0.0208 (10)	0.0176 (9)	−0.0045 (8)	−0.0009 (8)	−0.0015 (8)
C11	0.0244 (11)	0.0292 (12)	0.0262 (11)	−0.0067 (9)	−0.0030 (9)	0.0018 (9)
C12	0.0265 (11)	0.0341 (13)	0.0247 (11)	−0.0072 (10)	−0.0071 (9)	0.0027 (9)
C13	0.0280 (11)	0.0201 (10)	0.0181 (10)	−0.0034 (8)	−0.0033 (8)	0.0018 (8)
C14	0.0342 (12)	0.0264 (12)	0.0195 (10)	−0.0110 (9)	−0.0011 (9)	−0.0015 (8)
C15	0.0360 (13)	0.0226 (11)	0.0203 (10)	−0.0070 (9)	0.0042 (9)	−0.0042 (8)
C16	0.0315 (12)	0.0203 (11)	0.0219 (10)	−0.0025 (9)	0.0005 (9)	0.0010 (8)
C17	0.0348 (12)	0.0205 (11)	0.0231 (11)	−0.0080 (9)	0.0015 (9)	−0.0016 (8)
C18	0.0260 (11)	0.0236 (11)	0.0203 (10)	−0.0068 (9)	0.0008 (8)	−0.0027 (8)
C19	0.0336 (12)	0.0250 (12)	0.0320 (12)	−0.0099 (10)	−0.0008 (10)	−0.0082 (9)
C20	0.0343 (13)	0.0346 (13)	0.0267 (11)	−0.0146 (10)	−0.0075 (10)	−0.0081 (10)
C21	0.0258 (11)	0.0324 (13)	0.0220 (11)	−0.0098 (9)	−0.0007 (9)	−0.0021 (9)
C22	0.0282 (11)	0.0237 (11)	0.0252 (11)	−0.0052 (9)	−0.0006 (9)	−0.0063 (9)
C23	0.0261 (11)	0.0269 (12)	0.0236 (11)	−0.0071 (9)	−0.0045 (9)	−0.0074 (9)
C24	0.0322 (13)	0.0454 (16)	0.0372 (14)	−0.0042 (11)	−0.0143 (11)	−0.0033 (12)
S1′	0.0233 (3)	0.0244 (3)	0.0192 (2)	−0.0058 (2)	−0.0031 (2)	0.0010 (2)
O1′	0.0288 (9)	0.0474 (11)	0.0299 (9)	−0.0071 (8)	−0.0058 (7)	0.0000 (8)
O2′	0.0231 (9)	0.0504 (12)	0.0405 (11)	−0.0009 (8)	−0.0048 (8)	0.0061 (8)
O3′	0.0216 (7)	0.0276 (8)	0.0200 (7)	−0.0079 (6)	−0.0011 (6)	−0.0002 (6)
O4′	0.0309 (9)	0.0383 (10)	0.0192 (8)	−0.0050 (7)	−0.0038 (7)	−0.0029 (7)
O5′	0.0312 (9)	0.0232 (8)	0.0311 (9)	−0.0088 (7)	−0.0046 (7)	0.0023 (6)
N1′	0.0264 (10)	0.0315 (11)	0.0270 (10)	−0.0065 (8)	−0.0029 (8)	0.0076 (8)
N2′	0.0214 (9)	0.0258 (10)	0.0188 (8)	−0.0025 (7)	−0.0037 (7)	−0.0031 (7)
C1′	0.0250 (11)	0.0389 (14)	0.0186 (10)	−0.0036 (10)	0.0003 (9)	0.0041 (9)
C2′	0.0254 (11)	0.0362 (14)	0.0245 (11)	−0.0044 (10)	0.0001 (9)	0.0031 (10)
C3′	0.0320 (13)	0.0372 (14)	0.0260 (12)	−0.0002 (11)	0.0043 (10)	0.0019 (10)
C4′	0.0482 (17)	0.0344 (15)	0.0467 (17)	−0.0011 (13)	0.0068 (14)	−0.0007 (12)
C5′	0.0491 (18)	0.0444 (18)	0.060 (2)	−0.0168 (14)	0.0031 (15)	−0.0084 (15)
C6′	0.0356 (15)	0.0487 (18)	0.0520 (17)	−0.0157 (13)	−0.0054 (13)	0.0007 (14)
C7′	0.0292 (12)	0.0395 (15)	0.0292 (12)	−0.0070 (11)	−0.0008 (10)	0.0046 (10)
C8′	0.0248 (12)	0.0422 (15)	0.0323 (13)	−0.0055 (10)	−0.0053 (10)	0.0067 (11)
C9′	0.0330 (13)	0.0342 (13)	0.0224 (11)	−0.0049 (10)	−0.0003 (10)	0.0009 (9)
C10′	0.0222 (10)	0.0295 (12)	0.0185 (10)	−0.0059 (9)	−0.0027 (8)	0.0000 (8)
C11′	0.0236 (11)	0.0256 (11)	0.0267 (11)	−0.0035 (9)	−0.0027 (9)	−0.0017 (9)
C12′	0.0227 (11)	0.0254 (11)	0.0254 (11)	−0.0030 (9)	−0.0006 (9)	−0.0044 (9)
C13′	0.0235 (10)	0.0245 (11)	0.0178 (10)	−0.0066 (8)	−0.0005 (8)	−0.0025 (8)
C14′	0.0311 (12)	0.0262 (12)	0.0228 (11)	−0.0009 (9)	−0.0070 (9)	−0.0080 (9)
C15′	0.0261 (11)	0.0321 (12)	0.0198 (10)	−0.0067 (9)	−0.0049 (9)	−0.0051 (9)
C16′	0.0214 (10)	0.0252 (11)	0.0209 (10)	−0.0074 (8)	−0.0025 (8)	−0.0026 (8)
C17′	0.0239 (10)	0.0227 (11)	0.0200 (10)	−0.0057 (8)	−0.0015 (8)	−0.0041 (8)
C18′	0.0201 (10)	0.0235 (11)	0.0226 (10)	−0.0039 (8)	−0.0058 (8)	0.0017 (8)
C19′	0.0285 (12)	0.0235 (11)	0.0342 (12)	−0.0032 (9)	−0.0086 (10)	−0.0053 (9)
C20′	0.0305 (12)	0.0259 (12)	0.0389 (14)	−0.0104 (10)	−0.0138 (10)	0.0009 (10)
C21′	0.0239 (11)	0.0348 (13)	0.0276 (12)	−0.0092 (9)	−0.0134 (9)	0.0103 (10)
C22′	0.0234 (11)	0.0358 (13)	0.0236 (11)	−0.0022 (9)	−0.0055 (9)	−0.0021 (9)

C23′	0.0248 (11)	0.0257 (11)	0.0239 (11)	−0.0057 (9)	−0.0051 (9)	−0.0021 (8)
C24′	0.0281 (13)	0.0547 (17)	0.0358 (14)	−0.0165 (12)	−0.0121 (11)	0.0109 (12)

Geometric parameters (Å, º)

S1—O4	1.4332 (17)	S1′—O4′	1.4337 (17)
S1—O5	1.4337 (17)	S1′—O5′	1.4378 (17)
S1—N2	1.6368 (19)	S1′—N2′	1.6263 (18)
S1—C18	1.758 (2)	S1′—C18′	1.758 (2)
O1—C1	1.240 (3)	O1′—C1′	1.231 (3)
O2—C8	1.407 (3)	O2′—C8′	1.404 (3)
O2—H2	0.9160	O2′—H2′	0.9026
O3—C10	1.449 (2)	O3′—C13′	1.452 (2)
O3—C13	1.456 (2)	O3′—C10′	1.453 (3)
N1—C1	1.356 (3)	N1′—C1′	1.363 (3)
N1—C9	1.452 (3)	N1′—C9′	1.449 (3)
N1—C8	1.477 (3)	N1′—C8′	1.466 (3)
N2—C17	1.481 (3)	N2′—C17′	1.480 (3)
N2—C14	1.487 (3)	N2′—C14′	1.488 (3)
C1—C2	1.474 (3)	C1′—C2′	1.488 (4)
C2—C7	1.387 (3)	C2′—C7′	1.382 (3)
C2—C3	1.390 (3)	C2′—C3′	1.389 (3)
C3—C4	1.394 (3)	C3′—C4′	1.385 (4)
C3—H3	0.9500	C3′—H3′	0.9500
C4—C5	1.391 (4)	C4′—C5′	1.381 (4)
C4—H4	0.9500	C4′—H4′	0.9500
C5—C6	1.393 (4)	C5′—C6′	1.396 (4)
C5—H5	0.9500	C5′—H5′	0.9500
C6—C7	1.383 (3)	C6′—C7′	1.379 (4)
C6—H6	0.9500	C6′—H6′	0.9500
C7—C8	1.511 (3)	C7′—C8′	1.511 (4)
C8—H8	1.0000	C8′—H8′	1.0000
C9—C10	1.511 (3)	C9′—C10′	1.510 (3)
C9—H9A	0.9900	C9′—H9′A	0.9900
C9—H9B	0.9900	C9′—H9′B	0.9900
C10—C11	1.516 (3)	C10′—C11′	1.526 (3)
C10—C15	1.563 (3)	C10′—C15′	1.557 (3)
C11—C12	1.325 (3)	C11′—C12′	1.323 (3)
C11—H11	0.9500	C11′—H11′	0.9500
C12—C13	1.502 (3)	C12′—C13′	1.512 (3)
C12—H12	0.9500	C12′—H12′	0.9500
C13—C14	1.509 (3)	C13′—C14′	1.507 (3)
C13—C16	1.565 (3)	C13′—C16′	1.563 (3)
C14—H14A	0.9900	C14′—H14C	0.9900
C14—H14B	0.9900	C14′—H14D	0.9900
C15—C16	1.546 (3)	C15′—C16′	1.540 (3)
C15—H15A	0.9900	C15′—H15C	0.9900
C15—H15B	0.9900	C15′—H15D	0.9900

C16—C17	1.525 (3)	C16′—C17′	1.529 (3)
C16—H16	1.0000	C16′—H16′	1.0000
C17—H17A	0.9900	C17′—H17C	0.9900
C17—H17B	0.9900	C17′—H17D	0.9900
C18—C19	1.388 (3)	C18′—C19′	1.389 (3)
C18—C23	1.391 (3)	C18′—C23′	1.392 (3)
C19—C20	1.387 (3)	C19′—C20′	1.383 (3)
C19—H19	0.9500	C19′—H19′	0.9500
C20—C21	1.392 (3)	C20′—C21′	1.391 (4)
C20—H20	0.9500	C20′—H20′	0.9500
C21—C22	1.389 (3)	C21′—C22′	1.388 (3)
C21—C24	1.504 (3)	C21′—C24′	1.515 (3)
C22—C23	1.387 (3)	C22′—C23′	1.389 (3)
C22—H22	0.9500	C22′—H22′	0.9500
C23—H23	0.9500	C23′—H23′	0.9500
C24—H24A	0.9800	C24′—H24D	0.9800
C24—H24B	0.9800	C24′—H24E	0.9800
C24—H24C	0.9800	C24′—H24F	0.9800
O4—S1—O5	120.45 (10)	O4′—S1′—O5′	120.20 (10)
O4—S1—N2	106.71 (10)	O4′—S1′—N2′	105.39 (10)
O5—S1—N2	105.53 (10)	O5′—S1′—N2′	106.73 (10)
O4—S1—C18	107.32 (11)	O4′—S1′—C18′	108.51 (10)
O5—S1—C18	109.11 (10)	O5′—S1′—C18′	107.32 (10)
N2—S1—C18	107.01 (10)	N2′—S1′—C18′	108.20 (10)
C8—O2—H2	108.3	C8′—O2′—H2′	108.3
C10—O3—C13	95.72 (15)	C13′—O3′—C10′	95.37 (15)
C1—N1—C9	123.97 (18)	C1′—N1′—C9′	123.9 (2)
C1—N1—C8	113.04 (18)	C1′—N1′—C8′	113.8 (2)
C9—N1—C8	122.98 (17)	C9′—N1′—C8′	122.0 (2)
C17—N2—C14	109.96 (16)	C17′—N2′—C14′	110.14 (16)
C17—N2—S1	119.69 (15)	C17′—N2′—S1′	121.96 (14)
C14—N2—S1	118.46 (14)	C14′—N2′—S1′	119.12 (14)
O1—C1—N1	125.2 (2)	O1′—C1′—N1′	125.3 (2)
O1—C1—C2	127.7 (2)	O1′—C1′—C2′	128.7 (2)
N1—C1—C2	107.04 (18)	N1′—C1′—C2′	106.0 (2)
C7—C2—C3	121.9 (2)	C7′—C2′—C3′	121.8 (2)
C7—C2—C1	108.71 (19)	C7′—C2′—C1′	108.7 (2)
C3—C2—C1	129.4 (2)	C3′—C2′—C1′	129.6 (2)
C2—C3—C4	117.1 (2)	C4′—C3′—C2′	117.2 (3)
C2—C3—H3	121.5	C4′—C3′—H3′	121.4
C4—C3—H3	121.5	C2′—C3′—H3′	121.4
C5—C4—C3	120.9 (2)	C5′—C4′—C3′	121.3 (3)
C5—C4—H4	119.5	C5′—C4′—H4′	119.3
C3—C4—H4	119.5	C3′—C4′—H4′	119.3
C4—C5—C6	121.5 (2)	C4′—C5′—C6′	121.0 (3)
C4—C5—H5	119.2	C4′—C5′—H5′	119.5
C6—C5—H5	119.2	C6′—C5′—H5′	119.5

C7—C6—C5	117.5 (2)	C7′—C6′—C5′	117.8 (3)
C7—C6—H6	121.3	C7′—C6′—H6′	121.1
C5—C6—H6	121.3	C5′—C6′—H6′	121.1
C6—C7—C2	121.1 (2)	C6′—C7′—C2′	120.8 (3)
C6—C7—C8	129.4 (2)	C6′—C7′—C8′	129.4 (2)
C2—C7—C8	109.48 (19)	C2′—C7′—C8′	109.8 (2)
O2—C8—N1	112.16 (17)	O2′—C8′—N1′	112.0 (2)
O2—C8—C7	114.70 (18)	O2′—C8′—C7′	114.4 (2)
N1—C8—C7	101.68 (17)	N1′—C8′—C7′	101.48 (19)
O2—C8—H8	109.3	O2′—C8′—H8′	109.6
N1—C8—H8	109.3	N1′—C8′—H8′	109.6
C7—C8—H8	109.3	C7′—C8′—H8′	109.6
N1—C9—C10	113.26 (17)	N1′—C9′—C10′	113.6 (2)
N1—C9—H9A	108.9	N1′—C9′—H9′A	108.9
C10—C9—H9A	108.9	C10′—C9′—H9′A	108.9
N1—C9—H9B	108.9	N1′—C9′—H9′B	108.9
C10—C9—H9B	108.9	C10′—C9′—H9′B	108.9
H9A—C9—H9B	107.7	H9′A—C9′—H9′B	107.7
O3—C10—C9	111.77 (17)	O3′—C10′—C9′	112.69 (18)
O3—C10—C11	101.29 (16)	O3′—C10′—C11′	100.79 (17)
C9—C10—C11	118.54 (18)	C9′—C10′—C11′	117.59 (19)
O3—C10—C15	100.25 (15)	O3′—C10′—C15′	100.44 (16)
C9—C10—C15	115.28 (18)	C9′—C10′—C15′	114.75 (19)
C11—C10—C15	107.33 (18)	C11′—C10′—C15′	108.40 (18)
C12—C11—C10	106.5 (2)	C12′—C11′—C10′	106.32 (19)
C12—C11—H11	126.7	C12′—C11′—H11′	126.8
C10—C11—H11	126.7	C10′—C11′—H11′	126.8
C11—C12—C13	105.4 (2)	C11′—C12′—C13′	105.22 (19)
C11—C12—H12	127.3	C11′—C12′—H12′	127.4
C13—C12—H12	127.3	C13′—C12′—H12′	127.4
O3—C13—C12	102.11 (16)	O3′—C13′—C14′	113.05 (18)
O3—C13—C14	111.92 (18)	O3′—C13′—C12′	101.73 (16)
C12—C13—C14	125.30 (19)	C14′—C13′—C12′	124.03 (19)
O3—C13—C16	100.04 (16)	O3′—C13′—C16′	99.92 (16)
C12—C13—C16	107.30 (18)	C14′—C13′—C16′	106.76 (17)
C14—C13—C16	107.29 (17)	C12′—C13′—C16′	108.74 (17)
N2—C14—C13	103.49 (17)	N2′—C14′—C13′	103.46 (17)
N2—C14—H14A	111.1	N2′—C14′—H14C	111.1
C13—C14—H14A	111.1	C13′—C14′—H14C	111.1
N2—C14—H14B	111.1	N2′—C14′—H14D	111.1
C13—C14—H14B	111.1	C13′—C14′—H14D	111.1
H14A—C14—H14B	109.0	H14C—C14′—H14D	109.0
C16—C15—C10	100.84 (17)	C16′—C15′—C10′	100.90 (17)
C16—C15—H15A	111.6	C16′—C15′—H15C	111.6
C10—C15—H15A	111.6	C10′—C15′—H15C	111.6
C16—C15—H15B	111.6	C16′—C15′—H15D	111.6
C10—C15—H15B	111.6	C10′—C15′—H15D	111.6
H15A—C15—H15B	109.4	H15C—C15′—H15D	109.4

C17—C16—C15	119.1 (2)	C17′—C16′—C15′	118.39 (18)
C17—C16—C13	101.38 (17)	C17′—C16′—C13′	101.21 (16)
C15—C16—C13	101.55 (17)	C15′—C16′—C13′	101.62 (17)
C17—C16—H16	111.2	C17′—C16′—H16′	111.5
C15—C16—H16	111.2	C15′—C16′—H16′	111.5
C13—C16—H16	111.2	C13′—C16′—H16′	111.5
N2—C17—C16	101.58 (18)	N2′—C17′—C16′	100.82 (16)
N2—C17—H17A	111.5	N2′—C17′—H17C	111.6
C16—C17—H17A	111.5	C16′—C17′—H17C	111.6
N2—C17—H17B	111.5	N2′—C17′—H17D	111.6
C16—C17—H17B	111.5	C16′—C17′—H17D	111.6
H17A—C17—H17B	109.3	H17C—C17′—H17D	109.4
C19—C18—C23	120.8 (2)	C19′—C18′—C23′	120.5 (2)
C19—C18—S1	120.11 (18)	C19′—C18′—S1′	119.70 (17)
C23—C18—S1	119.01 (17)	C23′—C18′—S1′	119.76 (17)
C20—C19—C18	119.2 (2)	C20′—C19′—C18′	119.4 (2)
C20—C19—H19	120.4	C20′—C19′—H19′	120.3
C18—C19—H19	120.4	C18′—C19′—H19′	120.3
C19—C20—C21	121.0 (2)	C19′—C20′—C21′	120.9 (2)
C19—C20—H20	119.5	C19′—C20′—H20′	119.5
C21—C20—H20	119.5	C21′—C20′—H20′	119.5
C22—C21—C20	118.8 (2)	C22′—C21′—C20′	119.0 (2)
C22—C21—C24	119.4 (2)	C22′—C21′—C24′	120.3 (2)
C20—C21—C24	121.7 (2)	C20′—C21′—C24′	120.7 (2)
C23—C22—C21	121.2 (2)	C21′—C22′—C23′	120.9 (2)
C23—C22—H22	119.4	C21′—C22′—H22′	119.6
C21—C22—H22	119.4	C23′—C22′—H22′	119.6
C22—C23—C18	119.0 (2)	C22′—C23′—C18′	119.2 (2)
C22—C23—H23	120.5	C22′—C23′—H23′	120.4
C18—C23—H23	120.5	C18′—C23′—H23′	120.4
C21—C24—H24A	109.5	C21′—C24′—H24D	109.5
C21—C24—H24B	109.5	C21′—C24′—H24E	109.5
H24A—C24—H24B	109.5	H24D—C24′—H24E	109.5
C21—C24—H24C	109.5	C21′—C24′—H24F	109.5
H24A—C24—H24C	109.5	H24D—C24′—H24F	109.5
H24B—C24—H24C	109.5	H24E—C24′—H24F	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O3	1.00	2.63	3.206 (3)	117
C12—H12···O5^{i}	0.95	2.47	3.333 (3)	151
C14—H14*A*···O5′^{ii}	0.99	2.62	3.506 (3)	149
C23—H23···O5′^{ii}	0.95	2.41	3.195 (3)	139
C14′—H14*D*···O4	0.99	2.58	3.482 (3)	151
C15′—H15*C*···O2^{iii}	0.99	2.62	3.585 (3)	165
C16′—H16′···O4′^{iv}	1.00	2.53	3.422 (3)	149
C19′—H19′···O4	0.95	2.34	3.078 (3)	134

O2—H2···O1^{v}	0.92	1.85	2.756 (2)	172
O2′—H2′···O1′^{vi}	0.90	1.95	2.840 (3)	171

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