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Intermolecular interactions and disorder in six isostructural celecoxib solvates

Andrew D. Bond[a,b]* and Changquan C. Sun[c]

[a]Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW, England, [b]Department of Pharmacy, University of Copenhagen, Universitetsparken 2, Copenhagen, DK-2100, Denmark, and [c]Department of Pharmaceutics, University of Minnesota, Minneapolis, MN 5545, USA. *Correspondence e-mail: adb29@cam.ac.uk

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Six isostructural crystalline solvates of the active pharmaceutical ingredient celecoxib {4-[5-(4-methylphenyl)-3-(trifluoromethyl)pyrazol-1-yl]benzenesulfonamide; $C_{17}H_{14}F_3N_3O_2S$} are described, containing dimethylformamide (DMF, C_3H_7NO, **1**), dimethylacetamide (DMA, C_4H_9NO, **2**), *N*-methylpyrrolidin-2-one (NMP, C_5H_9NO, **3**), tetramethylurea (TMU, $C_5H_{12}N_2O$, **4**), 1,3-dimethyl-3,4,5,6-tetrahydropyrimidin-2(1*H*)-one (DMPU, $C_6H_{12}N_2O$, **5**) or dimethyl sulfoxide (DMSO, C_2H_6OS, **6**). The host celecoxib structure contains one-dimensional channel voids accommodating the solvent molecules, which accept hydrogen bonds from the NH_2 groups of two celecoxib molecules. The solvent binding sites have local twofold rotation symmetry, which is consistent with the point symmetry of the solvent molecule in **4** and **5**, but introduces orientational disorder for the solvent molecules in **1**, **2**, **3** and **6**. Despite the isostructurality of **1**–**6**, the unit-cell volume and solvent-accessible void space show significant variation. In particular, **4** and **5** show an enlarged and skewed unit cell, which can be attributed to a specific interaction between an N—CH_3 group in the solvent molecule and the toluene group of celecoxib. Intermolecular interaction energies calculated using the *PIXEL* method show that the total interaction energy between the celecoxib and solvent molecules is broadly correlated with the molecular volume of the solvent, except in **6**, where the increased polarity of the S=O bond leads to greater overall stabilization compared to the similarly-sized DMF molecule in **1**. In the structures showing disorder, the most stable orientations of the solvent molecules make C—H···O contacts to the S=O groups of celecoxib.

1. Introduction

Understanding the structures and properties of crystalline solids can be of significant importance for active pharmaceutical ingredients (APIs) (Sun, 2009). Solid-form screening is an integral part of most pre-formulation activities (Morissette *et al.*, 2004), with an aim to establish the range of solid forms that can exist for a given API. These generally include both polymorphs and multicomponent forms, which may variously be described as salts, cocrystals, solvates, *etc.* (Aitipamula *et al.*, 2012).

The API of interest in this work is the anti-inflammatory drug celecoxib (see Scheme 1). To date, there is only one polymorph (Form III) of celecoxib for which a single-crystal X-ray structure has been reported (Dev *et al.*, 1999; Wang *et al.*, 2019) in the Cambridge Structural Database (CSD; Groom *et al.*, 2016), although several polymorphs are established in the literature (Dev *et al.*, 1999; Lu *et al.*, 2006; Wang & Sun, 2019). Crystal structures are known for numerous multicomponent forms, including with pyrrolidin-2-one, caprolactam, valerolactam (Bolla *et al.*, 2014), pyridin-2(1*H*)-one (Bolla & Nangia, 2019), nicotinamide (Zhang *et al.*, 2017) and bis-(proline) (as a zwitterion; Li *et al.*, 2018). Some celecoxib

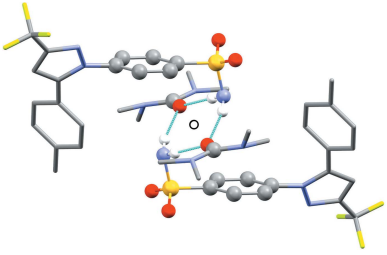


Table 1
Experimental details.

For all structures: monoclinic, $P2_1/c$, $Z = 4$. Experiments were carried out at 298 K with Cu $K\alpha$ radiation using a Bruker D8-QUEST PHOTON-100 diffractometer. Absorption was corrected for by multi-scan methods (*SADABS*; Bruker, 2016). H atoms were treated by a mixture of independent and constrained refinement.

	1	**2**	**3**
Crystal data			
Chemical formula	$C_{17}H_{14}F_3N_3O_2S\cdot C_3H_7NO$	$C_{17}H_{14}F_3N_3O_2S\cdot C_4H_9NO$	$C_{17}H_{14}F_3N_3O_2S\cdot C_5H_9NO$
M_r	454.47	468.49	480.50
a, b, c (Å)	11.8973 (4), 8.8360 (3), 21.8286 (7)	11.9584 (3), 9.2028 (2), 21.2811 (6)	11.9978 (4), 9.0896 (3), 21.9732 (8)
β (°)	103.4537 (13)	103.3826 (12)	101.358 (2)
V (Å^3)	2231.75 (13)	2278.41 (10)	2349.36 (14)
μ (mm^{-1})	1.77	1.75	1.71
Crystal size (mm)	0.16 × 0.16 × 0.14	0.20 × 0.18 × 0.18	0.20 × 0.18 × 0.18
Data collection			
T_{min}, T_{max}	0.440, 0.753	0.608, 0.753	0.593, 0.753
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16627, 3940, 3362	38939, 4032, 3394	24378, 4146, 3112
R_{int}	0.053	0.041	0.047
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.596	0.597	0.596
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.056, 0.149, 1.08	0.047, 0.129, 1.03	0.048, 0.136, 1.03
No. of reflections	3940	4032	4146
No. of parameters	346	345	389
No. of restraints	35	26	103
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.37	0.22, −0.29	0.22, −0.24

	4	**5**	**6**
Crystal data			
Chemical formula	$C_{17}H_{14}F_3N_3O_2S\cdot C_5H_{12}N_2O$	$C_{17}H_{14}F_3N_3O_2S\cdot C_6H_{12}N_2O$	$C_{17}H_{14}F_3N_3O_2S\cdot C_2H_6OS$
M_r	497.54	509.55	459.50
a, b, c (Å)	12.4050 (3), 8.9351 (2), 22.5727 (6)	12.4495 (17), 8.7822 (13), 22.656 (3)	11.9884 (3), 9.0230 (3), 20.8537 (6)
β (°)	98.6702 (13)	97.861 (5)	100.3908 (9)
V (Å^3)	2473.36 (11)	2453.9 (6)	2218.78 (11)
μ (mm^{-1})	1.66	1.68	2.63
Crystal size (mm)	0.16 × 0.14 × 0.14	0.20 × 0.20 × 0.18	0.14 × 0.12 × 0.12
Data collection			
T_{min}, T_{max}	0.657, 0.753	0.526, 0.753	0.476, 0.753
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	27591, 4397, 3339	25201, 4318, 3733	22464, 3916, 3520
R_{int}	0.034	0.031	0.042
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.597	0.597	0.596
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.142, 1.04	0.040, 0.118, 1.02	0.044, 0.126, 1.04
No. of reflections	4397	4318	3916
No. of parameters	349	364	318
No. of restraints	15	29	15
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.20	0.25, −0.21	0.29, −0.28

Computer programs: *APEX3* (Bruker, 2018), *SAINT* (Bruker, 2018), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*) and *Mercury* (Macrae *et al.*, 2020).

cocrystals with 4,4′-bipyridine and 1,2-bis(pyridin-4-yl)ethylene have also been reported to form isostructural solvates (*i.e.* isostructural three-component crystals) when combined with acetone, THF or 1,4-dioxane (Wang *et al.*, 2014).

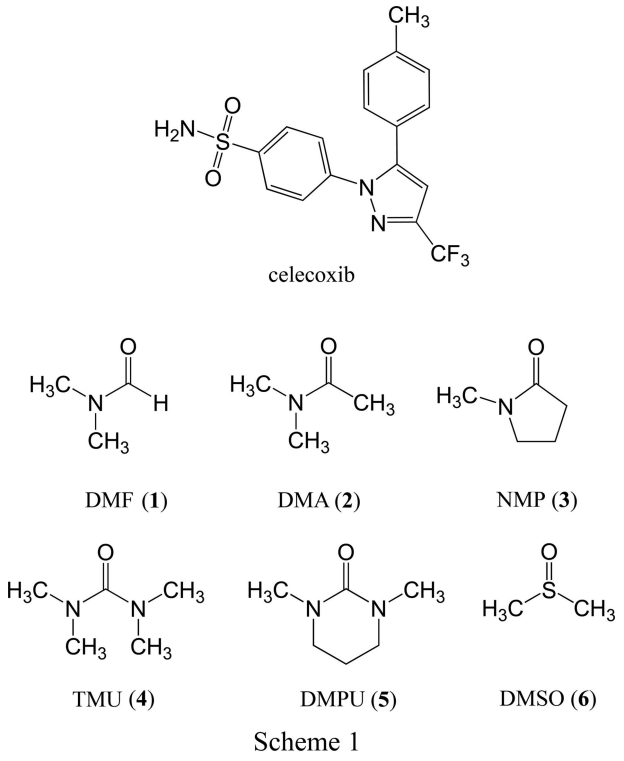
We were initially interested in studying solvates of celecoxib as part of a broader structure–property correlation exercise to understand and address its pharmaceutical deficiencies, *e.g.* high punch sticking propensity (Wang *et al.*, 2020; Paul *et al.*, 2017, 2020), amorphous phase stability (Wang & Sun, 2019), poor flowability (Chen *et al.*, 2020) and high elastic flexibility (Wang *et al.*, 2019). In the course of this work, we identified a group of six solvates (see Scheme 1) that form an isostructural group, different from any of the multicomponent celecoxib crystal structures in the CSD. We describe the new structure type in this paper and explore aspects of the isostructurality, including variation of the unit-cell parameters, disorder of the solvent molecules, and the intermolecular interactions between the solvent and celecoxib molecules.

2. Experimental

2.1. Synthesis and crystallization

Single crystals suitable for X-ray analysis were obtained by slow cooling of a warm solution of celecoxib in either di-

methylformamide (DMF, **1**), dimethylacetamide (DMA, **2**), *N*-methylpyrrolidin-2-one (NMP, **3**), tetramethylurea (TMU, **4**), 1,3-dimethyl-3,4,5,6-tetrahydropyrimidin-2(1*H*)-one (DMPU, **5**) or dimethyl sulfoxide (DMSO, **6**). The DMF (**1**) and DMA (**2**) solvates have been prepared previously (Chawla *et al.*, 2003), but structural details were not provided. A powder X-ray diffraction pattern published by Chawla *et al.* (2003) clearly matches that simulated from the crystal structure of **2**. The match to **1** is less clear, but additional thermal analysis is broadly consistent with our observations, so it seems probable that the structures described herein are consistent with the previously studied material.



Scheme 1

2.2. Refinement of 1–6

H atoms bound to C atoms were placed in idealized positions and refined using a riding model, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C). For the methyl group (C11) in celecoxib, the H atoms were allowed to rotate around the local threefold axis. H atoms of the NH_2 groups were located in difference Fourier maps, then refined with isotropic displacement parameters, with the N—H and H···H distances restrained to 0.86 (1) and 1.50 (1) Å, respectively. All of the structures display rotational disorder of the CF_3 group. This was modelled in each case as two sets of three F atoms, with site-occupancy factors constrained to sum to unity. To ensure a regular geometry, the C—F distances were restrained to a common refined value and the F···F distances were restrained to 1.633 times that value. All F atoms were refined with anisotropic ADPs. This produces highly distorted (prolate) ellipsoids in several cases, despite the inclusion of two sets of atomic sites, indicating that the rotational disorder is extensive. Given this rotational disorder, the distorted ellipsoids were considered to be an acceptable compromise to model the electron density in this region. For the disordered solvent molecules in **1**, **2**, **3** and **6**, two sets of atoms were refined, with site-occupancy factors summing to unity, and with appropriate geometrical restraints. Anisotropic ADPs were applied to all non-H atoms and H atoms were placed in idealized positions and refined as riding. The structure and refinement details are presented in Table 1.

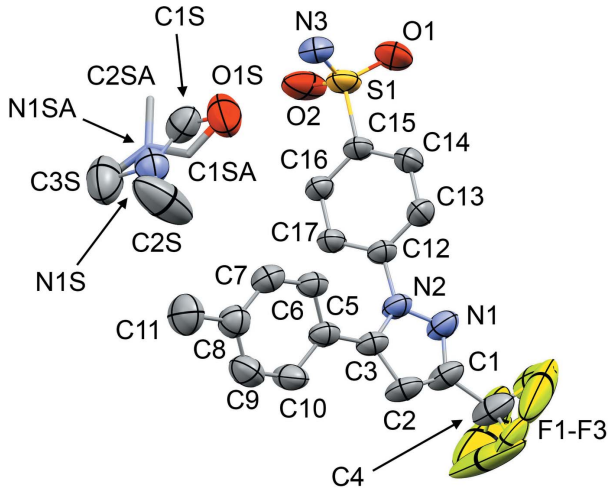


Figure 1
The molecular structure of **1**, with displacement ellipsoids at the 50% probability level. H atoms have been omitted. The second disorder component of the DMF molecule [site-occupancy factor = 0.221 (7)] is shown in outline only. Atoms O1*S* and C3*S* are common to both DMF components.

2.3. Computational details

The crystal structures were energy-minimized with dispersion-corrected density functional theory (DFT-D) using the *CASTEP* module (Clark *et al.*, 2005) in *Materials Studio* (Accelrys, 2011). The PBE functional (Perdew *et al.*, 1996) was applied with a plane-wave cut-off energy of 520 eV, in combination with the Grimme semi-empirical dispersion correction (Grimme, 2006). The unit-cell parameters were constrained to the experimental values and the space group $P2_1/c$ was imposed. Only one component of the rotationally-disordered CF_3 group was included (arbitrarily). For the structures with disordered solvent molecules, separate models were minimized for each disorder component. In each case, minimization produced only small geometrical deviations from the starting structure, as expected for high-quality single-crystal structures (van de Streek & Neumann, 2010). The purpose of the optimization step is to place the structures on a common basis for comparison, particularly for the disordered structures, where the results of the crystallographic refinement are generally less precise. The DFT-D-optimized structures were then used as input for the *PIXEL* module of the *CSP* package (Gavezzotti, 2002, 2003, 2011). The calculated pairwise interaction energies are estimated to have an accuracy within a range of *ca* ±3 kJ mol^{-1}.

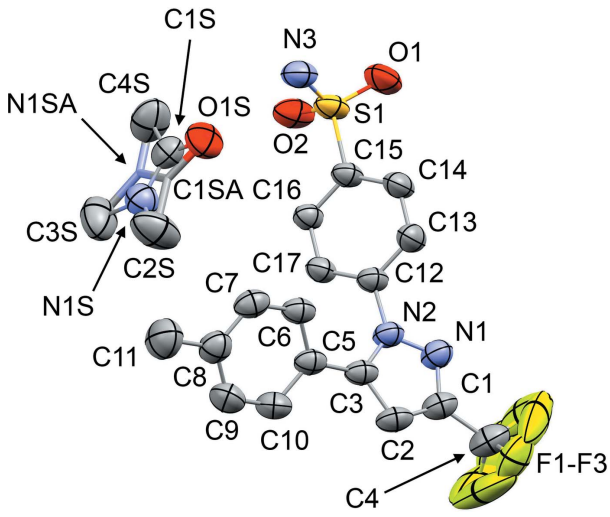


Figure 2
The molecular structure of **2**, with displacement ellipsoids at the 50% probability level. H atoms have been omitted. The second disorder component of the DMA molecule [site-occupancy factor = 0.464 (8)] is shown in outline only. Atoms O1*S*, C2*S*, C3*S* and C4*S* are common to both DMA components.

3. Results and discussion

3.1. Description of the crystal structures

The molecular structures of **1**–**6** are shown in Figs. 1–6. In the crystal structures, the celecoxib molecules are arranged into pairs around inversion centres with two solvent molecules accepting N—H···O hydrogen bonds (Fig. 7). The local symmetry of this unit is effectively 2/*m* (C_{2h}), where the C═O (or S═O) group of each solvent molecule is approximately aligned along the local twofold rotation axis. For the TMU and DMPU molecules in **4** and **5**, which themselves show twofold rotational point symmetry, this produces an ordered crystal-

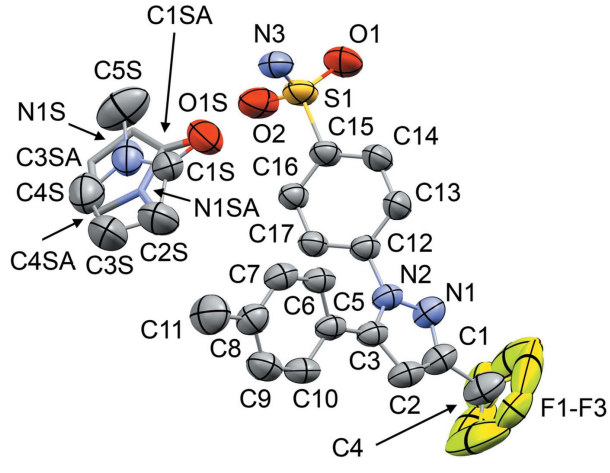


Figure 3
The molecular structure of **3**, with displacement ellipsoids at the 50% probability level. H atoms have been omitted. The second disorder component of the NMP molecule [site-occupancy factor = 0.321 (8)] is shown in outline only. Atoms C2*SA* and C5*SA* are not labelled, C2*SA* is directly below C5*S* and C5*SA* is hidden behind C2*S*.

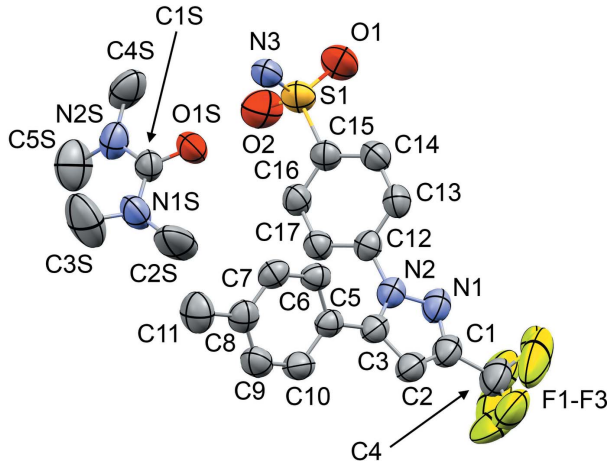


Figure 4
The molecular structure of **4**, with displacement ellipsoids at the 50% probability level. H atoms have been omitted. Disorder is not evident for the TMU molecule.

lographic result. The DMPU molecule displays minor conformational disorder of its six-membered ring (atoms C3*S*/C3*SA* in Fig. 5), but the parts of the molecule involved in binding to celecoxib are ordered and consistent for TMU and DMPU. For DMF (**1**), DMA (**2**), NMP (**3**) and DMSO (**6**), which do not possess twofold rotational symmetry, the crystal structure is disordered, with the molecules adopting two alternative orientations related by the local twofold axis. However, the full crystallographic environment of each solvent molecule is not twofold symmetric. Hence, the two orientations of the disordered solvent molecules have different total interaction energies (§3.3). With the solvent molecules removed from the structures, the void space between the celecoxib molecules defines one-dimensional (1D) channels along the *b* axis (Fig. 8). The solvent-accessible volume spans a considerable range for **1**–**6** (Table 2), constituting approximately 21–28% of the unit-cell volume.

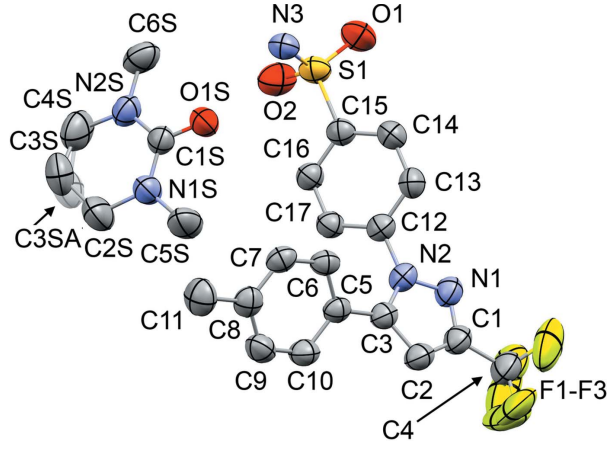


Figure 5
The molecular structure of **5**, with displacement ellipsoids at the 50% probability level. H atoms have been omitted. The alternative positions C3*S* and C3*SA* [site-occupancy factors = 0.584 (16):0.416 (16)] are shown for the DMPU molecule.

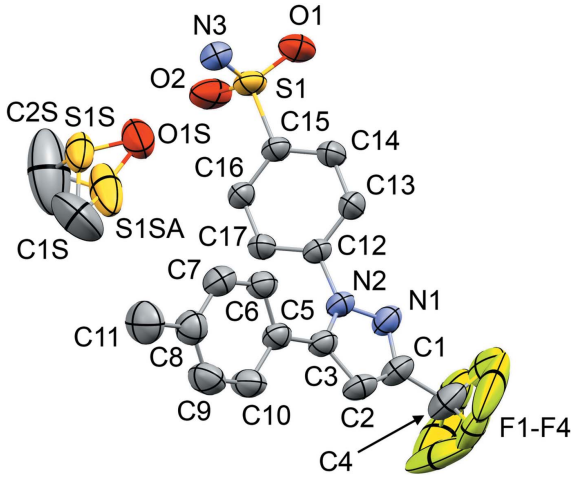


Figure 6
The molecular structure of **6**, with displacement ellipsoids at the 50% probability level. H atoms have been omitted. Atoms C1*S* and C2*S* are common to both disorder components for the DMSO molecule. The relatively large displacement ellipsoid of atom C2*S* was retained in preference to multiple atom sites for simplicity of the model.

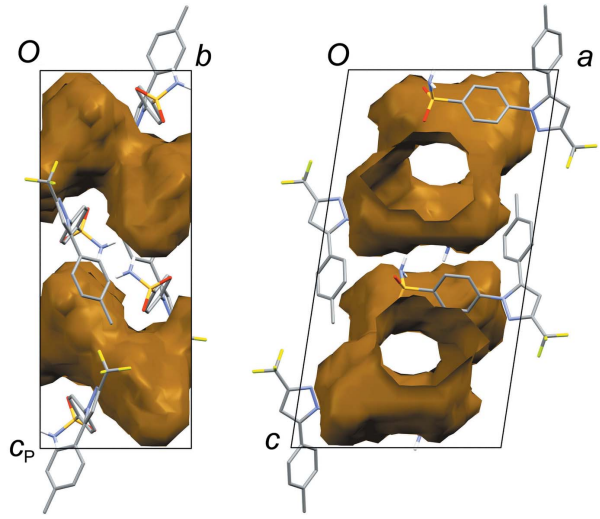


Figure 8
Views of the 1D voids running along the *b* axis in the celecoxib framework structure, after removing the solvent molecules. Structure **6** is shown. The voids are generated using *Mercury* (contact surface, probe radius 1.2 Å; Macrae *et al.*, 2020).

3.2. Variation of the unit-cell parameters

Despite the isostructural nature of the solvates, the unit-cell parameters differ quite significantly, with a difference of *ca* 250 Å^3 between the smallest (**6**) and largest (**4**) volumes. Plotting the *b* or *c* axis of **1**–**6** by ascending length (see supporting information) shows an approximately linear change in each case, but plotting the *a* axis in a similar manner shows a clear discontinuity, with the *a* axis in **4** and **5** being approximately 0.5 Å longer than in **1**, **2**, **3** and **6**. A similar pattern is seen for the β angle, indicating a relative skewing of the *ac* plane in **4** and **5**. Comparing representative structures in projection along the *b* axis (Fig. 9) indicates a reason for this observation. Common to structures **4** and **5**, but not present in **1**, **2**, **3** or **6**, is an N—CH_3 group in the solvent molecule that points approximately along the *a* axis and is directed towards a neighbouring toluene ring of celecoxib. The interaction pushes the toluene ring away from the position seen in the structures that do not have this N—CH_3 group. The celecoxib molecules are 'anchored' by their hydrogen-bonding NH_2 groups, which retain essentially identical positions in all structures, so the effect of pushing away the toluene ring is a relative rotation of the celecoxib molecules (Fig. 9). This serves to elongate both the *a* and the *c* axes, and to skew the unit cell. The other CH_3 groups in TMU (**4**) or DMPU (**5**) adopt positions that are seen in one or more of the other structures, and they do not make any clearly comparable intermolecular contacts to celecoxib.

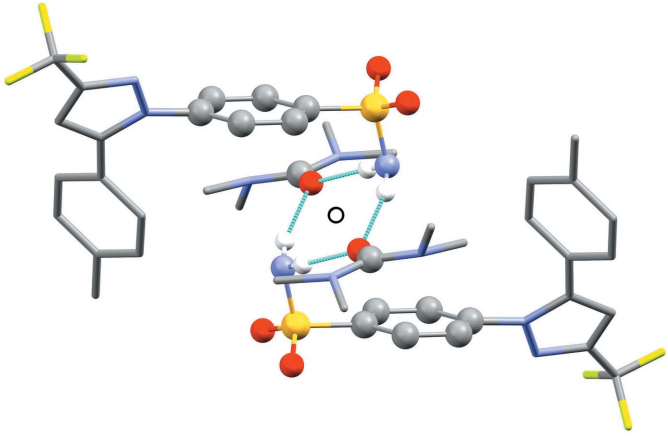


Figure 7
Hydrogen-bonded motif with two solvent molecules (TMU is shown) accepting N—H···O hydrogen bonds from two celecoxib molecules across a crystallographic inversion centre (indicated by the open circle). H atoms not involved in hydrogen bonding have been omitted. The atoms shown in ball-and-stick style conform to local 2/*m* (C_{2h}) point symmetry.

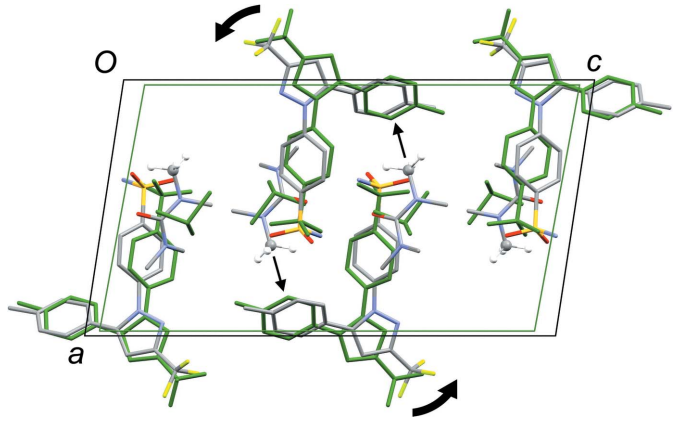


Figure 9
Projection of the structures of **4** (standard colour) and **6** (green) along the *b* axis. The highlighted N—CH_3···π interaction in **4** [C2*S*···centroid(C5–C10) = 3.825 Å] causes the celecoxib molecules to rotate outwards relative to each other, as indicated by the thick arrows, causing expansion and skewing of the unit cell compared to **6**.

Table 2
Intermolecular interaction energies between the celecoxib and solvent molecules [$E(\mathrm{tot})_{\mathrm{cel-solv}}$] and between the solvent molecules [$E(\mathrm{tot})_{\mathrm{solv-solv}}$], calculated using the *PIXEL* method, together with the unit-cell volume (V_{cell}), void volume (V_{void}) and solvent molecular volume (V_{solv}).

	Solvent	V_{cell} (Å^3)	V_{void} (Å^3)[a]	V_{solv} (Å^3)[b]	Disorder component	$E(\mathrm{tot})_{\mathrm{cel-solv}}$ (kJ mol^{-1})	$E(\mathrm{tot})_{\mathrm{solv-solv}}$ (kJ mol^{-1})
1	DMF	2231.8	485.4 (21.7%)	76.7	**A**	−144.0	+3.8
					B	−132.2	+5.1
2	DMA	2278.4	481.8 (21.1%)	93.2	**A**	−160.5	+2.4
					B	−162.1	+3.3
3	NMP	2349.4	617.5 (25.0%)	100.1	**A**	−170.7	+1.9
					B	−160.1	+1.5
4	TMU	2473.4	572.3 (24.4%)	121.8	–	−155.1	+0.7
5	DMPU	2453.9	692.1 (28.2%)	127.9	**A**	−180.5	−1.9
					B	−187.1	−3.0
6	DMSO	2218.8	466.5 (21.0%)	71.7	**A**	−168.9	+4.6
					B	−164.3	+4.5

Notes: (*a*) the voids were generated using *Mercury* (Macrae *et al.*, 2020) as a contact surface with probe radius of 1.2 Å and (*b*) molecular volumes are derived from van der Waals surfaces, calculated in *Materials Studio* (Accelrys, 2011) as a Connolly surface generated with zero probe radius.

3.3. Interactions between the solvent molecules and celecoxib

On account of the isostructurality, the pairwise intermolecular interactions in each structure can be directly matched. Table 2 lists the total interaction energy between the celecoxib and solvent molecules, based on an equivalent set of interactions in each structure. For **1**–**5**, the total celecoxib–solvent interaction energy broadly increases with the molecular volume of the solvent, with **2** (DMA) and **3** (NMP) being closely comparable. The DMSO molecule in **6** has a significantly more stabilizing total interaction with celecoxib, compared to the similarly-sized DMF molecule in **1**, due to the increased polarity of the S═O bond. For example, the two independent pairwise interactions including the hydrogen bonds to celecoxib are both approximately −50 kJ mol^{-1} in **1** (varying slightly for the two disorder components), but approximately −57 and −68 kJ mol^{-1} in **6**. The N—$CH_3\cdots\pi$ interaction highlighted in Fig. 9 belongs to the celecoxib–solvent pair within the asymmetric unit (as shown in Figs. 4 and 5). Since *PIXEL* energies refer to total pairwise intermolecular interactions, any specific features of the N—$CH_3\cdots\pi$ interaction are masked by the total interaction energy. Table 2 also lists the total interaction energy between solvent molecules, based on three equivalent significant interactions in each structure. The interaction between the two solvent molecules involved in the hydrogen-bonded motif (Fig. 7) is repulsive, due to the destabilizing Coulombic O$\cdots$O interaction. The only other significant interactions between solvent molecules are along the 2_1 screw axis parallel to *b*, which are slightly stabilizing. The extent to which these interactions mitigate the destabilizing O$\cdots$O interaction increases with the molecular volume of the solvent, and the overall solvent–solvent interaction is slightly stabilizing for the largest molecule, *i.e.* DMPU (**5**).

The difference between the total interaction energies with the celecoxib framework for the two disorder components of the solvent molecules in each structure is also shown in Table 2. The most significant difference within a single structure is seen for DMF (**1**), where the two orientations exchange the positions of the C—H and N—CH_3 groups (Fig. 1). Approximately two thirds of the energy difference arises from the interactions of the DMF molecule with the two celecoxib molecules in the hydrogen-bonding motif (Fig. 7), where the more stable DMF

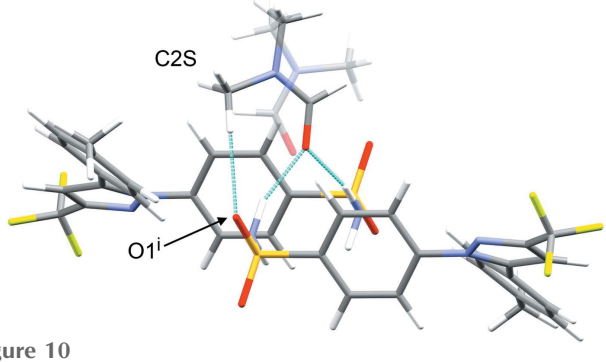


Figure 10
The most stable orientation of the disordered DMF molecule in **1**, highlighting the C—H$\cdots$O contact to an S═O group of celecoxib [symmetry code: (i) $-x+1, -y+1, -z+1$]. The less stable DMF orientation is shown as semi-transparent.

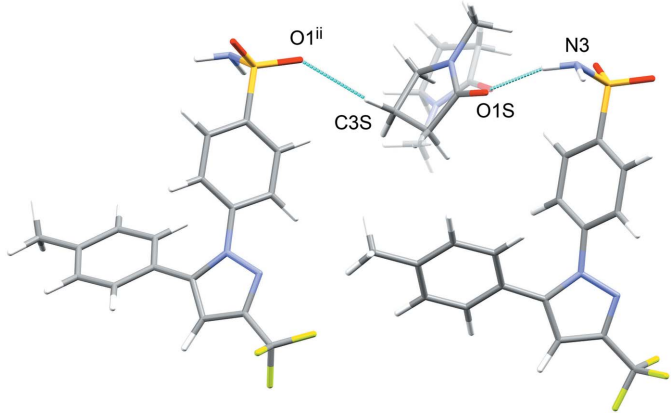


Figure 11
The most stable orientation of the disordered NMP molecule in **3**. A short C—H$\cdots$O contact is made to an S═O group of the neighbouring celecoxib molecule [symmetry code: (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$]. The less stable NMP orientation for **3** is shown as semi-transparent. A comparable C—H$\cdots$O contact is seen for the most stable disorder component of DMPU in **5**.

orientation brings the CH_3 group of atom C2*S* into close proximity to O1 in one of the S═O bonds (Fig. 10). For DMA (**2**), the disorder components have essentially the same molecular footprint (the positions of atoms O1*S*, C2*S*, C3*S* and C4*S* are common to both DMA components; Fig. 2), and the total interaction energies of the two components with the celecoxib framework are the same within the expected precision of the calculations. For NMP (**3**), the two solvent orientations are geometrically comparable, except for the positions of C3*S*/C3*SA* (Fig. 3). However, one orientation is noticeably more stable than the other. A significant energy difference also exists for the two orientations of the DMPU molecule in **5**, for which the principal geometrical difference is the position of one CH_2 group (C3*S*/C3*SA*), with accompanying differences in the positions of the H atoms on the neighbouring CH_2 groups. Comparing the most stable disorder components for **3** and **5**, they share a common position for one CH_2 group (C3*S* in **3** and C2*S* in **5**) that is not seen in the other disorder components. This introduces a short C—H···O contact to an S═O group of the neighbouring celecoxib molecule (Fig. 11). The *PIXEL* energies confirm that the interaction with this celecoxib molecule is significantly more stabilizing when this contact is present than when it is not. For the DMSO molecules in **6**, the difference between the two solvent orientations involves only the position of the S atom, and the interaction energies with the celecoxib framework are comparable.

4. Conclusion

This set of six isostructural celecoxib solvates includes small solvent molecules that can accept hydrogen bonds. The host celecoxib framework is consistent within the set, but it shows quite substantial flexibility in its unit-cell parameters and solvent-accessible void space, and can therefore accommodate solvent molecules of varying size and shape. The crystallographic disorder in several of the structures is understandable on the basis of the local twofold symmetry of the solvent binding site, compared to the point symmetry of the solvent molecules. In the absence of any additional hydrogen-bond donors in the solvent molecules, the next most stabilizing interactions between the solvent molecules and the celecoxib framework are C—H···O contacts to the S═O groups. The consideration of *PIXEL* interaction energies, in combination with geometrical analysis of the crystal structures, is helpful in drawing these conclusions.

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Intermolecular interactions and disorder in six isostructural celecoxib solvates

Andrew D. Bond and Changquan C. Sun

Computing details

For all structures, data collection: *APEX3* (Bruker, 2018); cell refinement: *SAINT* (Bruker, 2018); data reduction: *SAINT* (Bruker, 2018); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *SHELXL2018* (Sheldrick, 2015b).

4-[5-(4-Methylphenyl)-3-(trifluoromethyl)pyrazol-1-yl]benzenesulfonamide dimethylformamide monosolvate (1)

Crystal data

$C_{17}H_{14}F_3N_3O_2S{\cdot}C_3H_7NO$
M_r = 454.47
Monoclinic, $P2_1/c$
a = 11.8973 (4) Å
b = 8.8360 (3) Å
c = 21.8286 (7) Å
β = 103.4537 (13)°
V = 2231.75 (13) Å^3
Z = 4
$F(000)$ = 944
D_x = 1.353 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9864 reflections
θ = 3.8–66.7°
μ = 1.77 mm^{-1}
T = 298 K
Block, colourless
0.16 × 0.16 × 0.14 mm

Data collection

Bruker D8-QUEST PHOTON-100 diffractometer
Radiation source: Incoatec IμS Cu microsource
ω and φ–scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.440, T_{max} = 0.753
16627 measured reflections
3940 independent reflections
3362 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 66.9°, θ_{min} = 3.8°
h = −14→13
k = −6→10
l = −26→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.149
S = 1.08
3940 reflections
346 parameters
35 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 1.4975P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 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}	Occ. (<1)
S1	0.43324 (5)	0.72236 (9)	0.57626 (3)	0.0657 (2)	
O1	0.42145 (18)	0.6803 (3)	0.63714 (10)	0.0855 (7)	
O2	0.37685 (17)	0.8553 (3)	0.54695 (13)	0.0960 (8)	
N1	0.99334 (18)	0.8579 (3)	0.65536 (10)	0.0662 (6)	
N2	0.93631 (16)	0.8092 (3)	0.59763 (10)	0.0549 (5)	
N3	0.3870 (2)	0.5829 (4)	0.53040 (14)	0.0787 (7)	
H1N	0.388 (3)	0.602 (4)	0.4916 (7)	0.105 (13)*	
H2N	0.420 (3)	0.501 (3)	0.5478 (13)	0.096 (13)*	
C1	1.1007 (2)	0.8764 (4)	0.64939 (14)	0.0674 (8)	
C2	1.1140 (2)	0.8403 (3)	0.59008 (14)	0.0647 (7)	
H2A	1.181655	0.845345	0.575755	0.078*	
C3	1.00633 (19)	0.7950 (3)	0.55629 (12)	0.0525 (6)	
C4	1.1897 (3)	0.9281 (5)	0.70607 (18)	0.0929 (11)	
F1	1.2098 (12)	1.0702 (8)	0.7055 (8)	0.214 (10)	0.430 (12)
F2	1.1623 (7)	0.9023 (18)	0.7598 (3)	0.161 (8)	0.430 (12)
F3	1.2858 (6)	0.8657 (12)	0.7111 (4)	0.103 (4)	0.430 (12)
F1A	1.1645 (9)	1.0570 (9)	0.7240 (3)	0.133 (4)	0.570 (12)
F2A	1.2070 (13)	0.8394 (12)	0.7517 (5)	0.260 (9)	0.570 (12)
F3A	1.2861 (7)	0.952 (2)	0.6907 (6)	0.255 (8)	0.570 (12)
C5	0.97223 (19)	0.7359 (3)	0.49193 (12)	0.0525 (6)	
C6	0.8879 (2)	0.6253 (3)	0.47364 (12)	0.0552 (6)	
H6A	0.848346	0.588556	0.502597	0.066*	
C7	0.8625 (2)	0.5699 (3)	0.41321 (13)	0.0622 (7)	
H7A	0.804405	0.497839	0.401835	0.075*	
C8	0.9204 (3)	0.6177 (4)	0.36884 (13)	0.0690 (7)	
C9	1.0055 (3)	0.7265 (4)	0.38758 (16)	0.0824 (9)	
H9A	1.046738	0.760708	0.358948	0.099*	
C10	1.0302 (3)	0.7845 (4)	0.44753 (15)	0.0719 (8)	
H10A	1.087112	0.858253	0.458519	0.086*	
C11	0.8925 (4)	0.5548 (5)	0.30287 (16)	0.1031 (12)	
H11A	0.953139	0.580762	0.282434	0.155*	
H11B	0.820812	0.596789	0.279639	0.155*	
H11C	0.885819	0.446641	0.304506	0.155*	
C12	0.81447 (19)	0.7846 (3)	0.58947 (11)	0.0505 (6)	
C13	0.7788 (2)	0.6962 (4)	0.63299 (13)	0.0666 (8)	
H13A	0.832849	0.649861	0.665177	0.080*	
C14	0.6617 (2)	0.6764 (4)	0.62874 (13)	0.0650 (7)	
H14A	0.636730	0.616960	0.658131	0.078*	
C15	0.58275 (19)	0.7452 (3)	0.58074 (11)	0.0517 (6)	

C16	0.61940 (19)	0.8334 (3)	0.53691 (12)	0.0528 (6)	
H16A	0.565515	0.879102	0.504437	0.063*	
C17	0.73656 (19)	0.8539 (3)	0.54135 (11)	0.0522 (6)	
H17A	0.761968	0.913581	0.512178	0.063*	
O1S	0.4484 (3)	0.6595 (3)	0.41413 (12)	0.1112 (9)	0.779 (7)
N1S	0.4652 (5)	0.8198 (6)	0.3374 (3)	0.0814 (14)	0.779 (7)
C1S	0.4091 (4)	0.7692 (6)	0.3785 (2)	0.0842 (15)	0.779 (7)
H1S	0.340031	0.814639	0.381342	0.101*	0.779 (7)
C2S	0.5679 (8)	0.7485 (9)	0.3315 (5)	0.182 (4)	0.779 (7)
H2S	0.597691	0.798903	0.299680	0.272*	0.779 (7)
H3S	0.623841	0.753451	0.371019	0.272*	0.779 (7)
H4S	0.552215	0.644533	0.319836	0.272*	0.779 (7)
C3S	0.4288 (5)	0.9452 (6)	0.2954 (2)	0.1336 (18)	0.779 (7)
H5S	0.483661	0.960581	0.269917	0.200*	0.779 (7)
H6S	0.354239	0.923789	0.268657	0.200*	0.779 (7)
H7S	0.424206	1.034917	0.319466	0.200*	0.779 (7)
O1SA	0.4484 (3)	0.6595 (3)	0.41413 (12)	0.1112 (9)	0.221 (7)
N1SA	0.4178 (12)	0.829 (2)	0.3395 (9)	0.071 (5)	0.221 (7)
C1SA	0.4898 (12)	0.7281 (18)	0.3715 (7)	0.104 (6)	0.221 (7)
H8S	0.562389	0.707947	0.364335	0.124*	0.221 (7)
C2SA	0.3100 (13)	0.847 (2)	0.3560 (9)	0.127 (9)	0.221 (7)
H9S	0.265236	0.922855	0.329773	0.191*	0.221 (7)
H10S	0.268906	0.752317	0.349949	0.191*	0.221 (7)
H11S	0.322819	0.876604	0.399329	0.191*	0.221 (7)
C3SA	0.4288 (5)	0.9452 (6)	0.2954 (2)	0.1336 (18)	0.221 (7)
H12S	0.356405	0.997211	0.281819	0.200*	0.221 (7)
H13S	0.487444	1.015830	0.315055	0.200*	0.221 (7)
H14S	0.449868	0.900206	0.259591	0.200*	0.221 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0357 (3)	0.0825 (5)	0.0850 (5)	0.0007 (3)	0.0262 (3)	0.0128 (4)
O1	0.0602 (12)	0.1233 (19)	0.0855 (14)	−0.0024 (12)	0.0422 (10)	0.0075 (13)
O2	0.0436 (10)	0.0949 (17)	0.158 (2)	0.0214 (11)	0.0402 (12)	0.0396 (15)
N1	0.0417 (11)	0.0888 (17)	0.0647 (13)	−0.0017 (11)	0.0055 (9)	−0.0132 (12)
N2	0.0319 (9)	0.0713 (14)	0.0600 (12)	−0.0019 (9)	0.0079 (8)	−0.0031 (10)
N3	0.0513 (14)	0.099 (2)	0.0838 (19)	−0.0207 (14)	0.0110 (12)	0.0098 (16)
C1	0.0359 (12)	0.0794 (19)	0.0827 (18)	−0.0013 (12)	0.0050 (12)	−0.0194 (15)
C2	0.0318 (11)	0.0718 (18)	0.0902 (19)	−0.0041 (12)	0.0138 (12)	−0.0160 (15)
C3	0.0332 (11)	0.0561 (14)	0.0680 (15)	−0.0006 (10)	0.0116 (10)	−0.0031 (11)
C4	0.0530 (19)	0.114 (3)	0.104 (3)	−0.012 (2)	0.0043 (17)	−0.040 (3)
F1	0.171 (14)	0.098 (7)	0.294 (19)	−0.048 (7)	−0.111 (12)	−0.013 (8)
F2	0.077 (4)	0.35 (2)	0.064 (5)	−0.069 (7)	0.022 (4)	−0.068 (9)
F3	0.051 (4)	0.148 (7)	0.090 (4)	0.035 (4)	−0.027 (3)	−0.033 (4)
F1A	0.154 (7)	0.140 (7)	0.079 (4)	0.028 (5)	−0.023 (3)	−0.059 (4)
F2A	0.266 (15)	0.195 (8)	0.209 (12)	−0.077 (9)	−0.169 (11)	0.082 (8)
F3A	0.070 (5)	0.44 (2)	0.268 (11)	−0.106 (8)	0.058 (6)	−0.239 (12)

C5	0.0348 (11)	0.0567 (14)	0.0670 (15)	0.0027 (10)	0.0142 (10)	0.0012 (11)
C6	0.0398 (12)	0.0607 (15)	0.0665 (15)	−0.0018 (11)	0.0152 (11)	0.0008 (12)
C7	0.0461 (13)	0.0643 (16)	0.0738 (17)	−0.0016 (12)	0.0088 (12)	−0.0046 (13)
C8	0.0632 (16)	0.0773 (19)	0.0665 (16)	0.0027 (15)	0.0148 (13)	−0.0028 (14)
C9	0.081 (2)	0.099 (2)	0.078 (2)	−0.0124 (18)	0.0380 (17)	0.0037 (18)
C10	0.0604 (17)	0.078 (2)	0.0825 (19)	−0.0217 (15)	0.0281 (14)	−0.0037 (15)
C11	0.111 (3)	0.123 (3)	0.075 (2)	−0.008 (3)	0.0220 (19)	−0.014 (2)
C12	0.0316 (11)	0.0640 (15)	0.0564 (13)	−0.0008 (10)	0.0109 (9)	0.0004 (11)
C13	0.0420 (13)	0.092 (2)	0.0632 (15)	0.0021 (13)	0.0067 (11)	0.0215 (14)
C14	0.0475 (14)	0.087 (2)	0.0633 (15)	−0.0051 (13)	0.0182 (11)	0.0211 (14)
C15	0.0334 (11)	0.0649 (15)	0.0596 (14)	−0.0006 (10)	0.0168 (10)	0.0046 (11)
C16	0.0342 (11)	0.0638 (15)	0.0603 (14)	0.0030 (11)	0.0108 (10)	0.0097 (12)
C17	0.0365 (11)	0.0623 (15)	0.0594 (14)	−0.0023 (11)	0.0142 (10)	0.0096 (11)
O1S	0.138 (2)	0.111 (2)	0.0815 (16)	−0.0067 (18)	0.0190 (15)	0.0189 (15)
N1S	0.090 (4)	0.079 (3)	0.074 (3)	−0.003 (3)	0.017 (3)	0.001 (2)
C1S	0.072 (3)	0.102 (4)	0.073 (3)	0.008 (2)	0.007 (2)	−0.015 (3)
C2S	0.188 (8)	0.154 (7)	0.255 (10)	0.052 (6)	0.156 (8)	0.077 (7)
C3S	0.167 (5)	0.112 (3)	0.104 (3)	−0.014 (3)	−0.006 (3)	0.025 (3)
O1SA	0.138 (2)	0.111 (2)	0.0815 (16)	−0.0067 (18)	0.0190 (15)	0.0189 (15)
N1SA	0.071 (9)	0.080 (8)	0.060 (7)	−0.013 (7)	0.012 (6)	0.003 (6)
C1SA	0.101 (10)	0.116 (10)	0.096 (9)	−0.004 (8)	0.029 (8)	0.001 (8)
C2SA	0.097 (14)	0.16 (2)	0.117 (15)	0.056 (14)	0.005 (11)	−0.033 (13)
C3SA	0.167 (5)	0.112 (3)	0.104 (3)	−0.014 (3)	−0.006 (3)	0.025 (3)

Geometric parameters (Å, º)

S1—O1	1.418 (2)	C11—H11C	0.9600
S1—O2	1.428 (2)	C12—C17	1.372 (3)
S1—N3	1.602 (3)	C12—C13	1.372 (4)
S1—C15	1.770 (2)	C13—C14	1.385 (4)
N1—C1	1.324 (3)	C13—H13A	0.9300
N1—N2	1.355 (3)	C14—C15	1.376 (4)
N2—C3	1.369 (3)	C14—H14A	0.9300
N2—C12	1.435 (3)	C15—C16	1.381 (3)
N3—H1N	0.866 (10)	C16—C17	1.386 (3)
N3—H2N	0.869 (10)	C16—H16A	0.9300
C1—C2	1.378 (4)	C17—H17A	0.9300
C1—C4	1.501 (4)	O1S—C1S	1.262 (5)
C2—C3	1.380 (3)	N1S—C1S	1.314 (6)
C2—H2A	0.9300	N1S—C2S	1.407 (9)
C3—C5	1.465 (4)	N1S—C3S	1.440 (6)
C4—F2A	1.246 (7)	C1S—H1S	0.9300
C4—F3	1.250 (6)	C2S—H2S	0.9600
C4—F1A	1.263 (6)	C2S—H3S	0.9600
C4—F1	1.278 (8)	C2S—H4S	0.9600
C4—F3A	1.285 (7)	C3S—H5S	0.9600
C4—F2	1.309 (7)	C3S—H6S	0.9600
C5—C10	1.382 (4)	C3S—H7S	0.9600

C5—C6	1.391 (3)	O1SA—C1SA	1.299 (10)
C6—C7	1.373 (4)	N1SA—C1SA	1.321 (10)
C6—H6A	0.9300	N1SA—C2SA	1.419 (12)
C7—C8	1.379 (4)	N1SA—C3SA	1.432 (9)
C7—H7A	0.9300	C1SA—H8S	0.9300
C8—C9	1.387 (4)	C2SA—H9S	0.9600
C8—C11	1.507 (4)	C2SA—H10S	0.9600
C9—C10	1.372 (4)	C2SA—H11S	0.9600
C9—H9A	0.9300	C3SA—H12S	0.9600
C10—H10A	0.9300	C3SA—H13S	0.9600
C11—H11A	0.9600	C3SA—H14S	0.9600
C11—H11B	0.9600		

O1—S1—O2	119.78 (15)	H11A—C11—H11C	109.5
O1—S1—N3	106.84 (15)	H11B—C11—H11C	109.5
O2—S1—N3	107.20 (17)	C17—C12—C13	121.4 (2)
O1—S1—C15	107.17 (12)	C17—C12—N2	120.7 (2)
O2—S1—C15	106.99 (12)	C13—C12—N2	117.8 (2)
N3—S1—C15	108.46 (13)	C12—C13—C14	119.6 (2)
C1—N1—N2	103.5 (2)	C12—C13—H13A	120.2
N1—N2—C3	113.10 (19)	C14—C13—H13A	120.2
N1—N2—C12	115.86 (19)	C15—C14—C13	119.6 (2)
C3—N2—C12	131.0 (2)	C15—C14—H14A	120.2
S1—N3—H1N	112 (2)	C13—C14—H14A	120.2
S1—N3—H2N	108 (2)	C14—C15—C16	120.5 (2)
H1N—N3—H2N	118.7 (18)	C14—C15—S1	119.44 (18)
N1—C1—C2	112.8 (2)	C16—C15—S1	120.08 (18)
N1—C1—C4	117.9 (3)	C15—C16—C17	120.0 (2)
C2—C1—C4	129.2 (3)	C15—C16—H16A	120.0
C1—C2—C3	105.9 (2)	C17—C16—H16A	120.0
C1—C2—H2A	127.0	C12—C17—C16	119.0 (2)
C3—C2—H2A	127.0	C12—C17—H17A	120.5
N2—C3—C2	104.6 (2)	C16—C17—H17A	120.5
N2—C3—C5	126.1 (2)	C1S—N1S—C2S	120.0 (5)
C2—C3—C5	129.2 (2)	C1S—N1S—C3S	124.9 (5)
F2A—C4—F1A	109.0 (7)	C2S—N1S—C3S	115.2 (5)
F3—C4—F1	105.4 (7)	O1S—C1S—N1S	120.5 (5)
F2A—C4—F3A	108.7 (6)	O1S—C1S—H1S	119.7
F1A—C4—F3A	102.9 (6)	N1S—C1S—H1S	119.7
F3—C4—F2	104.9 (6)	N1S—C2S—H2S	109.5
F1—C4—F2	105.4 (7)	N1S—C2S—H3S	109.5
F2A—C4—C1	114.9 (5)	H2S—C2S—H3S	109.5
F3—C4—C1	113.2 (4)	N1S—C2S—H4S	109.5
F1A—C4—C1	111.0 (4)	H2S—C2S—H4S	109.5
F1—C4—C1	112.9 (7)	H3S—C2S—H4S	109.5
F3A—C4—C1	109.7 (5)	N1S—C3S—H5S	109.5
F2—C4—C1	114.2 (4)	N1S—C3S—H6S	109.5
C10—C5—C6	117.5 (2)	H5S—C3S—H6S	109.5

C10—C5—C3	119.3 (2)	N1S—C3S—H7S	109.5
C6—C5—C3	123.1 (2)	H5S—C3S—H7S	109.5
C7—C6—C5	120.6 (2)	H6S—C3S—H7S	109.5
C7—C6—H6A	119.7	C1SA—N1SA—C2SA	116.9 (10)
C5—C6—H6A	119.7	C1SA—N1SA—C3SA	133.7 (10)
C6—C7—C8	122.1 (3)	C2SA—N1SA—C3SA	108.8 (10)
C6—C7—H7A	119.0	O1SA—C1SA—N1SA	112.8 (9)
C8—C7—H7A	119.0	O1SA—C1SA—H8S	123.6
C7—C8—C9	117.1 (3)	N1SA—C1SA—H8S	123.6
C7—C8—C11	121.5 (3)	N1SA—C2SA—H9S	109.5
C9—C8—C11	121.4 (3)	N1SA—C2SA—H10S	109.5
C10—C9—C8	121.3 (3)	H9S—C2SA—H10S	109.5
C10—C9—H9A	119.3	N1SA—C2SA—H11S	109.5
C8—C9—H9A	119.3	H9S—C2SA—H11S	109.5
C9—C10—C5	121.4 (3)	H10S—C2SA—H11S	109.5
C9—C10—H10A	119.3	N1SA—C3SA—H12S	109.5
C5—C10—H10A	119.3	N1SA—C3SA—H13S	109.5
C8—C11—H11A	109.5	H12S—C3SA—H13S	109.5
C8—C11—H11B	109.5	N1SA—C3SA—H14S	109.5
H11A—C11—H11B	109.5	H12S—C3SA—H14S	109.5
C8—C11—H11C	109.5	H13S—C3SA—H14S	109.5

C1—N1—N2—C3	0.9 (3)	C6—C7—C8—C9	−0.7 (4)
C1—N1—N2—C12	−177.8 (2)	C6—C7—C8—C11	179.4 (3)
N2—N1—C1—C2	−0.4 (3)	C7—C8—C9—C10	−0.5 (5)
N2—N1—C1—C4	−178.9 (3)	C11—C8—C9—C10	179.4 (3)
N1—C1—C2—C3	−0.2 (4)	C8—C9—C10—C5	0.8 (5)
C4—C1—C2—C3	178.1 (3)	C6—C5—C10—C9	0.1 (4)
N1—N2—C3—C2	−1.0 (3)	C3—C5—C10—C9	176.5 (3)
C12—N2—C3—C2	177.4 (3)	N1—N2—C12—C17	125.6 (3)
N1—N2—C3—C5	175.8 (2)	C3—N2—C12—C17	−52.8 (4)
C12—N2—C3—C5	−5.8 (4)	N1—N2—C12—C13	−51.3 (3)
C1—C2—C3—N2	0.7 (3)	C3—N2—C12—C13	130.4 (3)
C1—C2—C3—C5	−176.0 (3)	C17—C12—C13—C14	−0.3 (4)
N1—C1—C4—F2A	62.5 (11)	N2—C12—C13—C14	176.6 (3)
C2—C1—C4—F2A	−115.7 (11)	C12—C13—C14—C15	0.3 (5)
N1—C1—C4—F3	141.5 (7)	C13—C14—C15—C16	0.1 (4)
C2—C1—C4—F3	−36.8 (8)	C13—C14—C15—S1	−178.9 (2)
N1—C1—C4—F1A	−61.7 (8)	O1—S1—C15—C14	21.2 (3)
C2—C1—C4—F1A	120.1 (7)	O2—S1—C15—C14	150.9 (2)
N1—C1—C4—F1	−98.9 (10)	N3—S1—C15—C14	−93.8 (3)
C2—C1—C4—F1	82.8 (11)	O1—S1—C15—C16	−157.7 (2)
N1—C1—C4—F3A	−174.7 (10)	O2—S1—C15—C16	−28.1 (3)
C2—C1—C4—F3A	7.0 (11)	N3—S1—C15—C16	87.3 (3)
N1—C1—C4—F2	21.5 (9)	C14—C15—C16—C17	−0.4 (4)
C2—C1—C4—F2	−156.8 (8)	S1—C15—C16—C17	178.6 (2)
N2—C3—C5—C10	152.5 (3)	C13—C12—C17—C16	0.0 (4)
C2—C3—C5—C10	−31.4 (4)	N2—C12—C17—C16	−176.8 (2)

N2—C3—C5—C6	−31.4 (4)	C15—C16—C17—C12	0.4 (4)
C2—C3—C5—C6	144.7 (3)	C2S—N1S—C1S—O1S	2.0 (10)
C10—C5—C6—C7	−1.3 (4)	C3S—N1S—C1S—O1S	−179.0 (5)
C3—C5—C6—C7	−177.5 (2)	C2SA—N1SA—C1SA—O1SA	0 (3)
C5—C6—C7—C8	1.6 (4)	C3SA—N1SA—C1SA—O1SA	170 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H1*N*···O1Sa	0.87 (1)	2.05 (2)	2.880 (4)	161 (4)
N3—H2*N*···O1Sa^{i}	0.87 (1)	2.13 (2)	2.964 (4)	160 (3)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

4-[5-(4-Methylphenyl)-3-(trifluoromethyl)pyrazol-1-yl]benzenesulfonamide dimethylacetamide monosolvate (2)

Crystal data

$C_{17}H_{14}F_3N_3O_2S·C_4H_9NO$
M_r = 468.49
Monoclinic, $P2_1/c$
a = 11.9584 (3) Å
b = 9.2028 (2) Å
c = 21.2811 (6) Å
β = 103.3826 (12)°
V = 2278.41 (10) Å^3
Z = 4
$F(000)$ = 976
D_x = 1.366 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9399 reflections
θ = 3.8–66.8°
μ = 1.75 mm^{-1}
T = 298 K
Block, colourless
0.20 × 0.18 × 0.18 mm

Data collection

Bruker D8-QUEST PHOTON-100 diffractometer
Radiation source: Incoatec IμS Cu microsource
ω and φ–scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.608, T_{max} = 0.753
38939 measured reflections
4032 independent reflections
3394 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 66.9°, θ_{min} = 3.8°
h = −14→14
k = −10→10
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.129
S = 1.03
4032 reflections
345 parameters
26 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0707P)^2 + 0.7443P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 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}	Occ. (<1)
S1	0.43445 (4)	0.72988 (6)	0.57506 (3)	0.05785 (19)	
O1	0.42323 (14)	0.6964 (2)	0.63856 (8)	0.0779 (5)	
O2	0.37684 (12)	0.85394 (17)	0.54250 (9)	0.0743 (5)	
N1	0.99144 (14)	0.8711 (2)	0.65110 (9)	0.0609 (4)	
N2	0.93377 (13)	0.81638 (19)	0.59372 (8)	0.0527 (4)	
N3	0.39037 (16)	0.5913 (2)	0.53096 (11)	0.0669 (5)	
H1N	0.393 (2)	0.609 (3)	0.4914 (6)	0.083 (9)*	
H2N	0.424 (2)	0.515 (2)	0.5502 (10)	0.094 (9)*	
C1	1.09752 (17)	0.8884 (2)	0.64353 (11)	0.0598 (5)	
C2	1.10928 (16)	0.8464 (2)	0.58289 (11)	0.0589 (5)	
H2A	1.175547	0.850068	0.567120	0.071*	
C3	1.00221 (15)	0.7981 (2)	0.55086 (10)	0.0506 (5)	
C4	1.1872 (2)	0.9455 (3)	0.69911 (14)	0.0815 (7)	
F1	1.2294 (9)	1.0652 (10)	0.6860 (6)	0.207 (7)	0.516 (10)
F2	1.2715 (5)	0.8604 (7)	0.7157 (3)	0.106 (2)	0.516 (10)
F3	1.1513 (5)	0.9639 (15)	0.7510 (4)	0.165 (5)	0.516 (10)
F1A	1.2840 (6)	0.9624 (18)	0.6835 (6)	0.193 (7)	0.484 (10)
F2A	1.2026 (13)	0.8676 (12)	0.7487 (5)	0.241 (9)	0.484 (10)
F3A	1.1649 (8)	1.0709 (8)	0.7164 (3)	0.124 (3)	0.484 (10)
C5	0.96681 (15)	0.7310 (2)	0.48700 (10)	0.0502 (5)	
C6	0.88913 (16)	0.6162 (2)	0.47387 (10)	0.0534 (5)	
H6A	0.854233	0.583021	0.505929	0.064*	
C7	0.86344 (17)	0.5516 (2)	0.41421 (11)	0.0599 (5)	
H7A	0.810159	0.476258	0.406339	0.072*	
C8	0.91479 (19)	0.5955 (3)	0.36545 (11)	0.0657 (6)	
C9	0.9924 (2)	0.7091 (3)	0.37893 (12)	0.0745 (7)	
H9A	1.028377	0.740852	0.347052	0.089*	
C10	1.0178 (2)	0.7761 (3)	0.43806 (12)	0.0653 (6)	
H10A	1.069851	0.852738	0.445453	0.078*	
C11	0.8864 (3)	0.5227 (4)	0.30007 (14)	0.1002 (9)	
H11A	0.929940	0.567241	0.272607	0.150*	
H11B	0.905441	0.421342	0.305008	0.150*	
H11C	0.805808	0.533181	0.281054	0.150*	
C12	0.81326 (15)	0.7913 (2)	0.58638 (9)	0.0491 (4)	
C13	0.77851 (18)	0.7144 (3)	0.63396 (11)	0.0626 (6)	
H13A	0.832718	0.675882	0.668465	0.075*	
C14	0.66275 (18)	0.6949 (3)	0.63017 (11)	0.0620 (6)	
H14A	0.638480	0.642754	0.662026	0.074*	
C15	0.58320 (16)	0.7530 (2)	0.57884 (10)	0.0497 (5)	

C16	0.61849 (16)	0.8294 (2)	0.53087 (10)	0.0501 (4)	
H16A	0.564382	0.867533	0.496216	0.060*	
C17	0.73436 (16)	0.8488 (2)	0.53465 (10)	0.0502 (4)	
H17A	0.758911	0.900046	0.502652	0.060*	
O1S	0.44913 (16)	0.63401 (19)	0.40777 (9)	0.0833 (5)	0.536 (8)
N1S	0.4762 (4)	0.7912 (5)	0.3367 (2)	0.0707 (15)	0.536 (8)
C1S	0.4097 (4)	0.7432 (5)	0.3738 (2)	0.0634 (15)	0.536 (8)
C2S	0.2989 (2)	0.8268 (4)	0.37048 (15)	0.0999 (10)	0.536 (8)
H1S	0.293223	0.904700	0.339905	0.150*	0.536 (8)
H2S	0.234527	0.762574	0.357160	0.150*	0.536 (8)
H3S	0.299015	0.865895	0.412316	0.150*	0.536 (8)
C3S	0.4369 (3)	0.9272 (4)	0.29637 (16)	0.1110 (11)	0.536 (8)
H4S	0.492151	0.951005	0.271683	0.167*	0.536 (8)
H5S	0.363604	0.909132	0.267630	0.167*	0.536 (8)
H6S	0.430222	1.006712	0.324457	0.167*	0.536 (8)
C4S	0.5805 (3)	0.7081 (4)	0.3364 (2)	0.1148 (12)	0.536 (8)
H7S	0.621272	0.753693	0.307813	0.172*	0.536 (8)
H8S	0.628586	0.705337	0.379286	0.172*	0.536 (8)
H9S	0.559878	0.610896	0.321895	0.172*	0.536 (8)
O1SA	0.44913 (16)	0.63401 (19)	0.40777 (9)	0.0833 (5)	0.464 (8)
N1SA	0.4034 (4)	0.8269 (5)	0.3446 (2)	0.0649 (17)	0.464 (8)
C1SA	0.4749 (4)	0.7183 (6)	0.3645 (3)	0.0628 (17)	0.464 (8)
C2SA	0.5805 (3)	0.7081 (4)	0.3364 (2)	0.1148 (12)	0.464 (8)
H10S	0.578131	0.784138	0.305225	0.172*	0.464 (8)
H11S	0.648469	0.718398	0.370407	0.172*	0.464 (8)
H12S	0.581462	0.615473	0.315826	0.172*	0.464 (8)
C3SA	0.4369 (3)	0.9272 (4)	0.29637 (16)	0.1110 (11)	0.464 (8)
H13S	0.380184	1.002320	0.284804	0.167*	0.464 (8)
H14S	0.510255	0.970064	0.314987	0.167*	0.464 (8)
H15S	0.441652	0.873150	0.258486	0.167*	0.464 (8)
C4SA	0.2989 (2)	0.8268 (4)	0.37048 (15)	0.0999 (10)	0.464 (8)
H16S	0.251945	0.908935	0.353710	0.150*	0.464 (8)
H17S	0.256497	0.738875	0.357782	0.150*	0.464 (8)
H18S	0.320425	0.832472	0.416762	0.150*	0.464 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0393 (3)	0.0633 (3)	0.0779 (4)	0.0051 (2)	0.0279 (2)	0.0130 (2)
O1	0.0628 (9)	0.1012 (12)	0.0821 (11)	0.0023 (9)	0.0422 (8)	0.0135 (9)
O2	0.0459 (8)	0.0694 (10)	0.1140 (13)	0.0175 (7)	0.0316 (8)	0.0227 (9)
N1	0.0464 (9)	0.0686 (11)	0.0664 (11)	−0.0031 (8)	0.0106 (8)	−0.0032 (9)
N2	0.0359 (8)	0.0599 (10)	0.0626 (10)	−0.0017 (7)	0.0120 (7)	0.0023 (8)
N3	0.0487 (10)	0.0682 (12)	0.0864 (15)	−0.0057 (9)	0.0207 (10)	0.0117 (11)
C1	0.0424 (11)	0.0569 (12)	0.0785 (14)	−0.0031 (9)	0.0107 (10)	−0.0039 (10)
C2	0.0363 (10)	0.0558 (11)	0.0861 (15)	−0.0016 (8)	0.0175 (9)	−0.0017 (10)
C3	0.0376 (9)	0.0455 (10)	0.0708 (12)	0.0016 (8)	0.0167 (9)	0.0040 (9)
C4	0.0555 (14)	0.0839 (19)	0.100 (2)	−0.0101 (14)	0.0084 (13)	−0.0165 (16)

F1	0.159 (9)	0.135 (7)	0.260 (12)	−0.105 (6)	−0.090 (7)	0.070 (7)
F2	0.068 (3)	0.130 (5)	0.102 (4)	0.033 (3)	−0.020 (2)	−0.022 (3)
F3	0.080 (3)	0.289 (13)	0.130 (6)	−0.044 (5)	0.034 (4)	−0.126 (8)
F1A	0.068 (4)	0.303 (15)	0.218 (11)	−0.082 (6)	0.057 (5)	−0.167 (11)
F2A	0.273 (15)	0.216 (10)	0.146 (9)	−0.144 (9)	−0.133 (9)	0.112 (8)
F3A	0.144 (6)	0.109 (5)	0.091 (4)	0.026 (4)	−0.030 (3)	−0.048 (3)
C5	0.0358 (9)	0.0483 (10)	0.0684 (12)	0.0056 (8)	0.0157 (8)	0.0052 (9)
C6	0.0414 (10)	0.0500 (11)	0.0717 (13)	0.0019 (8)	0.0189 (9)	0.0050 (9)
C7	0.0447 (10)	0.0526 (11)	0.0816 (14)	0.0021 (9)	0.0128 (10)	−0.0020 (10)
C8	0.0521 (12)	0.0740 (14)	0.0701 (14)	0.0056 (11)	0.0122 (10)	−0.0017 (11)
C9	0.0664 (14)	0.0906 (17)	0.0732 (15)	−0.0061 (13)	0.0300 (12)	0.0042 (13)
C10	0.0552 (12)	0.0673 (14)	0.0776 (15)	−0.0114 (10)	0.0241 (11)	0.0021 (11)
C11	0.098 (2)	0.122 (2)	0.0806 (18)	−0.0092 (19)	0.0205 (15)	−0.0189 (18)
C12	0.0371 (9)	0.0512 (10)	0.0615 (11)	−0.0002 (8)	0.0163 (8)	0.0032 (9)
C13	0.0460 (11)	0.0772 (14)	0.0633 (12)	0.0024 (10)	0.0099 (9)	0.0218 (11)
C14	0.0494 (11)	0.0743 (14)	0.0662 (13)	−0.0018 (10)	0.0215 (10)	0.0220 (11)
C15	0.0387 (9)	0.0516 (10)	0.0630 (12)	0.0026 (8)	0.0204 (8)	0.0069 (9)
C16	0.0384 (9)	0.0534 (11)	0.0598 (11)	0.0044 (8)	0.0141 (8)	0.0110 (9)
C17	0.0429 (10)	0.0512 (10)	0.0603 (11)	0.0014 (8)	0.0201 (8)	0.0102 (9)
O1S	0.0909 (12)	0.0720 (11)	0.0897 (12)	0.0050 (10)	0.0262 (10)	0.0162 (9)
N1S	0.070 (3)	0.069 (3)	0.074 (3)	−0.002 (2)	0.017 (2)	0.007 (2)
C1S	0.058 (3)	0.064 (3)	0.065 (3)	−0.001 (3)	0.007 (2)	−0.008 (2)
C2S	0.0733 (17)	0.128 (3)	0.097 (2)	0.0294 (18)	0.0171 (15)	−0.0117 (19)
C3S	0.146 (3)	0.0861 (19)	0.091 (2)	−0.015 (2)	0.006 (2)	0.0259 (17)
C4S	0.095 (2)	0.116 (3)	0.153 (3)	0.028 (2)	0.068 (2)	0.039 (2)
O1SA	0.0909 (12)	0.0720 (11)	0.0897 (12)	0.0050 (10)	0.0262 (10)	0.0162 (9)
N1SA	0.064 (3)	0.061 (3)	0.064 (3)	0.007 (2)	0.003 (2)	0.000 (2)
C1SA	0.060 (3)	0.059 (3)	0.068 (4)	−0.002 (3)	0.010 (3)	0.003 (3)
C2SA	0.095 (2)	0.116 (3)	0.153 (3)	0.028 (2)	0.068 (2)	0.039 (2)
C3SA	0.146 (3)	0.0861 (19)	0.091 (2)	−0.015 (2)	0.006 (2)	0.0259 (17)
C4SA	0.0733 (17)	0.128 (3)	0.097 (2)	0.0294 (18)	0.0171 (15)	−0.0117 (19)

Geometric parameters (Å, º)

S1—O1	1.4223 (16)	C13—C14	1.380 (3)
S1—O2	1.4274 (16)	C13—H13A	0.9300
S1—N3	1.599 (2)	C14—C15	1.380 (3)
S1—C15	1.7747 (19)	C14—H14A	0.9300
N1—C1	1.325 (3)	C15—C16	1.383 (3)
N1—N2	1.353 (2)	C16—C17	1.381 (3)
N2—C3	1.370 (2)	C16—H16A	0.9300
N2—C12	1.432 (2)	C17—H17A	0.9300
N3—H1N	0.864 (9)	O1S—C1S	1.264 (5)
N3—H2N	0.865 (9)	N1S—C1S	1.318 (5)
C1—C2	1.385 (3)	N1S—C4S	1.464 (5)
C1—C4	1.496 (3)	N1S—C3S	1.529 (5)
C2—C3	1.378 (3)	C1S—C2S	1.519 (5)
C2—H2A	0.9300	C2S—H1S	0.9600

C3—C5	1.463 (3)	C2S—H2S	0.9600
C4—F2A	1.254 (5)	C2S—H3S	0.9600
C4—F3A	1.258 (5)	C3S—H4S	0.9600
C4—F2	1.261 (4)	C3S—H5S	0.9600
C4—F1	1.270 (5)	C3S—H6S	0.9600
C4—F3	1.285 (6)	C4S—H7S	0.9600
C4—F1A	1.286 (5)	C4S—H8S	0.9600
C5—C10	1.386 (3)	C4S—H9S	0.9600
C5—C6	1.392 (3)	O1SA—C1SA	1.295 (5)
C6—C7	1.371 (3)	N1SA—C1SA	1.320 (6)
C6—H6A	0.9300	N1SA—C4SA	1.477 (5)
C7—C8	1.383 (3)	N1SA—C3SA	1.502 (5)
C7—H7A	0.9300	C1SA—C2SA	1.519 (5)
C8—C9	1.384 (3)	C2SA—H10S	0.9600
C8—C11	1.510 (4)	C2SA—H11S	0.9600
C9—C10	1.371 (3)	C2SA—H12S	0.9600
C9—H9A	0.9300	C3SA—H13S	0.9600
C10—H10A	0.9300	C3SA—H14S	0.9600
C11—H11A	0.9600	C3SA—H15S	0.9600
C11—H11B	0.9600	C4SA—H16S	0.9600
C11—H11C	0.9600	C4SA—H17S	0.9600
C12—C13	1.376 (3)	C4SA—H18S	0.9600
C12—C17	1.379 (3)		

O1—S1—O2	119.56 (10)	C12—C13—H13A	120.2
O1—S1—N3	107.11 (11)	C14—C13—H13A	120.2
O2—S1—N3	107.25 (11)	C13—C14—C15	119.62 (18)
O1—S1—C15	107.28 (10)	C13—C14—H14A	120.2
O2—S1—C15	106.98 (9)	C15—C14—H14A	120.2
N3—S1—C15	108.24 (9)	C14—C15—C16	120.60 (17)
C1—N1—N2	103.72 (17)	C14—C15—S1	119.31 (14)
N1—N2—C3	112.86 (15)	C16—C15—S1	120.09 (15)
N1—N2—C12	116.63 (16)	C17—C16—C15	119.75 (18)
C3—N2—C12	130.47 (17)	C17—C16—H16A	120.1
S1—N3—H1N	110.1 (18)	C15—C16—H16A	120.1
S1—N3—H2N	108.5 (19)	C12—C17—C16	119.27 (17)
H1N—N3—H2N	119.3 (17)	C12—C17—H17A	120.4
N1—C1—C2	112.74 (19)	C16—C17—H17A	120.4
N1—C1—C4	118.5 (2)	C1S—N1S—C4S	117.4 (4)
C2—C1—C4	128.7 (2)	C1S—N1S—C3S	117.4 (4)
C3—C2—C1	105.53 (18)	C4S—N1S—C3S	125.2 (3)
C3—C2—H2A	127.2	O1S—C1S—N1S	114.3 (4)
C1—C2—H2A	127.2	O1S—C1S—C2S	129.4 (4)
N2—C3—C2	105.14 (18)	N1S—C1S—C2S	116.3 (4)
N2—C3—C5	125.55 (17)	C1S—C2S—H1S	109.5
C2—C3—C5	129.17 (18)	C1S—C2S—H2S	109.5
F2A—C4—F3A	106.2 (6)	H1S—C2S—H2S	109.5
F2—C4—F1	105.5 (4)	C1S—C2S—H3S	109.5

F2—C4—F3	104.2 (5)	H1S—C2S—H3S	109.5
F1—C4—F3	107.7 (6)	H2S—C2S—H3S	109.5
F2A—C4—F1A	108.8 (5)	N1S—C3S—H4S	109.5
F3A—C4—F1A	103.2 (5)	N1S—C3S—H5S	109.5
F2A—C4—C1	113.8 (4)	H4S—C3S—H5S	109.5
F3A—C4—C1	113.0 (3)	N1S—C3S—H6S	109.5
F2—C4—C1	112.5 (3)	H4S—C3S—H6S	109.5
F1—C4—C1	112.3 (4)	H5S—C3S—H6S	109.5
F3—C4—C1	113.9 (3)	N1S—C4S—H7S	109.5
F1A—C4—C1	111.2 (4)	N1S—C4S—H8S	109.5
C10—C5—C6	117.7 (2)	H7S—C4S—H8S	109.5
C10—C5—C3	119.25 (18)	N1S—C4S—H9S	109.5
C6—C5—C3	122.89 (18)	H7S—C4S—H9S	109.5
C7—C6—C5	120.77 (19)	H8S—C4S—H9S	109.5
C7—C6—H6A	119.6	C1SA—N1SA—C4SA	114.9 (4)
C5—C6—H6A	119.6	C1SA—N1SA—C3SA	115.4 (4)
C6—C7—C8	121.6 (2)	C4SA—N1SA—C3SA	129.6 (4)
C6—C7—H7A	119.2	O1SA—C1SA—N1SA	116.0 (4)
C8—C7—H7A	119.2	O1SA—C1SA—C2SA	126.8 (4)
C7—C8—C9	117.3 (2)	N1SA—C1SA—C2SA	117.2 (4)
C7—C8—C11	121.1 (2)	C1SA—C2SA—H10S	109.5
C9—C8—C11	121.5 (2)	C1SA—C2SA—H11S	109.5
C10—C9—C8	121.7 (2)	H10S—C2SA—H11S	109.5
C10—C9—H9A	119.2	C1SA—C2SA—H12S	109.5
C8—C9—H9A	119.2	H10S—C2SA—H12S	109.5
C9—C10—C5	120.9 (2)	H11S—C2SA—H12S	109.5
C9—C10—H10A	119.6	N1SA—C3SA—H13S	109.5
C5—C10—H10A	119.6	N1SA—C3SA—H14S	109.5
C8—C11—H11A	109.5	H13S—C3SA—H14S	109.5
C8—C11—H11B	109.5	N1SA—C3SA—H15S	109.5
H11A—C11—H11B	109.5	H13S—C3SA—H15S	109.5
C8—C11—H11C	109.5	H14S—C3SA—H15S	109.5
H11A—C11—H11C	109.5	N1SA—C4SA—H16S	109.5
H11B—C11—H11C	109.5	N1SA—C4SA—H17S	109.5
C13—C12—C17	121.16 (17)	H16S—C4SA—H17S	109.5
C13—C12—N2	118.05 (17)	N1SA—C4SA—H18S	109.5
C17—C12—N2	120.72 (16)	H16S—C4SA—H18S	109.5
C12—C13—C14	119.60 (19)	H17S—C4SA—H18S	109.5

C1—N1—N2—C3	0.5 (2)	C7—C8—C9—C10	−0.1 (4)
C1—N1—N2—C12	−177.59 (17)	C11—C8—C9—C10	179.5 (3)
N2—N1—C1—C2	0.1 (2)	C8—C9—C10—C5	0.6 (4)
N2—N1—C1—C4	−178.8 (2)	C6—C5—C10—C9	−0.2 (3)
N1—C1—C2—C3	−0.6 (3)	C3—C5—C10—C9	175.6 (2)
C4—C1—C2—C3	178.1 (2)	N1—N2—C12—C13	−50.1 (3)
N1—N2—C3—C2	−0.9 (2)	C3—N2—C12—C13	132.2 (2)
C12—N2—C3—C2	176.86 (19)	N1—N2—C12—C17	126.8 (2)
N1—N2—C3—C5	175.06 (18)	C3—N2—C12—C17	−50.9 (3)

C12—N2—C3—C5	−7.2 (3)	C17—C12—C13—C14	−0.3 (3)
C1—C2—C3—N2	0.9 (2)	N2—C12—C13—C14	176.6 (2)
C1—C2—C3—C5	−174.9 (2)	C12—C13—C14—C15	−0.2 (4)
N1—C1—C4—F2A	59.7 (11)	C13—C14—C15—C16	0.7 (3)
C2—C1—C4—F2A	−119.0 (11)	C13—C14—C15—S1	−178.95 (18)
N1—C1—C4—F3A	−61.5 (7)	O1—S1—C15—C14	20.1 (2)
C2—C1—C4—F3A	119.8 (7)	O2—S1—C15—C14	149.50 (18)
N1—C1—C4—F2	122.4 (5)	N3—S1—C15—C14	−95.2 (2)
C2—C1—C4—F2	−56.3 (6)	O1—S1—C15—C16	−159.56 (17)
N1—C1—C4—F1	−118.7 (9)	O2—S1—C15—C16	−30.12 (19)
C2—C1—C4—F1	62.6 (9)	N3—S1—C15—C16	85.17 (18)
N1—C1—C4—F3	4.0 (8)	C14—C15—C16—C17	−0.6 (3)
C2—C1—C4—F3	−174.7 (8)	S1—C15—C16—C17	179.03 (15)
N1—C1—C4—F1A	−177.1 (9)	C13—C12—C17—C16	0.4 (3)
C2—C1—C4—F1A	4.2 (10)	N2—C12—C17—C16	−176.44 (18)
N2—C3—C5—C10	149.9 (2)	C15—C16—C17—C12	0.0 (3)
C2—C3—C5—C10	−35.1 (3)	C4S—N1S—C1S—O1S	4.0 (6)
N2—C3—C5—C6	−34.5 (3)	C3S—N1S—C1S—O1S	−177.4 (3)
C2—C3—C5—C6	140.5 (2)	C4S—N1S—C1S—C2S	−176.8 (4)
C10—C5—C6—C7	−0.7 (3)	C3S—N1S—C1S—C2S	1.8 (6)
C3—C5—C6—C7	−176.33 (18)	C4SA—N1SA—C1SA—O1SA	−5.6 (6)
C5—C6—C7—C8	1.2 (3)	C3SA—N1SA—C1SA—O1SA	177.7 (4)
C6—C7—C8—C9	−0.8 (3)	C4SA—N1SA—C1SA—C2SA	176.6 (4)
C6—C7—C8—C11	179.6 (2)	C3SA—N1SA—C1SA—C2SA	−0.1 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H1*N*···O1Sa	0.86 (1)	2.06 (1)	2.894 (3)	163 (2)
N3—H2*N*···O1Sa^{i}	0.87 (1)	2.08 (1)	2.920 (3)	162 (3)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

4-[5-(4-Methylphenyl)-3-(trifluoromethyl)pyrazol-1-yl]benzenesulfonamide *N*-methylpyrrolidin-2-one monosolvate (3)

Crystal data

$C_{17}H_{14}F_3N_3O_2S·C_5H_9NO$
M_r = 480.50
Monoclinic, $P2_1/c$
a = 11.9978 (4) Å
b = 9.0896 (3) Å
c = 21.9732 (8) Å
β = 101.358 (2)°
V = 2349.36 (14) Å^3
Z = 4
$F(000)$ = 1000
D_x = 1.358 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9878 reflections
θ = 3.8–66.5°
μ = 1.71 mm^{-1}
T = 298 K
Block, colourless
0.20 × 0.18 × 0.18 mm

Data collection

Bruker D8-QUEST PHOTON-100 diffractometer
Radiation source: Incoatec IμS Cu microsource
ω and φ–scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.593, T_{max} = 0.753
24378 measured reflections
4146 independent reflections
3112 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 66.8°, θ_{min} = 3.8°
h = −14→14
k = −10→9
l = −24→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.136
S = 1.03
4146 reflections
389 parameters
103 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2 + 0.6367P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015b)
Extinction coefficient: 0.0093 (5)

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.42443 (5)	0.72995 (8)	0.57323 (3)	0.0743 (3)	
O1	0.40662 (15)	0.6918 (3)	0.63344 (9)	0.0970 (6)	
O2	0.37053 (14)	0.8572 (2)	0.54265 (10)	0.0974 (6)	
N1	0.97465 (15)	0.8705 (2)	0.65213 (9)	0.0718 (5)	
N2	0.92235 (13)	0.8146 (2)	0.59662 (8)	0.0600 (5)	
N3	0.38435 (16)	0.5916 (3)	0.52861 (10)	0.0796 (6)	
H1N	0.393 (3)	0.614 (3)	0.4911 (7)	0.119*	
H2N	0.421 (2)	0.514 (2)	0.5457 (12)	0.119*	
C1	1.08126 (19)	0.8883 (3)	0.64533 (12)	0.0728 (6)	
C2	1.09811 (18)	0.8453 (3)	0.58771 (12)	0.0687 (6)	
H2A	1.165852	0.848585	0.573206	0.082*	
C3	0.99450 (16)	0.7967 (2)	0.55607 (10)	0.0565 (5)	
C4	1.1659 (3)	0.9471 (4)	0.69872 (16)	0.1011 (10)	
F1	1.2535 (9)	0.994 (2)	0.6765 (5)	0.222 (8)	0.507 (13)
F3	1.1276 (7)	1.0600 (9)	0.7205 (3)	0.134 (3)	0.507 (13)
F2	1.1967 (14)	0.8585 (8)	0.7407 (5)	0.232 (9)	0.507 (13)
F1A	1.1958 (8)	1.0844 (6)	0.6935 (7)	0.182 (7)	0.493 (13)
F2A	1.2593 (4)	0.8749 (8)	0.7101 (3)	0.108 (3)	0.493 (13)
F3A	1.1318 (6)	0.9433 (19)	0.7522 (4)	0.194 (8)	0.493 (13)

C5	0.96376 (16)	0.7310 (2)	0.49422 (10)	0.0560 (5)	
C6	0.88572 (16)	0.6174 (2)	0.48013 (11)	0.0590 (5)	
H6A	0.848432	0.582550	0.510538	0.071*	
C7	0.86273 (17)	0.5559 (3)	0.42205 (11)	0.0653 (6)	
H7A	0.809584	0.480362	0.413807	0.078*	
C8	0.9163 (2)	0.6029 (3)	0.37558 (12)	0.0733 (6)	
C9	0.9950 (2)	0.7151 (3)	0.38973 (13)	0.0833 (8)	
H9A	1.033100	0.748272	0.359382	0.100*	
C10	1.0182 (2)	0.7789 (3)	0.44766 (12)	0.0733 (7)	
H10A	1.070912	0.854952	0.455685	0.088*	
C11	0.8899 (3)	0.5348 (4)	0.31160 (14)	0.1128 (11)	
H11A	0.935098	0.581327	0.285594	0.169*	
H11B	0.907036	0.431568	0.314617	0.169*	
H11C	0.810760	0.548188	0.293943	0.169*	
C12	0.80263 (16)	0.7899 (2)	0.58845 (10)	0.0561 (5)	
C13	0.76268 (19)	0.7091 (3)	0.63267 (11)	0.0715 (6)	
H13A	0.813363	0.667305	0.665627	0.086*	
C14	0.64752 (19)	0.6904 (3)	0.62788 (11)	0.0740 (7)	
H14A	0.620015	0.635728	0.657536	0.089*	
C15	0.57292 (17)	0.7531 (2)	0.57887 (11)	0.0615 (6)	
C16	0.61338 (17)	0.8324 (2)	0.53439 (10)	0.0597 (5)	
H16A	0.562852	0.873081	0.501098	0.072*	
C17	0.72897 (16)	0.8514 (2)	0.53925 (10)	0.0582 (5)	
H17A	0.756691	0.905349	0.509478	0.070*	
O1S	0.46487 (18)	0.6396 (2)	0.41492 (10)	0.0977 (6)	0.679 (8)
N1S	0.3890 (4)	0.8101 (5)	0.34400 (18)	0.0848 (14)	0.679 (8)
C1S	0.4695 (5)	0.7240 (8)	0.3717 (3)	0.0727 (16)	0.679 (8)
C2S	0.5661 (7)	0.7546 (11)	0.3406 (4)	0.122 (3)	0.679 (8)
H2S1	0.624984	0.807865	0.368541	0.146*	0.679 (8)
H2S2	0.598100	0.662814	0.329412	0.146*	0.679 (8)
C3S	0.5277 (6)	0.8373 (13)	0.2880 (4)	0.177 (4)	0.679 (8)
H3S1	0.520389	0.776555	0.251096	0.212*	0.679 (8)
H3S2	0.580123	0.916926	0.284945	0.212*	0.679 (8)
C4S	0.4020 (6)	0.9032 (9)	0.2952 (4)	0.117 (3)	0.679 (8)
H4S1	0.405189	1.006227	0.306865	0.140*	0.679 (8)
H4S2	0.343951	0.887895	0.258223	0.140*	0.679 (8)
C5S	0.2769 (6)	0.8127 (10)	0.3636 (4)	0.144 (3)	0.679 (8)
H5S1	0.227545	0.881874	0.338547	0.216*	0.679 (8)
H5S2	0.243357	0.716451	0.358569	0.216*	0.679 (8)
H5S3	0.287600	0.841352	0.406450	0.216*	0.679 (8)
O1SA	0.46487 (18)	0.6396 (2)	0.41492 (10)	0.0977 (6)	0.321 (8)
N1SA	0.4849 (10)	0.7734 (12)	0.3361 (5)	0.129 (4)	0.321 (8)
C1SA	0.4263 (10)	0.7305 (16)	0.3763 (6)	0.086 (5)	0.321 (8)
C2SA	0.3286 (12)	0.8325 (19)	0.3689 (8)	0.127 (6)	0.321 (8)
H2S3	0.257860	0.777722	0.361922	0.152*	0.321 (8)
H2S4	0.332888	0.891552	0.406092	0.152*	0.321 (8)
C3SA	0.3331 (13)	0.9204 (19)	0.3193 (8)	0.182 (8)	0.321 (8)
H3S3	0.326878	1.022754	0.330697	0.218*	0.321 (8)

H3S4	0.270203	0.897681	0.285595	0.218*	0.321 (8)
C4SA	0.4571 (13)	0.8927 (16)	0.2963 (7)	0.096 (4)	0.321 (8)
H4S3	0.447513	0.866133	0.252777	0.116*	0.321 (8)
H4S4	0.509558	0.974392	0.305894	0.116*	0.321 (8)
C5SA	0.5910 (16)	0.693 (2)	0.3311 (11)	0.151 (8)	0.321 (8)
H5S4	0.624693	0.737444	0.299464	0.227*	0.321 (8)
H5S5	0.643550	0.697079	0.370117	0.227*	0.321 (8)
H5S6	0.573025	0.591953	0.320419	0.227*	0.321 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0452 (3)	0.0899 (5)	0.0951 (5)	0.0062 (3)	0.0318 (3)	0.0201 (3)
O1	0.0704 (11)	0.1386 (17)	0.0948 (12)	0.0002 (11)	0.0471 (9)	0.0159 (12)
O2	0.0537 (9)	0.0935 (13)	0.1515 (17)	0.0230 (9)	0.0360 (10)	0.0376 (12)
N1	0.0572 (11)	0.0795 (14)	0.0772 (12)	−0.0030 (9)	0.0096 (9)	−0.0089 (10)
N2	0.0441 (9)	0.0647 (11)	0.0712 (11)	−0.0021 (8)	0.0115 (8)	−0.0004 (9)
N3	0.0570 (11)	0.0913 (16)	0.0933 (15)	−0.0123 (10)	0.0214 (11)	0.0146 (12)
C1	0.0527 (13)	0.0696 (15)	0.0930 (17)	−0.0038 (11)	0.0070 (11)	−0.0111 (13)
C2	0.0451 (11)	0.0639 (14)	0.0979 (17)	−0.0047 (10)	0.0157 (11)	−0.0069 (13)
C3	0.0431 (10)	0.0484 (11)	0.0788 (14)	0.0005 (9)	0.0137 (9)	0.0035 (10)
C4	0.075 (2)	0.109 (3)	0.116 (3)	−0.0200 (19)	0.0116 (18)	−0.032 (2)
F1	0.134 (6)	0.34 (2)	0.207 (8)	−0.145 (9)	0.058 (6)	−0.142 (11)
F3	0.170 (6)	0.118 (5)	0.092 (4)	−0.016 (4)	−0.024 (3)	−0.040 (3)
F2	0.257 (16)	0.166 (7)	0.194 (13)	−0.029 (9)	−0.151 (12)	0.050 (8)
F1A	0.141 (8)	0.079 (4)	0.273 (14)	−0.039 (4)	−0.092 (8)	0.003 (5)
F2A	0.060 (3)	0.127 (5)	0.123 (5)	0.016 (3)	−0.017 (2)	−0.022 (4)
F3A	0.099 (5)	0.37 (2)	0.115 (6)	−0.071 (7)	0.028 (4)	−0.102 (10)
C5	0.0396 (10)	0.0501 (11)	0.0794 (14)	0.0040 (8)	0.0148 (9)	0.0049 (10)
C6	0.0464 (11)	0.0529 (12)	0.0806 (14)	−0.0008 (9)	0.0196 (10)	0.0030 (11)
C7	0.0496 (12)	0.0584 (13)	0.0879 (16)	−0.0026 (10)	0.0134 (11)	−0.0041 (12)
C8	0.0614 (13)	0.0784 (16)	0.0801 (15)	0.0018 (12)	0.0143 (11)	−0.0048 (13)
C9	0.0771 (16)	0.097 (2)	0.0826 (17)	−0.0118 (14)	0.0327 (13)	0.0055 (15)
C10	0.0592 (13)	0.0724 (15)	0.0925 (18)	−0.0155 (11)	0.0254 (12)	0.0022 (13)
C11	0.116 (2)	0.131 (3)	0.093 (2)	−0.018 (2)	0.0238 (18)	−0.024 (2)
C12	0.0432 (10)	0.0579 (12)	0.0692 (13)	0.0010 (9)	0.0162 (9)	0.0030 (10)
C13	0.0549 (13)	0.0855 (17)	0.0734 (14)	0.0030 (11)	0.0111 (10)	0.0234 (13)
C14	0.0591 (13)	0.0916 (18)	0.0756 (15)	−0.0006 (12)	0.0239 (11)	0.0270 (13)
C15	0.0459 (11)	0.0686 (14)	0.0750 (14)	0.0044 (10)	0.0242 (10)	0.0100 (11)
C16	0.0471 (11)	0.0610 (13)	0.0733 (13)	0.0056 (9)	0.0176 (9)	0.0131 (11)
C17	0.0489 (11)	0.0581 (13)	0.0712 (13)	0.0009 (9)	0.0205 (9)	0.0117 (10)
O1S	0.0985 (14)	0.1014 (15)	0.0988 (13)	0.0077 (12)	0.0332 (11)	0.0285 (12)
N1S	0.095 (3)	0.075 (3)	0.077 (2)	−0.005 (2)	−0.001 (2)	0.005 (2)
C1S	0.065 (3)	0.083 (3)	0.069 (3)	−0.010 (3)	0.011 (2)	0.003 (3)
C2S	0.100 (4)	0.154 (6)	0.120 (4)	−0.013 (5)	0.044 (4)	0.032 (5)
C3S	0.116 (5)	0.270 (8)	0.140 (5)	−0.050 (5)	0.014 (4)	0.093 (5)
C4S	0.118 (6)	0.109 (5)	0.112 (4)	−0.008 (4)	−0.005 (4)	0.021 (4)
C5S	0.082 (4)	0.169 (7)	0.185 (7)	0.015 (4)	0.037 (4)	−0.061 (5)

O1SA	0.0985 (14)	0.1014 (15)	0.0988 (13)	0.0077 (12)	0.0332 (11)	0.0285 (12)
N1SA	0.143 (9)	0.119 (7)	0.129 (8)	−0.005 (7)	0.038 (7)	0.011 (6)
C1SA	0.090 (9)	0.072 (6)	0.095 (8)	0.006 (7)	0.011 (6)	−0.008 (6)
C2SA	0.122 (10)	0.136 (9)	0.112 (8)	0.010 (8)	−0.003 (8)	−0.021 (7)
C3SA	0.189 (11)	0.170 (11)	0.174 (11)	0.010 (9)	0.007 (8)	−0.009 (9)
C4SA	0.128 (9)	0.078 (6)	0.080 (6)	0.041 (7)	0.011 (7)	0.030 (5)
C5SA	0.158 (13)	0.129 (11)	0.193 (14)	0.051 (9)	0.099 (10)	0.031 (10)

Geometric parameters (Å, º)

S1—O1	1.4240 (18)	C14—C15	1.381 (3)
S1—O2	1.4271 (18)	C14—H14A	0.9300
S1—N3	1.609 (2)	C15—C16	1.377 (3)
S1—C15	1.774 (2)	C16—C17	1.381 (3)
N1—C1	1.327 (3)	C16—H16A	0.9300
N1—N2	1.356 (2)	C17—H17A	0.9300
N2—C3	1.369 (3)	O1S—C1S	1.230 (5)
N2—C12	1.430 (2)	N1S—C1S	1.297 (6)
N3—H1N	0.875 (10)	N1S—C4S	1.399 (7)
N3—H2N	0.875 (10)	N1S—C5S	1.492 (8)
C1—C2	1.377 (3)	C1S—C2S	1.483 (9)
C1—C4	1.492 (4)	C2S—C3S	1.379 (11)
C2—C3	1.372 (3)	C2S—H2S1	0.9700
C2—H2A	0.9300	C2S—H2S2	0.9700
C3—C5	1.464 (3)	C3S—C4S	1.659 (11)
C4—F2	1.226 (6)	C3S—H3S1	0.9700
C4—F3	1.258 (5)	C3S—H3S2	0.9700
C4—F2A	1.279 (5)	C4S—H4S1	0.9700
C4—F1A	1.310 (6)	C4S—H4S2	0.9700
C4—F1	1.315 (6)	C5S—H5S1	0.9600
C4—F3A	1.320 (7)	C5S—H5S2	0.9600
C5—C6	1.387 (3)	C5S—H5S3	0.9600
C5—C10	1.388 (3)	O1SA—C1SA	1.209 (8)
C6—C7	1.371 (3)	N1SA—C1SA	1.293 (9)
C6—H6A	0.9300	N1SA—C4SA	1.392 (9)
C7—C8	1.378 (3)	N1SA—C5SA	1.492 (11)
C7—H7A	0.9300	C1SA—C2SA	1.478 (11)
C8—C9	1.383 (4)	C2SA—C3SA	1.361 (14)
C8—C11	1.512 (4)	C2SA—H2S3	0.9700
C9—C10	1.376 (4)	C2SA—H2S4	0.9700
C9—H9A	0.9300	C3SA—C4SA	1.682 (14)
C10—H10A	0.9300	C3SA—H3S3	0.9700
C11—H11A	0.9600	C3SA—H3S4	0.9700
C11—H11B	0.9600	C4SA—H4S3	0.9700
C11—H11C	0.9600	C4SA—H4S4	0.9700
C12—C17	1.373 (3)	C5SA—H5S4	0.9600
C12—C13	1.377 (3)	C5SA—H5S5	0.9600
C13—C14	1.375 (3)	C5SA—H5S6	0.9600

C13—H13A	0.9300

O1—S1—O2	119.86 (12)	C16—C15—S1	120.12 (17)
O1—S1—N3	107.11 (12)	C14—C15—S1	119.57 (16)
O2—S1—N3	107.05 (13)	C15—C16—C17	120.0 (2)
O1—S1—C15	107.24 (11)	C15—C16—H16A	120.0
O2—S1—C15	107.02 (10)	C17—C16—H16A	120.0
N3—S1—C15	108.11 (11)	C12—C17—C16	119.40 (19)
C1—N1—N2	103.29 (18)	C12—C17—H17A	120.3
N1—N2—C3	112.96 (16)	C16—C17—H17A	120.3
N1—N2—C12	116.57 (17)	C1S—N1S—C4S	122.7 (5)
C3—N2—C12	130.41 (18)	C1S—N1S—C5S	120.2 (5)
S1—N3—H1N	109 (2)	C4S—N1S—C5S	117.1 (6)
S1—N3—H2N	108 (2)	O1S—C1S—N1S	126.6 (5)
H1N—N3—H2N	116.4 (17)	O1S—C1S—C2S	129.1 (5)
N1—C1—C2	112.9 (2)	N1S—C1S—C2S	104.3 (5)
N1—C1—C4	118.5 (2)	C3S—C2S—C1S	109.1 (7)
C2—C1—C4	128.6 (2)	C3S—C2S—H2S1	109.9
C3—C2—C1	105.9 (2)	C1S—C2S—H2S1	109.9
C3—C2—H2A	127.0	C3S—C2S—H2S2	109.9
C1—C2—H2A	127.0	C1S—C2S—H2S2	109.9
N2—C3—C2	105.0 (2)	H2S1—C2S—H2S2	108.3
N2—C3—C5	125.23 (18)	C2S—C3S—C4S	106.1 (6)
C2—C3—C5	129.7 (2)	C2S—C3S—H3S1	110.5
F2—C4—F3	109.1 (6)	C4S—C3S—H3S1	110.5
F2A—C4—F1A	105.2 (4)	C2S—C3S—H3S2	110.5
F2—C4—F1	110.5 (6)	C4S—C3S—H3S2	110.5
F3—C4—F1	104.7 (6)	H3S1—C3S—H3S2	108.7
F2A—C4—F3A	103.0 (6)	N1S—C4S—C3S	95.5 (5)
F1A—C4—F3A	104.0 (6)	N1S—C4S—H4S1	112.7
F2—C4—C1	114.5 (4)	C3S—C4S—H4S1	112.7
F3—C4—C1	110.4 (4)	N1S—C4S—H4S2	112.7
F2A—C4—C1	113.9 (4)	C3S—C4S—H4S2	112.7
F1A—C4—C1	115.4 (5)	H4S1—C4S—H4S2	110.1
F1—C4—C1	107.2 (4)	N1S—C5S—H5S1	109.5
F3A—C4—C1	114.1 (4)	N1S—C5S—H5S2	109.5
C6—C5—C10	117.6 (2)	H5S1—C5S—H5S2	109.5
C6—C5—C3	123.13 (19)	N1S—C5S—H5S3	109.5
C10—C5—C3	119.17 (19)	H5S1—C5S—H5S3	109.5
C7—C6—C5	121.0 (2)	H5S2—C5S—H5S3	109.5
C7—C6—H6A	119.5	C1SA—N1SA—C4SA	124.8 (9)
C5—C6—H6A	119.5	C1SA—N1SA—C5SA	119.3 (10)
C6—C7—C8	121.7 (2)	C4SA—N1SA—C5SA	115.9 (10)
C6—C7—H7A	119.1	O1SA—C1SA—N1SA	120.0 (9)
C8—C7—H7A	119.1	O1SA—C1SA—C2SA	133.8 (10)
C7—C8—C9	117.4 (2)	N1SA—C1SA—C2SA	105.1 (9)
C7—C8—C11	121.3 (2)	C3SA—C2SA—C1SA	107.5 (11)
C9—C8—C11	121.3 (2)	C3SA—C2SA—H2S3	110.2

C10—C9—C8	121.6 (2)	C1SA—C2SA—H2S3	110.2
C10—C9—H9A	119.2	C3SA—C2SA—H2S4	110.2
C8—C9—H9A	119.2	C1SA—C2SA—H2S4	110.2
C9—C10—C5	120.7 (2)	H2S3—C2SA—H2S4	108.5
C9—C10—H10A	119.6	C2SA—C3SA—C4SA	109.3 (10)
C5—C10—H10A	119.6	C2SA—C3SA—H3S3	109.8
C8—C11—H11A	109.5	C4SA—C3SA—H3S3	109.8
C8—C11—H11B	109.5	C2SA—C3SA—H3S4	109.8
H11A—C11—H11B	109.5	C4SA—C3SA—H3S4	109.8
C8—C11—H11C	109.5	H3S3—C3SA—H3S4	108.3
H11A—C11—H11C	109.5	N1SA—C4SA—C3SA	92.5 (8)
H11B—C11—H11C	109.5	N1SA—C4SA—H4S3	113.2
C17—C12—C13	120.86 (19)	C3SA—C4SA—H4S3	113.2
C17—C12—N2	120.66 (18)	N1SA—C4SA—H4S4	113.2
C13—C12—N2	118.40 (19)	C3SA—C4SA—H4S4	113.2
C14—C13—C12	119.7 (2)	H4S3—C4SA—H4S4	110.6
C14—C13—H13A	120.1	N1SA—C5SA—H5S4	109.5
C12—C13—H13A	120.1	N1SA—C5SA—H5S5	109.5
C13—C14—C15	119.7 (2)	H5S4—C5SA—H5S5	109.5
C13—C14—H14A	120.1	N1SA—C5SA—H5S6	109.5
C15—C14—H14A	120.1	H5S4—C5SA—H5S6	109.5
C16—C15—C14	120.31 (19)	H5S5—C5SA—H5S6	109.5

C1—N1—N2—C3	0.4 (2)	C3—N2—C12—C17	−52.0 (3)
C1—N1—N2—C12	−177.00 (19)	N1—N2—C12—C13	−52.1 (3)
N2—N1—C1—C2	−0.2 (3)	C3—N2—C12—C13	131.1 (2)
N2—N1—C1—C4	−179.1 (2)	C17—C12—C13—C14	−0.5 (4)
N1—C1—C2—C3	−0.1 (3)	N2—C12—C13—C14	176.4 (2)
C4—C1—C2—C3	178.7 (3)	C12—C13—C14—C15	−0.1 (4)
N1—N2—C3—C2	−0.5 (2)	C13—C14—C15—C16	0.9 (4)
C12—N2—C3—C2	176.5 (2)	C13—C14—C15—S1	−179.5 (2)
N1—N2—C3—C5	176.31 (19)	O1—S1—C15—C16	−160.02 (19)
C12—N2—C3—C5	−6.7 (3)	O2—S1—C15—C16	−30.2 (2)
C1—C2—C3—N2	0.4 (3)	N3—S1—C15—C16	84.8 (2)
C1—C2—C3—C5	−176.2 (2)	O1—S1—C15—C14	20.4 (2)
N1—C1—C4—F2	74.9 (11)	O2—S1—C15—C14	150.2 (2)
C2—C1—C4—F2	−103.9 (11)	N3—S1—C15—C14	−94.8 (2)
N1—C1—C4—F3	−48.7 (7)	C14—C15—C16—C17	−1.0 (4)
C2—C1—C4—F3	132.5 (6)	S1—C15—C16—C17	179.36 (18)
N1—C1—C4—F2A	133.1 (5)	C13—C12—C17—C16	0.4 (3)
C2—C1—C4—F2A	−45.7 (7)	N2—C12—C17—C16	−176.5 (2)
N1—C1—C4—F1A	−105.2 (9)	C15—C16—C17—C12	0.4 (3)
C2—C1—C4—F1A	76.1 (10)	C4S—N1S—C1S—O1S	179.7 (7)
N1—C1—C4—F1	−162.2 (10)	C5S—N1S—C1S—O1S	−0.4 (11)
C2—C1—C4—F1	19.0 (11)	C4S—N1S—C1S—C2S	1.3 (9)
N1—C1—C4—F3A	15.1 (9)	C5S—N1S—C1S—C2S	−178.9 (6)
C2—C1—C4—F3A	−163.6 (9)	O1S—C1S—C2S—C3S	169.9 (9)
N2—C3—C5—C6	−34.0 (3)	N1S—C1S—C2S—C3S	−11.7 (10)

C2—C3—C5—C6	142.0 (2)	C1S—C2S—C3S—C4S	15.9 (10)
N2—C3—C5—C10	149.0 (2)	C1S—N1S—C4S—C3S	7.5 (9)
C2—C3—C5—C10	−35.0 (3)	C5S—N1S—C4S—C3S	−172.3 (6)
C10—C5—C6—C7	−0.5 (3)	C2S—C3S—C4S—N1S	−13.7 (9)
C3—C5—C6—C7	−177.62 (19)	C4SA—N1SA—C1SA—O1SA	−169.5 (15)
C5—C6—C7—C8	0.5 (3)	C5SA—N1SA—C1SA—O1SA	10 (3)
C6—C7—C8—C9	0.2 (3)	C4SA—N1SA—C1SA—C2SA	1 (2)
C6—C7—C8—C11	−179.7 (3)	C5SA—N1SA—C1SA—C2SA	−179.9 (16)
C7—C8—C9—C10	−0.8 (4)	O1SA—C1SA—C2SA—C3SA	174 (2)
C11—C8—C9—C10	179.1 (3)	N1SA—C1SA—C2SA—C3SA	6 (2)
C8—C9—C10—C5	0.7 (4)	C1SA—C2SA—C3SA—C4SA	−9 (2)
C6—C5—C10—C9	−0.1 (3)	C1SA—N1SA—C4SA—C3SA	−5 (2)
C3—C5—C10—C9	177.2 (2)	C5SA—N1SA—C4SA—C3SA	175.2 (16)
N1—N2—C12—C17	124.9 (2)	C2SA—C3SA—C4SA—N1SA	8 (2)

4-[5-(4-Methylphenyl)-3-(trifluoromethyl)pyrazol-1-yl]benzenesulfonamide tetramethylurea monosolvate (4)

Crystal data

$C_{17}H_{14}F_3N_3O_2S·C_5H_{12}N_2O$
M_r = 497.54
Monoclinic, $P2_1/c$
a = 12.4050 (3) Å
b = 8.9351 (2) Å
c = 22.5727 (6) Å
β = 98.6702 (13)°
V = 2473.36 (11) Å^3
Z = 4
$F(000)$ = 1040
D_x = 1.336 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9948 reflections
θ = 3.6–66.8°
μ = 1.66 mm^{-1}
T = 298 K
Block, colourless
0.16 × 0.14 × 0.14 mm

Data collection

Bruker D8-QUEST PHOTON-100 diffractometer
Radiation source: Incoatec IμS Cu microsource
ω and φ–scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.657, T_{max} = 0.753
27591 measured reflections
4397 independent reflections
3339 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 66.9°, θ_{min} = 3.6°
h = −14→14
k = −9→10
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.142
S = 1.03
4397 reflections
349 parameters
15 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0714P)^2 + 0.619P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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}	Occ. (<1)
S1	0.42251 (5)	0.73033 (8)	0.57691 (3)	0.0805 (2)	
O1	0.39736 (16)	0.6847 (3)	0.63369 (8)	0.1108 (7)	
O2	0.37201 (15)	0.8603 (2)	0.54817 (10)	0.1070 (6)	
N1	0.94939 (17)	0.8747 (2)	0.65960 (9)	0.0771 (5)	
N2	0.90320 (14)	0.8185 (2)	0.60585 (8)	0.0655 (5)	
N3	0.39387 (16)	0.5931 (3)	0.53183 (9)	0.0769 (5)	
H1N	0.408 (2)	0.620 (2)	0.4968 (7)	0.092 (8)*	
H2N	0.422 (2)	0.5081 (18)	0.5463 (10)	0.091 (9)*	
C1	1.0536 (2)	0.8897 (3)	0.65326 (12)	0.0769 (6)	
C2	1.07521 (19)	0.8457 (2)	0.59772 (11)	0.0736 (6)	
H2A	1.142114	0.847511	0.583867	0.088*	
C3	0.97680 (17)	0.7985 (2)	0.56714 (10)	0.0623 (5)	
C4	1.1316 (3)	0.9460 (4)	0.70503 (15)	0.1027 (9)	
F1	1.1353 (12)	1.0922 (5)	0.7124 (5)	0.157 (4)	0.541 (17)
F2	1.1137 (7)	0.8917 (13)	0.7567 (3)	0.129 (3)	0.541 (17)
F3	1.2325 (4)	0.9085 (16)	0.7014 (3)	0.139 (3)	0.541 (17)
F1A	1.0843 (7)	1.0587 (14)	0.7295 (4)	0.151 (4)	0.459 (17)
F2A	1.1571 (16)	0.8507 (12)	0.7464 (6)	0.211 (8)	0.459 (17)
F3A	1.2167 (10)	0.999 (2)	0.6878 (6)	0.195 (6)	0.459 (17)
C5	0.95104 (16)	0.7317 (2)	0.50748 (10)	0.0586 (5)	
C6	0.88179 (16)	0.6091 (2)	0.49569 (10)	0.0599 (5)	
H6A	0.847648	0.569658	0.526178	0.072*	
C7	0.86323 (16)	0.5455 (2)	0.43971 (10)	0.0645 (5)	
H7A	0.816579	0.463763	0.433008	0.077*	
C8	0.91224 (18)	0.6002 (3)	0.39311 (10)	0.0698 (6)	
C9	0.9805 (2)	0.7221 (3)	0.40481 (11)	0.0769 (6)	
H9A	1.013960	0.761633	0.374068	0.092*	
C10	1.00050 (18)	0.7867 (3)	0.46071 (11)	0.0719 (6)	
H10A	1.047615	0.867941	0.467234	0.086*	
C11	0.8907 (3)	0.5301 (4)	0.33170 (12)	0.0992 (9)	
H11A	0.880615	0.607387	0.301832	0.149*	
H11B	0.826048	0.469671	0.328501	0.149*	
H11C	0.951543	0.468655	0.325674	0.149*	
C12	0.78759 (17)	0.7950 (2)	0.59725 (10)	0.0614 (5)	
C13	0.7437 (2)	0.7113 (3)	0.63911 (10)	0.0731 (6)	
H13A	0.788827	0.668236	0.671245	0.088*	
C14	0.6324 (2)	0.6922 (3)	0.63282 (11)	0.0742 (6)	
H14A	0.602035	0.635395	0.660624	0.089*	
C15	0.56598 (18)	0.7575 (2)	0.58518 (10)	0.0663 (5)	

C16	0.61042 (18)	0.8404 (3)	0.54350 (10)	0.0677 (6)
H16A	0.565409	0.883539	0.511356	0.081*
C17	0.72232 (18)	0.8594 (2)	0.54957 (10)	0.0645 (5)
H17A	0.752950	0.915223	0.521583	0.077*
O1S	0.47057 (13)	0.6652 (2)	0.42142 (8)	0.0869 (5)
N1S	0.53109 (19)	0.7639 (3)	0.34089 (9)	0.0902 (7)
N2S	0.34946 (17)	0.7769 (3)	0.35146 (9)	0.0835 (6)
C1S	0.45072 (18)	0.7314 (3)	0.37302 (10)	0.0662 (5)
C2S	0.6425 (3)	0.7372 (5)	0.36927 (19)	0.1527 (18)
H1S	0.648920	0.759700	0.411246	0.229*
H2S	0.691099	0.800189	0.351168	0.229*
H3S	0.660995	0.634216	0.364152	0.229*
C3S	0.5154 (4)	0.7437 (6)	0.27663 (17)	0.1638 (19)
H4S	0.444587	0.701588	0.263666	0.246*
H5S	0.570328	0.677299	0.266065	0.246*
H6S	0.520929	0.838723	0.257482	0.246*
C4S	0.2627 (2)	0.7334 (4)	0.38412 (15)	0.1158 (11)
H7S	0.275181	0.633146	0.398838	0.174*
H8S	0.194159	0.737855	0.357951	0.174*
H9S	0.261118	0.800385	0.417233	0.174*
C5S	0.3256 (3)	0.9007 (4)	0.31098 (17)	0.1307 (13)
H10S	0.389073	0.962898	0.312511	0.196*
H11S	0.266742	0.958313	0.322455	0.196*
H12S	0.305013	0.863733	0.270950	0.196*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0617 (4)	0.1053 (5)	0.0791 (4)	0.0079 (3)	0.0257 (3)	0.0038 (3)
O1	0.0878 (13)	0.174 (2)	0.0789 (12)	−0.0065 (13)	0.0414 (10)	−0.0020 (12)
O2	0.0733 (11)	0.1056 (14)	0.1441 (17)	0.0316 (10)	0.0231 (11)	0.0122 (12)
N1	0.0803 (14)	0.0787 (13)	0.0671 (12)	−0.0039 (10)	−0.0060 (10)	−0.0047 (9)
N2	0.0632 (11)	0.0658 (10)	0.0646 (11)	0.0004 (8)	−0.0002 (9)	−0.0018 (8)
N3	0.0641 (12)	0.0997 (16)	0.0694 (13)	−0.0055 (10)	0.0177 (10)	0.0149 (11)
C1	0.0785 (16)	0.0685 (14)	0.0775 (16)	−0.0091 (11)	−0.0084 (12)	0.0016 (11)
C2	0.0640 (13)	0.0687 (13)	0.0842 (16)	−0.0067 (10)	−0.0016 (12)	0.0056 (12)
C3	0.0584 (12)	0.0541 (11)	0.0718 (13)	−0.0011 (9)	0.0011 (10)	0.0056 (9)
C4	0.105 (3)	0.102 (2)	0.090 (2)	−0.017 (2)	−0.0200 (18)	−0.0046 (19)
F1	0.203 (9)	0.081 (3)	0.151 (6)	−0.031 (4)	−0.085 (6)	−0.011 (3)
F2	0.107 (4)	0.204 (8)	0.067 (3)	−0.033 (4)	−0.017 (3)	0.026 (3)
F3	0.072 (3)	0.216 (9)	0.120 (5)	−0.011 (4)	−0.017 (2)	−0.032 (5)
F1A	0.161 (6)	0.174 (8)	0.105 (5)	−0.063 (5)	−0.022 (4)	−0.045 (5)
F2A	0.241 (16)	0.148 (6)	0.191 (12)	−0.029 (8)	−0.137 (10)	0.055 (7)
F3A	0.153 (9)	0.234 (13)	0.181 (7)	−0.127 (9)	−0.026 (7)	−0.018 (9)
C5	0.0477 (10)	0.0579 (11)	0.0687 (13)	0.0040 (8)	0.0040 (9)	0.0062 (9)
C6	0.0502 (11)	0.0598 (11)	0.0704 (13)	0.0029 (9)	0.0114 (9)	0.0042 (10)
C7	0.0518 (11)	0.0650 (12)	0.0766 (14)	0.0043 (9)	0.0090 (10)	−0.0057 (10)
C8	0.0587 (13)	0.0789 (14)	0.0716 (14)	0.0134 (11)	0.0096 (11)	−0.0012 (11)

C9	0.0662 (14)	0.0926 (17)	0.0750 (16)	0.0034 (12)	0.0201 (12)	0.0121 (13)
C10	0.0594 (13)	0.0722 (14)	0.0838 (16)	−0.0075 (10)	0.0099 (11)	0.0081 (12)
C11	0.111 (2)	0.112 (2)	0.0752 (17)	0.0125 (17)	0.0173 (15)	−0.0116 (15)
C12	0.0612 (12)	0.0616 (12)	0.0603 (12)	0.0029 (9)	0.0063 (10)	−0.0038 (9)
C13	0.0757 (15)	0.0789 (15)	0.0624 (13)	0.0044 (11)	0.0028 (11)	0.0115 (11)
C14	0.0751 (15)	0.0834 (15)	0.0661 (14)	−0.0015 (12)	0.0171 (11)	0.0101 (11)
C15	0.0611 (12)	0.0744 (13)	0.0651 (13)	0.0054 (10)	0.0155 (10)	−0.0010 (10)
C16	0.0613 (13)	0.0782 (14)	0.0637 (13)	0.0107 (10)	0.0098 (10)	0.0073 (11)
C17	0.0635 (13)	0.0675 (13)	0.0629 (12)	0.0039 (10)	0.0110 (10)	0.0074 (10)
O1S	0.0702 (10)	0.1191 (14)	0.0737 (11)	0.0058 (9)	0.0183 (8)	0.0310 (10)
N1S	0.0824 (14)	0.1250 (18)	0.0674 (13)	0.0110 (12)	0.0246 (11)	0.0276 (12)
N2S	0.0707 (13)	0.1075 (16)	0.0687 (12)	0.0160 (11)	−0.0010 (10)	−0.0045 (11)
C1S	0.0650 (13)	0.0789 (14)	0.0540 (12)	0.0045 (10)	0.0064 (10)	0.0001 (10)
C2S	0.0701 (19)	0.237 (5)	0.159 (3)	0.011 (2)	0.042 (2)	0.090 (3)
C3S	0.201 (5)	0.215 (5)	0.088 (2)	0.045 (4)	0.061 (3)	0.020 (3)
C4S	0.0594 (16)	0.177 (3)	0.109 (2)	0.0090 (18)	0.0084 (15)	−0.019 (2)
C5S	0.140 (3)	0.116 (3)	0.128 (3)	0.052 (2)	−0.007 (2)	0.016 (2)

Geometric parameters (Å, º)

S1—O1	1.4236 (19)	C11—H11A	0.9600
S1—O2	1.428 (2)	C11—H11B	0.9600
S1—N3	1.599 (2)	C11—H11C	0.9600
S1—C15	1.778 (2)	C12—C17	1.372 (3)
N1—C1	1.329 (3)	C12—C13	1.380 (3)
N1—N2	1.357 (2)	C13—C14	1.377 (3)
N2—C3	1.367 (3)	C13—H13A	0.9300
N2—C12	1.433 (3)	C14—C15	1.382 (3)
N3—H1N	0.870 (9)	C14—H14A	0.9300
N3—H2N	0.876 (9)	C15—C16	1.376 (3)
C1—C2	1.378 (3)	C16—C17	1.385 (3)
C1—C4	1.487 (4)	C16—H16A	0.9300
C2—C3	1.375 (3)	C17—H17A	0.9300
C2—H2A	0.9300	O1S—C1S	1.234 (3)
C3—C5	1.464 (3)	N1S—C1S	1.350 (3)
C4—F2A	1.269 (7)	N1S—C3S	1.446 (4)
C4—F3A	1.271 (7)	N1S—C2S	1.452 (4)
C4—F3	1.310 (6)	N2S—C1S	1.340 (3)
C4—F2	1.312 (6)	N2S—C5S	1.437 (4)
C4—F1	1.317 (5)	N2S—C4S	1.447 (4)
C4—F1A	1.327 (7)	C2S—H1S	0.9600
C5—C10	1.388 (3)	C2S—H2S	0.9600
C5—C6	1.393 (3)	C2S—H3S	0.9600
C6—C7	1.373 (3)	C3S—H4S	0.9600
C6—H6A	0.9300	C3S—H5S	0.9600
C7—C8	1.381 (3)	C3S—H6S	0.9600
C7—H7A	0.9300	C4S—H7S	0.9600
C8—C9	1.381 (3)	C4S—H8S	0.9600

C8—C11	1.508 (3)	C4S—H9S	0.9600
C9—C10	1.375 (3)	C5S—H10S	0.9600
C9—H9A	0.9300	C5S—H11S	0.9600
C10—H10A	0.9300	C5S—H12S	0.9600
O1—S1—O2	120.07 (13)	C8—C11—H11C	109.5
O1—S1—N3	107.20 (13)	H11A—C11—H11C	109.5
O2—S1—N3	107.12 (13)	H11B—C11—H11C	109.5
O1—S1—C15	107.23 (12)	C17—C12—C13	121.2 (2)
O2—S1—C15	107.49 (12)	C17—C12—N2	120.33 (19)
N3—S1—C15	107.12 (10)	C13—C12—N2	118.46 (19)
C1—N1—N2	103.2 (2)	C14—C13—C12	119.3 (2)
N1—N2—C3	112.76 (18)	C14—C13—H13A	120.3
N1—N2—C12	117.02 (18)	C12—C13—H13A	120.3
C3—N2—C12	130.17 (18)	C13—C14—C15	120.0 (2)
S1—N3—H1N	108.0 (17)	C13—C14—H14A	120.0
S1—N3—H2N	113.0 (18)	C15—C14—H14A	120.0
H1N—N3—H2N	117.2 (16)	C16—C15—C14	120.4 (2)
N1—C1—C2	113.3 (2)	C16—C15—S1	119.96 (18)
N1—C1—C4	118.5 (3)	C14—C15—S1	119.65 (18)
C2—C1—C4	128.2 (3)	C15—C16—C17	119.8 (2)
C3—C2—C1	105.3 (2)	C15—C16—H16A	120.1
C3—C2—H2A	127.3	C17—C16—H16A	120.1
C1—C2—H2A	127.3	C12—C17—C16	119.4 (2)
N2—C3—C2	105.5 (2)	C12—C17—H17A	120.3
N2—C3—C5	124.54 (18)	C16—C17—H17A	120.3
C2—C3—C5	129.9 (2)	C1S—N1S—C3S	120.9 (3)
F2A—C4—F3A	110.5 (6)	C1S—N1S—C2S	117.3 (2)
F3—C4—F2	104.6 (5)	C3S—N1S—C2S	113.4 (3)
F3—C4—F1	104.2 (5)	C1S—N2S—C5S	123.8 (3)
F2—C4—F1	105.1 (6)	C1S—N2S—C4S	117.5 (2)
F2A—C4—F1A	106.2 (7)	C5S—N2S—C4S	115.7 (3)
F3A—C4—F1A	106.5 (6)	O1S—C1S—N2S	121.2 (2)
F2A—C4—C1	114.4 (6)	O1S—C1S—N1S	120.9 (2)
F3A—C4—C1	111.0 (6)	N2S—C1S—N1S	117.9 (2)
F3—C4—C1	112.2 (5)	N1S—C2S—H1S	109.5
F2—C4—C1	113.4 (5)	N1S—C2S—H2S	109.5
F1—C4—C1	116.2 (4)	H1S—C2S—H2S	109.5
F1A—C4—C1	107.9 (4)	N1S—C2S—H3S	109.5
C10—C5—C6	117.6 (2)	H1S—C2S—H3S	109.5
C10—C5—C3	119.70 (19)	H2S—C2S—H3S	109.5
C6—C5—C3	122.65 (19)	N1S—C3S—H4S	109.5
C7—C6—C5	121.0 (2)	N1S—C3S—H5S	109.5
C7—C6—H6A	119.5	H4S—C3S—H5S	109.5
C5—C6—H6A	119.5	N1S—C3S—H6S	109.5
C6—C7—C8	121.5 (2)	H4S—C3S—H6S	109.5
C6—C7—H7A	119.2	H5S—C3S—H6S	109.5
C8—C7—H7A	119.2	N2S—C4S—H7S	109.5

C9—C8—C7	117.5 (2)	N2S—C4S—H8S	109.5
C9—C8—C11	121.5 (2)	H7S—C4S—H8S	109.5
C7—C8—C11	121.0 (2)	N2S—C4S—H9S	109.5
C10—C9—C8	121.8 (2)	H7S—C4S—H9S	109.5
C10—C9—H9A	119.1	H8S—C4S—H9S	109.5
C8—C9—H9A	119.1	N2S—C5S—H10S	109.5
C9—C10—C5	120.7 (2)	N2S—C5S—H11S	109.5
C9—C10—H10A	119.7	H10S—C5S—H11S	109.5
C5—C10—H10A	119.7	N2S—C5S—H12S	109.5
C8—C11—H11A	109.5	H10S—C5S—H12S	109.5
C8—C11—H11B	109.5	H11S—C5S—H12S	109.5
H11A—C11—H11B	109.5		

C1—N1—N2—C3	0.2 (2)	C7—C8—C9—C10	0.6 (3)
C1—N1—N2—C12	−177.43 (18)	C11—C8—C9—C10	179.9 (2)
N2—N1—C1—C2	0.1 (3)	C8—C9—C10—C5	−0.8 (4)
N2—N1—C1—C4	−178.4 (2)	C6—C5—C10—C9	0.5 (3)
N1—C1—C2—C3	−0.4 (3)	C3—C5—C10—C9	177.6 (2)
C4—C1—C2—C3	177.9 (3)	N1—N2—C12—C17	124.6 (2)
N1—N2—C3—C2	−0.5 (2)	C3—N2—C12—C17	−52.6 (3)
C12—N2—C3—C2	176.8 (2)	N1—N2—C12—C13	−53.0 (3)
N1—N2—C3—C5	176.31 (18)	C3—N2—C12—C13	129.8 (2)
C12—N2—C3—C5	−6.4 (3)	C17—C12—C13—C14	0.0 (4)
C1—C2—C3—N2	0.5 (2)	N2—C12—C13—C14	177.6 (2)
C1—C2—C3—C5	−176.1 (2)	C12—C13—C14—C15	−0.5 (4)
N1—C1—C4—F2A	75.1 (12)	C13—C14—C15—C16	0.7 (4)
C2—C1—C4—F2A	−103.1 (12)	C13—C14—C15—S1	179.24 (19)
N1—C1—C4—F3A	−159.1 (11)	O1—S1—C15—C16	−161.84 (19)
C2—C1—C4—F3A	22.7 (11)	O2—S1—C15—C16	−31.5 (2)
N1—C1—C4—F3	158.1 (7)	N3—S1—C15—C16	83.4 (2)
C2—C1—C4—F3	−20.2 (8)	O1—S1—C15—C14	19.6 (2)
N1—C1—C4—F2	39.8 (7)	O2—S1—C15—C14	150.0 (2)
C2—C1—C4—F2	−138.4 (6)	N3—S1—C15—C14	−95.2 (2)
N1—C1—C4—F1	−82.2 (10)	C14—C15—C16—C17	−0.4 (3)
C2—C1—C4—F1	99.6 (10)	S1—C15—C16—C17	−179.00 (17)
N1—C1—C4—F1A	−42.8 (8)	C13—C12—C17—C16	0.2 (3)
C2—C1—C4—F1A	139.0 (8)	N2—C12—C17—C16	−177.30 (19)
N2—C3—C5—C10	143.2 (2)	C15—C16—C17—C12	0.0 (3)
C2—C3—C5—C10	−40.8 (3)	C5S—N2S—C1S—O1S	153.9 (3)
N2—C3—C5—C6	−39.8 (3)	C4S—N2S—C1S—O1S	−5.7 (4)
C2—C3—C5—C6	136.2 (2)	C5S—N2S—C1S—N1S	−24.3 (4)
C10—C5—C6—C7	−0.2 (3)	C4S—N2S—C1S—N1S	176.1 (2)
C3—C5—C6—C7	−177.20 (19)	C3S—N1S—C1S—O1S	137.6 (3)
C5—C6—C7—C8	0.1 (3)	C2S—N1S—C1S—O1S	−8.5 (4)
C6—C7—C8—C9	−0.3 (3)	C3S—N1S—C1S—N2S	−44.2 (4)
C6—C7—C8—C11	−179.6 (2)	C2S—N1S—C1S—N2S	169.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H1*N*···O1*S*	0.87 (1)	2.01 (1)	2.872 (3)	168 (2)
N3—H2*N*···O1*S*^{i}	0.88 (1)	2.10 (1)	2.955 (3)	164 (2)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

4-[5-(4-Methylphenyl)-3-(trifluoromethyl)pyrazol-1-yl]benzenesulfonamide 1,3-dimethyltetrahydropyrimidin-2(1*H*)-one monosolvate (5)

Crystal data

$C_{17}H_{14}F_3N_3O_2S{\cdot}C_6H_{12}N_2O$
M_r = 509.55
Monoclinic, $P2_1/c$
a = 12.4495 (17) Å
b = 8.7822 (13) Å
c = 22.656 (3) Å
β = 97.861 (5)°
V = 2453.9 (6) Å^3
Z = 4
$F(000)$ = 1064
D_x = 1.379 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9925 reflections
θ = 3.6–66.6°
μ = 1.68 mm^{-1}
T = 298 K
Block, colourless
0.20 × 0.20 × 0.18 mm

Data collection

Bruker D8-QUEST PHOTON-100 diffractometer
Radiation source: Incoatec IμS Cu microsource
ω and φ–scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.526, T_{max} = 0.753
25201 measured reflections
4318 independent reflections
3733 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 66.9°, θ_{min} = 3.6°
h = −14→14
k = −10→10
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.118
S = 1.02
4318 reflections
364 parameters
29 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0598P)^2 + 0.786P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.41794 (4)	0.72483 (6)	0.57289 (2)	0.06125 (17)	

O1	0.38898 (13)	0.6787 (2)	0.62889 (7)	0.0869 (5)	
O2	0.37005 (12)	0.85770 (18)	0.54431 (8)	0.0818 (5)	
N1	0.94062 (13)	0.86685 (19)	0.66122 (7)	0.0622 (4)	
N2	0.89648 (12)	0.81202 (17)	0.60722 (7)	0.0542 (4)	
N3	0.39091 (13)	0.5856 (2)	0.52759 (8)	0.0620 (4)	
H1N	0.4063 (19)	0.611 (2)	0.4926 (6)	0.083 (7)*	
H2N	0.4186 (19)	0.5013 (18)	0.5434 (9)	0.087 (8)*	
C1	1.04450 (16)	0.8842 (2)	0.65569 (9)	0.0611 (5)	
C2	1.06875 (15)	0.8419 (2)	0.59995 (9)	0.0595 (5)	
H2A	1.136063	0.844931	0.586550	0.071*	
C3	0.97180 (14)	0.79438 (19)	0.56875 (8)	0.0508 (4)	
C4	1.1196 (2)	0.9403 (3)	0.70779 (11)	0.0805 (7)	
F1	1.1215 (13)	1.0863 (6)	0.7165 (5)	0.146 (4)	0.537 (19)
F2	1.1088 (6)	0.8746 (13)	0.7582 (3)	0.106 (2)	0.537 (19)
F3	1.2216 (4)	0.9050 (16)	0.7002 (4)	0.123 (3)	0.537 (19)
F1A	1.0755 (7)	1.0643 (9)	0.7306 (4)	0.112 (2)	0.463 (19)
F2A	1.1290 (12)	0.8452 (12)	0.7514 (5)	0.140 (4)	0.463 (19)
F3A	1.2113 (8)	0.981 (2)	0.6962 (5)	0.162 (5)	0.463 (19)
C5	0.94815 (13)	0.7296 (2)	0.50877 (8)	0.0490 (4)	
C6	0.87851 (13)	0.6065 (2)	0.49599 (8)	0.0506 (4)	
H6A	0.843189	0.565111	0.525859	0.061*	
C7	0.86134 (14)	0.5453 (2)	0.43937 (8)	0.0539 (4)	
H7A	0.814361	0.463082	0.431819	0.065*	
C8	0.91219 (15)	0.6029 (2)	0.39355 (8)	0.0579 (5)	
C9	0.98180 (17)	0.7245 (2)	0.40657 (9)	0.0642 (5)	
H9A	1.017106	0.765364	0.376597	0.077*	
C10	1.00027 (16)	0.7868 (2)	0.46305 (9)	0.0597 (5)	
H10A	1.048129	0.868048	0.470546	0.072*	
C11	0.8913 (2)	0.5355 (3)	0.33191 (10)	0.0823 (7)	
H11A	0.841042	0.452615	0.331654	0.123*	
H11B	0.861432	0.612155	0.304201	0.123*	
H11C	0.958260	0.498922	0.320603	0.123*	
C12	0.78175 (14)	0.7888 (2)	0.59761 (8)	0.0505 (4)	
C13	0.73524 (16)	0.6991 (2)	0.63745 (8)	0.0598 (5)	
H13A	0.778399	0.652147	0.669010	0.072*	
C14	0.62451 (16)	0.6800 (2)	0.62994 (9)	0.0611 (5)	
H14A	0.592406	0.619688	0.656376	0.073*	
C15	0.56091 (15)	0.7510 (2)	0.58288 (8)	0.0523 (4)	
C16	0.60771 (14)	0.8393 (2)	0.54282 (8)	0.0534 (4)	
H16A	0.564691	0.885626	0.511055	0.064*	
C17	0.71903 (14)	0.8583 (2)	0.55034 (8)	0.0526 (4)	
H17A	0.751369	0.917624	0.523677	0.063*	
O1S	0.47338 (11)	0.66985 (18)	0.41995 (6)	0.0705 (4)	
N1S	0.54014 (13)	0.7997 (2)	0.34753 (8)	0.0687 (5)	
N2S	0.35615 (13)	0.7975 (2)	0.35315 (7)	0.0677 (5)	
C1S	0.45703 (15)	0.7530 (2)	0.37519 (8)	0.0549 (4)	
C2S	0.5267 (2)	0.8980 (4)	0.29596 (12)	0.1010 (9)	0.584 (16)
H1S	0.574357	0.864441	0.268074	0.121*	0.584 (16)

H2S	0.547167	1.001104	0.308134	0.121*	0.584 (16)
C3S	0.4159 (5)	0.8973 (14)	0.2668 (3)	0.091 (2)	0.584 (16)
H3S	0.406119	0.984954	0.240594	0.109*	0.584 (16)
H4S	0.405910	0.807169	0.241903	0.109*	0.584 (16)
C4S	0.3331 (2)	0.8996 (4)	0.30334 (14)	0.1001 (9)	0.584 (16)
H5S	0.265038	0.870624	0.279950	0.120*	0.584 (16)
H6S	0.325220	1.002247	0.317936	0.120*	0.584 (16)
C2SA	0.5267 (2)	0.8980 (4)	0.29596 (12)	0.1010 (9)	0.416 (16)
H7S	0.583895	0.973801	0.301486	0.121*	0.416 (16)
H8S	0.538350	0.837141	0.261690	0.121*	0.416 (16)
C3SA	0.4282 (8)	0.9749 (14)	0.2818 (5)	0.085 (3)	0.416 (16)
H9S	0.413220	0.985276	0.238792	0.102*	0.416 (16)
H10S	0.435769	1.076536	0.298529	0.102*	0.416 (16)
C4SA	0.3331 (2)	0.8996 (4)	0.30334 (14)	0.1001 (9)	0.416 (16)
H11S	0.284975	0.978559	0.314179	0.120*	0.416 (16)
H12S	0.293977	0.843185	0.270375	0.120*	0.416 (16)
C5S	0.65001 (19)	0.7594 (4)	0.37258 (13)	0.0941 (8)	
H13S	0.700024	0.800549	0.348052	0.141*	
H14S	0.665658	0.800556	0.412086	0.141*	
H15S	0.657044	0.650610	0.374190	0.141*	
C6S	0.26640 (17)	0.7537 (3)	0.38401 (12)	0.0850 (7)	
H16S	0.200077	0.793538	0.363098	0.128*	
H17S	0.262107	0.644691	0.385612	0.128*	
H18S	0.277552	0.793959	0.423776	0.128*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0469 (3)	0.0736 (3)	0.0663 (3)	0.0024 (2)	0.0187 (2)	0.0018 (2)
O1	0.0710 (9)	0.1265 (14)	0.0697 (9)	−0.0083 (9)	0.0335 (7)	−0.0009 (9)
O2	0.0571 (8)	0.0745 (10)	0.1146 (12)	0.0166 (7)	0.0140 (8)	0.0083 (9)
N1	0.0612 (10)	0.0664 (10)	0.0561 (9)	−0.0045 (8)	−0.0021 (7)	−0.0045 (8)
N2	0.0474 (8)	0.0569 (9)	0.0562 (8)	−0.0003 (7)	−0.0001 (7)	−0.0036 (7)
N3	0.0529 (9)	0.0713 (11)	0.0636 (10)	−0.0069 (8)	0.0145 (8)	0.0069 (9)
C1	0.0593 (11)	0.0561 (11)	0.0640 (11)	−0.0075 (9)	−0.0054 (9)	0.0017 (9)
C2	0.0486 (10)	0.0561 (11)	0.0717 (12)	−0.0060 (8)	0.0007 (9)	0.0029 (9)
C3	0.0467 (9)	0.0441 (9)	0.0604 (10)	0.0005 (7)	0.0030 (8)	0.0040 (8)
C4	0.0760 (16)	0.0854 (17)	0.0740 (15)	−0.0148 (14)	−0.0119 (12)	−0.0004 (13)
F1	0.196 (9)	0.068 (2)	0.142 (6)	−0.021 (4)	−0.092 (6)	−0.013 (3)
F2	0.082 (3)	0.170 (7)	0.061 (2)	−0.031 (3)	−0.009 (2)	0.013 (3)
F3	0.057 (3)	0.182 (7)	0.122 (4)	−0.022 (3)	−0.020 (2)	−0.041 (4)
F1A	0.129 (5)	0.109 (4)	0.092 (3)	−0.037 (3)	−0.013 (3)	−0.034 (3)
F2A	0.171 (9)	0.108 (4)	0.115 (7)	0.005 (4)	−0.070 (5)	0.025 (4)
F3A	0.120 (7)	0.245 (13)	0.124 (5)	−0.124 (8)	0.024 (5)	−0.056 (7)
C5	0.0396 (8)	0.0480 (9)	0.0588 (10)	0.0041 (7)	0.0045 (7)	0.0030 (8)
C6	0.0426 (9)	0.0489 (9)	0.0611 (10)	0.0006 (7)	0.0106 (7)	0.0009 (8)
C7	0.0417 (9)	0.0531 (10)	0.0666 (11)	0.0024 (8)	0.0061 (8)	−0.0053 (8)
C8	0.0500 (10)	0.0625 (11)	0.0611 (11)	0.0122 (9)	0.0074 (8)	−0.0015 (9)

C9	0.0592 (11)	0.0728 (13)	0.0635 (12)	0.0017 (10)	0.0187 (9)	0.0100 (10)
C10	0.0515 (10)	0.0564 (11)	0.0712 (12)	−0.0069 (8)	0.0088 (9)	0.0048 (9)
C11	0.0911 (16)	0.0916 (17)	0.0652 (13)	0.0070 (13)	0.0144 (11)	−0.0116 (12)
C12	0.0474 (9)	0.0500 (9)	0.0540 (10)	0.0011 (7)	0.0062 (7)	−0.0047 (8)
C13	0.0597 (11)	0.0641 (12)	0.0540 (10)	0.0018 (9)	0.0021 (8)	0.0093 (9)
C14	0.0606 (11)	0.0673 (12)	0.0564 (10)	−0.0048 (9)	0.0119 (9)	0.0082 (9)
C15	0.0489 (10)	0.0545 (10)	0.0547 (10)	0.0024 (8)	0.0113 (8)	−0.0018 (8)
C16	0.0468 (9)	0.0559 (10)	0.0574 (10)	0.0050 (8)	0.0066 (8)	0.0041 (8)
C17	0.0504 (10)	0.0516 (10)	0.0565 (10)	0.0012 (8)	0.0099 (8)	0.0062 (8)
O1S	0.0572 (8)	0.0912 (10)	0.0638 (8)	0.0037 (7)	0.0115 (6)	0.0201 (8)
N1S	0.0546 (9)	0.0859 (12)	0.0663 (10)	0.0040 (8)	0.0103 (8)	0.0207 (9)
N2S	0.0514 (9)	0.0873 (12)	0.0622 (10)	0.0056 (8)	−0.0001 (7)	0.0004 (9)
C1S	0.0515 (10)	0.0621 (11)	0.0503 (10)	0.0026 (8)	0.0047 (8)	−0.0013 (8)
C2S	0.0911 (18)	0.124 (2)	0.0878 (17)	−0.0044 (17)	0.0131 (14)	0.0457 (17)
C3S	0.113 (4)	0.102 (5)	0.056 (3)	0.016 (4)	0.001 (2)	0.014 (3)
C4S	0.0854 (18)	0.101 (2)	0.105 (2)	0.0151 (15)	−0.0189 (15)	0.0244 (16)
C2SA	0.0911 (18)	0.124 (2)	0.0878 (17)	−0.0044 (17)	0.0131 (14)	0.0457 (17)
C3SA	0.106 (5)	0.073 (5)	0.073 (5)	0.008 (4)	0.007 (4)	0.017 (4)
C4SA	0.0854 (18)	0.101 (2)	0.105 (2)	0.0151 (15)	−0.0189 (15)	0.0244 (16)
C5S	0.0536 (12)	0.132 (2)	0.0985 (18)	0.0083 (13)	0.0174 (12)	0.0368 (17)
C6S	0.0485 (12)	0.1091 (19)	0.0972 (17)	0.0005 (12)	0.0088 (11)	−0.0092 (15)

Geometric parameters (Å, º)

S1—O1	1.4246 (15)	C13—H13A	0.9300
S1—O2	1.4250 (16)	C14—C15	1.386 (3)
S1—N3	1.6020 (19)	C14—H14A	0.9300
S1—C15	1.7783 (19)	C15—C16	1.382 (3)
N1—C1	1.325 (3)	C16—C17	1.383 (3)
N1—N2	1.359 (2)	C16—H16A	0.9300
N2—C3	1.373 (2)	C17—H17A	0.9300
N2—C12	1.430 (2)	O1S—C1S	1.244 (2)
N3—H1N	0.869 (9)	N1S—C1S	1.345 (2)
N3—H2N	0.873 (9)	N1S—C2SA	1.444 (3)
C1—C2	1.389 (3)	N1S—C2S	1.444 (3)
C1—C4	1.486 (3)	N1S—C5S	1.451 (3)
C2—C3	1.377 (3)	N2S—C1S	1.344 (2)
C2—H2A	0.9300	N2S—C4SA	1.439 (3)
C3—C5	1.466 (3)	N2S—C4S	1.439 (3)
C4—F3A	1.259 (6)	N2S—C6S	1.449 (3)
C4—F2A	1.286 (7)	C2S—C3S	1.446 (6)
C4—F1	1.297 (5)	C2S—H1S	0.9700
C4—F2	1.302 (6)	C2S—H2S	0.9700
C4—F3	1.341 (6)	C3S—C4S	1.407 (6)
C4—F1A	1.353 (7)	C3S—H3S	0.9700
C5—C10	1.389 (3)	C3S—H4S	0.9700
C5—C6	1.391 (2)	C4S—H5S	0.9700
C6—C7	1.380 (3)	C4S—H6S	0.9700

C6—H6A	0.9300	C2SA—C3SA	1.398 (9)
C7—C8	1.384 (3)	C2SA—H7S	0.9700
C7—H7A	0.9300	C2SA—H8S	0.9700
C8—C9	1.381 (3)	C3SA—C4SA	1.495 (10)
C8—C11	1.506 (3)	C3SA—H9S	0.9700
C9—C10	1.382 (3)	C3SA—H10S	0.9700
C9—H9A	0.9300	C4SA—H11S	0.9700
C10—H10A	0.9300	C4SA—H12S	0.9700
C11—H11A	0.9600	C5S—H13S	0.9600
C11—H11B	0.9600	C5S—H14S	0.9600
C11—H11C	0.9600	C5S—H15S	0.9600
C12—C17	1.379 (3)	C6S—H16S	0.9600
C12—C13	1.383 (3)	C6S—H17S	0.9600
C13—C14	1.376 (3)	C6S—H18S	0.9600

O1—S1—O2	119.78 (11)	C14—C15—S1	119.76 (14)
O1—S1—N3	107.27 (10)	C15—C16—C17	119.49 (17)
O2—S1—N3	107.20 (10)	C15—C16—H16A	120.3
O1—S1—C15	107.11 (9)	C17—C16—H16A	120.3
O2—S1—C15	107.54 (9)	C12—C17—C16	119.59 (17)
N3—S1—C15	107.40 (8)	C12—C17—H17A	120.2
C1—N1—N2	103.60 (15)	C16—C17—H17A	120.2
N1—N2—C3	112.59 (15)	C1S—N1S—C2SA	123.21 (19)
N1—N2—C12	117.39 (15)	C1S—N1S—C2S	123.21 (19)
C3—N2—C12	129.94 (15)	C1S—N1S—C5S	119.20 (17)
S1—N3—H1N	109.8 (16)	C2SA—N1S—C5S	117.44 (19)
S1—N3—H2N	110.4 (17)	C2S—N1S—C5S	117.44 (19)
H1N—N3—H2N	117.6 (15)	C1S—N2S—C4SA	123.2 (2)
N1—C1—C2	113.06 (16)	C1S—N2S—C4S	123.2 (2)
N1—C1—C4	118.6 (2)	C1S—N2S—C6S	119.13 (18)
C2—C1—C4	128.3 (2)	C4SA—N2S—C6S	117.4 (2)
C3—C2—C1	105.28 (17)	C4S—N2S—C6S	117.4 (2)
C3—C2—H2A	127.4	O1S—C1S—N2S	120.91 (18)
C1—C2—H2A	127.4	O1S—C1S—N1S	120.55 (17)
N2—C3—C2	105.47 (16)	N2S—C1S—N1S	118.54 (17)
N2—C3—C5	124.35 (15)	N1S—C2S—C3S	111.4 (4)
C2—C3—C5	130.11 (17)	N1S—C2S—H1S	109.4
F3A—C4—F2A	110.8 (7)	C3S—C2S—H1S	109.4
F1—C4—F2	107.8 (6)	N1S—C2S—H2S	109.4
F1—C4—F3	104.4 (5)	C3S—C2S—H2S	109.4
F2—C4—F3	102.9 (5)	H1S—C2S—H2S	108.0
F3A—C4—F1A	106.0 (6)	C4S—C3S—C2S	117.5 (5)
F2A—C4—F1A	103.2 (6)	C4S—C3S—H3S	107.9
F3A—C4—C1	114.8 (5)	C2S—C3S—H3S	107.9
F2A—C4—C1	112.1 (6)	C4S—C3S—H4S	107.9
F1—C4—C1	116.4 (4)	C2S—C3S—H4S	107.9
F2—C4—C1	114.9 (4)	H3S—C3S—H4S	107.2
F3—C4—C1	109.0 (4)	C3S—C4S—N2S	111.6 (4)

F1A—C4—C1	109.0 (4)	C3S—C4S—H5S	109.3
C10—C5—C6	117.86 (17)	N2S—C4S—H5S	109.3
C10—C5—C3	119.72 (16)	C3S—C4S—H6S	109.3
C6—C5—C3	122.35 (16)	N2S—C4S—H6S	109.3
C7—C6—C5	120.60 (17)	H5S—C4S—H6S	108.0
C7—C6—H6A	119.7	C3SA—C2SA—N1S	118.4 (4)
C5—C6—H6A	119.7	C3SA—C2SA—H7S	107.7
C6—C7—C8	121.74 (17)	N1S—C2SA—H7S	107.7
C6—C7—H7A	119.1	C3SA—C2SA—H8S	107.7
C8—C7—H7A	119.1	N1S—C2SA—H8S	107.7
C9—C8—C7	117.43 (18)	H7S—C2SA—H8S	107.1
C9—C8—C11	121.7 (2)	C2SA—C3SA—C4SA	114.8 (6)
C7—C8—C11	120.9 (2)	C2SA—C3SA—H9S	108.6
C8—C9—C10	121.61 (18)	C4SA—C3SA—H9S	108.6
C8—C9—H9A	119.2	C2SA—C3SA—H10S	108.6
C10—C9—H9A	119.2	C4SA—C3SA—H10S	108.6
C9—C10—C5	120.76 (18)	H9S—C3SA—H10S	107.5
C9—C10—H10A	119.6	N2S—C4SA—C3SA	116.8 (4)
C5—C10—H10A	119.6	N2S—C4SA—H11S	108.1
C8—C11—H11A	109.5	C3SA—C4SA—H11S	108.1
C8—C11—H11B	109.5	N2S—C4SA—H12S	108.1
H11A—C11—H11B	109.5	C3SA—C4SA—H12S	108.1
C8—C11—H11C	109.5	H11S—C4SA—H12S	107.3
H11A—C11—H11C	109.5	N1S—C5S—H13S	109.5
H11B—C11—H11C	109.5	N1S—C5S—H14S	109.5
C17—C12—C13	121.06 (17)	H13S—C5S—H14S	109.5
C17—C12—N2	120.19 (16)	N1S—C5S—H15S	109.5
C13—C12—N2	118.72 (16)	H13S—C5S—H15S	109.5
C14—C13—C12	119.36 (17)	H14S—C5S—H15S	109.5
C14—C13—H13A	120.3	N2S—C6S—H16S	109.5
C12—C13—H13A	120.3	N2S—C6S—H17S	109.5
C13—C14—C15	119.85 (18)	H16S—C6S—H17S	109.5
C13—C14—H14A	120.1	N2S—C6S—H18S	109.5
C15—C14—H14A	120.1	H16S—C6S—H18S	109.5
C16—C15—C14	120.65 (17)	H17S—C6S—H18S	109.5
C16—C15—S1	119.58 (14)		

C1—N1—N2—C3	0.4 (2)	C3—N2—C12—C13	129.1 (2)
C1—N1—N2—C12	−176.62 (16)	C17—C12—C13—C14	−0.5 (3)
N2—N1—C1—C2	−0.2 (2)	N2—C12—C13—C14	177.77 (17)
N2—N1—C1—C4	−178.68 (18)	C12—C13—C14—C15	−0.2 (3)
N1—C1—C2—C3	−0.1 (2)	C13—C14—C15—C16	0.9 (3)
C4—C1—C2—C3	178.2 (2)	C13—C14—C15—S1	179.45 (15)
N1—N2—C3—C2	−0.5 (2)	O1—S1—C15—C16	−159.85 (16)
C12—N2—C3—C2	176.06 (17)	O2—S1—C15—C16	−29.88 (18)
N1—N2—C3—C5	176.51 (16)	N3—S1—C15—C16	85.20 (16)
C12—N2—C3—C5	−6.9 (3)	O1—S1—C15—C14	21.56 (19)
C1—C2—C3—N2	0.4 (2)	O2—S1—C15—C14	151.52 (16)

C1—C2—C3—C5	−176.41 (18)	N3—S1—C15—C14	−93.40 (17)
N1—C1—C4—F3A	−167.1 (10)	C14—C15—C16—C17	−0.8 (3)
C2—C1—C4—F3A	14.7 (10)	S1—C15—C16—C17	−179.37 (14)
N1—C1—C4—F2A	65.3 (8)	C13—C12—C17—C16	0.6 (3)
C2—C1—C4—F2A	−112.9 (8)	N2—C12—C17—C16	−177.67 (16)
N1—C1—C4—F1	−81.5 (10)	C15—C16—C17—C12	0.1 (3)
C2—C1—C4—F1	100.3 (10)	C4SA—N2S—C1S—O1S	176.8 (2)
N1—C1—C4—F2	45.9 (6)	C4S—N2S—C1S—O1S	176.8 (2)
C2—C1—C4—F2	−132.4 (6)	C6S—N2S—C1S—O1S	3.2 (3)
N1—C1—C4—F3	160.7 (6)	C4SA—N2S—C1S—N1S	−3.6 (3)
C2—C1—C4—F3	−17.5 (7)	C4S—N2S—C1S—N1S	−3.6 (3)
N1—C1—C4—F1A	−48.3 (6)	C6S—N2S—C1S—N1S	−177.3 (2)
C2—C1—C4—F1A	133.4 (5)	C2SA—N1S—C1S—O1S	−179.0 (2)
N2—C3—C5—C10	144.19 (18)	C2S—N1S—C1S—O1S	−179.0 (2)
C2—C3—C5—C10	−39.6 (3)	C5S—N1S—C1S—O1S	−3.7 (3)
N2—C3—C5—C6	−39.0 (3)	C2SA—N1S—C1S—N2S	1.4 (3)
C2—C3—C5—C6	137.3 (2)	C2S—N1S—C1S—N2S	1.4 (3)
C10—C5—C6—C7	−0.7 (3)	C5S—N1S—C1S—N2S	176.7 (2)
C3—C5—C6—C7	−177.66 (16)	C1S—N1S—C2S—C3S	−19.3 (6)
C5—C6—C7—C8	0.1 (3)	C5S—N1S—C2S—C3S	165.2 (5)
C6—C7—C8—C9	0.3 (3)	N1S—C2S—C3S—C4S	41.2 (11)
C6—C7—C8—C11	−179.29 (18)	C2S—C3S—C4S—N2S	−43.3 (11)
C7—C8—C9—C10	−0.1 (3)	C1S—N2S—C4S—C3S	24.1 (6)
C11—C8—C9—C10	179.5 (2)	C6S—N2S—C4S—C3S	−162.1 (6)
C8—C9—C10—C5	−0.6 (3)	C1S—N1S—C2SA—C3SA	14.3 (8)
C6—C5—C10—C9	1.0 (3)	C5S—N1S—C2SA—C3SA	−161.1 (8)
C3—C5—C10—C9	178.00 (17)	N1S—C2SA—C3SA—C4SA	−25.6 (13)
N1—N2—C12—C17	123.84 (19)	C1S—N2S—C4SA—C3SA	−8.9 (8)
C3—N2—C12—C17	−52.6 (3)	C6S—N2S—C4SA—C3SA	164.9 (7)
N1—N2—C12—C13	−54.4 (2)	C2SA—C3SA—C4SA—N2S	23.2 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H1*N*···O1*S*	0.87 (1)	2.01 (1)	2.870 (2)	168 (2)
N3—H2*N*···O1*S*^{i}	0.87 (1)	2.11 (1)	2.958 (2)	164 (2)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

4-[5-(4-Methylphenyl)-3-(trifluoromethyl)pyrazol-1-yl]benzenesulfonamide dimethyl sulfoxide monosolvate (6)

Crystal data

$C_{17}H_{14}F_3N_3O_2S·C_2H_6OS$
M_r = 459.50
Monoclinic, $P2_1/c$
a = 11.9884 (3) Å
b = 9.0230 (3) Å
c = 20.8537 (6) Å
β = 100.3908 (9)°
V = 2218.78 (11) Å^3
Z = 4
$F(000)$ = 952
D_x = 1.376 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9824 reflections
θ = 4.0–66.8°

μ = 2.63 mm^{-1}
T = 298 K

Block, colourless
0.14 × 0.12 × 0.12 mm

Data collection

Bruker D8-QUEST PHOTON-100 diffractometer
Radiation source: Incoatec IμS Cu microsource
ω and φ–scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.476, T_{max} = 0.753
22464 measured reflections

3916 independent reflections
3520 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 66.8°, θ_{min} = 3.8°
h = −14→14
k = −10→10
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.126
S = 1.04
3916 reflections
318 parameters
15 restraints
Primary atom site location: dual

Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 0.7974P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.44222 (4)	0.73094 (6)	0.58322 (3)	0.05825 (19)	
O1	0.43028 (13)	0.6822 (2)	0.64670 (8)	0.0748 (5)	
O2	0.38751 (13)	0.8632 (2)	0.55698 (10)	0.0865 (6)	
N1	0.99161 (13)	0.8825 (2)	0.64689 (8)	0.0614 (4)	
N2	0.93516 (12)	0.8229 (2)	0.59031 (8)	0.0520 (4)	
N3	0.39656 (15)	0.5997 (3)	0.53365 (10)	0.0695 (5)	
H1N	0.403 (2)	0.621 (3)	0.4937 (7)	0.086 (8)*	
H2N	0.426 (2)	0.5160 (18)	0.5493 (10)	0.080 (8)*	
C1	1.09613 (16)	0.8974 (3)	0.63600 (11)	0.0616 (5)	
C2	1.10903 (15)	0.8487 (2)	0.57482 (11)	0.0584 (5)	
H2A	1.175041	0.849422	0.557261	0.070*	
C3	1.00368 (14)	0.7992 (2)	0.54545 (9)	0.0501 (4)	
C4	1.1841 (2)	0.9581 (3)	0.68942 (14)	0.0872 (8)	
F1	1.2791 (4)	0.8978 (10)	0.6941 (3)	0.103 (3)	0.435 (10)
F2	1.2022 (10)	1.0988 (6)	0.6870 (8)	0.217 (8)	0.435 (10)
F3	1.1604 (5)	0.9368 (15)	0.7500 (3)	0.128 (5)	0.435 (10)
F1A	1.2289 (11)	0.8568 (7)	0.7273 (6)	0.244 (8)	0.565 (10)
F2A	1.2654 (7)	1.0176 (14)	0.6642 (4)	0.198 (5)	0.565 (10)

F3A	1.1478 (4)	1.0607 (9)	0.7190 (3)	0.122 (3)	0.565 (10)
C5	0.96935 (15)	0.7264 (2)	0.48219 (9)	0.0504 (4)	
C6	0.88711 (16)	0.6159 (2)	0.47095 (10)	0.0550 (5)	
H6A	0.849346	0.587856	0.504251	0.066*	
C7	0.86100 (17)	0.5475 (2)	0.41090 (11)	0.0618 (5)	
H7A	0.804298	0.475879	0.404152	0.074*	
C8	0.9169 (2)	0.5827 (3)	0.36076 (11)	0.0689 (6)	
C9	1.0000 (2)	0.6903 (3)	0.37240 (12)	0.0794 (7)	
H9A	1.039563	0.715210	0.339438	0.095*	
C10	1.0259 (2)	0.7618 (3)	0.43164 (11)	0.0686 (6)	
H10A	1.081833	0.834444	0.437849	0.082*	
C11	0.8873 (3)	0.5063 (4)	0.29538 (13)	0.1020 (9)	
H11A	0.827940	0.435486	0.296642	0.153*	
H11B	0.861991	0.578628	0.262165	0.153*	
H11C	0.953037	0.456362	0.285822	0.153*	
C12	0.81593 (14)	0.7978 (2)	0.58644 (9)	0.0479 (4)	
C13	0.66715 (16)	0.6961 (3)	0.63440 (10)	0.0607 (5)	
H13A	0.642776	0.642659	0.667416	0.073*	
C14	0.78154 (16)	0.7171 (3)	0.63526 (10)	0.0618 (5)	
H14A	0.834895	0.676792	0.668636	0.074*	
C15	0.58944 (14)	0.7553 (2)	0.58406 (9)	0.0482 (4)	
C16	0.62439 (15)	0.8371 (2)	0.53513 (9)	0.0518 (5)	
H16A	0.571201	0.877375	0.501672	0.062*	
C17	0.73877 (15)	0.8585 (2)	0.53635 (9)	0.0519 (5)	
H17A	0.763427	0.913147	0.503771	0.062*	
O1S	0.47134 (17)	0.6580 (2)	0.41112 (8)	0.0915 (6)	
S1S	0.43698 (8)	0.68487 (10)	0.34114 (4)	0.0876 (4)	0.807 (3)
C1S	0.5584 (5)	0.6975 (8)	0.3078 (2)	0.198 (3)	0.807 (3)
H1S1	0.538075	0.715194	0.261751	0.298*	0.807 (3)
H1S2	0.604363	0.777903	0.327870	0.298*	0.807 (3)
H1S3	0.600290	0.606580	0.315160	0.298*	0.807 (3)
C2S	0.3926 (7)	0.8682 (6)	0.3303 (3)	0.235 (4)	0.807 (3)
H2S1	0.369592	0.888148	0.284653	0.352*	0.807 (3)
H2S2	0.329712	0.884567	0.352215	0.352*	0.807 (3)
H2S3	0.453870	0.932914	0.348210	0.352*	0.807 (3)
S1SA	0.5073 (7)	0.7789 (6)	0.3699 (2)	0.153 (3)	0.193 (3)
C1SA	0.5584 (5)	0.6975 (8)	0.3078 (2)	0.198 (3)	0.193 (3)
H1S4	0.582101	0.772639	0.280502	0.298*	0.193 (3)
H1S5	0.621958	0.635925	0.325183	0.298*	0.193 (3)
H1S6	0.500104	0.638050	0.282502	0.298*	0.193 (3)
C2SA	0.3926 (7)	0.8682 (6)	0.3303 (3)	0.235 (4)	0.193 (3)
H2S4	0.415844	0.945446	0.303989	0.352*	0.193 (3)
H2S5	0.344523	0.799568	0.302991	0.352*	0.193 (3)
H2S6	0.351645	0.910595	0.361412	0.352*	0.193 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0349 (3)	0.0718 (3)	0.0718 (3)	0.0014 (2)	0.0198 (2)	0.0103 (2)
O1	0.0589 (9)	0.1013 (12)	0.0720 (10)	−0.0075 (8)	0.0328 (7)	0.0038 (9)
O2	0.0450 (8)	0.0863 (12)	0.1343 (15)	0.0178 (8)	0.0321 (9)	0.0303 (11)
N1	0.0415 (8)	0.0819 (12)	0.0585 (9)	−0.0047 (8)	0.0026 (7)	−0.0073 (9)
N2	0.0328 (7)	0.0692 (10)	0.0534 (9)	−0.0038 (7)	0.0056 (6)	0.0012 (7)
N3	0.0484 (10)	0.0910 (15)	0.0675 (12)	−0.0139 (10)	0.0058 (8)	0.0101 (11)
C1	0.0364 (9)	0.0714 (13)	0.0740 (13)	−0.0043 (9)	0.0018 (9)	−0.0072 (10)
C2	0.0331 (9)	0.0646 (12)	0.0778 (13)	−0.0026 (8)	0.0111 (8)	−0.0024 (10)
C3	0.0348 (9)	0.0554 (11)	0.0603 (11)	−0.0001 (8)	0.0090 (8)	0.0042 (8)
C4	0.0521 (14)	0.105 (2)	0.0974 (19)	−0.0078 (14)	−0.0043 (13)	−0.0276 (18)
F1	0.040 (2)	0.168 (7)	0.091 (3)	0.032 (3)	−0.0195 (19)	−0.049 (4)
F2	0.174 (11)	0.084 (4)	0.322 (16)	−0.047 (6)	−0.146 (10)	0.020 (6)
F3	0.078 (3)	0.247 (12)	0.060 (3)	−0.047 (5)	0.013 (3)	−0.044 (5)
F1A	0.220 (11)	0.175 (6)	0.252 (12)	−0.035 (7)	−0.183 (10)	0.043 (7)
F2A	0.104 (4)	0.299 (12)	0.207 (7)	−0.129 (6)	0.070 (5)	−0.158 (8)
F3A	0.093 (3)	0.172 (7)	0.088 (3)	0.009 (3)	−0.016 (2)	−0.072 (4)
C5	0.0370 (9)	0.0566 (11)	0.0585 (11)	0.0029 (8)	0.0107 (8)	0.0044 (8)
C6	0.0441 (10)	0.0598 (11)	0.0622 (11)	−0.0024 (9)	0.0126 (8)	0.0030 (9)
C7	0.0505 (11)	0.0622 (12)	0.0717 (13)	−0.0031 (9)	0.0084 (9)	−0.0029 (10)
C8	0.0681 (13)	0.0755 (15)	0.0628 (12)	0.0020 (11)	0.0108 (10)	−0.0029 (11)
C9	0.0817 (16)	0.0945 (18)	0.0695 (14)	−0.0117 (14)	0.0335 (12)	−0.0008 (13)
C10	0.0602 (13)	0.0785 (15)	0.0713 (14)	−0.0154 (11)	0.0231 (11)	−0.0008 (11)
C11	0.118 (2)	0.115 (2)	0.0732 (16)	−0.010 (2)	0.0190 (15)	−0.0184 (16)
C12	0.0321 (8)	0.0598 (11)	0.0517 (10)	−0.0025 (8)	0.0077 (7)	0.0012 (8)
C13	0.0450 (10)	0.0801 (14)	0.0584 (11)	−0.0032 (10)	0.0134 (8)	0.0204 (10)
C14	0.0413 (10)	0.0853 (15)	0.0570 (11)	0.0001 (10)	0.0040 (8)	0.0206 (10)
C15	0.0343 (9)	0.0565 (10)	0.0553 (10)	−0.0003 (8)	0.0125 (7)	0.0025 (8)
C16	0.0359 (9)	0.0637 (12)	0.0556 (10)	0.0034 (8)	0.0072 (7)	0.0121 (9)
C17	0.0401 (9)	0.0631 (12)	0.0537 (10)	−0.0017 (8)	0.0119 (8)	0.0124 (9)
O1S	0.1077 (14)	0.1002 (14)	0.0645 (10)	−0.0028 (11)	0.0097 (9)	0.0122 (9)
S1S	0.1060 (7)	0.0805 (6)	0.0628 (5)	−0.0200 (5)	−0.0212 (4)	0.0063 (4)
C1S	0.224 (6)	0.257 (7)	0.130 (4)	−0.029 (5)	0.072 (4)	0.069 (4)
C2S	0.390 (10)	0.126 (4)	0.150 (4)	0.094 (5)	−0.056 (5)	0.011 (3)
S1SA	0.249 (8)	0.106 (3)	0.074 (3)	−0.082 (4)	−0.046 (3)	0.016 (2)
C1SA	0.224 (6)	0.257 (7)	0.130 (4)	−0.029 (5)	0.072 (4)	0.069 (4)
C2SA	0.390 (10)	0.126 (4)	0.150 (4)	0.094 (5)	−0.056 (5)	0.011 (3)

Geometric parameters (Å, º)

S1—O2	1.4227 (17)	C11—H11A	0.9600
S1—O1	1.4265 (16)	C11—H11B	0.9600
S1—N3	1.602 (2)	C11—H11C	0.9600
S1—C15	1.7755 (17)	C12—C14	1.375 (3)
N1—C1	1.320 (3)	C12—C17	1.378 (3)
N1—N2	1.361 (2)	C13—C15	1.379 (3)

N2—C3	1.369 (2)	C13—C14	1.381 (3)
N2—C12	1.435 (2)	C13—H13A	0.9300
N3—H1N	0.873 (9)	C14—H14A	0.9300
N3—H2N	0.870 (9)	C15—C16	1.384 (3)
C1—C2	1.384 (3)	C16—C17	1.380 (2)
C1—C4	1.493 (3)	C16—H16A	0.9300
C2—C3	1.375 (3)	C17—H17A	0.9300
C2—H2A	0.9300	O1S—S1S	1.4634 (18)
C3—C5	1.464 (3)	O1S—S1SA	1.499 (5)
C4—F3A	1.234 (4)	S1S—C1S	1.727 (5)
C4—F1	1.250 (5)	S1S—C2S	1.740 (5)
C4—F1A	1.263 (5)	C1S—H1S1	0.9600
C4—F2	1.291 (5)	C1S—H1S2	0.9600
C4—F2A	1.303 (6)	C1S—H1S3	0.9600
C4—F3	1.358 (6)	C2S—H2S1	0.9600
C5—C10	1.389 (3)	C2S—H2S2	0.9600
C5—C6	1.392 (3)	C2S—H2S3	0.9600
C6—C7	1.380 (3)	S1SA—C2SA	1.676 (9)
C6—H6A	0.9300	S1SA—C1SA	1.697 (9)
C7—C8	1.376 (3)	C1SA—H1S4	0.9600
C7—H7A	0.9300	C1SA—H1S5	0.9600
C8—C9	1.382 (4)	C1SA—H1S6	0.9600
C8—C11	1.512 (3)	C2SA—H2S4	0.9600
C9—C10	1.378 (3)	C2SA—H2S5	0.9600
C9—H9A	0.9300	C2SA—H2S6	0.9600
C10—H10A	0.9300		

O2—S1—O1	119.93 (11)	C8—C11—H11B	109.5
O2—S1—N3	106.97 (12)	H11A—C11—H11B	109.5
O1—S1—N3	106.92 (11)	C8—C11—H11C	109.5
O2—S1—C15	106.76 (9)	H11A—C11—H11C	109.5
O1—S1—C15	107.15 (9)	H11B—C11—H11C	109.5
N3—S1—C15	108.74 (9)	C14—C12—C17	121.48 (16)
C1—N1—N2	103.30 (16)	C14—C12—N2	118.09 (16)
N1—N2—C3	112.88 (14)	C17—C12—N2	120.38 (16)
N1—N2—C12	116.47 (15)	C15—C13—C14	119.33 (18)
C3—N2—C12	130.64 (16)	C15—C13—H13A	120.3
S1—N3—H1N	111.8 (18)	C14—C13—H13A	120.3
S1—N3—H2N	109.5 (17)	C12—C14—C13	119.51 (18)
H1N—N3—H2N	116.7 (16)	C12—C14—H14A	120.2
N1—C1—C2	113.18 (17)	C13—C14—H14A	120.2
N1—C1—C4	118.3 (2)	C13—C15—C16	120.99 (16)
C2—C1—C4	128.51 (19)	C13—C15—S1	119.56 (14)
C3—C2—C1	105.51 (17)	C16—C15—S1	119.43 (14)
C3—C2—H2A	127.2	C17—C16—C15	119.51 (17)
C1—C2—H2A	127.2	C17—C16—H16A	120.2
N2—C3—C2	105.12 (17)	C15—C16—H16A	120.2
N2—C3—C5	125.46 (16)	C12—C17—C16	119.18 (17)

C2—C3—C5	129.29 (18)	C12—C17—H17A	120.4
F3A—C4—F1A	112.3 (6)	C16—C17—H17A	120.4
F1—C4—F2	105.9 (5)	O1S—S1S—C1S	107.9 (2)
F3A—C4—F2A	104.4 (4)	O1S—S1S—C2S	108.1 (2)
F1A—C4—F2A	106.6 (5)	C1S—S1S—C2S	98.4 (4)
F1—C4—F3	101.9 (5)	S1S—C1S—H1S1	109.5
F2—C4—F3	103.9 (6)	S1S—C1S—H1S2	109.5
F3A—C4—C1	112.5 (3)	H1S1—C1S—H1S2	109.5
F1—C4—C1	114.2 (3)	S1S—C1S—H1S3	109.5
F1A—C4—C1	111.4 (3)	H1S1—C1S—H1S3	109.5
F2—C4—C1	115.7 (4)	H1S2—C1S—H1S3	109.5
F2A—C4—C1	109.2 (4)	S1S—C2S—H2S1	109.5
F3—C4—C1	113.8 (3)	S1S—C2S—H2S2	109.5
C10—C5—C6	117.66 (19)	H2S1—C2S—H2S2	109.5
C10—C5—C3	118.96 (18)	S1S—C2S—H2S3	109.5
C6—C5—C3	123.25 (17)	H2S1—C2S—H2S3	109.5
C7—C6—C5	120.73 (19)	H2S2—C2S—H2S3	109.5
C7—C6—H6A	119.6	O1S—S1SA—C2SA	109.7 (5)
C5—C6—H6A	119.6	O1S—S1SA—C1SA	107.7 (4)
C6—C7—C8	121.6 (2)	C2SA—S1SA—C1SA	102.1 (4)
C6—C7—H7A	119.2	S1SA—C1SA—H1S4	109.5
C8—C7—H7A	119.2	S1SA—C1SA—H1S5	109.5
C9—C8—C7	117.6 (2)	H1S4—C1SA—H1S5	109.5
C9—C8—C11	121.6 (2)	S1SA—C1SA—H1S6	109.5
C7—C8—C11	120.8 (2)	H1S4—C1SA—H1S6	109.5
C10—C9—C8	121.7 (2)	H1S5—C1SA—H1S6	109.5
C10—C9—H9A	119.2	S1SA—C2SA—H2S4	109.5
C8—C9—H9A	119.2	S1SA—C2SA—H2S5	109.5
C9—C10—C5	120.7 (2)	H2S4—C2SA—H2S5	109.5
C9—C10—H10A	119.6	S1SA—C2SA—H2S6	109.5
C5—C10—H10A	119.6	H2S4—C2SA—H2S6	109.5
C8—C11—H11A	109.5	H2S5—C2SA—H2S6	109.5

C1—N1—N2—C3	0.9 (2)	C3—C5—C6—C7	−177.68 (18)
C1—N1—N2—C12	−178.05 (18)	C5—C6—C7—C8	1.8 (3)
N2—N1—C1—C2	−0.4 (3)	C6—C7—C8—C9	−0.5 (3)
N2—N1—C1—C4	−178.7 (2)	C6—C7—C8—C11	179.9 (2)
N1—C1—C2—C3	−0.2 (3)	C7—C8—C9—C10	−0.7 (4)
C4—C1—C2—C3	177.9 (2)	C11—C8—C9—C10	178.9 (3)
N1—N2—C3—C2	−1.0 (2)	C8—C9—C10—C5	0.6 (4)
C12—N2—C3—C2	177.7 (2)	C6—C5—C10—C9	0.7 (3)
N1—N2—C3—C5	175.17 (18)	C3—C5—C10—C9	176.7 (2)
C12—N2—C3—C5	−6.1 (3)	N1—N2—C12—C14	−53.1 (3)
C1—C2—C3—N2	0.7 (2)	C3—N2—C12—C14	128.2 (2)
C1—C2—C3—C5	−175.3 (2)	N1—N2—C12—C17	124.4 (2)
N1—C1—C4—F3A	−40.1 (6)	C3—N2—C12—C17	−54.3 (3)
C2—C1—C4—F3A	141.8 (6)	C17—C12—C14—C13	−0.1 (3)
N1—C1—C4—F1	141.4 (6)	N2—C12—C14—C13	177.3 (2)

C2—C1—C4—F1	−36.6 (7)	C15—C13—C14—C12	0.7 (4)
N1—C1—C4—F1A	86.9 (10)	C14—C13—C15—C16	−1.0 (3)
C2—C1—C4—F1A	−91.1 (10)	C14—C13—C15—S1	−179.17 (18)
N1—C1—C4—F2	−95.3 (10)	O2—S1—C15—C13	144.31 (19)
C2—C1—C4—F2	86.7 (10)	O1—S1—C15—C13	14.6 (2)
N1—C1—C4—F2A	−155.6 (7)	N3—S1—C15—C13	−100.59 (19)
C2—C1—C4—F2A	26.4 (8)	O2—S1—C15—C16	−33.9 (2)
N1—C1—C4—F3	25.0 (7)	O1—S1—C15—C16	−163.53 (17)
C2—C1—C4—F3	−153.1 (7)	N3—S1—C15—C16	81.23 (19)
N2—C3—C5—C10	153.3 (2)	C13—C15—C16—C17	0.7 (3)
C2—C3—C5—C10	−31.4 (3)	S1—C15—C16—C17	178.82 (16)
N2—C3—C5—C6	−30.8 (3)	C14—C12—C17—C16	−0.2 (3)
C2—C3—C5—C6	144.4 (2)	N2—C12—C17—C16	−177.63 (18)
C10—C5—C6—C7	−1.8 (3)	C15—C16—C17—C12	0.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H1*N*···O1*S*	0.87 (1)	2.06 (1)	2.904 (3)	162 (2)
N3—H2*N*···O1*S*^{i}	0.87 (1)	2.07 (1)	2.930 (3)	167 (2)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.