

# Structural, Hirshfeld surface and three-dimensional interaction energy studies of 2-(6-iodo-4-oxo-3,4-dihydroquinazolin-3-yl)ethanesulfonyl fluoride

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Received 17 October 2022

Accepted 28 December 2022

Edited by A. S. Batsanov, University of Durham, United Kingdom

**Keywords:** Single-crystal structure; C—H...N and C—H...O hydrogen bonds; I...O halogen bond; Hirshfeld surface; intermolecular energies.

**CCDC reference:** 1987361

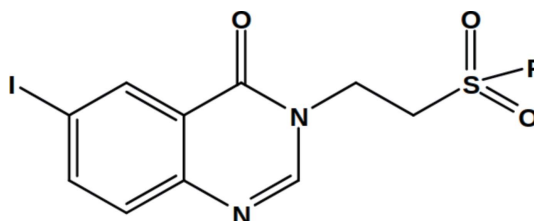
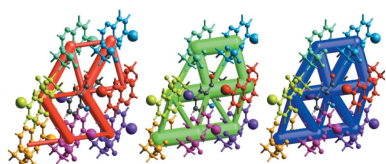
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In the crystal, molecules of the title compound, C<sub>10</sub>H<sub>8</sub>FIN<sub>2</sub>O<sub>3</sub>S, are connected through C—H...N and C—H...O hydrogen bonds, I...O halogen bonds,  $\pi$ – $\pi$  stacking interactions between the benzene and pyrimidine rings, and edge-to-edge electrostatic interactions, as shown by the analysis of the Hirshfeld surface and two-dimensional fingerprint plots, as well as intermolecular interaction energies calculated using the electron-density model at the HF/3–21 G level of theory.

## 1. Chemical context

Quinazoline is an aromatic heterocycle consisting of a benzene ring fused with a pyrimidine ring. Its derivatives are well known for their biological activities such as anti-analgesic, anti-inflammatory, anti-hypertensive, sedative, hypnotic, anti-histaminic, anti-tumor, anti-microbial, anti-convulsant, anti-bacterial, anti-fungal, enzyme inhibition, and anti-HIV activities (Kumar *et al.*, 1981; Baker *et al.*, 1952; Rewcastle *et al.*, 1995; Hitkari *et al.*, 1995; Bertelli *et al.*, 2000; Yang *et al.*, 2009; Cao *et al.*, 2009; De Clercq, 2001). Compounds bearing the quinazoline moiety also are potent cytotoxic agents (Ibrahim *et al.*, 1988; Riou *et al.*, 1991; Braña *et al.*, 1994; Helissey *et al.*, 1994), show anti-oxidant (Al-Amiery *et al.*, 2014) and insecticidal (Yang *et al.*, 2021) activities. In view of their therapeutic importance, we report herein the crystal structure, Hirshfeld surface and three-dimensional interaction energy studies of 2-(6-iodo-4-oxo-3,4-dihydroquinazolin-3-yl)ethanesulfonyl fluoride, (I).



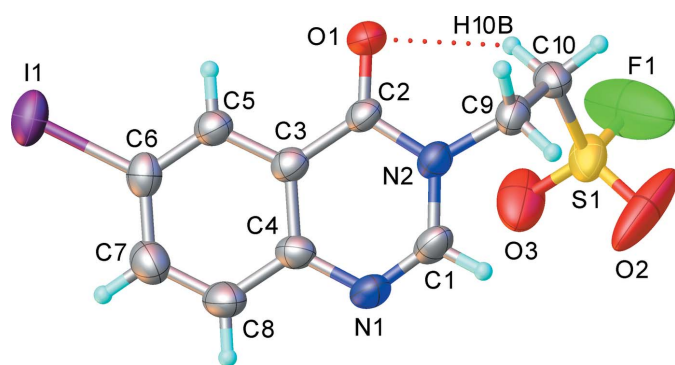
## 2. Structural commentary

The molecular structure of (I) (Fig. 1) shows an out-of-plane conformation of the (CH<sub>2</sub>)<sub>2</sub>SO<sub>2</sub>F side chain, the C9/C10/S1 fragment forming a dihedral angle of 76.1 (5)° with the



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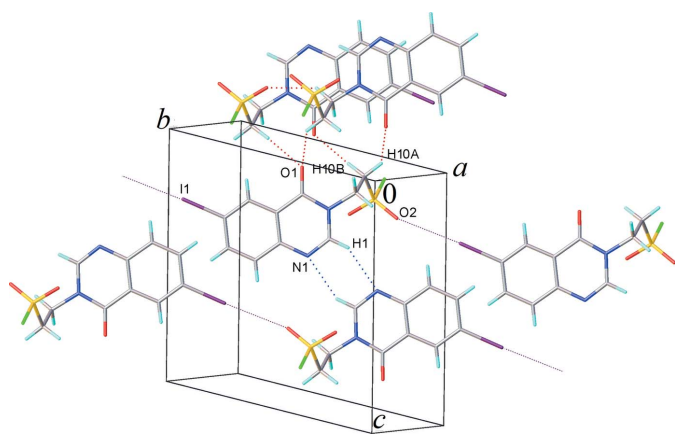
**Figure 1**  
Molecular structure of (I). The atomic displacement ellipsoids are drawn at the 50% probability level.

quinazoline (N1/N2/C1–C8) system mean plane, whereas the I1 and O1 substituents do not deviate appreciably from the latter plane. The molecule is stabilized by a weak intramolecular C10–H10B···O1 hydrogen bond, forming an *S*(6) ring motif. The S1 atom has a slightly distorted tetrahedral geometry. In the heterocycle, the N1=C1 bond [1.271 (8) Å] is essentially double, while those at the three-coordinate N2 atom are nominally single [C1–N2 = 1.359 (7), N2–C2 = 1.384 (6) Å].

The bond lengths and angles are in agreement with those in related structures (El-Hiti *et al.*, 2014; Al-Salahi *et al.*, 2012; Utayeva *et al.*, 2013; Priya *et al.*, 2011; Lakshminarayana *et al.*, 2009, 2022; Sreenatha *et al.*, 2018*a,b*, 2020, 2022).

### 3. Supramolecular features

In the crystal, each molecule donates three and accepts three intermolecular hydrogen bonds, *viz.* C1–H1···N1, C10–H10B···O1, C10–H10A···O1 (Table 1) and their inversion equivalents. Thus, each molecule participates in three centrosymmetric dimers with  $R_2^2(6)$ ,  $R_2^2(12)$  and  $R_2^2(12)$  ring motifs, respectively (Fig. 2). Molecules related by the *a* translation, form a continuous stack *via*  $\pi$ – $\pi$  interactions



**Figure 2**  
Intermolecular hydrogen (see Table 1) and halogen bonds in the structure of (I).

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

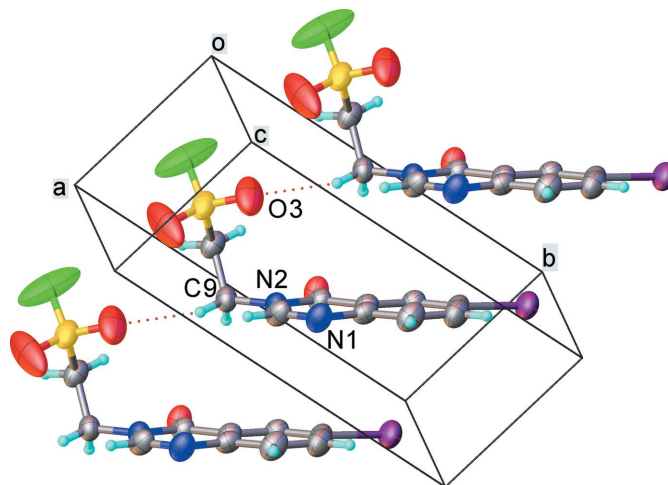
<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C1–H1···N1 <sup>i</sup>	0.93	2.46	3.284 (8)	148
C10–H10B···O1 <sup>ii</sup>	0.97	2.56	3.493 (7)	160
C10–H10A···O1 <sup>iii</sup>	0.97	2.45	3.151 (7)	129
C9–H9A···O3 <sup>iv</sup>	0.97	2.33	3.150 (8)	141
C10–H10B···O1	0.97	2.59	3.121 (7)	115

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

between the benzene and the pyrimidine rings (which are parallel within 1.5°), with a mean interplanar separation of 3.503 (4) Å (Fig. 3). The I1···O2(*x* – 1, *y* + 1, *z*) contact of 3.152 (6) Å is considerably shorter than the sum of the van der Waals radii of 3.61 Å (Batsanov, 1995; Rowland & Taylor, 1996) and can be described as a halogen bond (Metrangolo & Resnati, 2001), the nearly linear angle C6–I1···O2 = 175.9 (3)° being typical of such bonds.

### 4. Database survey

A survey of the Cambridge Structural Database (CSD version 5.41, update of October 2022; Groom *et al.*, 2016) revealed only one structure, namely (*Z*)-ethyl-2-cyano-2-(3*H*-quinazoline-4-ylidene)acetate (ACEZUE; Tulyasheva *et al.*, 2005), which shares such features of (I) as one two-coordinate (N1) and one three-coordinate (N2) nitrogen atom of the quinazoline ring system, as well as an exocyclic double bond at C2, although in this case the H atom at N2 is not substituted. Of the other comparable quinazoline derivatives, in 3-amino-6-bromo-1-methyl-2, 4-(1*H*,3*H*)-quinazolinedione (ABMQZD; Ardebili & While, 1978) both N atoms are three-coordinate, while in *N*-(5-methyl-1,2-oxazol-3-yl)-4-[(quinazolin-4-yl) level of theoryamino]benzene-1-sulfonamide and *N*-(3,4-dimethyl-1,2-oxazol-5-yl)-4-[(quinazolin-4-yl)amino]benzene-1-sulfonamide (GEYYOB, GEYYUH; Sunil Kumar *et al.*, 2018) both are two-coordinate.



**Figure 3**  
 $\pi$ – $\pi$  stacking in the structure of (I).

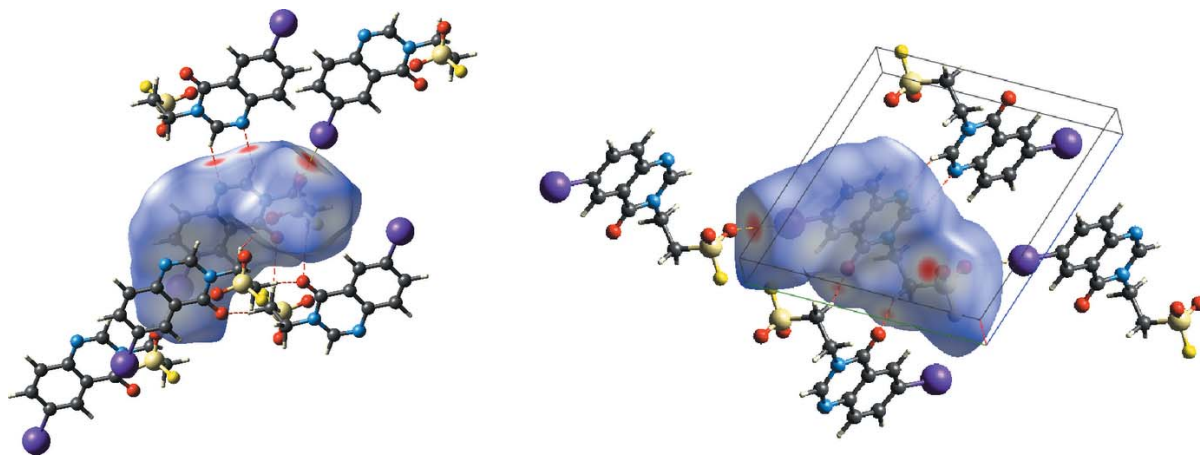


Figure 4

Different aspects of the three-dimensional Hirshfeld surface of (I) mapped over  $d_{\text{norm}}$ . Red spots indicate shortened contacts, revealing intermolecular hydrogen and halogen bonds

### 5. Hirshfeld surfaces and 2D fingerprint calculations

The Hirshfeld surfaces and two-dimensional fingerprint plots were calculated using *CrystalExplorer17.5* (Spackman *et al.*, 2009) to analyse the intermolecular interactions. The three-dimensional Hirshfeld surface mapped over the normalized contact distance ( $d_{\text{norm}}$ ) is shown in Fig. 4. The eight bright-red spots, indicating shortened contacts, correspond to the three pairs of intermolecular hydrogen bonds and one pair of halogen bonds discussed in Section 3. The two-dimensional fingerprint plots show the H...O contacts to be the most common (23.0%), followed by H...H (13.5%), H...C

(11.5%), H...I (9.9%), I...O (7.8%), H...F (6.7%), H...N (6.4%), I...F (4.0%), I...C (3.2%), O...O (2.2%) and C...N (1.9%) (including the reverse ones for all heteronuclear contacts). The characteristic spikes in the plots of the H...O and H...N contacts indicate intermolecular hydrogen bonds, those in the I...O plot indicate halogen bonds (Fig. 5).

### 6. Three-dimensional framework analysis of interaction energies

Quantification of intermolecular interactions energies is important for molecular recognition, protein modelling and drug design (Volkov & Coppens, 2004). We computed these energies for (I) with the HF/3-21G(d,p) electron-density model (Grimme, 2006), using *CrystalExplorer17.5* software. Eleven molecules surrounding the original one with shortest intermolecular atom–atom distances of 3.8 Å or less were included in the calculations. The total interaction energy ( $E_{\text{tot}}$ ) between each pair of molecules comprises coulombic ( $E_{\text{ele}}$ ), dispersion ( $E_{\text{dis}}$ ), polarization ( $E_{\text{pol}}$ ) and exchange-repulsion interaction energies ( $E_{\text{rep}}$ ) (Turner *et al.*, 2015, 2017). The  $E_{\text{ele}}$ ,  $E_{\text{dis}}$  and  $E_{\text{tot}}$  intermolecular energy frameworks for (I) are shown graphically in Fig. 6 and numerically in Fig. 7. The molecular stacks (Fig. 3, top line in the Fig. 7 table) are held

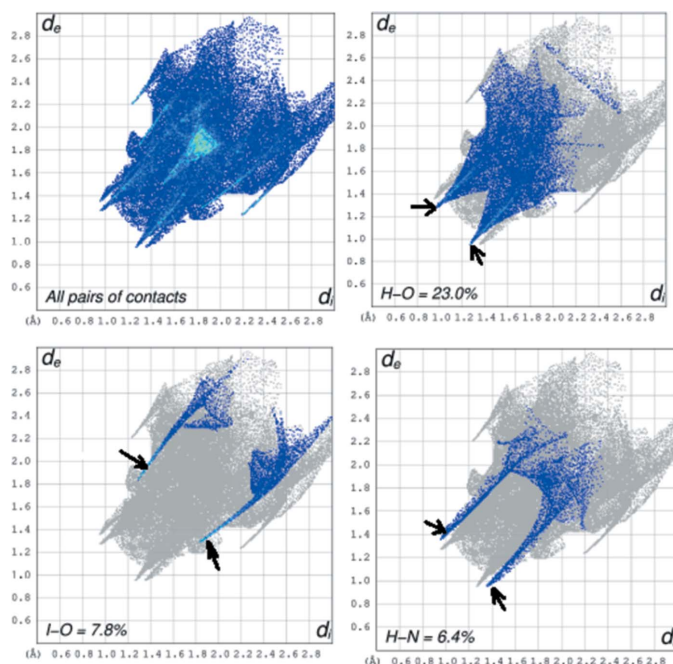


Figure 5

Selected two-dimensional fingerprint plots of structure (I);  $d_i$  and  $d_e$  are the distances from the Hirshfeld surface to the nearest internal and external atoms. Arrows indicate the 'spikes' characteristic of hydrogen and halogen bonds

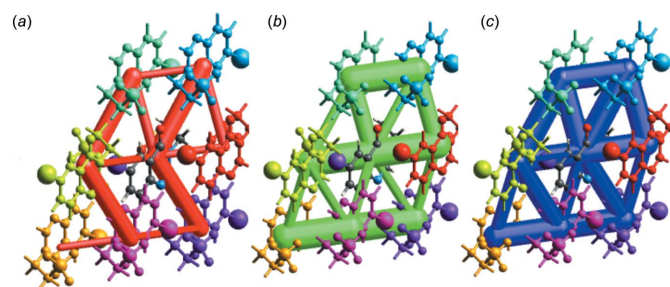


Figure 6

Intermolecular energy frameworks of (a)  $E_{\text{ele}}$ , (b)  $E_{\text{dis}}$  and (c)  $E_{\text{tot}}$  in the structure of (I), viewed down the  $b$  axis.

together mostly by dispersion (van der Waals) interactions, supported by the shortest C—H···O hydrogen bonds, while edge-to-edge intermolecular contacts (lines 5 to 8) have larger contributions of electrostatic interactions. The interaction between halogen-bonded molecules (line 3) is smaller than the above in absolute terms (10.8 kJ mol<sup>-1</sup>), but is remarkable given that only one pair of atoms is actually in contact.

### 7. Synthesis and crystallization

To an ice-cooled stirred suspension of NaH (60% suspension in mineral oil; 125 mg, 2.0 mmol, 2.0 equiv) and 6-iodoquinazolin-4(3*H*)-one (1.0 mmol, 1.0 equiv) in DMF (2 mL), a solution of 2-bromoethanesulfonyl fluoride (350 mg, 1.0 mmol, 1.0 equiv) in DMF (1 mL) was added, under an N<sub>2</sub> atmosphere. The reaction was heated at 353 K for 4 h under an N<sub>2</sub> atmosphere (monitored by TLC). After the complete conversion of the reactants as confirmed from TLC analysis, the reaction mixture was quenched with saturated NH<sub>4</sub>Cl solution (25 mL), extracted with EtOAc (25 mL) and the collected organic layer was further washed with water (25 mL) and brine (25 mL), then dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and concentrated under vacuum. Compound (I) was isolated by silica gel chromatography (using chloroform and methanol as mobile phase) and recrystallized from DMF.

### 8. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms were placed in idealized positions and refined using a riding model with C—H 0.93 Å for *sp*<sup>2</sup> and 0.97 Å for *sp*<sup>3</sup> C atoms, with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C) for both.

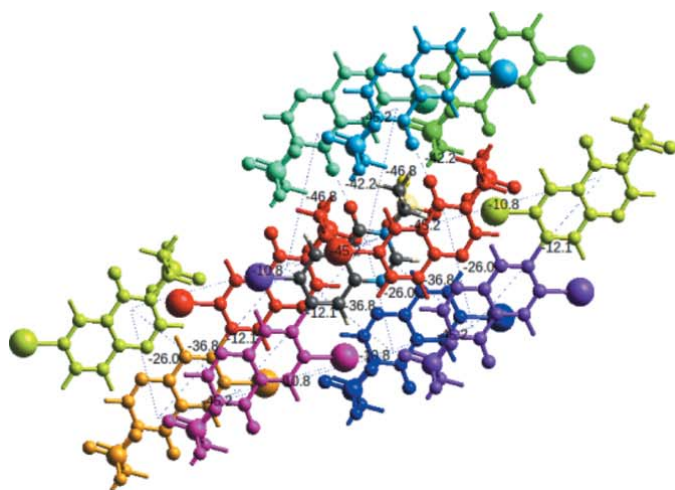
**Table 2**  
Experimental details.

Crystal data	
Chemical formula	C <sub>10</sub> H <sub>8</sub> FIN <sub>2</sub> O <sub>3</sub> S
<i>M</i> <sub>r</sub>	382.14
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	5.0230 (5), 11.3241 (11), 11.5509 (11)
$\alpha$ , $\beta$ , $\gamma$ (°)	103.081 (2), 96.742 (1), 97.860 (1)
<i>V</i> (Å <sup>3</sup> )	626.43 (11)
<i>Z</i>	2
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	2.74
Crystal size (mm)	0.34 × 0.30 × 0.27
Data collection	
Diffractometer	Bruker APEXII
Absorption correction	—
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	4073, 3207, 2315
<i>R</i> <sub>int</sub>	0.035
(sin $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.673
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.055, 0.166, 1.11
No. of reflections	3207
No. of parameters	164
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$ , $\Delta\rho_{min}$ (e Å <sup>-3</sup> )	0.88, -1.39

Computer programs: APEX2 and SAINT (Bruker, 2009), SHELXT (Sheldrick, 2015*a*), SHELXL2018/3 (Sheldrick, 2015*b*) and PLATON (Spek, 2020).

### Acknowledgements

The authors are thankful to Dr A. S. Jeevan Chakravarthy, C/O Professor H. ILA, New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur Post, Amruthahalli, Bengaluru – 560064, Karnataka, and to the Department of Engineering Physics, Adichunchanagiri Institute of Technology, Chikkamagaluru, Karnataka, India, for support.



**Figure 7**

Intermolecular energies (in kJ mol<sup>-1</sup>) and their components in the structure of (I). *N* is the number of molecules in a group, *Symop* is the symmetry operator, *R* is the distance between molecular centroids in Å.

Colour code	<i>N</i>	<i>Symop</i>	<i>R</i>	Electron Density	<i>E</i> <sub>ele</sub>	<i>E</i> <sub>pol</sub>	<i>E</i> <sub>dis</sub>	<i>E</i> <sub>rep</sub>	<i>E</i> <sub>tot</sub>
Orange	2	<i>x</i> , <i>y</i> , <i>z</i>	5.02	HF/3-21G	-13.0	-8.9	-59.8	34.1	-45.2
Yellow	1	- <i>x</i> , - <i>y</i> , - <i>z</i>	10.76	HF/3-21G	-2.7	-0.4	-8.5	4.3	-7.2
Light Green	2	<i>x</i> , <i>y</i> , <i>z</i>	13.00	HF/3-21G	-12.4	-2.2	-5.9	10.5	-10.8
Green	1	- <i>x</i> , - <i>y</i> , - <i>z</i>	14.58	HF/3-21G	-2.7	-0.1	-3.3	0.2	-5.7
Light Blue	1	- <i>x</i> , - <i>y</i> , - <i>z</i>	6.08	HF/3-21G	-17.9	-7.4	-37.0	17.4	-42.2
Blue	1	- <i>x</i> , - <i>y</i> , - <i>z</i>	8.69	HF/3-21G	-32.4	-10.7	-22.4	16.5	-46.8
Dark Blue	1	- <i>x</i> , - <i>y</i> , - <i>z</i>	7.28	HF/3-21G	-8.7	-4.2	-21.6	6.3	-26.0
Purple	1	- <i>x</i> , - <i>y</i> , - <i>z</i>	8.83	HF/3-21G	-31.4	-7.0	-19.1	21.0	-36.8
Pink	1	- <i>x</i> , - <i>y</i> , - <i>z</i>	8.64	HF/3-21G	-4.9	-0.5	-20.8	14.7	-12.1

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## supporting information

*Acta Cryst.* (2023). E79, 65-69 [https://doi.org/10.1107/S205698902201221X]

## Structural, Hirshfeld surface and three-dimensional interaction energy studies of 2-(6-iodo-4-oxo-3,4-dihydroquinazolin-3-yl)ethanesulfonyl fluoride

**D. P. Ganesha, N. R. Sreenatha, S. R. Shankara and B. N. Lakshminarayana**

### Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINTE* (Bruker, 2009); data reduction: *SAINTE* (Bruker, 2009); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *PLATON* (Spek, 2020); software used to prepare material for publication: *PLATON* (Spek, 2020).

### 2-(6-Iodo-4-oxo-3,4-dihydroquinazolin-3-yl)ethanesulfonyl fluoride

#### Crystal data

$C_{10}H_8FIN_2O_3S$	$Z = 2$
$M_r = 382.14$	$F(000) = 368$
Triclinic, $P\bar{1}$	$D_x = 2.026 \text{ Mg m}^{-3}$
$a = 5.0230 (5) \text{ \AA}$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$b = 11.3241 (11) \text{ \AA}$	Cell parameters from 3207 reflections
$c = 11.5509 (11) \text{ \AA}$	$\theta = 2.9\text{--}28.6^\circ$
$\alpha = 103.081 (2)^\circ$	$\mu = 2.74 \text{ mm}^{-1}$
$\beta = 96.742 (1)^\circ$	$T = 293 \text{ K}$
$\gamma = 97.860 (1)^\circ$	Block, colourless
$V = 626.43 (11) \text{ \AA}^3$	$0.34 \times 0.30 \times 0.27 \text{ mm}$

#### Data collection

Bruker APEXII diffractometer	2315 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{\text{int}} = 0.035$
Graphite monochromator	$\theta_{\text{max}} = 28.6^\circ$ , $\theta_{\text{min}} = 2.9^\circ$
SAINTE (Bruker, 2009) scans	$h = -6 \rightarrow 6$
4073 measured reflections	$k = -15 \rightarrow 15$
3207 independent reflections	$l = -15 \rightarrow 9$

#### Refinement

Refinement on $F^2$	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.055$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.166$	$(\Delta/\sigma)_{\text{max}} = 0.027$
$S = 1.11$	$\Delta\rho_{\text{max}} = 0.88 \text{ e \AA}^{-3}$
3207 reflections	$\Delta\rho_{\text{min}} = -1.39 \text{ e \AA}^{-3}$
164 parameters	Extinction correction: <i>SHELXL2018/3</i>
0 restraints	(Sheldrick, 2015b),
Hydrogen site location: inferred from neighbouring sites	$F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.075 (6)

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
II	0.12293 (8)	0.97164 (3)	0.27666 (4)	0.0627 (3)
S1	0.6688 (3)	0.23549 (14)	0.14355 (16)	0.0558 (4)
C4	0.6072 (11)	0.6675 (5)	0.4017 (4)	0.0400 (10)
O1	0.7389 (9)	0.6113 (4)	0.0952 (3)	0.0492 (9)
C6	0.3202 (11)	0.8380 (5)	0.3281 (5)	0.0452 (12)
N1	0.7570 (11)	0.5853 (5)	0.4409 (4)	0.0502 (11)
C3	0.5977 (10)	0.6826 (5)	0.2840 (4)	0.0374 (10)
C2	0.7379 (10)	0.6082 (4)	0.2009 (4)	0.0370 (10)
C1	0.8777 (12)	0.5224 (5)	0.3644 (5)	0.0473 (12)
H1	0.976779	0.467243	0.390691	0.057*
C10	0.8383 (12)	0.3422 (5)	0.0775 (5)	0.0466 (12)
H10A	0.946662	0.300744	0.022171	0.056*
H10B	0.705250	0.375036	0.031537	0.056*
C9	1.0223 (10)	0.4478 (5)	0.1700 (5)	0.0424 (11)
H9A	1.146034	0.414079	0.219643	0.051*
H9B	1.130812	0.496966	0.128183	0.051*
C5	0.4554 (11)	0.7690 (5)	0.2498 (5)	0.0416 (11)
H5	0.452220	0.780100	0.172336	0.050*
C7	0.3249 (13)	0.8216 (6)	0.4448 (6)	0.0554 (14)
H7	0.231139	0.867697	0.498211	0.066*
O3	0.4727 (11)	0.2855 (6)	0.2052 (7)	0.0900 (19)
O2	0.8528 (12)	0.1889 (8)	0.2130 (10)	0.139 (4)
N2	0.8762 (8)	0.5277 (4)	0.2479 (4)	0.0393 (9)
F1	0.532 (2)	0.1389 (6)	0.0379 (6)	0.167 (4)
C8	0.4670 (14)	0.7380 (6)	0.4805 (5)	0.0534 (14)
H8	0.470010	0.728088	0.558397	0.064*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
II	0.0622 (3)	0.0401 (3)	0.0873 (4)	0.01597 (19)	0.0067 (2)	0.0166 (2)
S1	0.0624 (8)	0.0382 (7)	0.0754 (11)	0.0114 (6)	0.0258 (8)	0.0219 (7)
C4	0.049 (2)	0.038 (3)	0.031 (2)	0.001 (2)	0.005 (2)	0.0078 (19)
O1	0.069 (2)	0.049 (2)	0.038 (2)	0.0201 (19)	0.0135 (17)	0.0178 (16)
C6	0.046 (3)	0.033 (3)	0.055 (3)	0.007 (2)	0.006 (2)	0.007 (2)
N1	0.072 (3)	0.048 (3)	0.034 (2)	0.017 (2)	0.003 (2)	0.0161 (19)
C3	0.042 (2)	0.034 (2)	0.036 (2)	0.0027 (19)	0.0040 (19)	0.0112 (19)
C2	0.045 (2)	0.031 (2)	0.036 (3)	0.0049 (19)	0.0046 (19)	0.0147 (19)
C1	0.062 (3)	0.040 (3)	0.039 (3)	0.011 (2)	-0.007 (2)	0.014 (2)

C10	0.064 (3)	0.038 (3)	0.042 (3)	0.010 (2)	0.018 (2)	0.012 (2)
C9	0.044 (2)	0.040 (3)	0.050 (3)	0.014 (2)	0.012 (2)	0.017 (2)
C5	0.050 (3)	0.038 (3)	0.037 (3)	0.006 (2)	0.005 (2)	0.012 (2)
C7	0.067 (4)	0.045 (3)	0.056 (3)	0.012 (3)	0.021 (3)	0.009 (3)
O3	0.078 (3)	0.079 (4)	0.142 (5)	0.028 (3)	0.065 (4)	0.053 (4)
O2	0.073 (4)	0.141 (7)	0.265 (11)	0.040 (4)	0.031 (5)	0.160 (8)
N2	0.044 (2)	0.036 (2)	0.040 (2)	0.0097 (18)	0.0016 (17)	0.0129 (17)
F1	0.280 (10)	0.083 (4)	0.098 (4)	-0.080 (5)	0.054 (5)	-0.009 (3)
C8	0.076 (4)	0.048 (3)	0.041 (3)	0.010 (3)	0.017 (3)	0.015 (2)

*Geometric parameters (Å, °)*

I1—C6	2.075 (5)	C2—N2	1.384 (6)
S1—O3	1.390 (6)	C1—N2	1.359 (7)
S1—O2	1.389 (6)	C1—H1	0.9300
S1—F1	1.467 (6)	C10—C9	1.521 (8)
S1—C10	1.748 (5)	C10—H10A	0.9700
C4—C3	1.404 (7)	C10—H10B	0.9700
C4—N1	1.393 (7)	C9—N2	1.462 (6)
C4—C8	1.392 (8)	C9—H9A	0.9700
O1—C2	1.230 (6)	C9—H9B	0.9700
C6—C5	1.363 (8)	C5—H5	0.9300
C6—C7	1.400 (9)	C7—C8	1.367 (9)
N1—C1	1.271 (8)	C7—H7	0.9300
C3—C5	1.387 (7)	C8—H8	0.9300
C3—C2	1.443 (7)		
O3—S1—O2	113.9 (5)	C9—C10—H10A	109.1
O3—S1—F1	108.8 (5)	S1—C10—H10A	109.1
O2—S1—F1	110.1 (6)	C9—C10—H10B	109.1
O3—S1—C10	110.6 (3)	S1—C10—H10B	109.1
O2—S1—C10	110.8 (3)	H10A—C10—H10B	107.8
F1—S1—C10	101.9 (3)	N2—C9—C10	114.0 (4)
C3—C4—N1	121.3 (5)	N2—C9—H9A	108.8
C3—C4—C8	118.8 (5)	C10—C9—H9A	108.8
N1—C4—C8	119.8 (5)	N2—C9—H9B	108.8
C5—C6—C7	119.6 (5)	C10—C9—H9B	108.8
C5—C6—I1	120.1 (4)	H9A—C9—H9B	107.7
C7—C6—I1	120.3 (4)	C6—C5—C3	121.0 (5)
C1—N1—C4	116.9 (4)	C6—C5—H5	119.5
C4—C3—C5	119.6 (5)	C3—C5—H5	119.5
C4—C3—C2	119.2 (4)	C8—C7—C6	120.2 (6)
C5—C3—C2	121.2 (4)	C8—C7—H7	119.9
O1—C2—N2	120.0 (5)	C6—C7—H7	119.9
O1—C2—C3	125.0 (4)	C1—N2—C2	121.1 (4)
N2—C2—C3	115.0 (4)	C1—N2—C9	120.1 (4)
N1—C1—N2	126.4 (5)	C2—N2—C9	118.8 (4)
N1—C1—H1	116.8	C7—C8—C4	120.8 (5)



N2—C1—H1	116.8	C7—C8—H8	119.6
C9—C10—S1	112.5 (4)	C4—C8—H8	119.6
C3—C4—N1—C1	-2.0 (8)	I1—C6—C5—C3	177.4 (4)
C8—C4—N1—C1	179.1 (6)	C4—C3—C5—C6	-1.2 (8)
N1—C4—C3—C5	-177.4 (5)	C2—C3—C5—C6	179.1 (5)
C8—C4—C3—C5	1.6 (8)	C5—C6—C7—C8	0.8 (9)
N1—C4—C3—C2	2.3 (7)	I1—C6—C7—C8	-176.6 (5)
C8—C4—C3—C2	-178.8 (5)	N1—C1—N2—C2	1.0 (9)
C4—C3—C2—O1	178.3 (5)	N1—C1—N2—C9	-179.1 (6)
C5—C3—C2—O1	-2.1 (8)	O1—C2—N2—C1	-179.9 (5)
C4—C3—C2—N2	-1.0 (7)	C3—C2—N2—C1	-0.6 (7)
C5—C3—C2—N2	178.7 (4)	O1—C2—N2—C9	0.2 (7)
C4—N1—C1—N2	0.3 (9)	C3—C2—N2—C9	179.5 (4)
O3—S1—C10—C9	70.2 (5)	C10—C9—N2—C1	106.4 (6)
O2—S1—C10—C9	-57.1 (7)	C10—C9—N2—C2	-73.7 (6)
F1—S1—C10—C9	-174.2 (6)	C6—C7—C8—C4	-0.4 (10)
S1—C10—C9—N2	-67.0 (5)	C3—C4—C8—C7	-0.7 (9)
C7—C6—C5—C3	0.0 (8)	N1—C4—C8—C7	178.2 (6)

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C1—H1...N1 <sup>i</sup>	0.93	2.46	3.284 (8)	148
C10—H10B...O1 <sup>ii</sup>	0.97	2.56	3.493 (7)	160
C10—H10A...O1 <sup>iii</sup>	0.97	2.45	3.151 (7)	129
C9—H9A...O3 <sup>iv</sup>	0.97	2.33	3.150 (8)	141
C10—H10B...O1	0.97	2.59	3.121 (7)	115

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