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Data Article

Synthesis, crystal structure and Hirshfeld surface analysis of 3-butyl-4-oxo-3,4-dihydroquinazoline-6-sulfonamide

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ABSTRACT

It was developed simple and efficient One-pot multicomponent synthesis (MCRs) sulfonamides in the series of 3-alkyl-quinazolines. The structure of the compound has been confirmed by IR and ^{1}H NMR spectroscopy as well as X-ray diffraction analysis. The crystal structure of 3-butyl-4-oxo-3,4-dihydroquinazoline-6-sulfonamide was determined by the single-crystal X-ray diffraction method at 294 K. The crystallographic study revealed disordering the butyl part. The Hirshfeld surface analysis revealed that in the structure the most significant contacts are H•••H (44%) and O•••H/H•••O (25.4%).

1. Rationale

Quinazolines are an interesting kind of heterocyclic compounds that are of great importance in medicinal chemistry. From compounds of this class, substances with pharmacological activity were obtained that are effective as antimicrobial [1–5], anti-inflammatory [6], antioxidant [7], and anticonvulsant [8]. In addition, compounds of this class are also chemically interesting. At the same time, heterocyclic compounds with sulfonamide groups (-S(=O)$_2$-NH-) are considered important chemical compounds in terms of chemical and biological activity. The development of sulfonamides is a fascinating and informative area in medicinal chemistry [9,10]. Its functional group has a long and rich history in organic chemistry and drug discovery [11]. Furthermore, sulfonamide moiety has a crucial functionality because of its wide variety of reported biological [12,13] and pharmacological activities such as anticancer [14], carbonic anhydrase inhibitory [15,16], antibacterial [17], antitumor [18], antihypertensive [19], anti-inflammatory [20], and antiprotozoal activities [21]. Sulfonamide has also been reported to possess good herbicidal [22] and corrosion inhibitory properties [23,24]. Preparations based on pyrimidines (quinazolines) fused with a benzene ring are widely used in agricultural and medical practice throughout the world. In particular, drugs based on compounds of this class are used against viruses, germs, colds and cancer, as well as stimulants and pesticides. Examples include erlotinib, gefitinib, vandetanib, lapatinib and afatinib (Fig. 1), which have been successfully used against various types of cancer in recent years. Therefore, it is very important to carry out targeted syntheses and chemical modifications of new, potentially biologically active compounds containing this pharmacophore -

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quinazoline ring, to determine their physicochemical and biological properties, and to create new drugs based on selected "candidate" compounds.

Therefore, our goal was focused on the synthesis of new heterocyclic compound, consisting quinazolinone fragment and the sulfonamide group (-S(=O)$_2$-NH-). To do this, we tested the reaction of quinazolin-4-one with present alkyl halides and synthesized quinazolin-4-one compounds with N-alkyl compounds in position 3. As a result of the reactions of the obtained N-alkyl derivatives with chlorosulfonic acid and subsequent treatment of the reaction mixture with concentrated ammonium hydroxide solution, 3-alkyl-4-oxo-3,4-dihydroquinazoline-6-sulfonamides [25]. The structure of the compound was determined using state-of-the art physical method of investigations by IR- and NMR- spectroscopy. The synthesis and crystal structure of the 3-butyl-4-oxo-3,4-dihydroquinazoline-6-sulfonamide is reported here (Fig. 2). The more prominent intermolecular contacts were quantified by using Hirshfeld surface analysis.

2. Procedure

2.1. Synthesis and crystallization

A mixture consisting of 3.5 g (0.03 mol, d=1.75 g/ml) of chlorosulfonic acid and 0.60 g (0.003 mol) of 3-butylquinazolin-4-one was heated for 4 h at 120-130°C. It was then cooled to 0-2°C temperature and aqueous solution of ammonia was added until the pH reached 8-9. The resulting precipitate was filtered off and washed with water. As a result, 3-butyl-4-oxo-3,4-dihydroquinazoline-6-sulfonamide is formed (Fig. S1). Quantity 0.5 g, yield 60.0%, R_f= 0.19 (chloroform:methanol - 10:1), melting point 173-174°C.

2.2. ^{1}H NMR and IR spectra

^{1}H NMR spectra were recorded on a Unity-400+ instrument (operating frequency 400 MHz, internal standard TMS, δ scale) solvents - DMSO-d6+CCl_4 (Fig. S2), IR spectra - on a System 2000 IR Fourier spectrometer in KBr tablets (Fig. S3). The purity of the products and the progress of the reaction were monitored by TLC on Silufol UV-254 in the system - chloroform: methanol - 10:1. Melting points were determined with an electro thermal melting point apparatus «MEL-TEMP» (USA).

^{1}H NMR spectrum (400 MHz, DMSO-d6): 8.56 (1H, s, J=1.8; H-2), 8.43 (1H, d; J=3.7; H-5), 8.14 (1H, dd J_1=2.17, J_2=8.5; H-7), 7.75 (1H, dd, H-8), 7.43 (2H, s, NH_2), 4.0 (2H, t, J=7.3; CH_2), 1.7 (2H, m; CH_2); 1.37 (2H, m; CH_2), 0.95 (3H, t, J=7.16; CH_3).

IR spectrum (KBr, ν, cm^{-1}): 3309 (NH_2), 1663 (C=O), 1605 (C=N), 1328, 1175 (SO_2), 773 (C-S).

2.3. Single crystal X-ray diffraction and refinement

Single crystal diffraction data were collected at a temperature of 294 K on a XtaLAB Synergy, Single source at home/near, HyPix3000 with CuKα radiation from a PhotonJet (Cu) X-ray Source microfocus tube. The structure was solved by direct methods with the program *SHELXS* [26] and refined by full-matrix least squares on F^2 using the *SHELXL* [27] package. Non-hydrogen atoms were refined anisotropically, and hydrogen atoms were refined using the riding model, except for the N-H atoms, which were located by a difference Fourier map and refined isotropically. The H atoms bonded to nitrogen were restrained to a N-H distance of 0.87 Å. Geometrical calculations were carried out using *PLATON* [28]. Crystal data and convergence results have been included in Table 1. Supplementary crystallographic data were deposited in CCDC (Cambridge Crystallographic Data Centre, No: 2190885). The data can be obtained free of charge via http:/www.ccdc.cam.ac.uk/conts/retrieving.html, or e-mail: deposit@ccdc.ac.uk

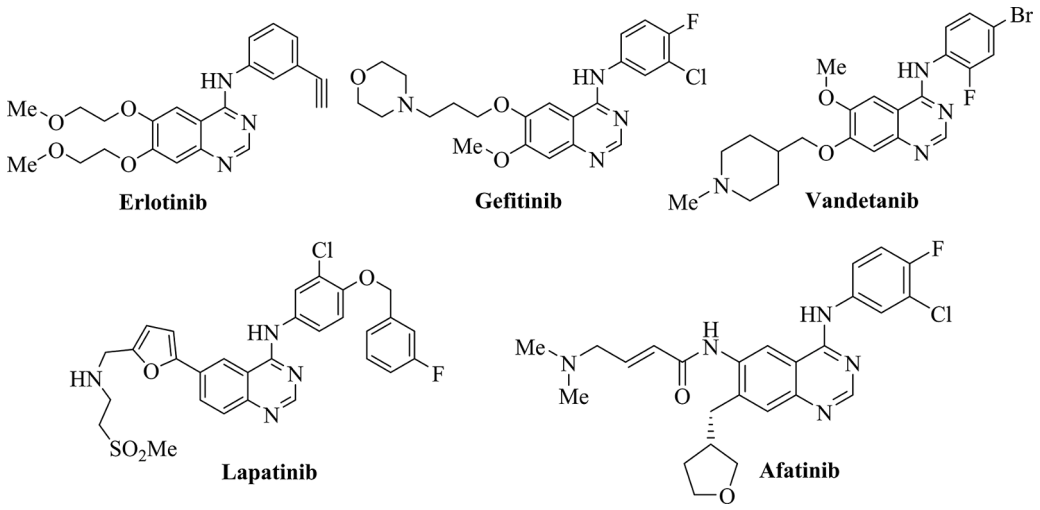

Fig. 1. Drugs based on compounds of pyrimidines (quinazolines) class.

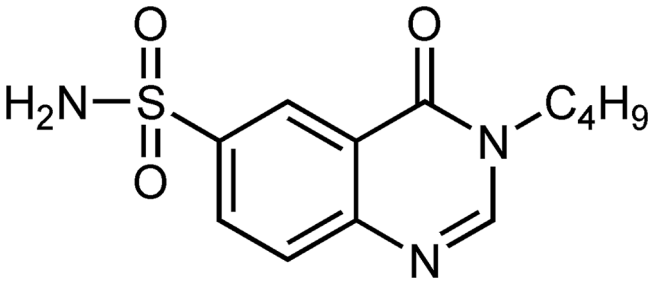

Fig. 2. Structure of title compound.

Table 1
Crystallographic data of the 3-butyl-4-oxo-3,4-dihydroquinazoline-6-sulfonamide.

Chemical formula: $C_{12}H_{15}N_3O_3S$	
Formula weight = 281.33	
T=294.2 K	
Crystal system: monoclinic	Space group: P-1
a= 8.41582(9)Å	α = 69.0966(11)°
b= 8.83995(11)Å	β = 76.6018(10)°
c= 9.71369(12)Å	γ = 81.7483(9)°
V= 655.244(13)	Z=2
Dx= 1.426 g/cm^3	
Radiation type: Cu Kα (λ = 1.54184 Å)	
μ(Cu Kα) = 2.286 mm^{-1}	F(000) = 296.0
Crystal size = 0.5 × 0.16 × 0.02 mm^3	
No. of reflections collected = 2527	
No. of independent reflections = 2449	
θ range for data collection: 4.96 to 71.247°	
Data/Restraints/Parameters = 2527/6/217	
Goodness-of-fit on F^2 = 1.037	
R indices [I>2σ(I)]: R1 = 0.0320, wR2 = 0.0326	
R indices (all data): R1 =0.0898, wR2 = 0.0903	
(Δ/σ)max = 0.002	
(Δρ)min = -0.33 eÅ^{-3}	(Δρ)max = 0.24 eÅ^{-3}
Measurement: Rigaku OD, XtaLAB Synergy, HyPix3000	
Programs systems: CrysAlisPro	
Structure determination: SHELXS	
Structure refinement program: SHELXL 2018/3	
CCDC deposition number: 2190885	

2.4. Hirshfeld surfaces calculations

The Hirshfeld surface analysis [29] and the associated two-dimensional (2D) fingerprint plot [30] were performed with CrystalExplorer17 [31]. The Hirshfeld surface for the title molecule, mapped with d_{norm} with the color scale of - 0.5391 (red) to 1.1141 (blue) is represented in Fig. 4. Colors with on the Hirshfeld surface encode contact distances (red - close, white - medium, blue - long) between atoms on either side of the surface.

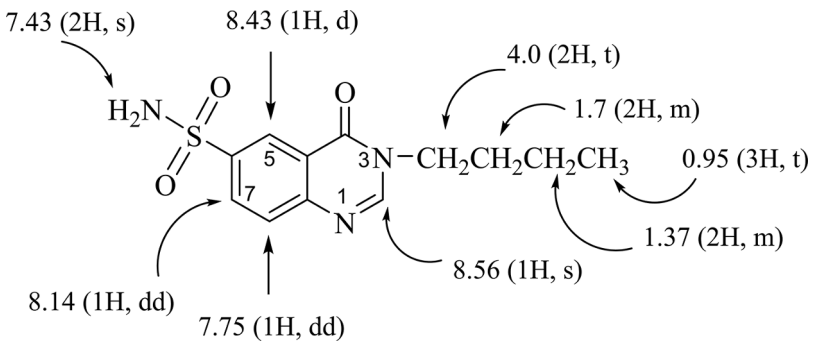

Fig. 3. Multiplicity of protons of 3-butyl-4-oxo-3,4-dihydroquinazoline-6-sulfonamide in 1H NMR spectra.

3. Data, value and validation

3.1. Spectra description

In the ^{1}H NMR spectrum of the 3-butyl-4-oxo-3,4-dihydroquinazoline-6-sulfonamide, the signals of the H_{Ar}-5 proton in the benzene ring is found at 8.43 ppm as doublet (d), H_{Ar}-7 proton signals at 8.14 ppm as doublet-of doublets (dd) and signal of proton of H_{Ar}-8 at 7.75 ppm also as doublet-of doublets and signal of proton in the position 2 of the pyrimidine ring at 8.56 ppm appeared as a singlet. In addition, two protons corresponding to NH_2 were visible in the region of 7.43 ppm. Also, the signal of the methyl group is found at 0.95 ppm as triplet (N3-CH_2-CH_2-CH_2-CH_3), proton signals of the methylene group of the N3-butyl fragment 1.37 ppm as multiplet (N3-CH_2-CH_2-CH_2-CH_3), and are found at 1.7 ppm as multiplet (N3-CH_2-CH_2-CH_2-CH_3), at 4.0 ppm as triplet (N3-CH_2-CH_2-CH_2-CH_3) of methylene groups (Fig. 3).

In IR spectrum, stretching vibrations of bonds were found in the areas: amino group at 3309 cm^{-1}, carbonyl group at 1663 cm^{-1}, C=N bond at 1605 cm^{-1}, SO_2 bond at 1328, 1175 cm^{-1}, C-S bond at 773 cm^{-1}. These results confirm the structure of title compound, which are consistent with the literature data.

3.2. Single crystal structure description

The title compound, $C_{12}H_{15}N_3O_3S$, crystallizes in the triclinic space group *P-1*. A displacement ellipsoid plot and the numbering scheme are provided in Fig. 4. The central aromatic quinazoline moiety is near planar with r.m.s. deviation 0.0258 Å, the largest deviation of 0.0462(11)Å from the that plane by an N3 atom (Fig. 5a). A search in the Cambridge Structural Database (CSD) [32] gave only one hit with more similar conformation for the aromatic quinazoline moiety: N-Methyl-6-sulfamoyl-9H-b-carboline-1-carboxamide (refcode: BATNOB) [33] (Fig. 5b). A comparative analysis of the geometry of the sulphonamide group of the title molecule from CSD with the most similar structures showed that the bond lengths and angles have close values (Table 2).

In the crystal revealed an intramolecular C5—H5•••O3 interaction, and molecules are linked by intermolecular N2—H2A···O2 and N2—H2B···O1 hydrogen bonds (Table 3), forming infinity chains propagating along the [1 0 3] direction and give rise to $R_2^2(8)$, $R_2^2(16)$, $C_2^2(10)$, $C_2^2(12)$ and $C_4^4(22)$ graph-set motifs [37] (Fig. 6).

The molecules in adjacent chains interact C—H···π stacking and S—O···π contacts (Fig. 7). They amount to C11B—H11C···*Cg*2 (*x*, *y*+1, *z*) = 3.796(6) Å, S—O2···*Cg*1 (1-*x*, 1-*y*, 1-*z*) = 3.9714(7) Å, S—O3···*Cg*1 (1-*x*, 1-*y*, 1-*z*) = 3.9714(7) Å and S—O3···*Cg*2 (1-*x*, 1-*y*, 1-*z*) = 4.0910(8) Å. *Cg*1 and *Cg*2 correspond to the ring centroids N1/C2/N3/C4/C4A/C8A and C4A/C5/C6/C7/C8/C8A, respectively.

3.3. Hirshfeld surface analysis

To further highlight to most relevant contacts of the title molecule in terms of close interactions, the three-dimensional Hirshfeld surface is depicted in Fig. 8. The Hirshfeld surface mapped with d_{norm} enables us to identify donor (red) and acceptor (blue) regions in the molecules. In investigated structure, the bright red spots appearing near atoms O and N, and H atoms, indicate their roles as the respective donors and acceptors (Table 3).

The two-dimensional fingerprint plot for all contacts is depicted in Fig. 9a and the decomposed plots show that the surface is dominated by H•••H (44.0%) contacts (Fig. 9 b). The pair of sharp spikes (Fig. 9 c) represents the O••H/H•••O contacts with a contribution of 25.4% which indicate the formation of N—H...O hydrogen bonds that can be clearly seen in Fig. 8, and a similar state for N—H...O hydrogen bonds was met in our previous investigations [38]. C•••H/H•••C interactions contribute 11.8% (Fig. 9 d),

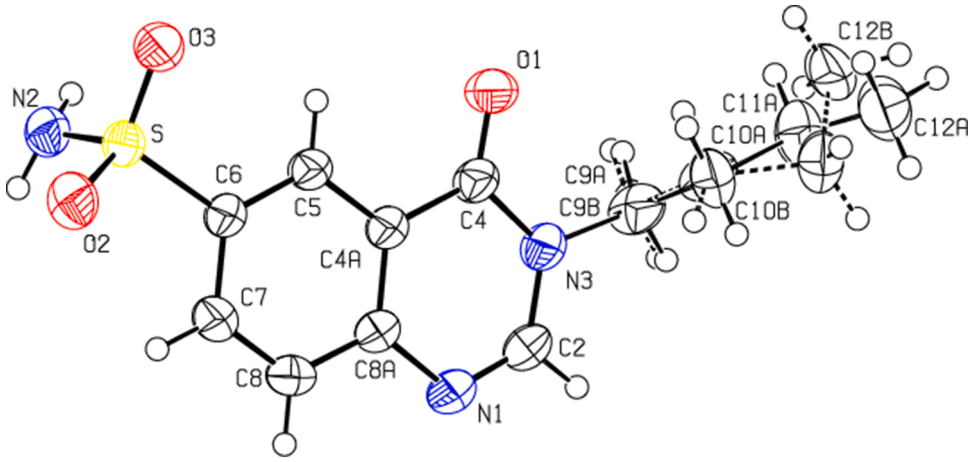

Fig. 4. Displacement ellipsoid plot of the 3-butyl-4-oxo-3,4-dihydroquinazoline-6-sulfonamide and atom-labeling scheme ellipsoids drawn at 50% probability, H atoms shown as fixed-size spheres.

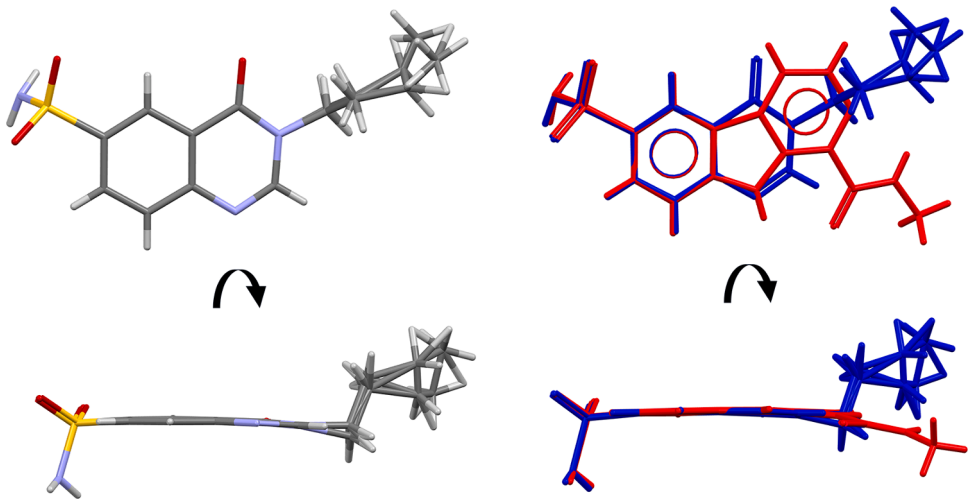

Fig. 5. (a) View the planarity (down) of the aromatic part of title molecule; (b) Structures overlay of title molecule (blue) and molecule of refcode: BATNOB (red) [33].

Table 2
Selected Bond Distances (Å) and Angles (°) for title compound and refcodes: BATNOB [33], AZUTUL [34], WOQVEF [35], YAWTUN [36].

Bond lengths				
Title molecule	BATNOB	AZUTUL	WOQVEF	YAWTUN
C6—S 1.7688(14)	C9—S 1.772(3)	C1—S 1.772(3)	C9—S1 1.758(3)	C10—S1 1.764(2)
O2—S 1.4364(12)	O2—S 1.437(2)	O1—S 1.436(4)	O1—S1 1.441(4)	O2—S1 1.440(2)
O3—S 1.4252(11)	O3—S 1.426(2)	O2—S 1.427(5)	O2—S1 1.439(2)	O1—S1 1.444(2)
N2—S 1.6073(14)	N2—S 1.618(3)	N1—S 1.600(6)	N1—S1 1.615(2)	N1—S1 1.620(2)
Bond angles				
O3—S—O2 119.22(7)	O3—S—O2 118.94(13)	O1—S1—O2 117.3(3)	O1—S1—O2 119.3(1)	O1—S1—O2 118.92(9)
O3—S—N2 107.21(7)	O3—S—N4 107.55(14)	O1—S1—N1 106.7(3)	O3—S1—N2 105.9(1)	O2—S1—N1 107.9(1)
O3—S—C6 108.43(7)	O3—S—C9 107.87(13)	O1—S1—C1 108.2(3)	O1—S1—C9 107.1(1)	O2—S1—C10 108.08(9)
N2—S—O2 106.34(7)	N4—S—O2 106.01(14)	N1—S1—O2 107.9(3)	N2—S1—O2 107.0(1)	N1—S1—O1 106.72(7)

Table 3
Hydrogen-bond and π-ring interactions geometries (Å, °) for title compound.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O2^{i}	0.88(3)	2.16(3)	3.0214 (18)	167(2)
N2—H2*B*···O1^{ii}	0.87(3)	2.05(3)	2.9086 (19)	170(2)
C5—H5···O3	0.93	2.59	2.9446 (17)	103

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

N•••H/H•••N contacts 10.3% (Fig. 9 e), O•••C/C•••O contacts 5.1% (Fig. 9 f) of the total Hirshfeld surface and the contributions of further contacts are only minor (Fig. 10).

4. Conclusions

Thus, as a result of the studies carried out simple and efficient one-pot two-stage methods for the synthesis of sulfonamides were developed. The structure of the compound has been confirmed by IR and ^{1}H NMR spectroscopy as well as X-ray diffraction analysis, and they are structural elements of both theoretical and practical importance in organic and bioorganic chemistry. The asymmetric unit of the title compound, $C_{12}H_{15}N_3O_3S$, comprises two molecules with disordered butyl moiety. In the crystal, the intermolecular N—H•••O hydrogen bonds lead to the formation of an infinity chain with $C_4^4(22)$ graph-set notation. The Hirshfeld surface analysis and the two-dimensional fingerprint plot revealed that H•••H and O•••H/H•••O contacts have a relevant contribution to the crystal packing.

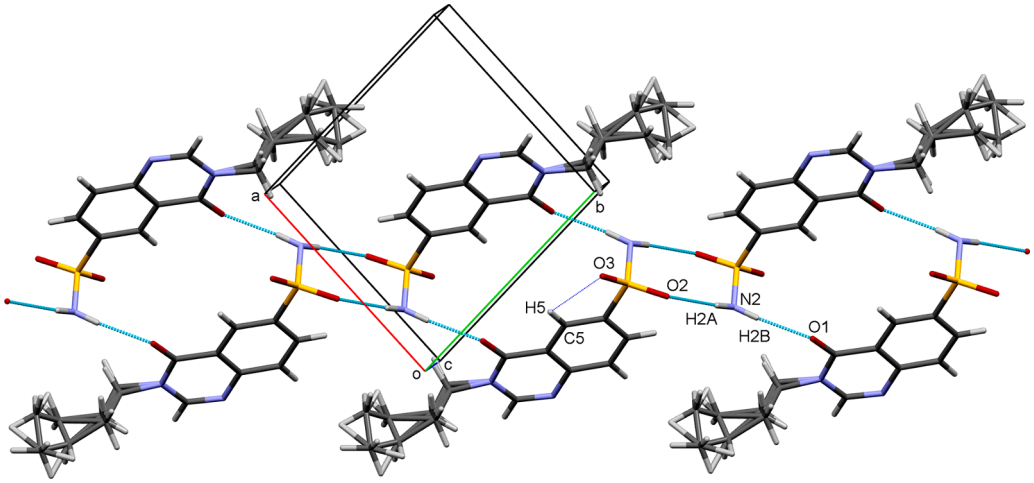

Fig. 6. Intramolecular C5—H5•••O3 hydrogen bonds (dark blue dashed lines) and intermolecular N2—H2A•••O2, N2—H2B•••O2 hydrogen bonds (blue dashed lines).

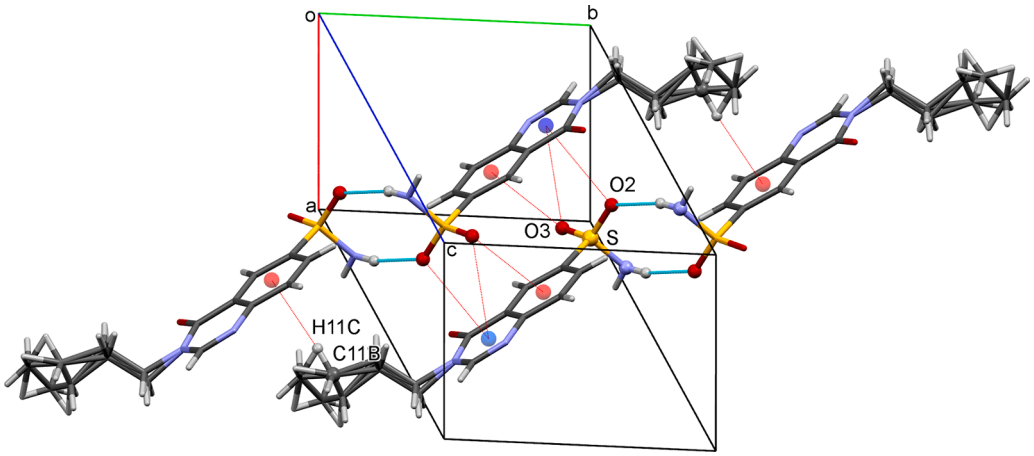

Fig. 7. Dashed red lines denote contacts C11B—H11C···Cg2, S—O2···Cg1, S—O3···Cg1 and S—O3···Cg1. Blue and red spheres correspond to the ring centroids Cg1 and Cg2, respectively.

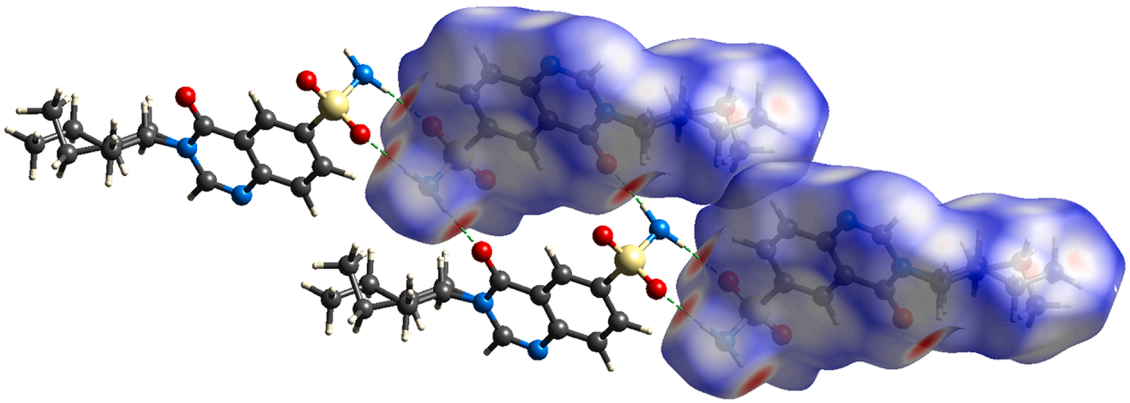

Fig. 8. The Hirshfeld surfaces of title compound mapped with dnorm, the red spots correspond to strong N—H···O hydrogen bonds.

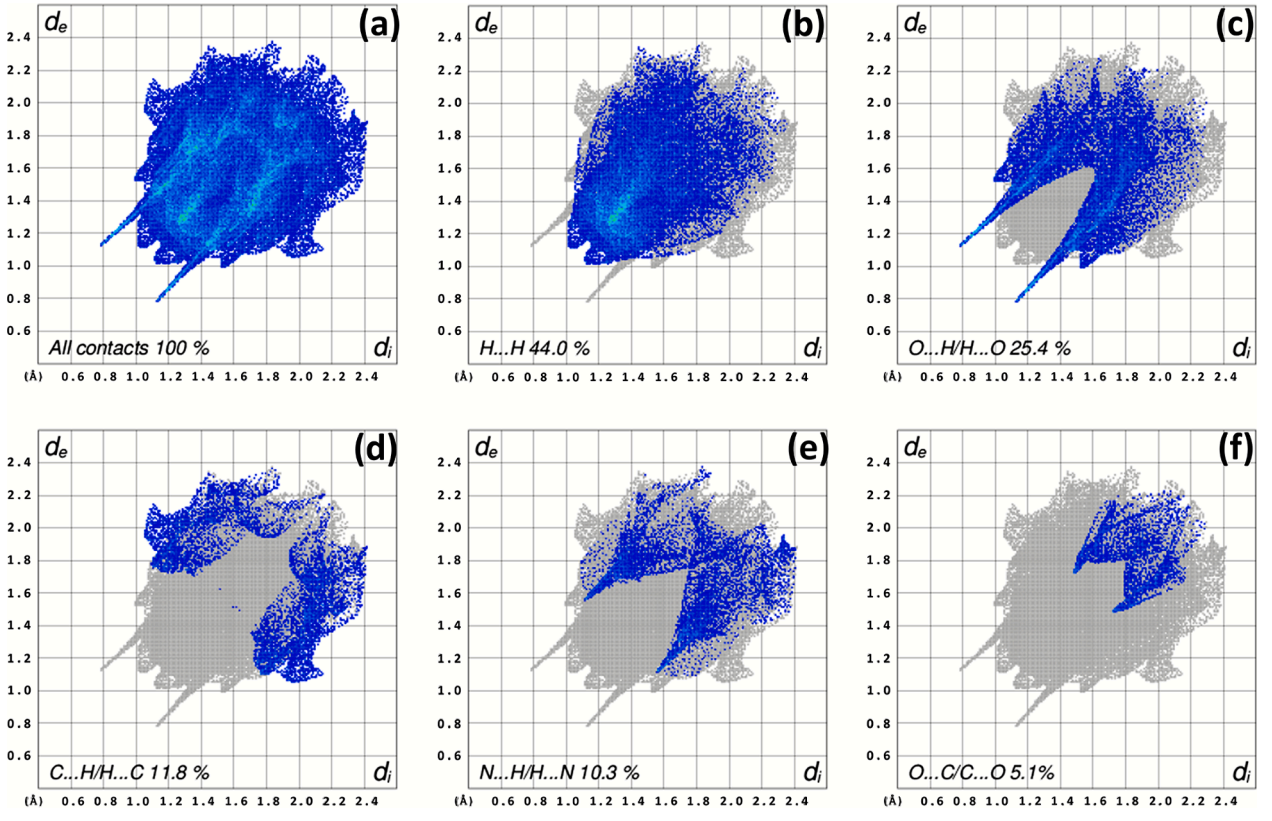

Fig. 9. Full two-dimensional fingerprint plots for title compound showing all interactions (a) and (b) H●●●H, (c) O●●●H/H●●●O, (d) C●●●H/H●●●C, (e) N●●●H/H●●●N, (f) O●●●C/C●●●O interactions. The di and de values are the closest internal and external distances (in Å) from a given point on the Hirshfeld surface.

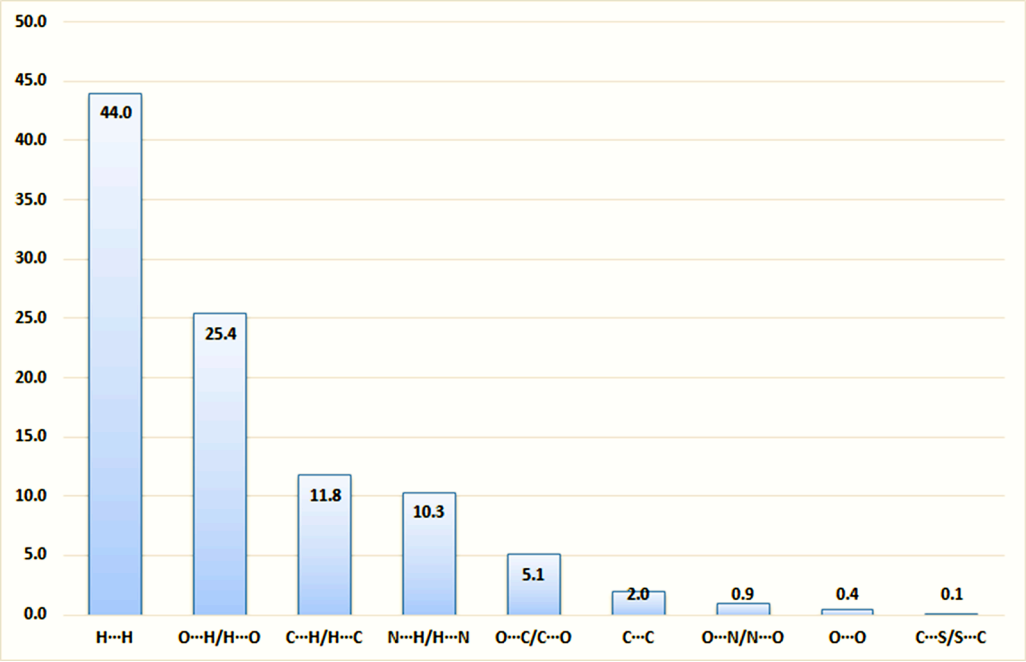

Fig. 10. Relative percentage significant contribute of close contacts to the Hirshfeld surface of title compound.

Specifications table

Subject area	*Organic Chemistry, Physical Chemistry, Single crystal X-ray crystallography.*
Compounds	*3-butyl-4-oxo-3,4-dihydroquinazoline-6-sulfonamide*
Data category	*Synthesized, crystallographic.*
Data acquisition format	*NMR, IR, CIF for crystallography.*
Data type	*Experimental.*
Procedure	*The title compound was synthesis and characterized by crystallographic studies.*
Data accessibility	*Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 2190885.* *URL:* https://summary.ccdc.cam.ac.uk/structure-summary-form

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

Acknowledgments

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.cdc.2022.100926.

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