

Hirshfeld Surface, Fingerprint Plot, Intermolecular Interaction and Crystal Packing Analysis of DCB-Tzol Compound

DCB-Tzol Bileşiğinin Hirshfeld Yüzeyi, Parmak İzi Grafiği, Moleküller Arası Etkileşim ve Kristal Paketlenme Analizi

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ÖZET

Bu çalışmada, 1-(benzoilmethyl)-4-[(2,4-dichlorobenzylidene)amino]-3-(2-thienylmethyl)-4,5-dihydro-1H-1,2,4-triazol-5-one (DCB-Tzol) bileşiğinin moleküller arası etkileşimleri ve kristal paketlenme özellikleri, CSD veri tabanından elde edilen kristal yapısı (CCDC 651492) temel alınarak Hirshfeld yüzey analizi, iki boyutlu parmak izi grafikleri ve fragment patch mapping yöntemleri kullanılarak incelenmiştir. d_{norm} yüzeyi, van der Waals yarıçapları toplamından daha kısa olan baskın C-H...O etkileşiminin yanı sıra zayıf C-H...Cl ve van der Waals temaslarını ortaya koymuştur. Parmak izi analizi, H...H (%35,4), C...H/H...C (%17.2), O...H/H...O (%12.0) ve Cl...H/H...Cl (%11.7) temaslarının yüzeye en büyük katkısı sağladığını göstermiştir. Hirshfeld yüzeyleri, parmak izi grafikleri, shape index ve fragment patch mapping analizlerinin birlikte değerlendirilmesi, DCB-Tzol'un moleküller arası temas ortamının ayrıntılı ve nicel bir tanımını sağlamakta ve yönlü ile dispersif etkileşimlerin kristal paketlenmesine göreceli katkılarını ortaya koymaktadır. Shape index yüzeyi, C-H... π etkileşimlerinin varlığını desteklerken, π ... π istiflenmesine işaret eden karakteristik bir desen gözlenmemiştir. Genel olarak, DCB-Tzol bileşiğinin kristal paketlenmesi, tek bir baskın kuvvetten ziyade çok merkezli zayıf moleküller arası etkileşimlerin birlikte oluşturduğu bir ağ tarafından yönetilmektedir.

Anahtar Kelimeler: 1,2,4-Triazol, Hirshfeld Yüzey Analizi, Kristal Paketlenme, Parmak İzi Haritası, Moleküler Arası Etkileşimler

ABSTRACT

In this study, the intermolecular interactions and crystal packing properties of the compound 1-(benzoilmethyl)-4-[(2,4-dichlorobenzylidene)amino]-3-(2-thienylmethyl)-4,5-dihydro-1H-1,2,4-triazol-5-one (DCB-Tzol) were investigated using Hirshfeld surface analysis, two-dimensional fingerprinting graphs, and fragment patch mapping methods, based on the crystal structure (CCDC 651492) obtained from the CSD database. The d_{norm} surface revealed the dominant C-H...O interaction, which falls below the sum of the van der Waals radii, along with weak C-H...Cl and van der Waals contacts. Fingerprint analysis showed that H...H (35.4%), C...H/H...C (17.2%), O...H/H...O (12.0%), and Cl...H/H...Cl (11.7%) contacts contributed the

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most to the surface. The combined analysis of Hirshfeld surfaces, fingerprint plots, shape index, and fragment patch mapping provides a detailed quantitative description of the intermolecular contact environment of DCB-Tzol and highlights the relative contributions of directional and dispersive interactions to its crystal packing. The shape index surface supports the presence of C–H $\cdots$ π interactions, while no characteristic pattern indicative of $\pi\cdots\pi$ stacking was observed. Overall, the crystal packing of the DCB-Tzol compound is governed by a network maintained by the cooperation of multicentric weak intermolecular interactions rather than a single dominant force.

Keywords: 1,2,4-Triazole, Hirshfeld surface analysis, Crystal packing, Fingerprint plot, Intermolecular interactions

INTRODUCTION

1,2,4-Triazole and its derivatives constitute an important class of nitrogen-containing heterocyclic compounds because of their diverse chemical and biological properties. In particular, 1,2,4-triazol-5-one derivatives have attracted considerable attention owing to their structural versatility, electron-rich heterocyclic framework, and ability to participate in various intermolecular interactions. Their molecular structures can be readily modified through substitution at different positions, providing useful systems for investigating the relationship between molecular structure and crystal packing. Previous studies have reported various biological and structural properties of 1,2,4-triazole derivatives, including antimicrobial, antifungal (Haddad et al., 2015), anti-inflammatory (Li et al., 2016), anticancer (Sun et al., 2019), and antioxidant activities (Zobo Mfomo et al., 2017). However, beyond their biological relevance, the structural features of these compounds make them suitable candidates for investigating intermolecular interactions and supramolecular organization in the crystalline state.

The properties and stability of molecular crystals are strongly influenced by the manner in which molecules are arranged and interconnected within the crystal lattice. Intermolecular hydrogen bonding, C–H $\cdots$ π contacts, $\pi\cdots\pi$ interactions, halogen-related contacts, and dispersive van der Waals interactions may act cooperatively to determine crystal packing and supramolecular architecture. Consequently, understanding the nature and relative contributions of intermolecular interactions is an important aspect of crystal engineering and supramolecular chemistry. Crystal engineering focuses on understanding intermolecular interactions in the context of crystal packing and using this knowledge to rationalize or design molecular solids with desired structural and physical properties (Desiraju, 2013). Therefore, detailed analysis of intermolecular contacts provides valuable information for establishing structure–packing relationships in molecular crystals.

Single-crystal X-ray diffraction (SC-XRD) provides precise information on molecular geometry, intermolecular distances, and crystal packing. Nevertheless, the interpretation of a crystal structure based solely on selected geometric parameters may not readily provide a quantitative overview of the relative contributions of different types of intermolecular contacts to the molecular surface. Hirshfeld surface analysis provides a complementary approach by partitioning the crystal space around a molecule and enabling intermolecular contacts to be visualized and quantified. The normalized contact distance (d_{norm}), together

with the internal (d_i) and external (d_e) distances, allows short contacts to be readily identified on the molecular surface. In addition, two-dimensional fingerprint plots provide a quantitative representation of the different intermolecular contact types and their relative contributions to the Hirshfeld surface (Spackman and Jayatilaka, 2009; Spackman et al., 2021). CrystalExplorer has subsequently become an established computational platform for the visualization and quantitative analysis of Hirshfeld surfaces, fingerprint plots, and intermolecular interactions in molecular crystals (Spackman et al., 2021).

The interpretation of Hirshfeld surfaces can be further complemented by surface descriptors such as the shape index and fragment patch mapping. The shape index is particularly useful for examining characteristic surface patterns associated with contacts involving aromatic systems, while fragment patch analysis enables different contact regions on the Hirshfeld surface to be visualized according to their interacting atomic fragments. Together with fingerprint plots, these approaches provide a more comprehensive description of the supramolecular environment of a molecule and help distinguish the relative roles of directional contacts and more diffuse dispersive interactions. Such analyses have been successfully applied to a wide range of molecular crystals, including heterocyclic and triazole-containing compounds, where $H\cdots H$, $C\cdots H/H\cdots C$, $O\cdots H/H\cdots O$, and halogen-involving contacts can make substantial contributions to crystal packing (Lazrak et al., 2023; Mescheryakova et al., 2026; Sancak et al., 2025a; Sancak et al., 2025b).

In this context, the 1-(benzoylmethyl)-4-[(2,4-dichlorobenzylidene)amino]-3-(2-thienylmethyl)-4,5-dihydro-1H-1,2,4-triazol-5-one compound (**DCB-Tzol**) represents an interesting molecular system for investigating the relationship between molecular structure and crystal packing. The molecule contains a 1,2,4-triazol-5-one ring together with benzoylmethyl, dichlorobenzylidene, and thienylmethyl groups, providing several potential sites for intermolecular contacts. The crystal structure of DCB-Tzol was previously reported by Ustabaş et al. and is available in the Cambridge Structural Database (CSD) under the accession number CCDC 651492 (Ustabaş et al., 2007).

In the present study, the previously reported crystal structure of **DCB-Tzol** was examined in detail using Hirshfeld surface analysis, two-dimensional fingerprint plots, shape-index mapping, and fragment patch analysis. The aim was to characterize the intermolecular contacts governing the crystal packing and to quantify their relative contributions to the Hirshfeld surface. Particular attention was given to $C-H\cdots O$ and $C-H\cdots Cl$ contacts, $H\cdots H$ and $C\cdots H/H\cdots C$ dispersive contacts, and possible aromatic interactions. This analysis provides a quantitative description of the supramolecular organization of DCB-Tzol and contributes to a better understanding of the intermolecular interaction patterns governing the crystal packing of 1,2,4-triazol-5-one derivatives.

MATERIALS AND METHODS

Crystal Structure

The crystal structure of the compound was first reported by Ustabaş et al. (Ustabaş et al., 2007). The XRD structure of this compound is registered in the Cambridge Structural Database (CSD) with accession number CCDC 651492. The molecular geometry used in this

study was obtained from the previously reported experimental single crystal XRD structure (Figure 1).

Computational Methodology

The crystal information file (CIF) of the molecule was obtained from CSD. Hirshfeld surface analysis, fingerprint analysis, crystal packing and visualization processes used for supramolecular analysis were performed using CrystalExplorer 21.5 (Spackman et al., 2021) and Mercury (Macrae et al., 2020) programs.

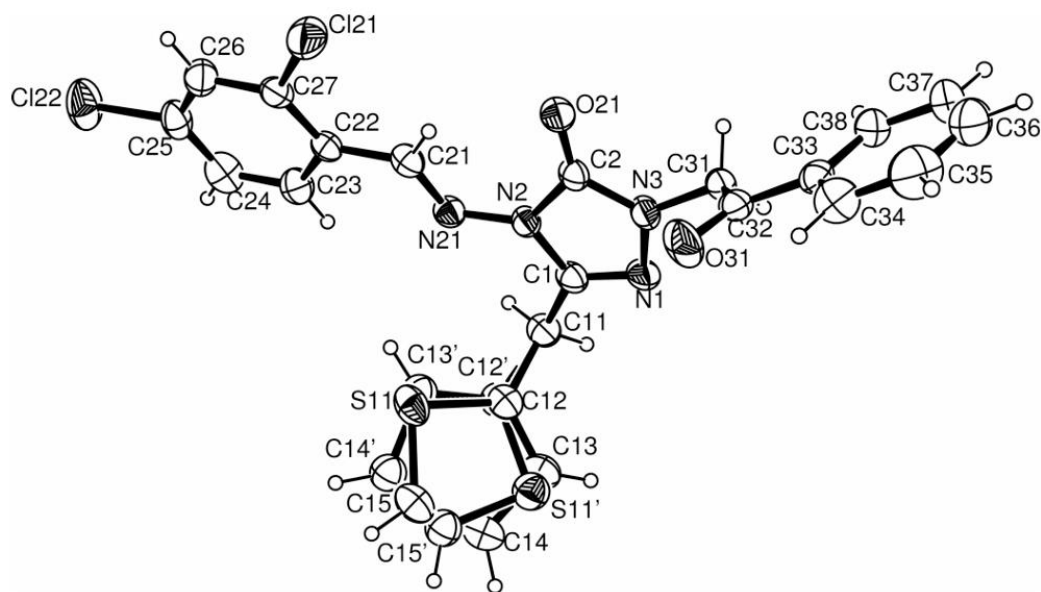


Figure 1. The DCB-Tzol molecule drawn at 30% probability level (Ustabaş et al., 2007).

RESULTS AND DISCUSSION

Hirshfeld Surface Analysis

Hirshfeld surface analysis is an important method that allows for the visualization and study of intermolecular interactions in crystal packing arrangements in two and three dimensions. These interactions include fundamental phenomena such as hydrogen bonds, $\pi \cdots \pi$ interactions, London dispersion forces, and dipole-dipole interactions. This analysis facilitates understanding the effect of these interactions on the stability of molecules within the crystalline structure (Sancak et al., 2025b). The Hirshfeld surface is constructed using an electron density weighting function based on an isovalue of 0.5. This isovalue represents the natural molecular boundary where the electron density contribution of the molecule under study is equal to the total electron density of the surrounding molecules.

In this section, d_i , d_e , d_{norm} , shape index, fragment patch surfaces, and the ratios of these surfaces were determined for the purpose of studying intermolecular interactions and contact points in the crystalline structure. The distance of an atom in the molecule to the point closest to the Hirshfeld surface is defined as d_i , and the distance between it and the nearest atom outside the surface is defined as d_e . The d_{norm} value is determined by the

van der Waals radii of the atoms and is calculated by normalizing the measurements with d_i (Spackman and Jayatilaka, 2009).

Table 1. Intermolecular interactions and van der Waals analysis

Interactions	Observed Distance (Å)	Sum of van der Waals radii (Å) (Mantina et al., 2009)	Difference (Δ , Å)	Character
C11–H11A...O21	2.649	2.72	–0.07	Weak H-bond
C13–H13...O21	2.533	2.72	–0.19	Moderate H-bond
C26–H26...O31	2.598	2.72	–0.12	Moderate–weak H-bond
C36–H36...Cl21	2.943	2.95	–0.01	Borderline van der Waals contact

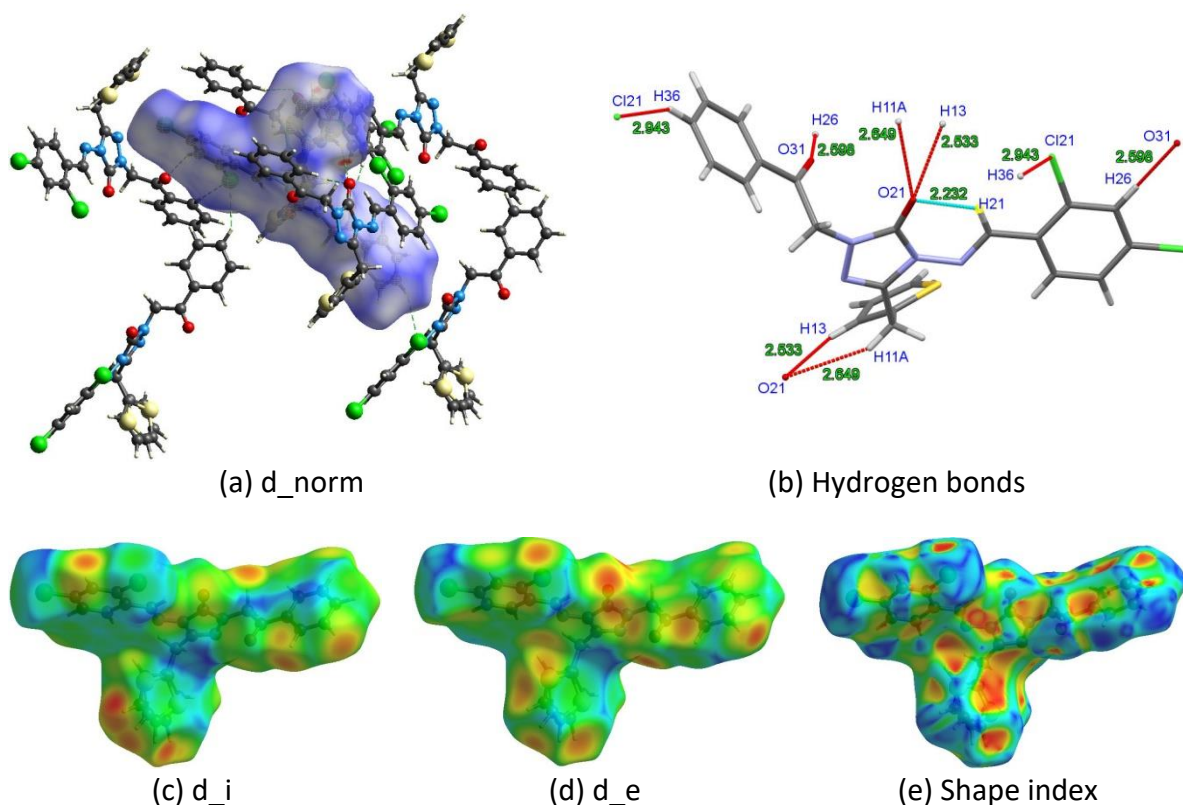


Figure 2. Hirshfeld surfaces and hydrogen bonds. Hirshfeld surface mapping ranges: (a) d_{norm} (–0.150 to 1.289), (c) d_i (0.914 to 2.572 Å), (d) d_e (0.918 to 2.633 Å), (e) shape index (–0.999 to 0.997 a.u.)

The blue regions on the d_{norm} surface show contacts longer than the sum of the van der Waals radii, while the white regions ($d_{\text{norm}} \approx 0$) show regions at the exact van der Waals contact distance (Özşanlı and Aygün, 2026). The red regions represent contacts shorter than the sum of the van der Waals radii, i.e., strong/moderate intermolecular interactions (Figure 2a). Several distinct red dots are seen on the surface, which correspond to hydrogen bond donor-acceptor pairs. All distances observed on the surface are below the sum of the van der

Waals radii ($\Delta < 0$); this confirms that all interactions have a true attractive nature. C13–H13...O21 ($\Delta = -0.19 \text{ \AA}$) represents the strongest interaction in this series and is compatible with a moderately strong C–H...O hydrogen bond. C36–H36...Cl21 ($\Delta = -0.01 \text{ \AA}$) is located almost exactly at the van der Waals contact boundary, indicating a very weak C–H...Cl interaction (Table 1 and Figure 2b). The fact that the surface is covered with large blue areas and contains a small number of red dots shows that the majority of the molecule is in van der Waals contact, while directional strong interactions remain localized.

The red circular dots on the d_i surface, showing the distance from the inside of the Hirshfeld surface to the atoms of the molecule, indicate the proximity of the molecule to its own atoms; these regions correspond to the convex parts of the molecule, especially where the hydrogen atoms are located (Figure 2c). The relatively homogeneous distribution in the aromatic ring regions indicates that the π system occupies a uniform area on the surface.

The prominent red areas in the upper region of the d_e surface, showing the distance from the outside of the Hirshfeld surface to the atoms of neighboring molecules, indicate that an atom of a neighboring molecule is very close to this surface point (Figure 2d). The blue/green tones on the aromatic rings indirectly support the idea that the π surfaces are relatively far from neighboring atoms, i.e., that there is no $\pi\cdots\pi$ stacking.

The shape index surface codes the local curvature of the surface between -1 (concave, red) and +1 (convex, blue) and is the most informative surface for detecting $\pi\cdots\pi$ and C–H... π interactions (Suhta et al., 2026). The red (concave) and adjacent blue (convex) patches together form a bicolor pattern that is a classic signature of C–H... π interactions. The hydrogen atom (convex, blue) of one molecule sits on the aromatic π surface (concave, red) of the neighboring molecule. The red-blue mosaic pattern seen in the shape index is prominent on the aromatic ring surfaces; this suggests that C–H... π interactions are active. If $\pi\cdots\pi$ stacking were present, large, flat, "hourglass funnel-shaped" interlocking red and blue patches would be seen on the opposing rings. Such a pattern is not observed in this structure, which is consistent with the absence of $\pi\cdots\pi$ stacking. The color variation across the entire surface of the molecule indicates the presence of numerous different types of intermolecular contacts, but none forming a dominant and uniform geometric pattern (Figure 2e).

Fragment patches divide the Hirshfeld surface into colored regions, where each color represents a specific pair of atomic interactions (Ali et al., 2026). The area ($\text{\AA}^2$) of each of the 19 patches identified on the surface directly expresses the area occupied by the relevant interaction on the molecular surface (Figure 3). The largest patch of the molecule is the magenta-colored $77.0 \text{ \AA}^2$ patch, corresponding to H...H dominant van der Waals contacts, which is consistent with H...H (35.4%) contacts in the fingerprint analysis. The second largest dominant interaction is the yellow-colored $71.6 \text{ \AA}^2$ patch, corresponding to C...H / H...C (17.2%) in the fingerprint analysis. Such large areas are generally associated with aromatic ring systems and hydrogen-rich surfaces, and usually define regions where H...H and C...H/H...C type dispersion interactions are concentrated. The smallest patch of the molecule was identified as $6.1 \text{ \AA}^2$.

The calculated surface volume of the molecule is $526.18 \text{ \AA}^3$, the unit cell volume is $4284.4 \text{ \AA}^3$, and the surface area is $470.57 \text{ \AA}^2$, revealing the spatial dimensions of the molecule

within the crystal structure. The globularity ratio, indicating the degree of sphericity of the molecule, is 0.670, suggesting moderate sphericity. This is a typical value expected for molecules containing large aromatic ring systems and side groups.

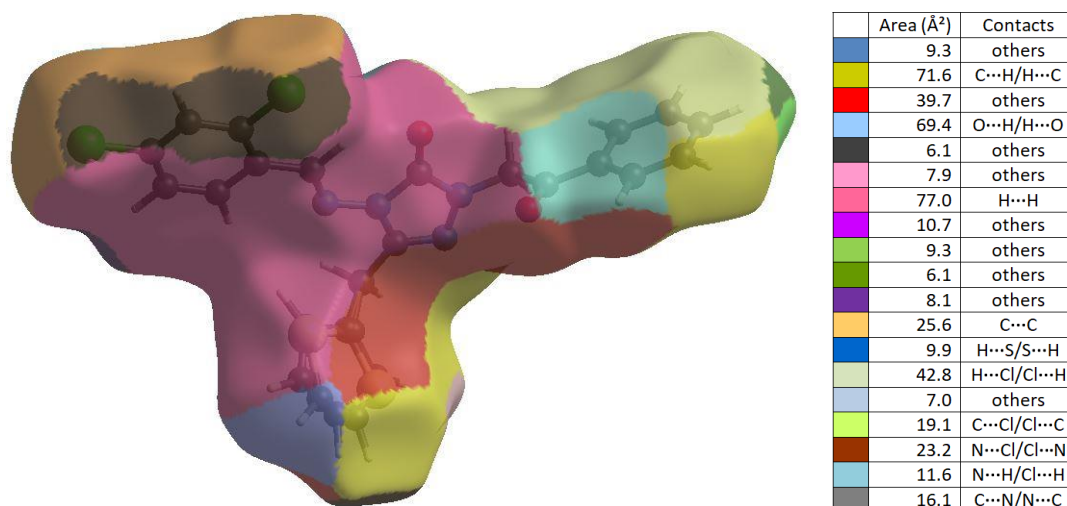


Figure 3. Fragment patches on the Hirshfeld surface

The asphericity ratio, indicating the degree of deviation from sphericity, is 0.242, suggesting that the molecule is not entirely planar but has a structure with distinct protrusions (Davydenko et al., 2025). When these four parameters are considered together, it is understood that the molecule has a moderately spherical, slightly elongated geometry with surface roughness. This structure allows for complementary packing with neighboring molecules in the crystal lattice and supports the observed intermolecular interactions.

Fingerprint surface analysis

2D fingerprint maps quantitatively reveal the type and relative contributions of intermolecular contacts in the crystal structure (Turner et al., 2014). The concentration of density in the central region across the entire contribution map indicates that the crystal packing consists largely of van der Waals-type contacts (Figure 4). The sharp protrusions observed in the fingerprint diagrams are characteristic of directional and short intermolecular interactions.

The most dominant contribution comes from H...H contacts, constituting 35.4% of the total surface area. This broad and widespread distribution indicates that the crystal structure has a high density of hydrogen atoms and that the molecular packing is significantly stabilized by dispersive van der Waals interactions. The high proportion of H...H contacts also supports the limited presence of strong classical hydrogen bonds in the structure.

C...H/H...C contacts constitute the second largest interaction group with a contribution of 17.2%. The characteristic wing-like distribution in the fingerprint map shows that these contacts are largely due to C–H... π and weak C–H...C interactions. This result is consistent with

the red-blue mosaic patterns observed on the shape index surface and supports the conclusion that aromatic ring systems make a significant contribution to the crystal packing.

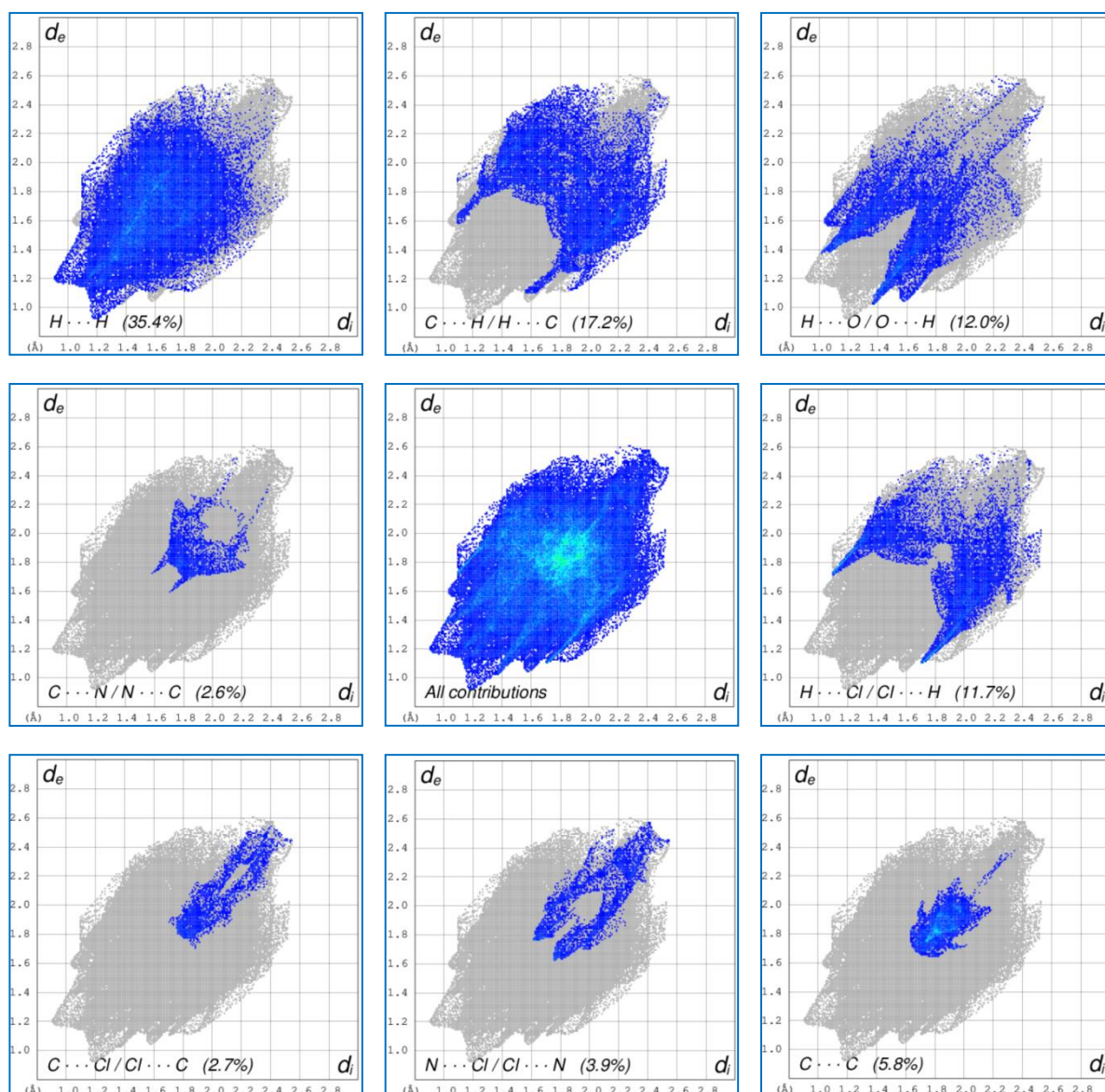


Figure 4. Two-dimensional fingerprint plots and relative contributions of intermolecular contacts

O...H/H...O contacts contribute a total of 12.0%. The prominent spikes in the map confirm the presence of directional C—H...O hydrogen bonds. In particular, a denser distribution has occurred in this region due to the short contact distance of the C13—H13...O21 interaction. These contacts are among the most important specific intermolecular interactions contributing to crystal stability.

Cl...H/H...Cl contacts contribute 11.7%. This distribution shows that chlorine atoms act as both weak hydrogen bond acceptors and dispersive contact centers. The thin spike regions

in the map are associated with weak C–H...Cl contacts and show interaction characteristics close to the van der Waals boundary.

The fact that C...C contacts contribute only 5.8% indicates that there is no significant $\pi\cdots\pi$ stacking in the structure. If strong aromatic stacking were present, more dense and symmetrical central regions would be observed in the fingerprint diagram. This result is also consistent with the absence of large complementary red-blue patches characteristic of $\pi\cdots\pi$ interactions on the shape index surface.

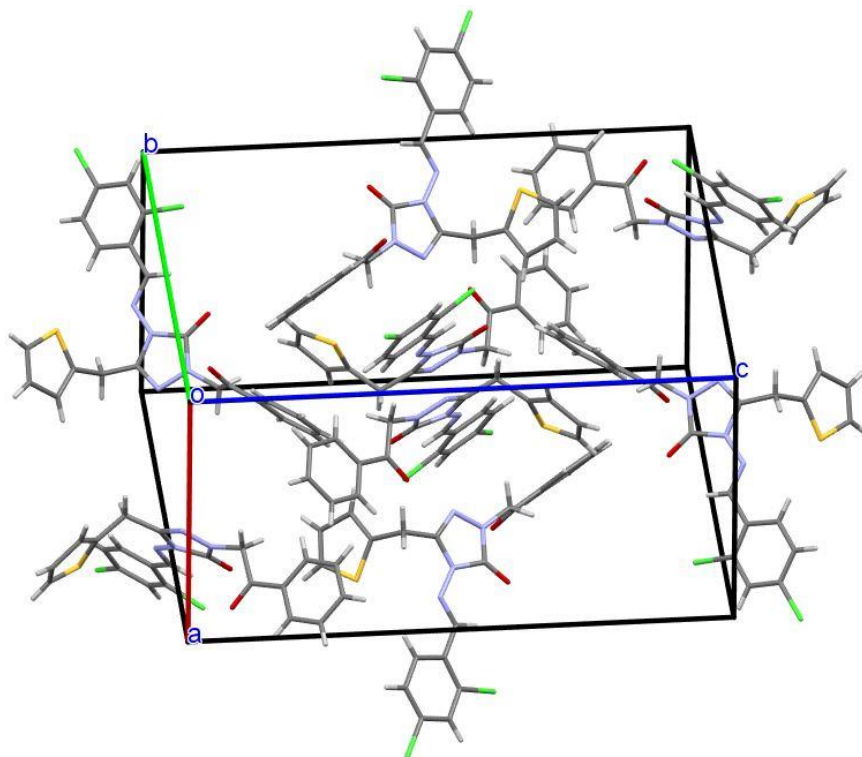


Figure 5. Molecular packing and unit cell representation of the title compound

N...Cl/Cl...N (3.9%) and C...Cl/Cl...C (2.7%) contacts have low contribution rates and contribute secondarily to crystal packing. Similarly, the fact that C...N/N...C contacts remain at 2.6% indicates that nitrogen atoms play a limited role in crystal organization.

Filtering fingerprint by element type quantitatively show the atom-based contact distributions on the Hirshfeld surface (Table 2). In this table, it is seen that the highest contribution comes from hydrogen atoms at 61.0%. This indicates that crystal packing is largely controlled by H-based van der Waals and dispersive interactions. In particular, the high value of H...H contacts at 35.4% confirms that a significant portion of the molecular surface is surrounded by hydrogen atoms and that crystal stability is largely due to weak dispersive forces.

Overall, fingerprint analysis reveals that the crystal structure is primarily stabilized by H...H dispersive contacts and C...H/H...C interactions; in addition, O...H/H...O and Cl...H/H...Cl contacts provide directional but moderately weak contributions. In contrast, the absence of

$\pi\cdots\pi$ stacking indicates that the crystal packing is driven by multicentric weak intermolecular contacts rather than aromatic aggregation (Figure 5).

Table 2. Percentage contributions of intermolecular contacts to the Hirshfeld surface

Outside atoms								
Inside atoms	Atoms	Cl	O	N	C	H	S	(%)
	C	1.4	0.6	1.3	5.8	9.7	.	18.7
	Cl	1.0	0.2	2.0	1.3	7.2	1.2	12.9
	H	4.5	5.3	1.2	7.5	35.4	0.3	54.3
	N	1.9	.	0.4	1.3	1.3	.	5.0
	O	0.1	.	.	0.5	6.7	.	7.2
	S	1.2	.	.	.	0.7	.	1.9
	(%)	10.1	6.1	4.9	16.4	61.0	1.5	100

CONCLUSIONS

In this study, the crystal packing properties of the **DCB-Tzol** compound were comprehensively investigated using Hirshfeld surface analysis, two-dimensional fingerprinting, and fragment patch mapping methods. The findings reveal that crystal stability arises not from any single dominant force, but from the cooperation of multicentric weak intermolecular interactions. $H\cdots H$ (35.4%) and $C\cdots H/H\cdots C$ (17.2%) contacts show the dominance of dispersive van der Waals interactions, while $C-H\cdots O$ (12.0%) and $C-H\cdots Cl$ (11.7%) hydrogen bonds contribute directionally to the crystal structure. Shape index analysis supports the presence of $C-H\cdots\pi$ interactions and suggests that $\pi\cdots\pi$ stacking is not effective in this structure. These results contribute to the understanding of the supramolecular organization of 1,2,4-triazol-5-one derivatives. From a crystal engineering standpoint, the dominant role of directional $C-H\cdots O$ and $C-H\cdots Cl$ contacts alongside dispersive $H\cdots H$ interactions indicates that the carbonyl and triazolone acceptor sites are the most promising synthons for supramolecular design in this compound, offering suitable targets for future co-crystal or salt engineering aimed at tuning solubility and packing efficiency. Furthermore, the absence of $\pi\cdots\pi$ stacking implies that crystal engineering strategies for this scaffold should rely on weak hydrogen-bond and van der Waals synthons rather than aromatic stacking motifs to control polymorphism and crystal habit. Overall, contacts involving hydrogen atoms ($H\cdots H$, $C\cdots H$, $O\cdots H$ and $Cl\cdots H$ contacts combined) account for over 76% of the total Hirshfeld surface, indicating that this crystal system is stabilized predominantly by numerous weak, additive interactions rather than by a single strong directional force. This quantitative distribution,

summarized in Table 2, provides a solid basis for rationalizing the packing motif and offers practical guidance for future crystal engineering and co-crystal design efforts targeting this scaffold.

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Author Contributions

The author solely conducted all stages of the study, including conceptualization, methodology, investigation, data analysis, writing of the original draft, review, and editing, and approved the final version of the manuscript.

Conflict of Interest

The author declares that there is no conflict of interest regarding the preparation, publication, and authorship of this study.

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Ethical Statement

No ethical committee approval is required for this study.