CRYSTAL STRUCTURE OF (E)-N'-((1H-PYRROL-2-YL)METHYLENE)-4-HYDROXYBENZOHYDRAZIDE

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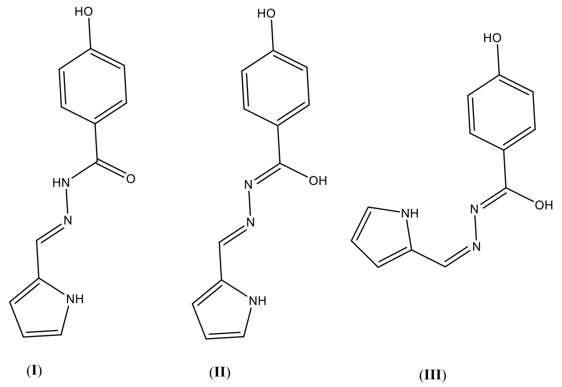
ABSTRACT

The title compound corresponds to an enaminone *E* isomer in the solid state. X-ray structure shows that this crystallizes in the orthorrombic system, with space group Pna2_1 with 2 independent molecules in the asymmetric unit in a non-centrosymmetric setting. The CNNC unit forms dihedral angles of 5.9(3)/2.1(3); 19.7(3)/17.6(3)° with the pyrrole and phenol rings for molecules A and B respectively. The main differences between both molecules is the dihedral torsion between rings, their mean planes form dihedral angles of 25.45(15) and 15.38(15)° for the molecules A and B. In the asymmetric unit, molecules are linked by two weak N – H···O hydrogen bonds with set graph-motif $R_2^2(16)$.The crystal structure of title compound generates a two dimensional supramolecular network lying parallel (110) with hydrogen bonds interactions between O – H···O and N – H···O along to [100] and [001] direction with graph set motifs $R_1^2(5)$, $R_2^2(10)$, $C_1^1(8)$ and $C_1^1(12)$. π-π stacking interactions are not observed. Hirshfeld surface analysis were used to verify the contributions of the different intermolecular interactions. Both molecules are essentially overlaid between them with RMSD = 0.0574; max D = 0.1211 Å considering inversion and flexibility.

Keywords: Hydrazide, X-ray diffracction, non-covalent interactions, Hirshfeld surface, energy framework.

1. INTRODUCTION

Weak interactions, such as hydrogen, halogen, chalcogen, pnicogen, tetrel and picosagen bonds were extensively used in the synthesis, catalysis, crystal engineering, drug delivery, etc. [1-11]. Among those, hydrogen bonding has turned out to be particularly suitable for design of organic and coordination compounds[12–19]. Herein, we found strong intermolecular hydrogen bonds in (E)-N'-((1H-pyrrol-2-yl)methylene)-4-hydroxybenzohydrazide (**I**) and other weak non-covalent interactions, which were analized by Hirshfeld surface analysis to observe all contributions of the different intermolecular interactions stabilizing final 2D organic framework network (Scheme 1).



(I) (II) (III)

Scheme 1.

2. EXPERIMENTAL

High purity (*E*)-*N*'-((1H-pyrrol-2-yl)methylene)-4-hydroxybenzohydrazide was prepared in the laboratory following the literature method[20]. A possible future solution to our inability to grow single-crystals is the use of very interesting and unusual glassware for reaction/crystallization apparatus (branched tube) recently developed by us[21]. For the molecular structure of title compound, H atoms were located in the difference Fourier map and refined freely with distances in the range of 0.88(4) – 0.99(3) Å, except for the atoms H5A and H3B, which were treated has riding model , with distances C5A–H5A and N3B–H3B of 0.951 and 0.88 Å and U_{iso}(H) fixed at $1.2U_{eq}$ of the parent C and N atoms respectively.

X-ray diffraction patterns of title compound were collected using a Bruker SMART APEX-II CCD area detector equipped with graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å) at 100 K. The diffraction frames were integrated using the APEX3 package[22]. The structure of were solved by intrinsic phasing[23] using the OLEX 2 program[24]. The structure was then refined with full-matrix least-square methods based on F^2 (*SHELXL-2014*)[23]. For (I), non-hydrogen atoms were refined with anisotropic displacement parameters. A summary of the details about crystal data, collection parameters and refinement are documented in Table 1, and additional crystallographic details are in the CIF files. ORTEP views were drawn using OLEX2 software[24]. CCDC 1917875 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via **www.ccdc.cam.as.uk/data_request/cif**.

Table 1. Crystal data parameters for compound (I)

Empirical Formula	$C_{12}H_{11}N_3O_2$
Formula mass, g mol^{-1}	229.24
Collection T, K	99.99
crystal system	orthorhombic
space group	Pna2_1
a (Å)	15.3668(9)
b (Å)	11.0969(8)
c (Å)	12.7075(10)
α,β, γ (°)	90
V (Å^3)	2166.9(3)
Z	8
ρ_{calcd} (gcm^{-3})	1.405
Crystal size (mm)	0.29 x 0.21 x 0.14
F(000)	960.0
abs coeff (mm^{-1})	0.099
2θ range (°)	4.528 to 52.024
range h,k,l	-17/18, -13/13, -15/15
No. total refl.	4264
No. unique refl.	4264
Comp. θ_{max} (%)	1.00/26.00
Max/min transmission	0.943,1.000
Data/Restraints/Parameters	4264/1/387
Final R [$I>2\sigma(I)$]	R_1 = 0.0368, wR_2 = 0.0820
R indices (all data)	R_1 = 0.0529, wR_2 = 0.0907
Goodness of fit / F^2	1.038
Largest diff. Peak/hole (eÅ^{-3})	0.18/-0.24

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3. RESULTS AND DISCUSSIONS

The title compound corresponds to an enaminone *E* isomer in the solid state. The crystal structure can be described in terms of discrete molecules with two independent molecules in the asymmetric unit. An analysis of normal probability plot[25] indicates that differences in the bond lengths and angles of these molecules are statistically insignificant. The average values will therefore be discussed. The sum of the angles around the N1 and N3 atoms [358.9 (3); 359.7(3)°] reflects a planar *sp2* geometry. All the distances and angles are normal[26,27] and comparable with similar compounds, refcode JOVQUI[28] and VETPAO[29] , included in CCDC data base[30]. The CNNC unit forms dihedral angles of 5.9(3)/2.1(3)°; 19.7(3)/17.6(3)° with the pyrrole and phenol rings for molecules A and B respectively. The main differences between both molecules is the dihedral torsion between rings, their mean planes form dihedral angles of 25.45(15) and 15.38(15)° for the molecules A and B. In the asymmetric unit, molecules are linked by two weak N–H···O hydrogen bonds with set graph-motif $R_2^2(16)$. The crystal structure of title compound generates a two dimensional supramolecular network lying parallel (110) with hydrogen bonds interactions between O – H···O and N – H···O along to [100] and [001] direction with graph set motifs $R_1^2(5)$, $R_2^2(10)$, $C_1^1(8)$ and $C_1^1(12)$. π-π stacking interactions are not observed. Both molecules are essentially overlaid between them with RMSD = 0.0574; max D = 0.1211 Å considering inversion and flexibility.

The molecular structure shows average dihedral angles of 20.1(4)° and 16.0(4)° between 4-hidroxyphenyl ring and -C(O)-NH- moiety and, 3.90(4)° between pyrrole ring and N2 atoms, 4.50(4)°, between carbonyl and -NH-N= fragment, respectively.

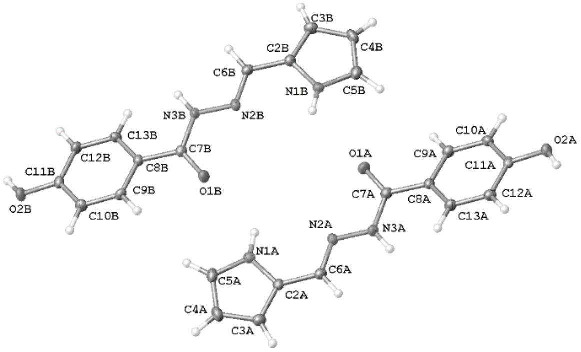

Figure 1. ORTEP plot of the title compound. Thermal ellipsoids were drawn with 30% of probability.

Half-normal probability plot analysis was used to (i) investigate the reliability of the s.u.'s and (ii) identify systematic geometrical differences in two molecules. A comparison of the bond distances and angles of the fitted residues, reveals that the two molecules do not show any significant geometrical differences (see Table 2)[31]. The slope plot of the bond angles is 0.4910 and the intercept is -0.0016, showed a straight line with an intercept of almost zero and a slope of less than unity indicating that the s.u.s are slightly overestimated. The largest difference (-0.80°) is between the C8A -C9A -C10A angle in the first molecule and C8B -C9B -C10B in the second molecule , with Diff/Sig of -1.89, (RMS Angle Fit = 0.336°, sample size of 23)[32].

Table 2. Bond distances and angles of the title compound.

Atom		Length/Å	Atom		Length/Å	Atom			Angle/°	Atom			Angle/°
O1A	C7A	1.238(4)	O1B	C7B	1.236(4)	C5A	N1A	C2A	109.0(3)	C5B	N1B	C2B	109.2(3)
O2A	C11A	1.360(4)	O2B	C11B	1.357(4)	C6A	N2A	N3A	116.0(3)	C6B	N2B	N3B	116.5(3)
N1A	C2A	1.373(5)	N1B	C2B	1.373(5)	C7A	N3A	N2A	118.5(3)	C7B	N3B	N2B	118.0(2)
N1A	C5A	1.363(4)	N1B	C5B	1.362(4)	N1A	C2A	C3A	107.9(3)	N1B	C2B	C3B	107.4(3)
N2A	N3A	1.380(4)	N2B	N3B	1.379(3)	N1A	C2A	C6A	122.6(3)	N1B	C2B	C6B	122.4(3)
N2A	C6A	1.278(4)	N2B	C6B	1.278(4)	C3A	C2A	C6A	129.4(3)	C3B	C2B	C6B	129.6(3)
N3A	C7A	1.353(5)	N3B	C7B	1.356(4)	C2A	C3A	C4A	107.2(3)	C2B	C3B	C4B	107.2(3)
C2A	C3A	1.378(5)	C2B	C3B	1.383(5)	C5A	C4A	C3A	107.6(3)	C5B	C4B	C3B	108.0(3)
C2A	C6A	1.440(5)	C2B	C6B	1.441(5)	N1A	C5A	C4A	108.3(3)	C4B	C5B	N1B	108.2(3)
C3A	C4A	1.406(5)	C3B	C4B	1.401(5)	N2A	C6A	C2A	119.6(3)	N2B	C6B	C2B	119.3(3)
C4A	C5A	1.369(5)	C4B	C5B	1.362(5)	O1A	C7A	N3A	121.3(3)	O1B	C7B	N3B	121.4(3)
C7A	C8A	1.482(5)	C7B	C8B	1.487(5)	O1A	C7A	C8A	122.3(3)	O1B	C7B	C8B	122.1(3)
C8A	C9A	1.393(5)	C8B	C9B	1.388(5)	N3A	C7A	C8A	116.4(3)	N3B	C7B	C8B	116.4(3)
C8A	C13A	1.401(4)	C8B	C13B	1.397(4)	C9A	C8A	C7A	118.6(3)	C9B	C8B	C7B	118.5(3)
C9A	C10A	1.384(4)	C9B	C10B	1.383(5)	C9A	C8A	C13A	118.9(3)	C9B	C8B	C13B	118.6(3)
C10A	C11A	1.394(4)	C10B	C11B	1.397(4)	C13A	C8A	C7A	122.5(3)	C13B	C8B	C7B	122.9(3)
C11A	C12A	1.392(5)	C11B	C12B	1.390(5)	C10A	C9A	C8A	120.5(3)	C10B	C9B	C8B	121.3(3)
C12A	C13A	1.380(5)	C12B	C13B	1.384(5)	C9A	C10A	C11A	120.0(3)	C9B	C10B	C11B	119.5(3)
						O2A	C11A	C10A	117.8(3)	O2B	C11B	C10B	117.6(3)
						O2A	C11A	C12A	122.3(3)	O2B	C11B	C12B	122.6(3)
						C12A	C11A	C10A	120.0(3)	C12B	C11B	C10B	119.8(3)
						C13A	C12A	C11A	119.8(3)	C13B	C12B	C11B	119.9(3)
						C12A	C13A	C8A	120.8(3)	C12B	C13B	C8B	120.8(3)

The crystal structure of title compound generates a two dimensional supramolecular network with hydrogen bonds interactions between O – H···O and N – H···O along to [100] and [001] direction with graph set motifs[33] visible $R_1^2(5)$, $R_2^2(10)$, $C_1^1(8)$ and $C_1^1(12)$ (see Figure 2 and Table 3).

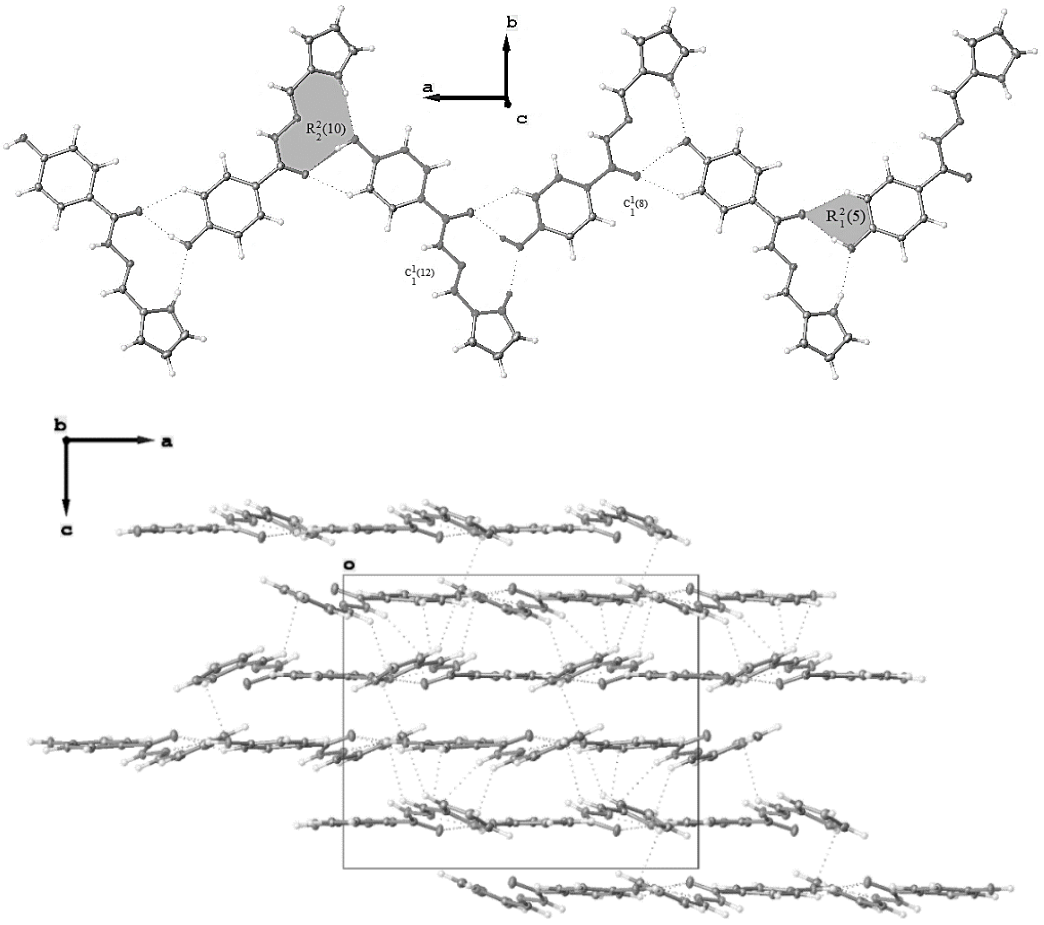

Figure 2. Crystal packing of the title compound showing graph set motifs (top) and intermolecular hydrogen bond between neighbor molecules (bottom).

Table 3 Hydrogen Bonds Interactions for title compound.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O2A	H2A	O1A[1]	0.88(4)	1.95(4)	2.819(3)	168(4)
N1A	H1A	O2A[2]	0.90(4)	2.25(4)	3.097(4)	156(4)
C6A	H6A	N1B[3]	0.97(3)	2.73(3)	3.389(5)	126(2)
C12A	H12A	O1A[1]	0.97(3)	2.35(3)	3.132(4)	137(3)
O2B	H2B	O1B[4]	0.90(5)	1.96(5)	2.814(3)	159(4)
O2B	H2B	N2B[4]	0.90(5)	2.31(5)	2.913(3)	124(4)
N1B	H1B	O2B[5]	0.88(4)	2.25(4)	3.103(4)	163(4)
C6B	H6B	N1A[6]	0.99(3)	2.67(4)	3.419(5)	133(3)
C12B	H12B	O1B[4]	0.94(3)	2.47(4)	3.179(4)	132(3)

[1] 1/2+X,3/2-Y,+Z; [2] -1/2+X,3/2-Y,+Z; [3] 3/2-X,-1/2+Y,-1/2+Z; [4] -1/2+X,1/2-Y,+Z; [5] 1/2+X,1/2-Y,+Z; [6] 1-X,1-Y,1/2+Z

A Hirshfeld surface analysis was conducted to verify the contributions of the different intermolecular interactions. This analysis was used to investigate the presence of hydrogen bonds and other weak intermolecular interactions in the crystal structure. The Hirshfeld surface analysis[34] was generated by CrystalExplorer 17.5[35] and comprised d_{norm} surface plots and 2D (two-dimensional) fingerprint plots[36]. The plots of the Hirshfeld surface confirms the presence of the non-covalent interaction described below (Figure 3), taking account that in the asymmetrical unit there are two units (A and B) a procedure described previously in the literature was used to a better analysis and understanding of this interactions[37]. As described above, a strong hydrogen bonding interaction is observed in the crystal structure generating a 2D-network in the crystal structure, where units "A" and "B" are interacting with N – H ···O hydrogen bond interaction, despite of both units are in different planes of the crystal, according to the symmetry elements on it. This are depicted in the Figure 3, where the both units are well defined and are interacting between them.

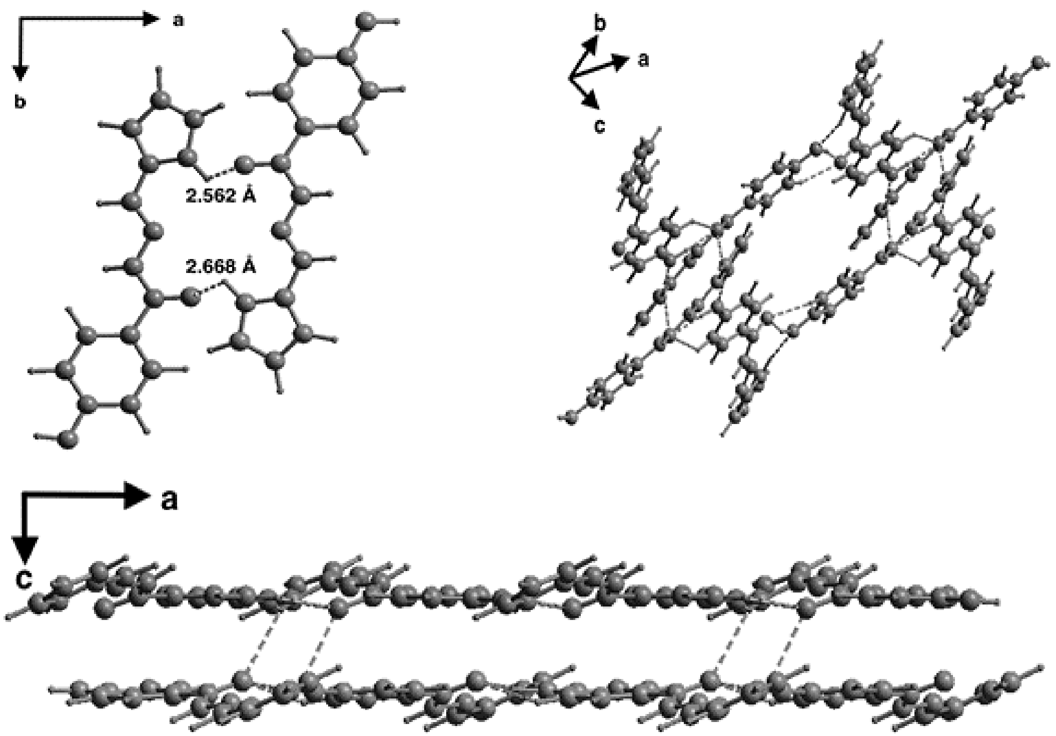

Figure 3. 2-D network generated for the title compound. Units A and B are defined by red and blue colours respectively.

In order to visualize and quantify the similarities and differences in intermolecular contacts across the crystal structure the Hirshfeld surface analysis was made for the molecules A and B present in the asymmetric unit independently (see Figure 4.).

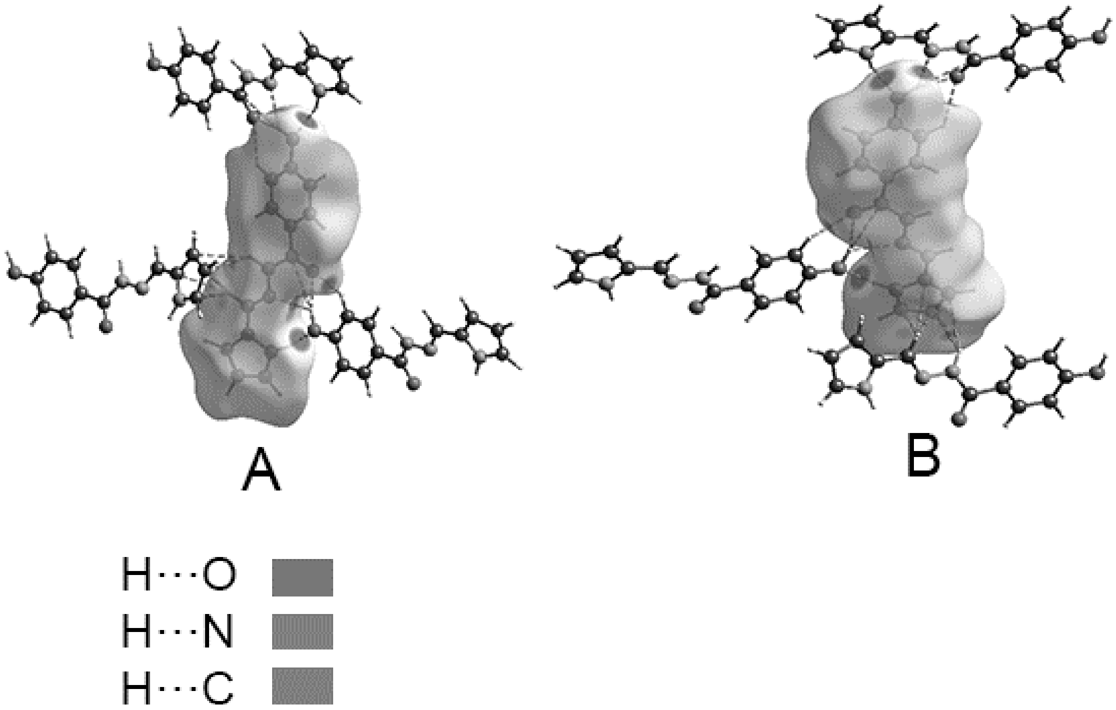

Figure 4. Hirshfeld surface of the title compound for each unit.

The weak intermolecular interactions are mainly constituted by H···O, H···N and H···C, the contribution for both units are depicted in Figure 5. Where the reciprocal contacts appear as a sharp wing for H···O, with $d_e + d_i \simeq 1.8$ Å, for H···N as a diffuse wing with $d_e + d_i \simeq 2.1$ Å and, H···C as asymmetrical wings with $d_e + d_i \simeq 2.9$ Å. In general, both units show a similar fingerprint plots except the H ··· C interaction. We can assume that this difference in the plot could be due to chirality of the crystal structure (non-centrosymmetric setting) or the antiparallel direction generated by the interactions in the both units.

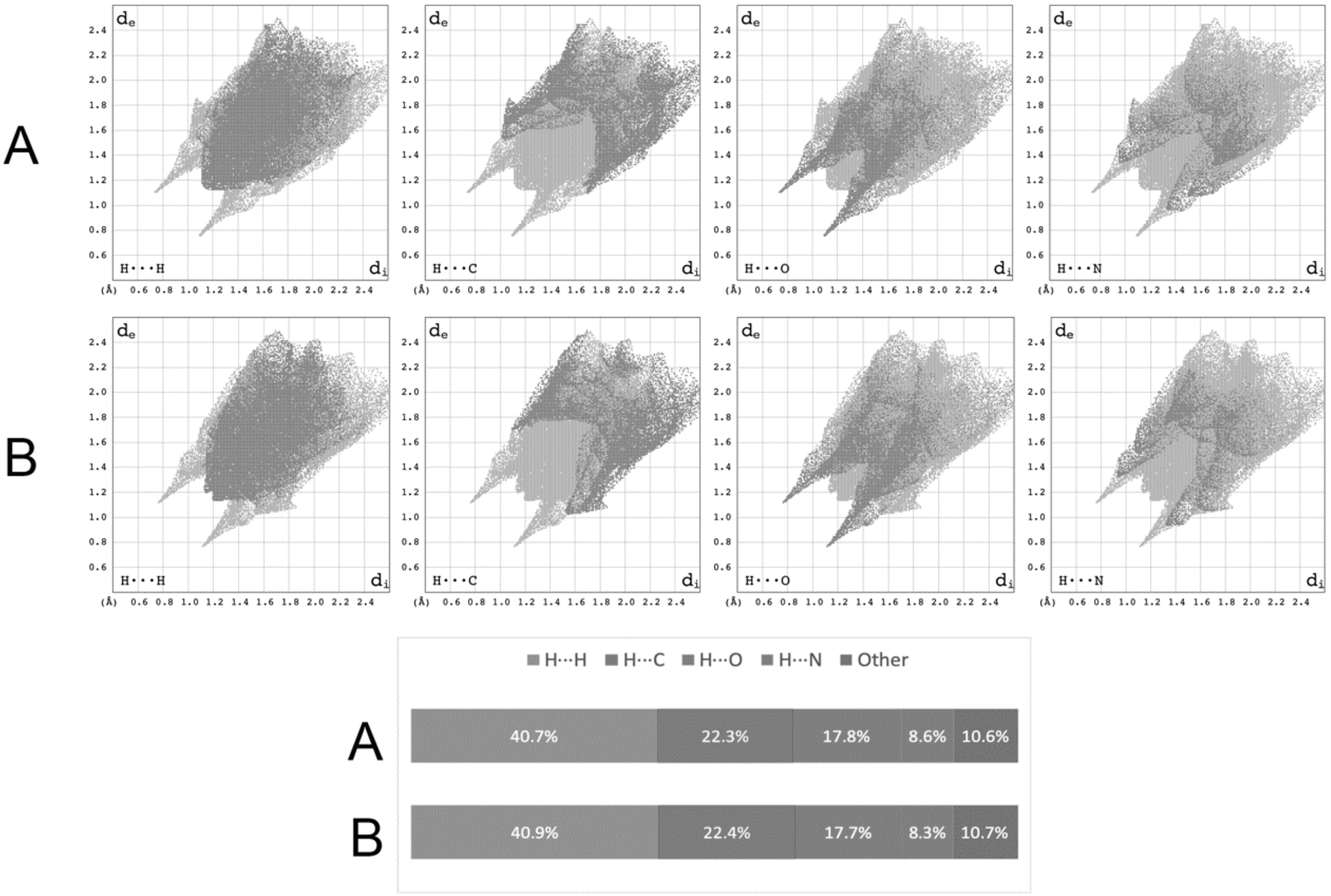

Figure 5. Fingerprint plots for units A and B (top) and weak interactions contributions (bottom).

Finally, energy framework was analysed to a better understanding of the packing of crystal structure and the supramolecular rearrangement. According to the tube direction, it can conclude that the formation of the framework is directed by the translational symmetry elements in each unit a long of *a* – axis due the strong hydrogen bond interaction O – H ···O and N – H ···O type directing the crystal structure layer by layer in the (110) plane disposing the molecular structure in an antiparallel *zig-zag* setting, according to the electrostatic (E_{ele}). The dispersion (E_{dis}) energy shows a hexagonal cage as a component of the framework energy being less dominating than (E_{ele}) (see Figure 6). This rearrangement allows the formation of another weak interactions in the crystal structure such as H ···π between the pyrrole ring and the H – CNN – H fragment. To the best of our knowledge already exists little examples of H ··· π weaks interactions between hydrogen and heterocycles[38,39].

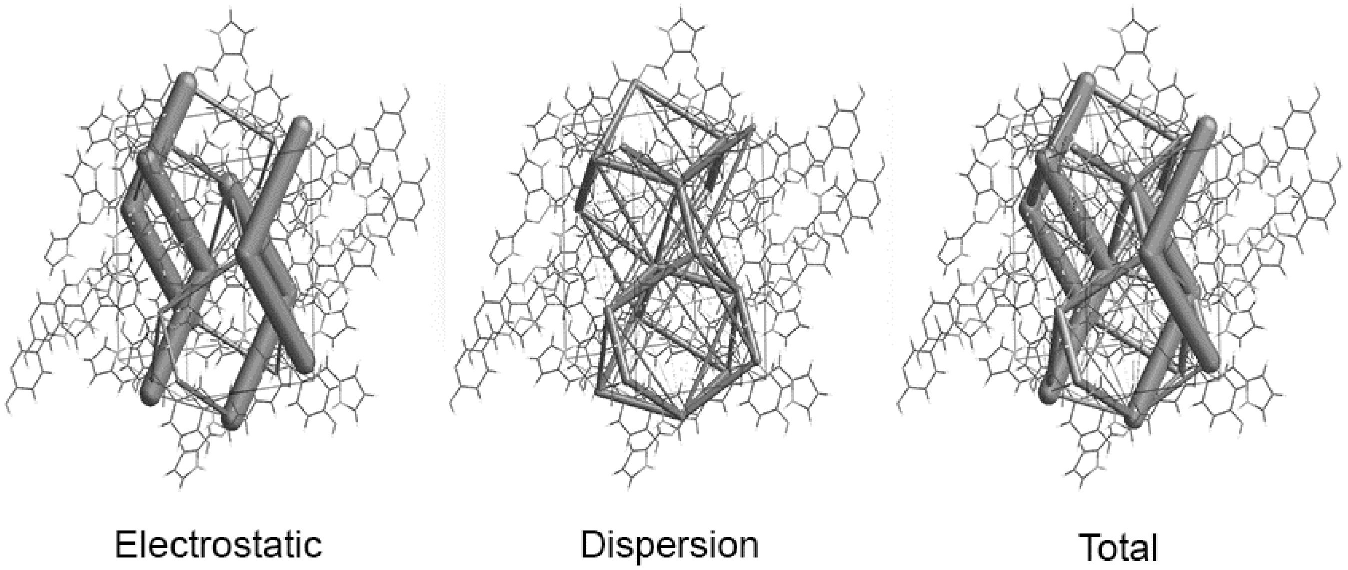

Figure 6. Energy framework diagrams for (E_{ele}), (E_{dis}) and (E_{tot}) for title compound.

CONCLUSIONS

In this study we offer the report of structural studies of the title compound, showing the *E* isomer in the solid state. The weak intermolecular interactions show a 2D supramolecular network. Both molecules are essentially overlaid between them with RMSD = 0.0574; max D = 0.1211 Å considering inversion and flexibility. The understanding of the crystal packing of this molecule allows to postulate this compound in some applications such as synthesis, catalysis, crystal engineering, pharmaceutical design, molecular biology, molecular recognition, materials.

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