SUPPLEMENTARY MATERIAL

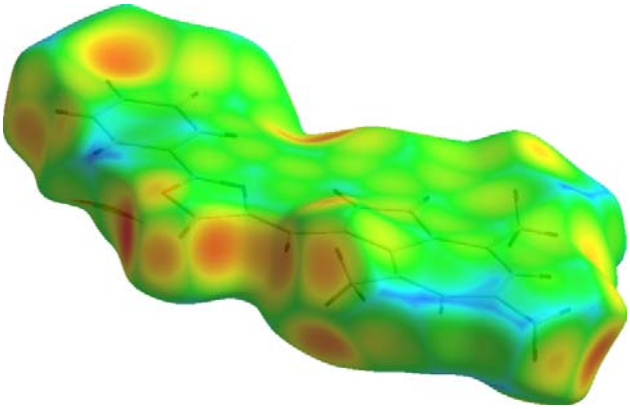

Figure S1. View of the Hirshfeld surface of **1** mapped with d_e.

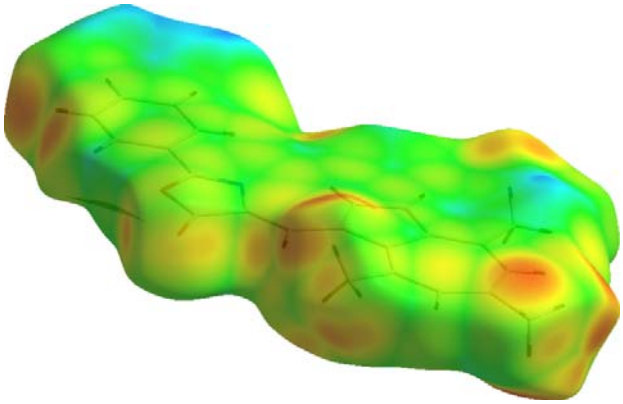

Figure S2. View of the Hirshfeld surface of **1** mapped with d_i.

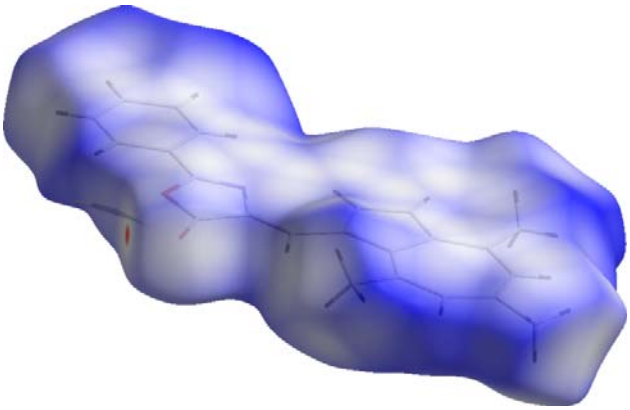

Figure S3. View of the Hirshfeld surface of **1** mapped with d_{norm}.

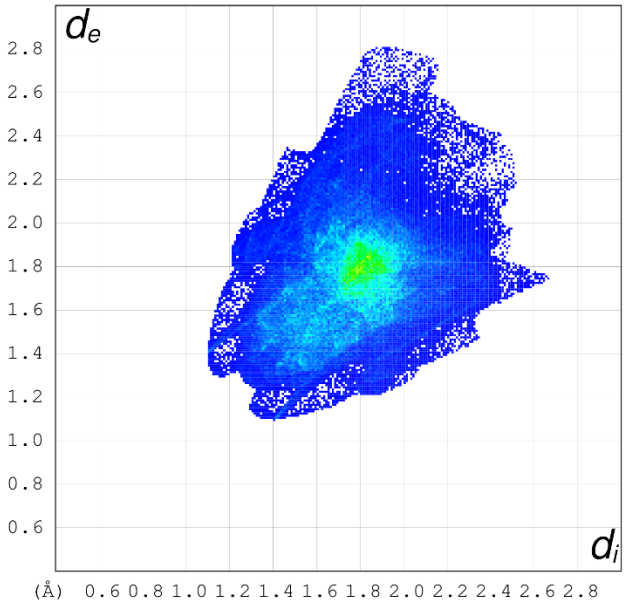

Figure S4. 2D fingerprint plots of d_e and d_i for **1**.

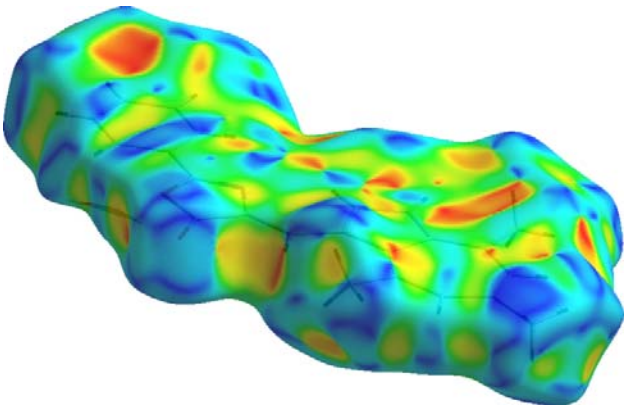

Figure S5. View of the Hirshfeld surface of **1** mapped with shape index, *S*.

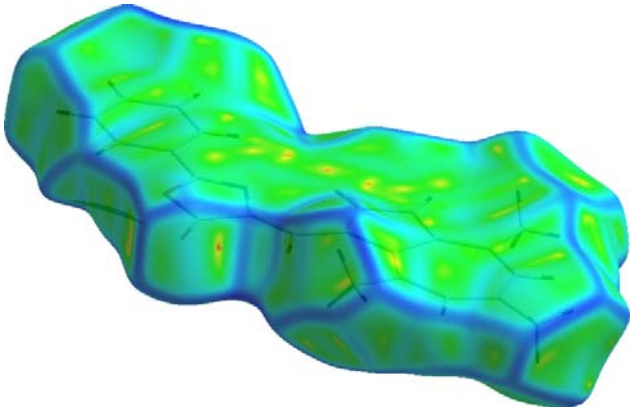

Figure S6. View of the Hirshfeld surface of 1 mapped with curvedness, *C*.

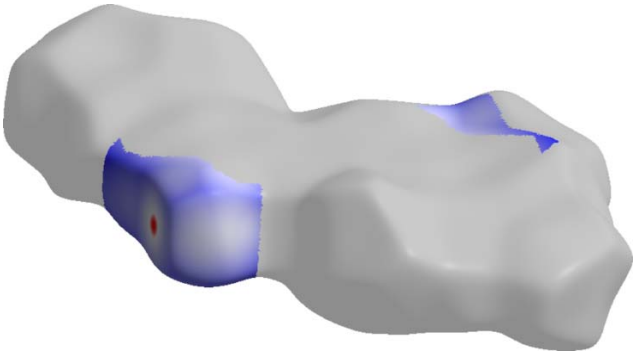

Figure S7. Fragment of the Hirshfeld surface of **1** mapped with d_{norm} showing O···H interactions.

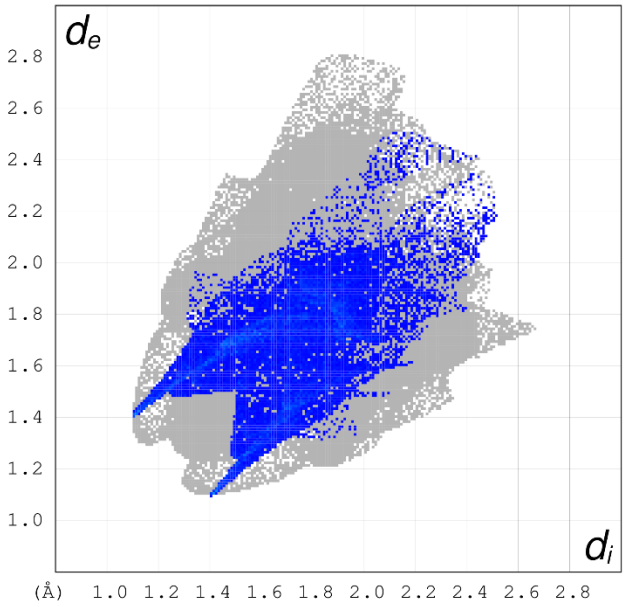

Figure S8. 2D fingerprint plots of d_e and d_i for **1** showing O···H interactions (11.0%).

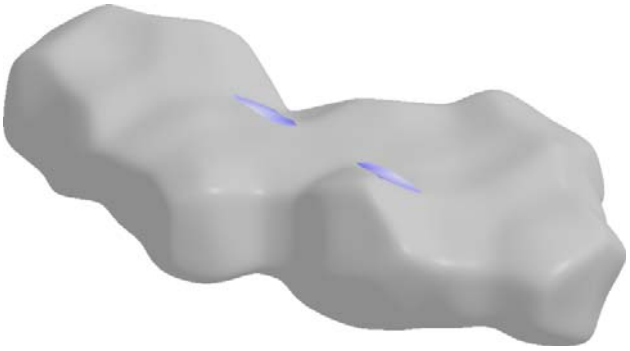

Figure S9. Fragment of the Hirshfeld surface of **1** mapped with d_{norm} showing N···H interactions.

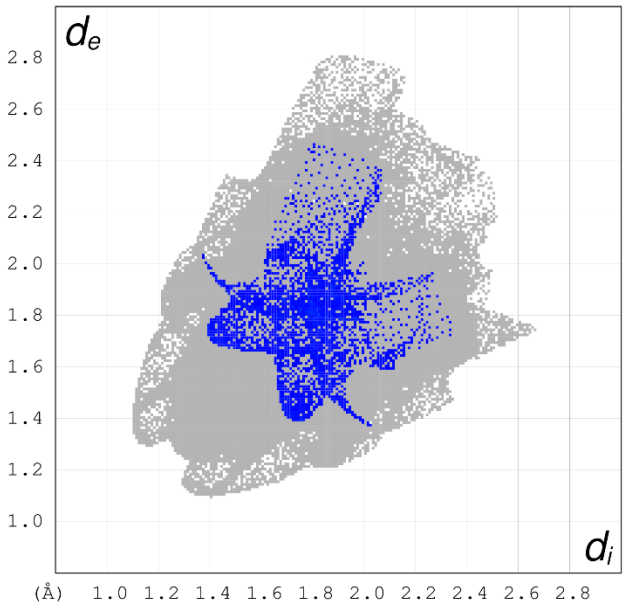

Figure S10. 2D fingerprint plots of d_e and d_i for **1** showing N···H interactions (2.7%).

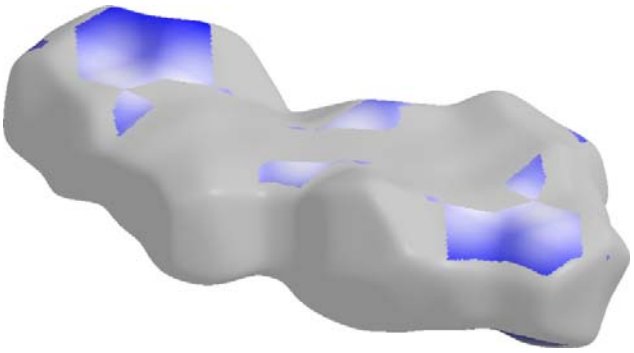

Figure S11. Fragment of the Hirshfeld surface of **1** mapped with d_{norm} showing C···H interactions.

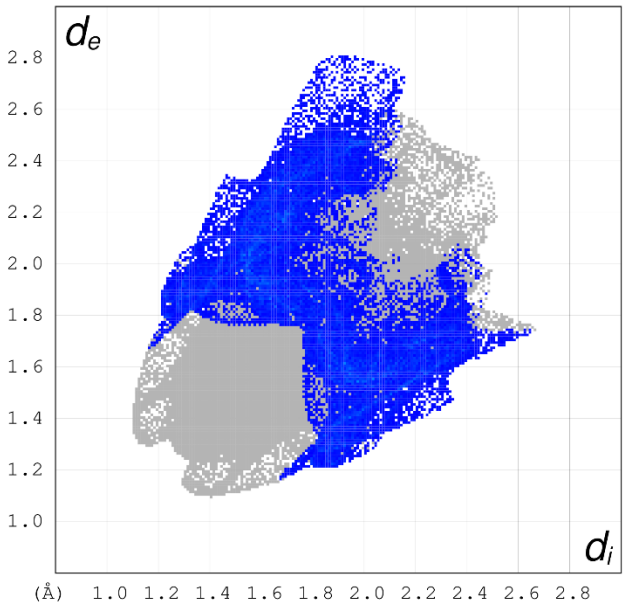

Figure S12. 2D fingerprint plots of d_e and d_i for **1** showing C···H interactions (18.5%).

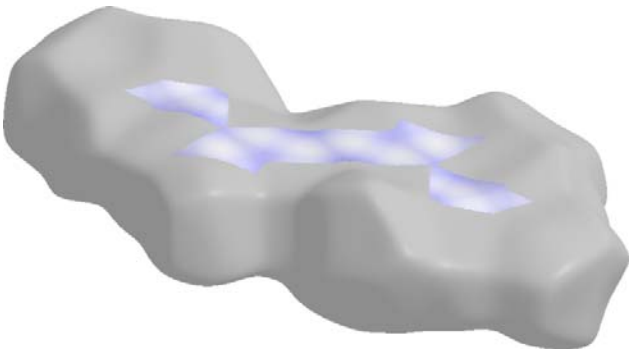

Figure S13. Fragment of the Hirshfeld surface of **1** mapped with d_{norm} showing C···C interactions.

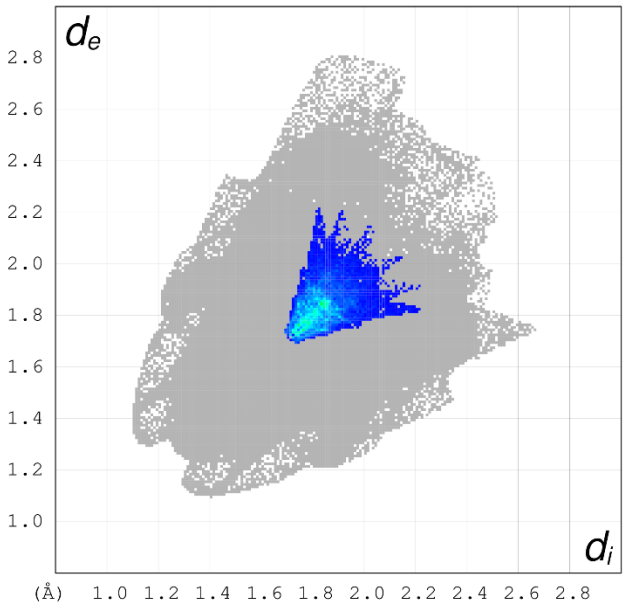

Figure S14. 2D fingerprint plots of d_e and d_i for **1** showing C···C interactions (8.5%).

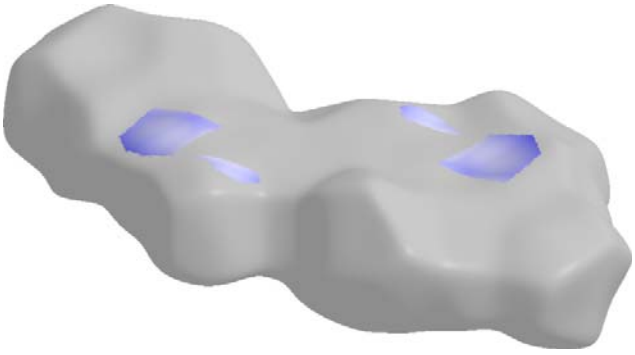

Figure S15. Fragment of the Hirshfeld surface of **1** mapped with d_{norm} showing C···O interactions.

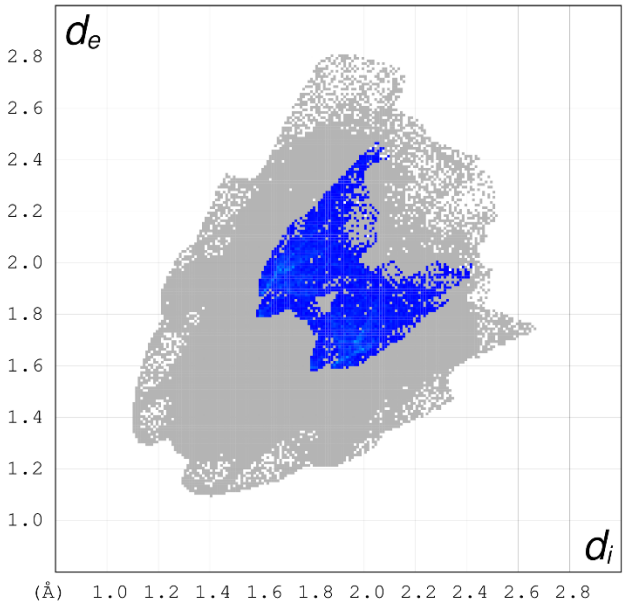

Figure S16. 2D fingerprint plots of d_e and d_i for **1** showing C···O interactions (6.0%).

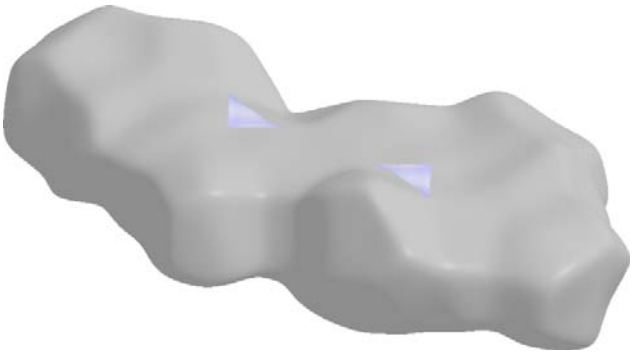

Figure S17. Fragment of the Hirshfeld surface of **1** mapped with d_{norm} showing C···N interactions.

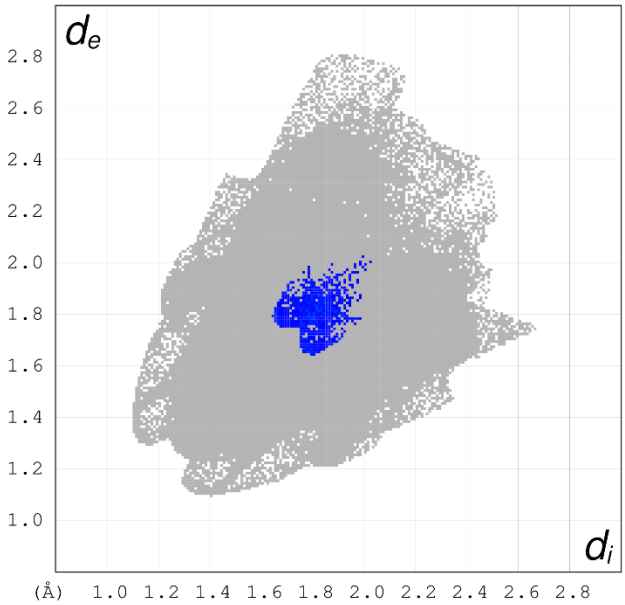

Figure S18. 2D fingerprint plots of d_e and d_i for **1** showing C···N interactions (1.0%).

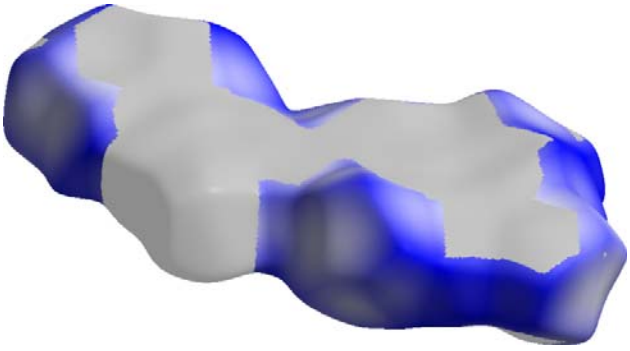

Figure S19. Fragment of the Hirshfeld surface of **1** mapped with d_{norm} showing H···H interactions.

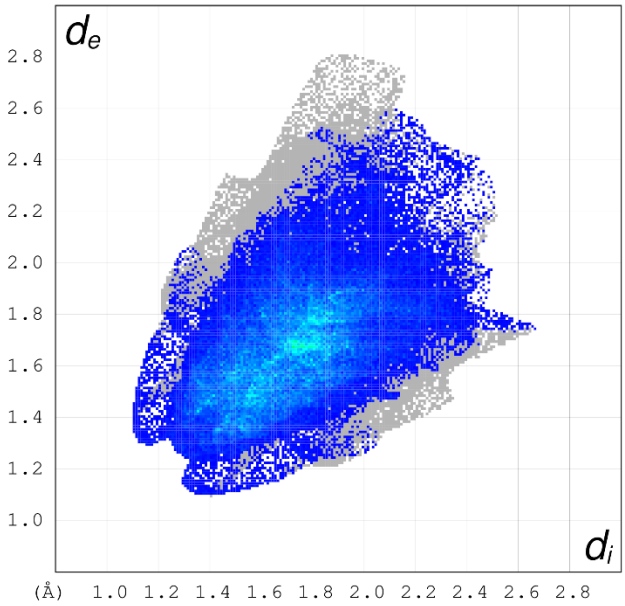

Figure S20. 2D fingerprint plots of d_e and d_i for **1** showing H···H interactions (52.4%).

Table S1. Interaction energies (kJ/mol) in the crystals of **1**.

	N	Symop	R*	Electron Density	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
	1	−x, −y, −z	4.68	B3LYP/6-31G(d,p)	−18.7	−6.0	−100.9	50.6	−80.9
	2	x+1/2, −y+1/2, z+1/2	10.09	B3LYP/6-31G(d,p)	−6.9	−2.8	−15.8	7.1	−18.8
	2	x+1/2, −y+1/2, z+1/2	13.44	B3LYP/6-31G(d,p)	−0.4	−0.8	−7.8	0.0	−7.9
	1	x+1/2, −y+1/2, z+1/2	11.12	B3LYP/6-31G(d,p)	1.1	−0.3	−5.8	0.3	−4.0
	2	−x+1/2, y+1/2, −z+1/2	11.30	B3LYP/6-31G(d,p)	−4.0	−1.1	−22.2	6.7	−20.2
	2	−x+1/2, y+1/2, −z+1/2	12.03	B3LYP/6-31G(d,p)	−4.6	−3.4	−14.1	0.0	−19.6
	1	−x, −y, −z	16.98	B3LYP/6-31G(d,p)	−0.1	−0.2	−6.2	0.0	−5.6
	1	−x, −y, −z	3.71	B3LYP/6-31G(d,p)	−20.0	−5.8	−120.9	61.3	−92.9
	2	−x+1/2, y+1/2, −z+1/2	12.15	B3LYP/6-31G(d,p)	−0.8	−0.3	−6.2	0.0	−6.5
	1	−x, −y, −z	12.75	B3LYP/6-31G(d,p)	1.4	−0.3	−6.8	0.0	−4.7
	1	x+1/2, −y+1/2, z+1/2	14.23	B3LYP/6-31G(d,p)	−0.4	−0.2	−1.6	0.0	−2.0

where:R is the distance between molecular centroids (mean atomic position) in Å; total energies (E_{tot}), are the sum of the four energy components (*i.e.*, E_{ele}, E_{pol}, E_{dis}, E_{rep}) scaled appropriately (1.057, 0.740, 0.871, and0.618, respectively); the colours on the first column correspond to those used for molecules representation in Figure S29.

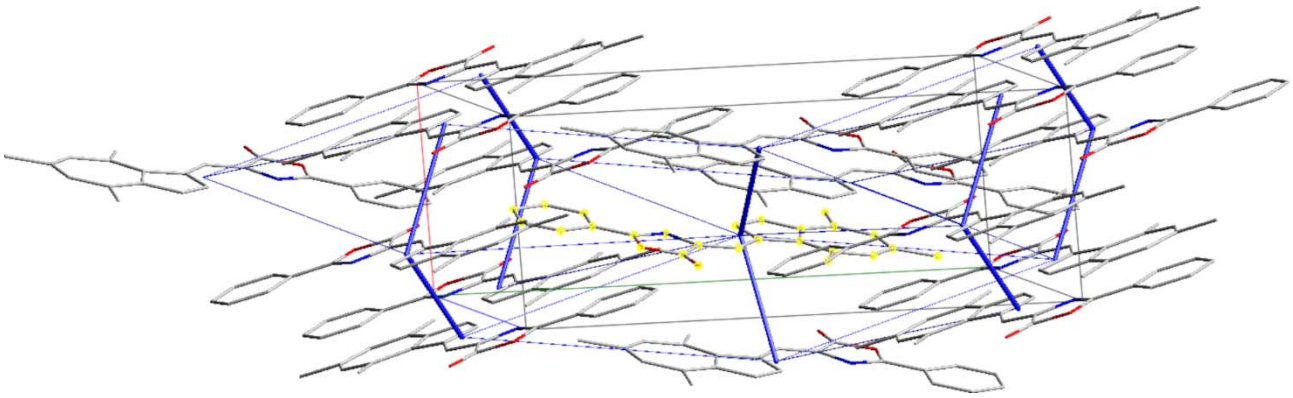

Figure S21. Energy-framework diagram for **1**. Hydrogen atoms were omitted for clarity. The total energy is represented by blue lines. A cut-off value of 10 kJ/mol was used for the representation.

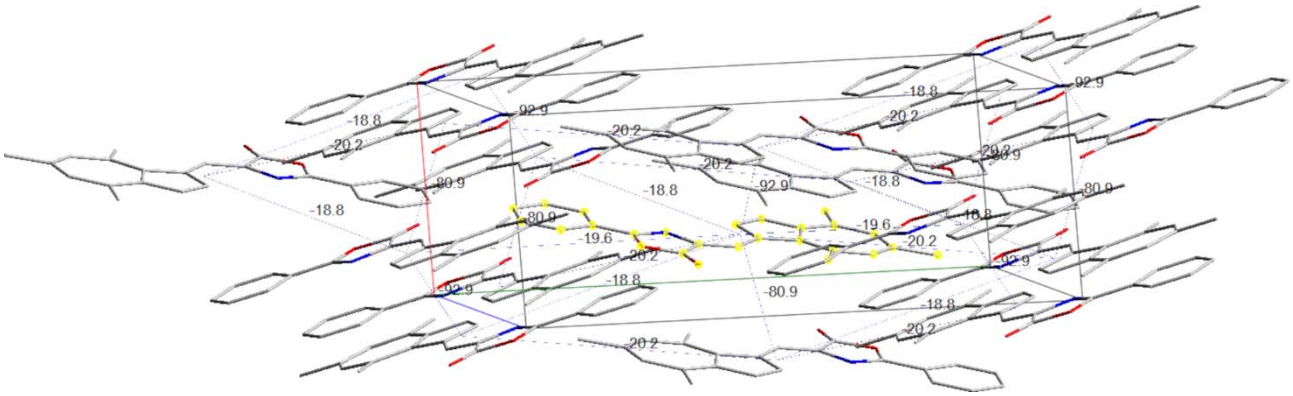

Figure S22. Energy-framework diagram for **1**. Hydrogen atoms were omitted for clarity. The total energy is provided in kJ/mol. A cut-off value of 10 kJ/mol was used for the representation.

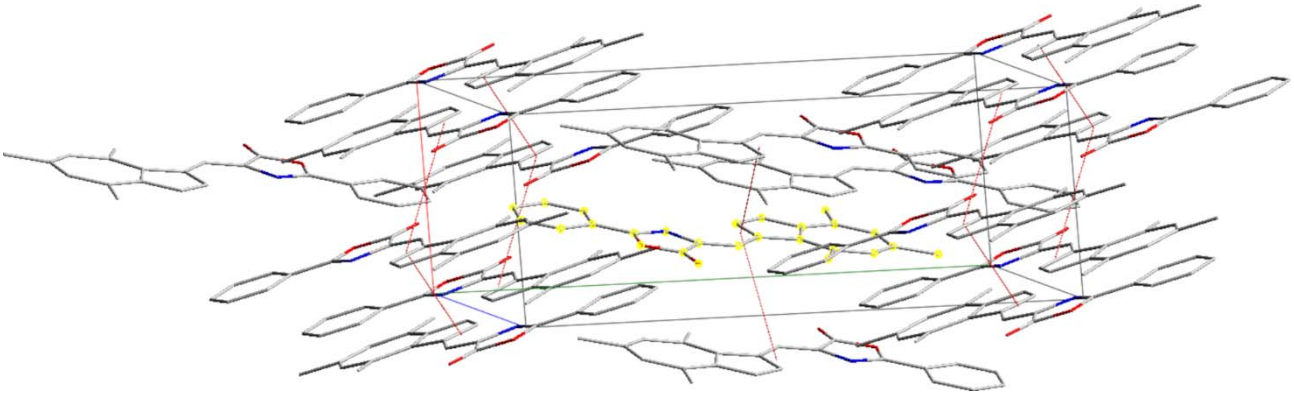

Figure S23. Energy-framework diagram for **1**. Hydrogen atoms were omitted for clarity. The Coulomb energy is represented by red lines. A cut-off value of 10 kJ/mol was used for the representation.

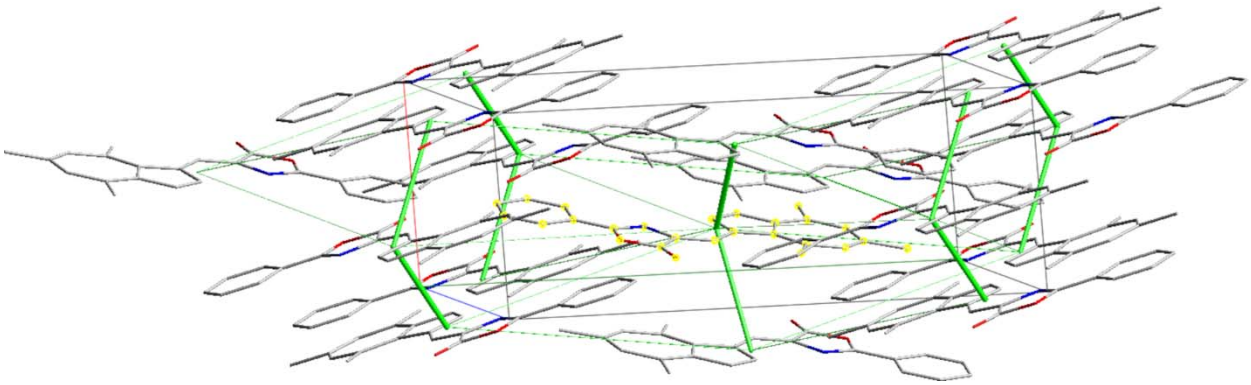

Figure S24. Energy-framework diagram for **1**. Hydrogen atoms were omitted for clarity. The dispersion energy is represented by red lines. A cut-off value of 10 kJ/mol was used for the representation.

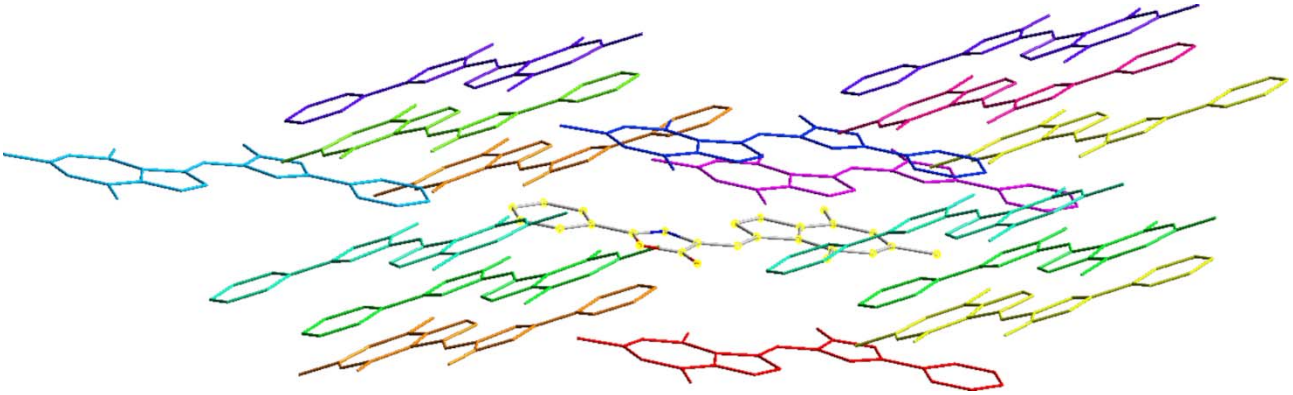

Figure S25. Interactions energies in the crystals of **1**. Hydrogen atoms were omitted for clarity. Values are listed in Table S1 (*vide infra).* Molecules containing atoms within 3.8 Å around the asymmetric unit (shown in the middle of the image) are represented.

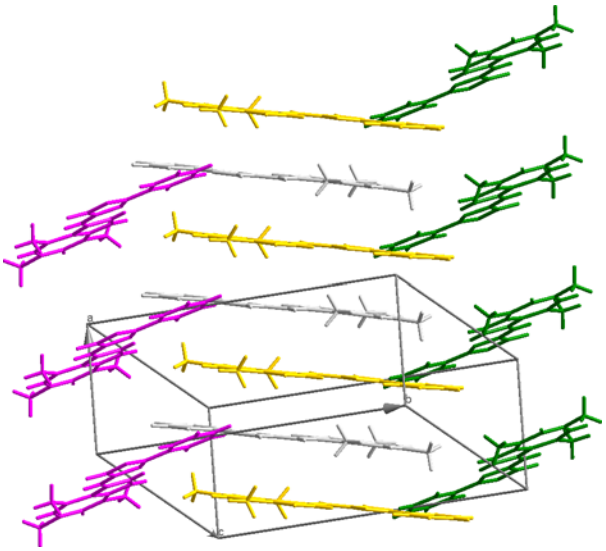

Figure S26. Perspective view of the crystal packing of **1**.

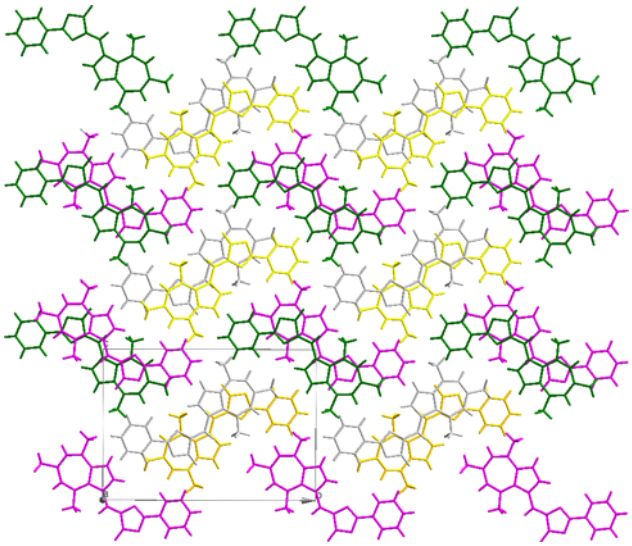

Figure S27. View along the *a* axis of the crystal packing of **1.**