STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 76 (2020)

Supporting information for article:

Charge density analysis of abiraterone acetate

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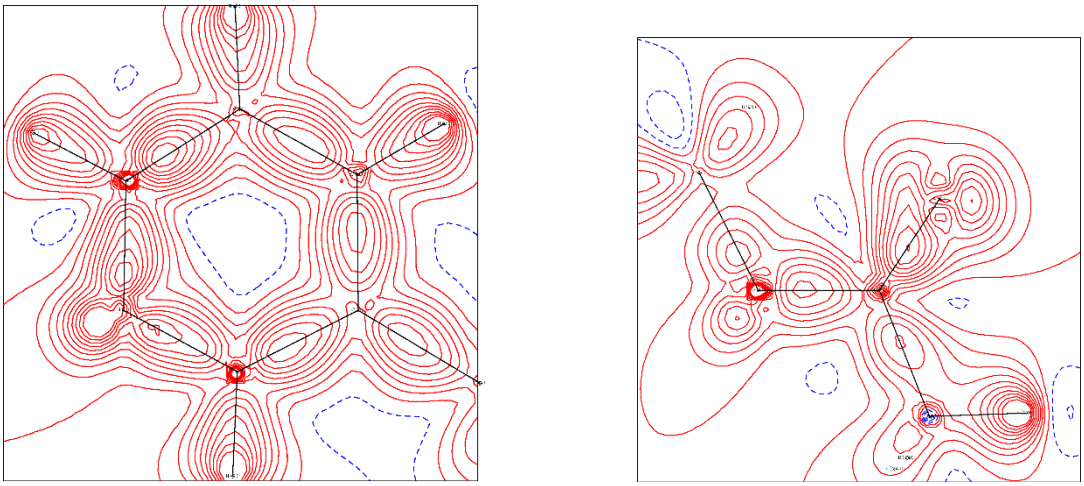


Figure S1 Experimental static deformation density in **1** depicted in the sections of (a) N(1), C(2), C(4); (b) O(1), O(2), C(24) atoms. The contour levels are equal to ±0.1, ±0.2, ±0.3, ±0.4, ±0.5, ±0.6, ±0.7, ±0.8, ±0.9, ±1.0 e Å^{-3}; the positive contours are shown with solid red line, the negative contours are dashed blue.

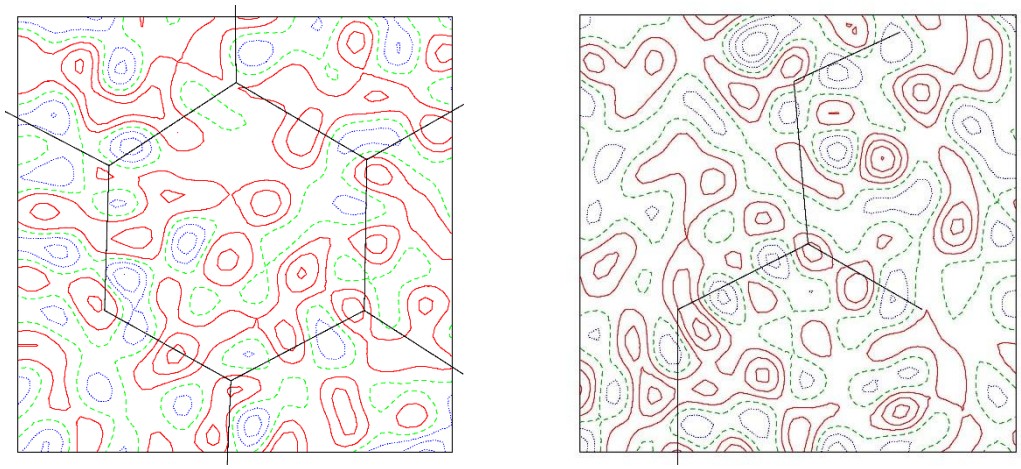


Figure S2 The residual density maps in the sections of (left) N(1), C(2) and C(4); (right) O(1), O(2) and C(24) atoms calculated using all data for **1**. The isocontours are drawn every 0.05 eÅ^{-3}; positive contours are shown in red, the negative contours are dashed blue.

The residual density maps of **1** are featureless (Figure S2).

The distribution of the residual density for **1** is of the Gaussian shape, and $d^f(0) = 2.68$ demonstrate good refinement. Figure S4 indicate low data quality at high angles that could be expected for a single crystal of **1** with low reflection ability.

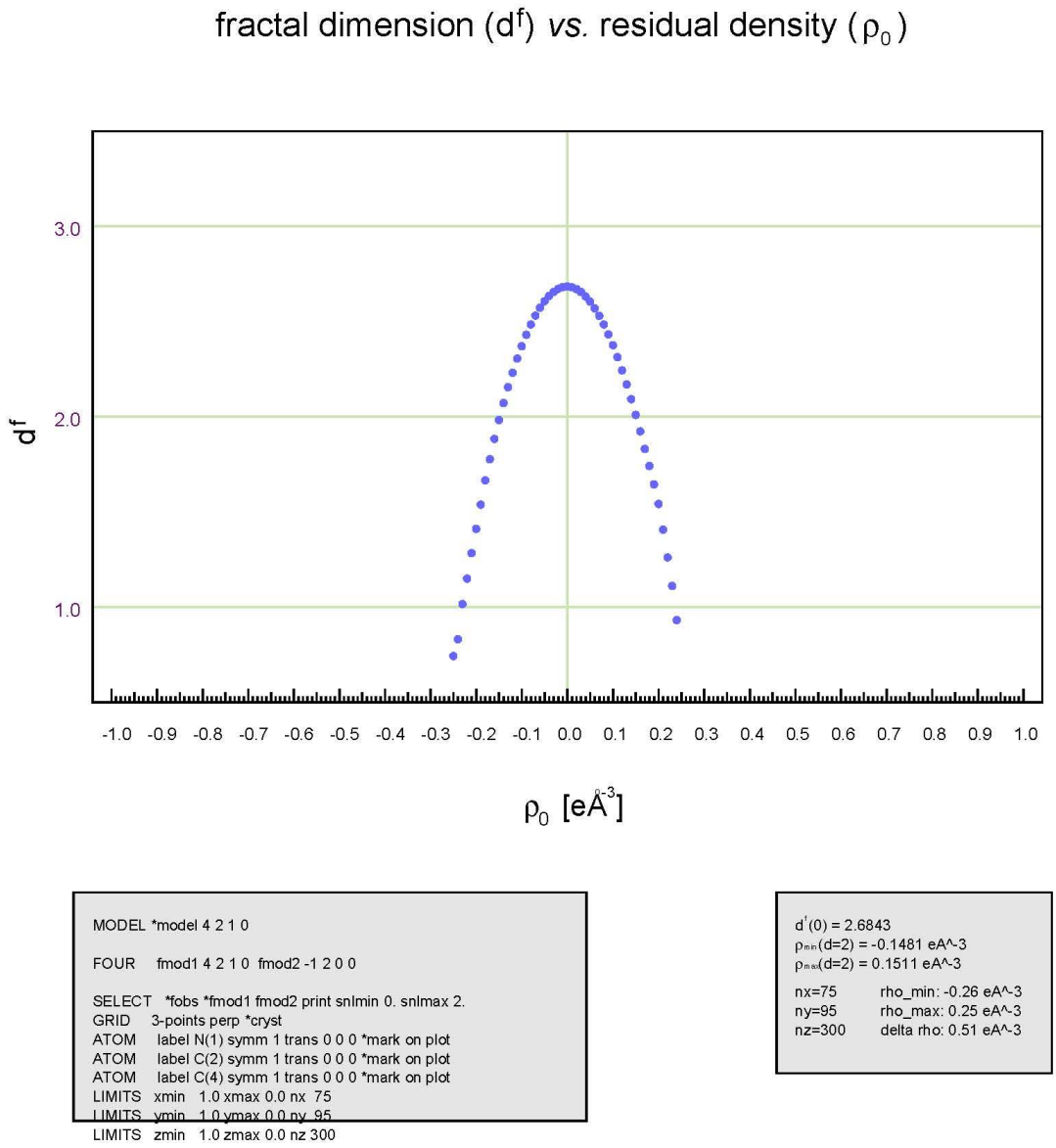
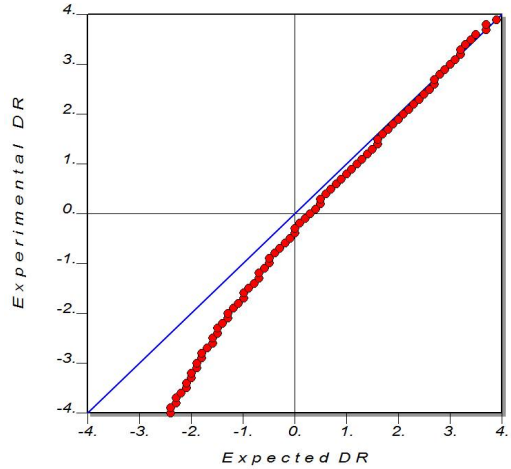
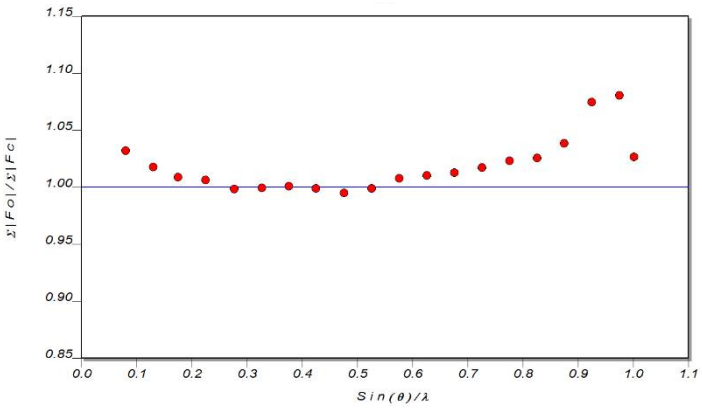


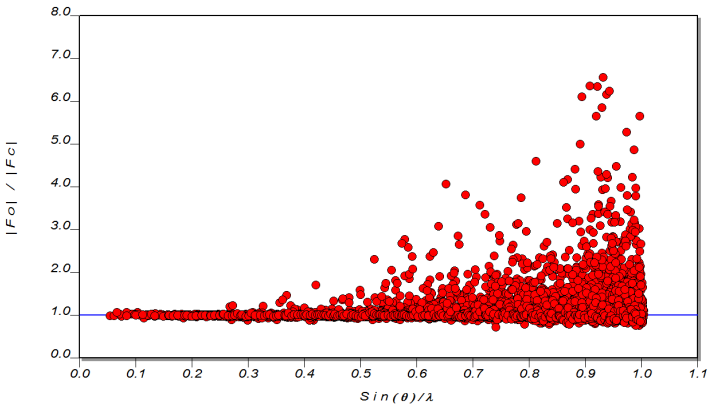
Figure S3 Plot of the fractal dimension d^f vs. the residual electron density (ρ_0) in the unit cell of **1**. No resolution cutoff was applied to the data used for the Fourier transformation.



(a)



(b)



(c)

Figure S4 (a) Normal probability plot plotted against full dataset of **1**; (b) Scale factor plot against resolution; (c) $|F_o|$ / $|F_c|$ against resolution.

Properties.

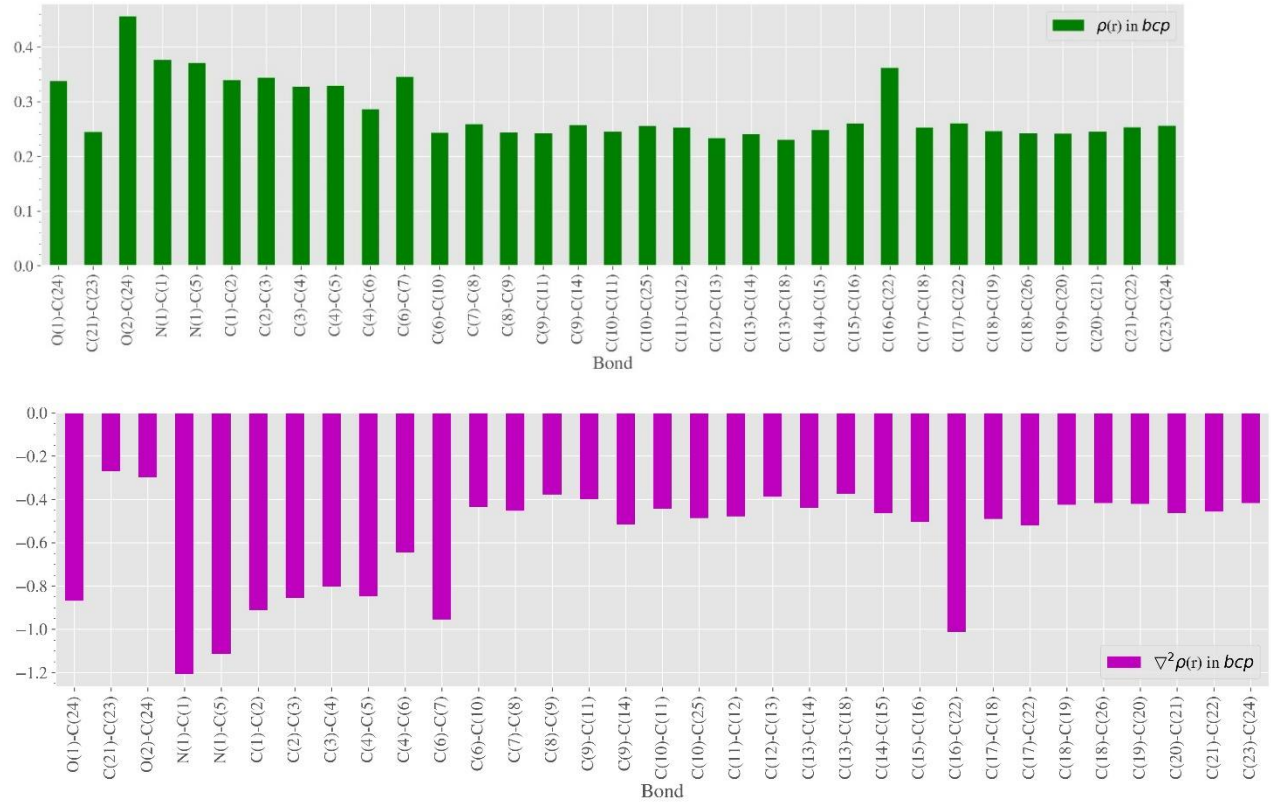


Figure S5 The values of electron density (upper diagram) and its Laplacian (lower diagram) in *bcp* in **1** [atomic units].

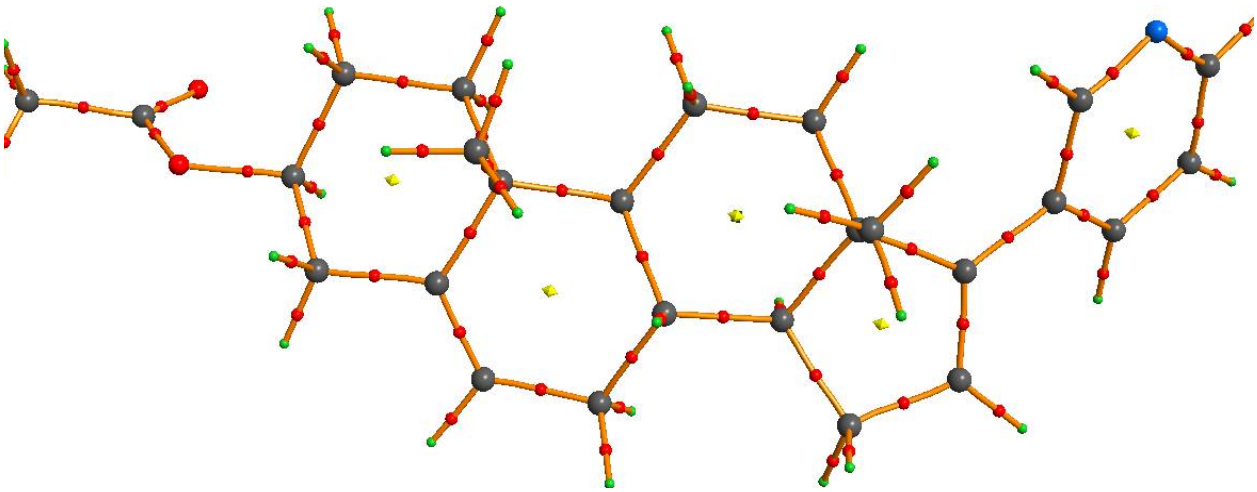


Figure S6 Molecular graph of **1**. Red and yellow circles denote CP (3,-1) and (3,+1).

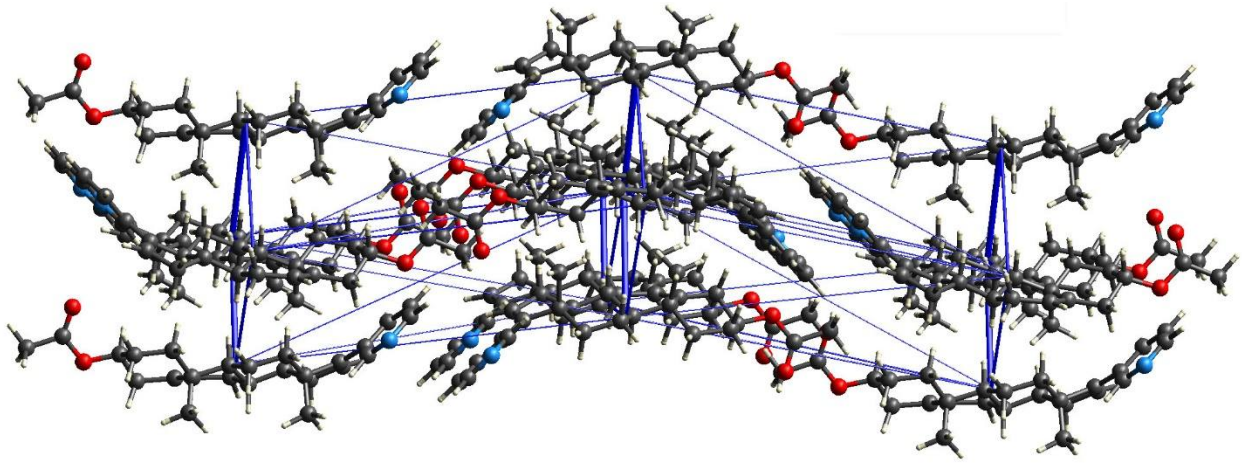


Figure S7 Energy framework diagram of crystal packing of **1**. The width of blue lines is proportional to the strength of bonding between adjacent molecules (E_{tot}).

Table S1 Characteristics of CPs in irreducible part of **1** [a.u.]

Type	Bond	ρ(r)	$\nabla^2\rho(r)$	g(r)	v(r)	h(r)
(3,-1)	O(1)-C(24)	0.34	-1.01	0.31	-0.88	-0.56
(3,-1)	C(21)-C(23)	0.25	-0.34	0.23	-0.54	-0.31
(3,-1)	O(2)-C(24)	0.45	-0.41	0.69	-1.49	-0.80
(3,-1)	N(1)-C(1)	0.37	-1.20	0.36	-1.02	-0.66
(3,+1)	C(3)-C(5)	0.02	0.20	0.04	-0.02	0.01
(3,-1)	N(1)-C(5)	0.37	-1.04	0.37	-1.00	-0.63
(3,-1)	C(1)-C(2)	0.34	-0.93	0.32	-0.87	-0.55
(3,-1)	C(1)-H(1)	0.29	-0.82	0.22	-0.65	-0.43
(3,-1)	C(2)-C(3)	0.34	-0.85	0.33	-0.88	-0.55
(3,-1)	C(2)-H(2)	0.31	-0.80	0.27	-0.73	-0.47
(3,-1)	C(3)-C(4)	0.33	-0.79	0.32	-0.83	-0.51
(3,-1)	C(3)-H(3)	0.32	-0.95	0.26	-0.77	-0.50
(3,-1)	C(4)-C(5)	0.33	-0.82	0.31	-0.83	-0.52
(3,-1)	C(4)-C(6)	0.29	-0.66	0.25	-0.67	-0.42
(3,-1)	C(5)-H(5)	0.30	-0.79	0.25	-0.70	-0.45
(3,-1)	C(6)-C(7)	0.35	-0.95	0.34	-0.91	-0.57
(3,+1)	C(8)-C(10)	0.04	0.26	0.06	-0.05	0.01
(3,-1)	C(6)-C(10)	0.25	-0.45	0.21	-0.53	-0.32
(3,-1)	C(7)-C(8)	0.26	-0.44	0.23	-0.57	-0.34
(3,-1)	C(7)-H(7)	0.28	-0.75	0.22	-0.63	-0.41
(3,-1)	C(8)-C(9)	0.25	-0.40	0.21	-0.52	-0.31
(3,-1)	C(8)-H(8A)	0.29	-0.72	0.25	-0.67	-0.43
(3,-1)	C(8)-H(8B)	0.28	-0.66	0.23	-0.63	-0.40
(3,-1)	C(9)-C(11)	0.25	-0.41	0.21	-0.52	-0.31
(3,+3)	C(9)-C(13)	0.00	0.07	0.00	0.00	0.00

(3,-1)	C(9)-C(14)	0.26	-0.52	0.30	-0.55	-0.34
(3,-1)	C(9)-H(9)	0.29	-0.72	0.24	-0.66	-0.42
(3,-1)	C(10)-C(11)	0.24	-0.42	0.20	-0.51	-0.31
(3,-1)	C(10)-C(25)	0.25	-0.45	0.21	-0.54	-0.32
(3,-1)	C(11)-C(12)	0.25	-0.45	0.21	-0.52	-0.32
(3,-1)	C(11)-H(11A)	0.28	-0.68	0.24	-0.65	-0.41
(3,-1)	C(11)-H(11B)	0.28	-0.71	0.23	-0.65	-0.41
(3,-1)	C(12)-C(13)	0.23	-0.40	0.18	-0.47	-0.28
(3,-1)	C(12)-H(12A)	0.27	-0.66	0.22	-0.60	-0.38
(3,-1)	C(12)-H(12B)	0.28	-0.69	0.23	-0.62	-0.40
(3,-1)	C(13)-C(14)	0.24	-0.46	0.19	-0.50	-0.31
(3,-1)	C(13)-C(18)	0.23	-0.38	0.18	-0.46	-0.28
(3,-1)	C(13)-H(13)	0.26	-0.58	0.21	-0.57	-0.36
(3,-1)	C(14)-C(15)	0.25	-0.46	0.20	-0.52	-0.32
(3,-1)	C(14)-H(14)	0.28	-0.70	0.22	-0.61	-0.39
(3,-1)	C(15)-C(16)	0.26	-0.50	0.23	-0.58	-0.35
(3,-1)	C(15)-H(15A)	0.27	-0.64	0.22	-0.60	-0.38
(3,-1)	C(15)-H(15B)	0.28	-0.68	0.23	-0.63	-0.40
(3,-1)	C(16)-C(22)	0.37	-1.03	0.37	-0.99	-0.62
(3,-1)	C(16)-H(16)	0.27	-0.59	0.23	-0.61	-0.38
(3,-1)	C(17)-C(26)	0.25	-0.48	0.21	-0.53	-0.33
(3,-1)	C(17)-C(22)	0.26	-0.50	0.22	-0.56	-0.34
(3,-1)	C(18)-C(19)	0.24	-0.39	0.21	-0.51	-0.30
(3,-1)	C(18)-C(26)	0.24	-0.41	0.20	-0.51	-0.31
(3,-1)	C(19)-C(20)	0.25	-0.43	0.21	-0.52	-0.31
(3,-1)	C(19)-H(19A)	0.27	-0.66	0.22	-0.61	-0.39
(3,-1)	C(19)-H(19B)	0.28	-0.68	0.22	-0.62	-0.39
(3,-1)	C(20)-C(21)	0.25	-0.49	0.21	-0.54	-0.33
(3,-1)	C(20)-H(20A)	0.28	-0.70	0.23	-0.63	-0.40
(3,-1)	C(20)-H(20B)	0.28	-0.67	0.22	-0.61	-0.39
(3,-1)	C(21)-C(22)	0.26	-0.50	0.22	-0.57	-0.35
(3,-1)	C(21)-H(21)	0.28	-0.74	0.22	-0.64	-0.41
(3,-1)	C(22)-H(22A)	0.28	-0.65	0.24	-0.64	-0.40
(3,-1)	C(22)-H(22B)	0.29	-0.71	0.24	-0.66	-0.42
(3,-1)	C(23)-C(24)	0.26	-0.46	0.22	-0.56	-0.34
(3,-1)	C(24)-H(24A)	0.29	-0.64	0.26	-0.68	-0.42
(3,-1)	C(24)-H(24B)	0.29	-0.58	0.26	-0.66	-0.40
(3,-1)	C(24)-H(24C)	0.30	-0.70	0.27	-0.71	-0.44
(3,-1)	C(25)-H(25A)	0.29	-0.74	0.24	-0.67	-0.43
(3,-1)	C(25)-H(25B)	0.28	-0.68	0.24	-0.65	-0.41
(3,-1)	C(25)-H(25C)	0.28	-0.61	0.24	-0.64	-0.40
(3,-1)	C(26)-H(26A)	0.28	-0.66	0.24	-0.65	-0.41
(3,-1)	C(26)-H(26B)	0.28	-0.62	0.24	-0.63	-0.39
(3,-1)	C(26)-H(26C)	0.27	-0.59	0.23	-0.61	-0.38

Table S2 Energies of pairwise intermolecular interactions in **1** calculated by UNI force field and energy decomposition of CE-B3LYP/6-31G(d,p) wavefunction (kJ/mol)

	UNI force field	CE-B3LYP/6-31G(d,p)				
Symmetry operation	E_{tot}	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
1-x, y+1/2, -z+3/2	-52.3	-11.0	-2.1	-79.0	45.8	-53.8
x+1, y, z	-32.1	-7.2	-2.5	-36.6	23.2	-27.1
-x+2, y+1/2, -z+3/2	-21.8	-2.1	-1.5	-44.2	23.8	-27.1
x+1/2, -y+1/2, -z+1	-13.8	-5.5	-1.2	-13.2	6.3	-14.3
-x+3/2, -y, z+1/2	-12.4	-7.3	-2.0	-5.9	6.7	-10.2
-x+1/2, -y, z+1/2	-12.3	-1.4	-0.3	-12.6	4.1	-10.2

Table S3 Atomic charges (Q, e) and volumes (V, Å^3), obtained within the QTAIM approach for **1**.

Atom	Q_{exp}	V_{AIM}	Atom	Q_{exp}	V_{AIM}
O(1)	-1.42	16.65	H(3)	0.01	6.49
O(2)	-1.58	22.20	H(5)	0.03	7.45
N(1)	-1.34	19.51	H(7)	0.05	7.38
C(1)	0.25	10.00	H(8A)	-0.01	7.32
C(2)	-0.21	15.49	H(8B)	0.04	7.22
C(3)	-0.10	10.58	H(9)	-0.06	6.87
C(4)	-0.05	11.10	H(11A)	0.04	6.78
C(5)	0.29	10.17	H(11B)	0.02	6.45
C(6)	0.21	8.78	H(12A)	0.03	7.69
C(7)	-0.14	12.42	H(12B)	0.00	6.68
C(8)	0.02	8.52	H(13)	-0.02	6.91
C(9)	0.03	6.20	H(14)	-0.06	7.99
C(10)	0.16	5.83	H(15A)	-0.03	7.47
C(11)	0.05	7.16	H(15B)	-0.09	9.05
C(12)	0.18	7.05	H(16)	-0.02	9.47
C(13)	0.17	6.33	H(19A)	0.08	7.81
C(14)	0.21	6.26	H(19B)	0.05	7.21
C(15)	0.21	6.87	H(20A)	-0.02	8.84
C(16)	-0.03	12.88	H(20B)	0.05	8.68
C(17)	0.06	9.26	H(21)	0.01	7.32
C(18)	0.22	5.78	H(22A)	-0.04	6.63
C(19)	-0.06	7.63	H(22B)	0.02	9.52
C(20)	0.22	7.55	H(24A)	0.16	5.19
C(21)	0.48	5.69	H(24B)	0.17	6.66
C(22)	0.02	7.28	H(24C)	0.10	6.02
C(23)	1.19	6.66	H(25A)	-0.11	9.67
C(24)	0.11	10.81	H(25B)	0.09	8.54
C(25)	0.14	8.05	H(25C)	0.08	9.98
C(26)	-0.05	8.84	H(26A)	-0.07	7.44
H(1)	-0.01	8.62	H(26B)	0.10	6.94
H(2)	0.09	7.62	H(26C)	0.08	6.40

Table S4 Contribution of various types of intermolecular interactions to the total packing energy and the area of molecular surface of **1**.

	E_{int}, kJ/mol	E_{int}, %	S, Ang^2	S, %
N…H	7.97	4.63	26.89	5.6
O…H	23.82	13.84	50.83	10.6
C…C	5.20	3.02	0.81	0.2
N…C	3.84	2.23	0.96	0.2
H…H	88.95	51.66	337.89	70.4

C…H	44.91	26.08	62.43	13.0

E_{int} was calculated for all *bcp* corresponding to intermolecular interactions as -0.5V(**r**) using EML correlation (Espinosa *et al.*, 1998). The molecular surface area was analysed using Voronoi tessellation implemented within ToposPro package (Blatov *et al.*, 2014).