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A Comparison of Electron Density from Hirshfeld-Atom Refinement, X-Ray Wavefunction Refinement and Multipole Refinement on Three Urea Derivatives

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Table S1. Bond lengths [Å] for murea obtained from the various models and methods.

	MM	HAR (+/-) [a]	HAR [a]	HAR (+/-) [b]	HAR [b]
O1-C1	1.2559(5)	1.2541(4)	1.2538(4)	1.2537(4)	1.2534(4)
C1-N1	1.3500(5)	1.3497(4)	1.3498(4)	1.3498(4)	1.3499(4)
C1-N2	1.3513(5)	1.3520(4)	1.3522(4)	1.3520(4)	1.3523(4)
N1-C11	1.4488(6)	1.4498(4)	1.4498(4)	1.4498(5)	1.4498(5)
N1-H1	1.009	1.016(9)	0.998(9)	1.01(1)	0.988(9)
N2-H2A	1.009	0.99(1)	0.97(1)	0.99(1)	0.97(1)
N2-H2B	1.009	1.008(9)	1.000(9)	1.011(9)	1.002(9)
C11-H11A	1.067	1.101(9)	1.100(9)	1.093(9)	1.094(9)
C11-H11B	1.066	1.09(1)	1.10(1)	1.08(1)	1.09(1)
C11-H11C	1.066	1.095(9)	1.090(9)	1.10(1)	1.09(1)

[a] HAR and HAR(+/-) were performed using the blyp/cc-pVTZ level of theory. [b] HAR and HAR(+/-) were performed using the blyp/cc-pVDZ level of theory. The bond distances N-H and C-H were set to average distances from neutron diffraction in the multipole refinement, but freely refined in both variations of HAR.

Table S2. Bond lengths [Å] for phurea obtained from the various models and methods.

	MM	HAR (+/-) [a]	HAR [a]	HAR (+/-) [b]	HAR [b]
O1-C1	1.2515(2)	1.2511(2)	1.2508(2)	1.2508(2)	1.2506(2)
C1-N1	1.3667(3)	1.3669(2)	1.3669(2)	1.3670(2)	1.3670(2)
C1-N2	1.3502(3)	1.3497(2)	1.3498(2)	1.3498(2)	1.3499(2)
N1-C11	1.4180(3)	1.4186(2)	1.4186(2)	1.4188(2)	1.4187(2)
C11-C12	1.4012(3)	1.4003(3)	1.4003(3)	1.4000(3)	1.4000(3)
C12-C13	1.3962(4)	1.3965(3)	1.3965(3)	1.3964(3)	1.3964(3)
C13-C14	1.4012(5)	1.3986(4)	1.3988(4)	1.3985(4)	1.3986(4)
C14-C15	1.3951(5)	1.3940(4)	1.3939(4)	1.3937(4)	1.3937(4)
C15-C16	1.3963(4)	1.3961(3)	1.3961(3)	1.3960(3)	1.3960(3)
C11-C16	1.3994(3)	1.3982(3)	1.3982(3)	1.3982(3)	1.3982(3)
N1-H1	1.009	1.014(5)	1.004(5)	1.012(6)	1.001(6)
N2-H2A	1.009	1.010(5)	0.990(5)	1.003(5)	0.986(5)
N2-H2B	1.009	1.000(6)	0.993(6)	0.992(6)	0.983(6)
C12-H12	1.081	1.094(4)	1.104(5)	1.093(5)	1.104(5)
C13-H13	1.083	1.097(6)	1.099(6)	1.097(7)	1.100(7)
C14-H14	1.082	1.104(6)	1.106(6)	1.099(6)	1.101(6)
C15-H15	1.080	1.093(5)	1.091(5)	1.082(5)	1.082(5)
C16-H16	1.082	1.094(6)	1.096(6)	1.090(7)	1.091(7)

[a] HAR and HAR(+/-) were performed using the blyp/cc-pVTZ level of theory. [b] HAR and HAR(+/-) were performed using the blyp/cc-pVDZ level of theory. The bond distances N-H and C-H were set to average distances from neutron diffraction in the multipole refinement, but freely refined in both variations of HAR.

Table S3. Bond lengths [Å] for dphurea obtained from the various models and methods.

	MM	HAR (+/-) [a]	HAR [a]	HAR (+/-) [b]	HAR [b]
O1-C1	1.2409(2)	1.2404(2)	1.2402(2)	1.2400(2)	1.2398(2)
C1-N1	1.3641(3)	1.3640(2)	1.3641(2)	1.3642(3)	1.3643(3)
C1-N2	1.3728(3)	1.3729(2)	1.3728(2)	1.3729(2)	1.3729(2)
N1-C11	1.4155(3)	1.4160(2)	1.4160(2)	1.4158(2)	1.4159(2)
N2-C21	1.4164(3)	1.4169(2)	1.4169(2)	1.4168(3)	1.4169(3)
C11-C12	1.4022(3)	1.4012(3)	1.4012(3)	1.4012(3)	1.4011(3)
C12-C13	1.3970(3)	1.3967(3)	1.3966(3)	1.3966(3)	1.3966(3)
C13-C14	1.3976(5)	1.3985(4)	1.3983(4)	1.3983(4)	1.3981(4)
C14-C15	1.4025(6)	1.3995(5)	1.3995(5)	1.3993(5)	1.3992(5)
C15-C16	1.3983(4)	1.3979(3)	1.3980(4)	1.3979(4)	1.3979(4)
C11-C16	1.4007(3)	1.4001(3)	1.4001(3)	1.4001(3)	1.4001(3)
C21-C22	1.4035(3)	1.4029(2)	1.4028(2)	1.4028(3)	1.4027(3)
C22-C23	1.4004(4)	1.3994(3)	1.3994(3)	1.3991(3)	1.3991(3)
C23-C24	1.3962(4)	1.3955(3)	1.3956(4)	1.3957(4)	1.3958(4)
C24-C25	1.3975(4)	1.3977(4)	1.3978(4)	1.3976(4)	1.3977(4)
C25-C26	1.3985(4)	1.3975(3)	1.3976(3)	1.3972(3)	1.3973(3)
C21-C26	1.4029(3)	1.4025(3)	1.4025(3)	1.4026(3)	1.4027(3)
N1-H1	1.008	1.014(5)	0.997(4)	1.008(5)	0.989(5)
N2-H2	1.007	0.997(5)	0.985(5)	0.994(5)	0.982(5)
C12-H12	1.082	1.095(5)	1.095(5)	1.094(6)	1.094(6)
C13-H13	1.082	1.092(5)	1.084(5)	1.089(6)	1.081(6)
C14-H14	1.081	1.108(6)	1.109(6)	1.101(6)	1.103(6)
C15-H15	1.082	1.117(6)	1.119(6)	1.120(6)	1.122(7)
C16-H16	1.080	1.095(5)	1.089(5)	1.097(5)	1.090(5)
C22-H22	1.083	1.088(5)	1.089(5)	1.074(5)	1.076(5)
C23-H23	1.084	1.105(5)	1.103(5)	1.097(5)	1.096(5)
C24-H24	1.081	1.099(6)	1.096(6)	1.100(6)	1.096(6)
C25-H25	1.082	1.107(6)	1.104(6)	1.109(6)	1.106(6)
C26-H26	1.081	1.092(5)	1.087(5)	1.086(5)	1.082(5)

[a] HAR and HAR(+/-) were performed using the blyp/cc-pVTZ level of theory. [b] HAR and HAR(+/-) were performed using the blyp/cc-pVDZ level of theory. The bond distances N-H and C-H were set to average distances from neutron diffraction in the multipole refinement, but freely refined in both variations of HAR.

Table S4. Topological parameters for murea obtained from the various models and methods.[a]

	ρ_{bcp} [b]				$\nabla^2\rho_{bcp}$ [c]			
	MM	HAR (+/-)	HAR	XWR	MM	HAR (+/-)	HAR	XWR
O1-C1	2.67(5)	2.61	2.65	2.67	-27.3(4)	-16.2	-18.1	-14.1
C1-N1	2.33(4)	2.30	2.27	2.33	-25.5(2)	-25.3	-24.6	-27.4
C1-N2	2.29(3)	2.28	2.25	2.26	-23.0(2)	-25.4	-24.2	-24.7
N1-C11	1.79(4)	1.78	1.77	1.80	-12.9(2)	-16.8	-16.6	-17.9
N1-H1	2.36(10)	2.30	2.41	2.41	-29.8(5)	-44.9	-44.8	-47.1
N2-H2A	2.33(10)	2.43	2.57	2.49	-32.6(5)	-50.6	-53.1	-54.6
N2-H2B	2.12(9)	2.33	2.38	2.36	-27.3(5)	-47.7	-47.1	-48.3
C11-H11A	1.90(5)	1.90	1.90	1.91	-19.8(1)	-25.7	-25.7	-15.0
C11-H11B	1.90(5)	1.93	1.91	1.87	-19.9(1)	-26.5	-25.9	-24.7
C11-H11C	1.90(5)	1.94	1.96	1.97	-19.7(1)	-26.7	-27.3	-28.5

[a] Basis-set calculations were performed using the blyp/cc-pVTZ level of theory. [b] ρ_{bcp} [in eÅ^{-3}] is electron density at the bond critical point [c] $\nabla^2\rho_{bcp}$ [in eÅ^{-5}] is a corresponding Laplacian. For evaluations of the wavefunctions standard deviations are not given.

Table S5. Topological parameters for phurea obtained from the various models and methods.[a]

	ρ_{bcp} [b]				$\nabla^2\rho_{bcp}$ [c]			
	MM	HAR (+/-)	HAR	XWR	MM	HAR (+/-)	HAR	XWR
O1-C1	2.65(3)	2.62	2.67	2.57	-34.3(2)	-15.6	-17.9	-13.5
C1-N1	2.21(2)	2.21	2.18	2.24	-19.0(1)	-24.0	-23.3	-26.5
C1-N2	2.30(2)	2.29	2.26	2.31	-22.5(1)	-25.4	-24.1	-26.4
N1-C11	1.84(2)	1.91	1.90	1.90	-10.9(1)	-18.9	-18.5	-17.8
C11-C12	2.06(2)	2.13	2.13	2.09	-14.5(1)	-24.3	-24.3	-22.6
C12-C13	2.11(2)	2.13	2.13	2.14	-17.9(1)	-24.3	-24.3	-24.5
C13-C14	2.09(2)	2.13	2.12	2.16	-14.8(1)	-24.3	-24.3	-25.4
C14-C15	2.09(3)	2.14	2.15	2.16	-15.2(1)	-24.7	-24.7	-25.1
C15-C16	2.11(3)	2.13	2.13	2.16	-17.9(1)	-24.3	-24.3	-25.5
C11-C16	2.16(2)	2.14	2.14	2.18	-17.7(1)	-24.6	-24.5	-25.7
N1-H1	2.00(4)	2.31	2.39	2.38	-32.6(3)	-45.5	-43.7	-46.7
N2-H2A	1.99(4)	2.33	2.45	2.41	-31.6(2)	-46.4	-47.3	-46.7
N2-H2B	2.05(5)	2.39	2.43	2.38	-29.8(3)	-49.0	-49.0	-52.0
C12-H12	1.92(2)	1.92	1.89	1.94	-18.7(1)	-26.3	-25.4	-28.4
C13-H13	1.95(2)	1.91	1.90	1.89	-19.7(1)	-26.0	-25.7	-25.1
C14-H14	1.96(2)	1.87	1.87	1.91	-19.0(1)	-25.0	-24.9	-26.4
C15-H15	1.96(2)	1.92	1.93	1.94	-19.9(1)	-26.3	-26.4	-27.3
C16-H16	1.92(2)	1.92	1.90	1.89	-18.6(1)	-26.1	-25.6	-25.4

[a] Basis-set calculations were performed using the blyp/cc-pVTZ level of theory. [b] ρ_{bcp} [in eÅ^{-3}] is electron density at the bond critical point and [c] $\nabla^2\rho_{bcp}$ [in eÅ^{-5}] is a corresponding Laplacian. For evaluations of the wavefunctions standard deviations are not given.

Table S6. Topological parameters for dphurea obtained from the various models and methods.[a]

	ρ_{bcp} [b]				$\nabla^2\rho_{bcp}$ [c]			
	MM	HAR (+/-)	HAR	XWR	MM	HAR (+/-)	HAR	XWR
O1-C1	2.71(3)	2.67	2.72	2.66	-27.3(2)	-14.0	-16.2	-14.0
C1-N1	2.25(2)	2.21	2.19	2.22	-20.0(1)	-23.6	-23.0	-24.9
C1-N2	2.18(2)	2.18	2.16	2.21	-18.6(1)	-23.2	-22.7	-25.7
N1-C11	1.89(2)	1.92	1.91	1.93	-10.2(1)	-19.0	-18.5	-19.8
N2-C21	1.90(2)	1.92	2.16	1.91	-11.2(1)	-18.6	-22.7	-18.7
C11-C12	2.00(2)	2.12	2.12	2.07	-13.3(1)	-24.2	-24.2	-22.1
C12-C13	2.05(2)	2.13	2.13	2.15	-15.0(1)	-24.3	-24.3	-25.6
C13-C14	2.11(2)	2.12	2.12	2.14	-16.6(1)	-24.2	-24.2	-24.9
C14-C15	2.10(3)	2.12	2.12	2.13	-15.2(1)	-24.1	-24.1	-24.5
C15-C16	2.04(2)	2.12	2.12	2.11	-14.9(1)	-24.2	-24.2	-23.2
C11-C16	2.01(2)	2.13	2.13	2.13	-13.2(1)	-24.3	-24.2	-24.3
C21-C22	1.93(2)	2.11	2.11	2.07	-10.5(1)	-23.9	-23.9	-22.2
C22-C23	2.01(2)	2.12	2.12	2.12	-13.1(1)	-24.0	-24.0	-24.1
C23-C24	2.09(2)	2.14	2.14	2.11	-15.9(1)	-24.6	-24.5	-23.6
C24-C25	2.04(3)	2.13	2.13	2.12	-15.2(1)	-24.3	-24.2	-24.5
C25-C26	2.01(2)	2.12	2.12	2.11	-13.3(1)	-24.2	-24.1	-23.4
C21-C26	2.01(2)	2.12	2.12	2.10	-13.1(1)	-24.1	-24.0	-22.9
N1-H1	2.02(4)	2.32	2.43	2.36	-27.1(2)	-46.0	-45.7	-48.9
N2-H2	2.00(4)	2.43	2.51	2.49	-26.3(2)	-49.8	-49.4	-49.2
C12-H12	1.86(2)	1.93	1.93	1.91	-16.3(1)	-26.3	-26.4	-25.3
C13-H13	1.85(2)	1.93	1.96	1.97	-17.4(1)	-26.6	-27.4	-28.1
C14-H14	1.80(2)	1.86	1.85	1.84	-14.6(1)	-24.7	-24.6	-24.4
C15-H15	1.85(2)	1.83	1.81	1.80	-17.5(1)	-23.8	-23.5	-23.1
C16-H16	1.87(2)	1.91	1.93	1.92	-16.6(1)	-26.0	-26.5	-26.2
C22-H22	1.81(2)	1.96	1.95	1.93	-16.5(1)	-27.1	-27.1	-26.2
C23-H23	1.85(2)	1.88	1.88	1.89	-17.6(1)	-25.3	-25.4	-25.2
C24-H24	1.94(2)	1.90	1.91	1.88	-20.2(1)	-25.6	-25.8	-24.6
C25-H25	1.85(2)	1.87	1.88	1.87	-17.6(1)	-24.9	-25.1	-25.2
C26-H26	1.81(2)	1.93	1.93	1.90	-16.1(1)	-26.3	-26.5	-25.4

[a] Basis-set calculations were performed using the blyp/cc-pVTZ level of theory. [b] ρ_{bcp} [in eÅ^{-3}] is electron density at the bond critical point and [c] $\nabla^2\rho_{bcp}$ [in eÅ^{-5}] is a corresponding Laplacian. For evaluations of the wavefunctions standard deviations are not given.

Table S7. Integrated atomic properties for murea obtained from the various models and methods.[a]

	V_{001} [b]				N_{001} [c]				Q [d]			
	MM	HAR (+/-)	HAR	XWR	MM	HAR (+/-)	HAR	XWR	MM	HAR (+/-)	HAR	XWR
O1	15.47	21.68	20.64	20.67	9.02	9.24	9.08	9.17	-1.02	-1.28	-1.12	-1.21
N1	14.15	14.35	14.13	14.44	8.02	8.10	8.09	8.13	-1.03	-1.12	-1.11	-1.15
N2	17.72	17.61	17.14	17.68	8.22	8.13	8.10	8.21	-1.22	-1.17	-1.13	-1.25
C1	4.45	4.72	4.70	4.40	4.26	4.22	4.21	4.09	1.74	1.77	1.79	1.91
C11	8.90	9.28	9.25	9.02	5.52	5.61	5.59	5.56	0.48	0.38	0.40	0.43
H1	3.85	3.98	4.76	4.56	0.66	0.54	0.63	0.59	0.34	0.45	0.35	0.39
H2A	3.18	3.97	4.53	4.23	0.58	0.54	0.61	0.56	0.42	0.44	0.37	0.43
H2B	3.01	3.89	4.38	4.23	0.53	0.52	0.57	0.54	0.47	0.47	0.41	0.44
H11A	7.29	7.29	7.51	7.31	1.05	0.96	0.98	0.97	-0.06	0.02	0.00	0.01
H11B	7.37	7.52	7.48	7.44	1.06	0.98	0.97	0.95	-0.06	0.00	0.01	0.02
H11C	7.10	7.02	7.03	7.32	1.05	0.95	0.94	1.02	-0.05	0.03	0.04	-0.04
Σ	92.48	101.32	101.56	101.30	39.97	39.79	39.78	39.78	0.004	0.00	0.00	0.00

[a] Basis-set calculations were performed using the blyp/cc-pVTZ level of theory. [b] V_{001} [in Å^3] is the basin volume cut at ρ=0.001 a.u and [c] N_{001} [in e] is the corresponding electron population, [d] atomic charge [in e].

Table S8. Integrated atomic properties for phurea obtained from the various models and methods.[a]

	V_{001} [b]				N_{001} [c]				Q [d]			
	MM	HAR (+/-)	HAR	XWR	MM	HAR (+/-)	HAR	XWR	MM	HAR (+/-)	HAR	XWR
O1	14.64	21.33	20.26	20.36	8.86	9.24	9.07	9.11	-0.86	-1.28	-1.11	-1.14
N1	14.65	14.13	13.99	14.05	8.13	8.11	8.10	8.11	-1.13	-1.12	-1.12	-1.12
N2	17.46	17.39	17.01	17.40	8.17	8.11	8.09	8.17	-1.18	-1.15	-1.13	-1.20
C1	5.70	4.78	4.80	4.85	4.52	4.23	4.22	4.19	1.48	1.77	1.78	1.80
C11	9.14	9.30	9.30	9.26	5.68	5.66	5.65	5.60	0.32	0.34	0.34	0.39
C12	10.71	12.05	11.95	12.13	5.97	5.99	5.97	6.03	0.03	0.00	0.01	-0.04
C13	10.77	12.33	12.42	12.61	5.91	5.98	5.99	6.02	0.09	0.00	-0.01	-0.04
C14	11.40	12.75	12.57	12.33	5.94	6.01	6.00	5.94	0.06	-0.03	-0.02	0.04
C15	11.28	12.55	12.40	12.57	5.91	6.00	5.99	5.98	0.09	-0.02	0.00	0.00
C16	10.96	12.20	12.35	12.59	5.98	5.98	5.99	6.05	0.02	0.00	-0.01	-0.07
H1	2.46	3.96	4.76	4.81	0.42	0.54	0.63	0.60	0.58	0.45	0.36	0.38
H2A	2.93	3.97	4.63	4.63	0.43	0.53	0.61	0.60	0.57	0.45	0.37	0.38
H2B	2.88	4.01	4.33	4.14	0.47	0.54	0.57	0.52	0.53	0.45	0.41	0.47
H12	7.39	6.95	6.92	6.87	1.11	0.94	0.92	0.89	-0.11	0.04	0.06	0.09
H13	8.56	7.52	7.50	7.51	1.13	0.96	0.96	0.95	-0.13	0.02	0.02	0.03
H14	8.33	7.47	7.59	7.64	1.10	0.95	0.96	0.96	-0.10	0.03	0.02	0.02
H15	7.77	7.36	7.52	7.44	1.14	0.95	0.96	0.94	-0.14	0.03	0.01	0.03
H16	8.26	7.36	7.60	7.69	1.11	0.95	0.97	0.97	-0.11	0.03	0.01	0.00
Σ	165.31	177.42	177.90	178.88	71.97	71.66	71.65	71.65	0.01	0.00	0.00	0.00

[a] Basis-set calculations were performed using the blyp/cc-pVTZ level of theory. [b] V_{001} [in Å^3] is the basin volume cut at ρ=0.001 a.u and [c] N_{001} [in e] is the corresponding electron population, [d] atomic charge [in e].

Table S9. Integrated atomic properties for dphurea obtained from the various models and methods.[a]

	V_{001} [b]				N_{001} [c]				Q [d]			
	MM	HAR (+/-)	HAR	XWR	MM	HAR (+/-)	HAR	XWR	MM	HAR (+/-)	HAR	XWR
O1	14.89	19.93	19.12	19.20	8.89	9.21	9.08	9.11	-0.90	-1.24	-1.11	-1.14
N1	13.46	14.08	13.90	14.23	8.02	8.11	8.11	8.12	-1.02	-1.13	-1.12	-1.14
N2	13.56	14.09	13.92	13.94	7.94	8.10	8.09	8.07	-0.94	-1.11	-1.11	-1.09
C1	5.08	4.85	4.87	4.96	4.61	4.24	4.24	4.24	1.39	1.75	1.75	1.75
C11	9.26	9.32	9.32	9.20	5.70	5.66	5.65	5.60	0.30	0.33	0.34	0.39
C12	11.01	12.05	11.94	11.89	6.00	5.98	5.96	5.95	0.00	0.00	0.02	0.03
C13	11.31	12.44	12.34	12.47	5.95	5.99	5.98	6.01	0.05	-0.01	0.01	-0.03
C14	11.79	12.72	12.63	13.02	6.04	6.01	6.00	6.05	-0.04	-0.03	-0.02	-0.07
C15	11.88	12.63	12.55	12.65	5.93	6.01	6.00	6.01	0.07	-0.03	-0.02	-0.03
C16	11.43	12.42	12.33	12.46	6.00	6.00	5.99	6.00	-0.01	-0.02	-0.01	-0.01
C21	9.41	9.43	9.34	9.28	5.70	5.68	5.66	5.62	0.30	0.31	0.33	0.37
C22	11.24	12.21	12.01	12.26	5.96	5.99	5.96	6.05	0.04	-0.01	0.02	-0.06
C23	10.64	12.61	12.42	12.40	5.90	6.01	5.99	5.94	0.10	-0.03	-0.01	0.04
C24	12.03	12.67	12.56	13.09	6.18	6.00	5.99	6.10	-0.18	-0.02	-0.01	-0.12
C25	11.90	12.58	12.48	12.69	5.92	6.01	5.99	6.01	0.08	-0.03	-0.01	-0.03
C26	11.85	12.50	12.37	12.44	5.97	6.00	5.99	5.95	0.02	-0.02	-0.01	0.03
H1	2.53	3.90	4.67	4.45	0.48	0.53	0.62	0.57	0.52	0.46	0.37	0.42
H2	3.07	4.01	4.59	4.67	0.49	0.55	0.62	0.62	0.51	0.44	0.37	0.37
H12	6.79	6.80	6.83	6.77	1.05	0.93	0.93	0.92	-0.05	0.05	0.05	0.06
H13	8.08	7.37	7.41	7.55	1.07	0.95	0.96	0.99	-0.07	0.03	0.02	-0.02
H14	8.33	7.54	7.58	7.46	1.05	0.95	0.95	0.91	-0.06	0.02	0.02	0.07
H15	7.71	7.47	7.64	7.63	1.07	0.94	0.95	0.94	-0.07	0.04	0.02	0.04
H16	7.87	7.36	7.55	7.70	1.04	0.95	0.97	0.99	-0.05	0.03	0.00	-0.02
H22	7.22	6.54	6.52	6.56	0.99	0.93	0.92	0.91	0.01	0.05	0.06	0.08
H23	7.48	7.20	7.52	7.37	0.99	0.92	0.95	0.92	0.00	0.05	0.02	0.06
H24	7.39	7.44	7.54	7.46	1.01	0.95	0.96	0.93	-0.01	0.03	0.01	0.04
H25	7.82	7.45	7.58	7.73	0.99	9.94	0.96	0.96	0.01	0.03	0.02	0.02
H26	7.47	7.13	7.58	7.62	0.98	0.94	0.98	0.98	0.01	0.04	0.00	0.00
Σ	262.48	276.73	277.12	279.18	111.92	111.48	111.47	111.47	0.01	0.00	0.00	0.00

[a] Basis-set calculations were performed using the blyp/cc-pVTZ level of theory. [b] V_{001} [in Å^3] is the basin volume cut at ρ=0.001 a.u and [c] N_{001} [in e] is the corresponding electron population, [d] atomic charge [in e].

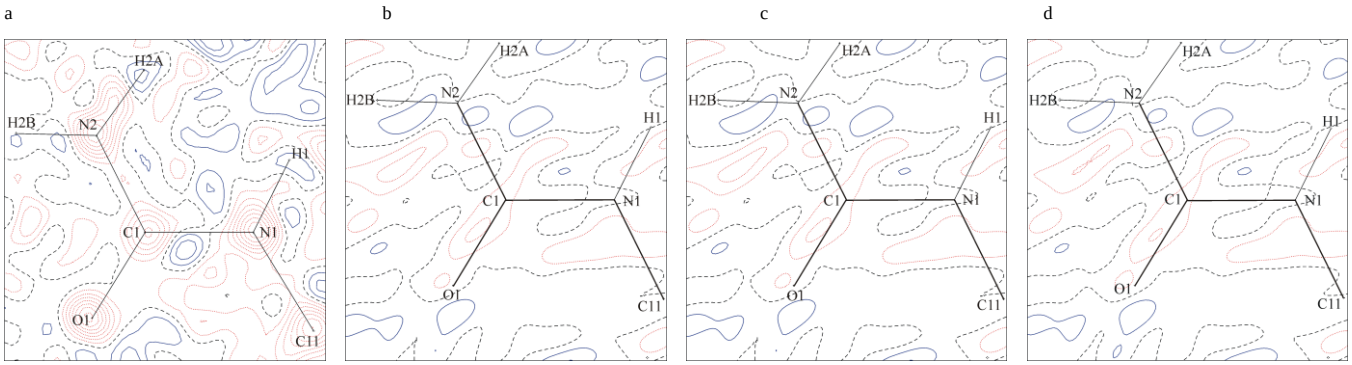

Figure S1. Residual electron density in the plane of the urea moiety for murea as obtained from *a*) multipole refinement (MM), *b*) Hirshfeld-atom refinement with point charges and dipoles (HAR +/-), *c*) Hirshfeld-atom refinement (HAR) and *d*) X-ray wavefunction refinement (XWR). Contour intervals are 0.05 eÅ^{-3}; positive, negative and zero contours are represented by solid blue, dotted red and dashed black lines, respectively.

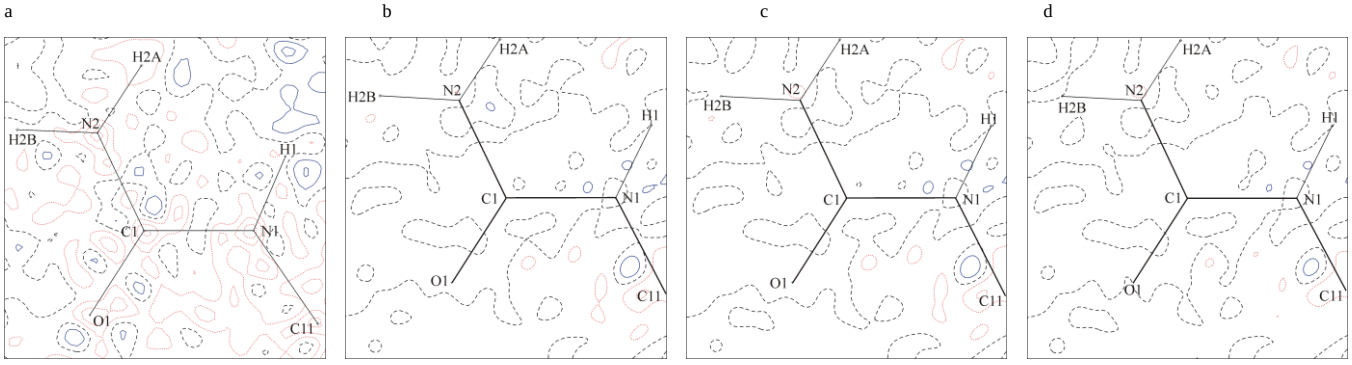

Figure S2. Residual electron density in the plane of the urea moiety for phurea as obtained from *a*) MM, *b*) HAR (+/-), *c*) HAR and *d*) XWR. Contour intervals and colours as in Figure S1.

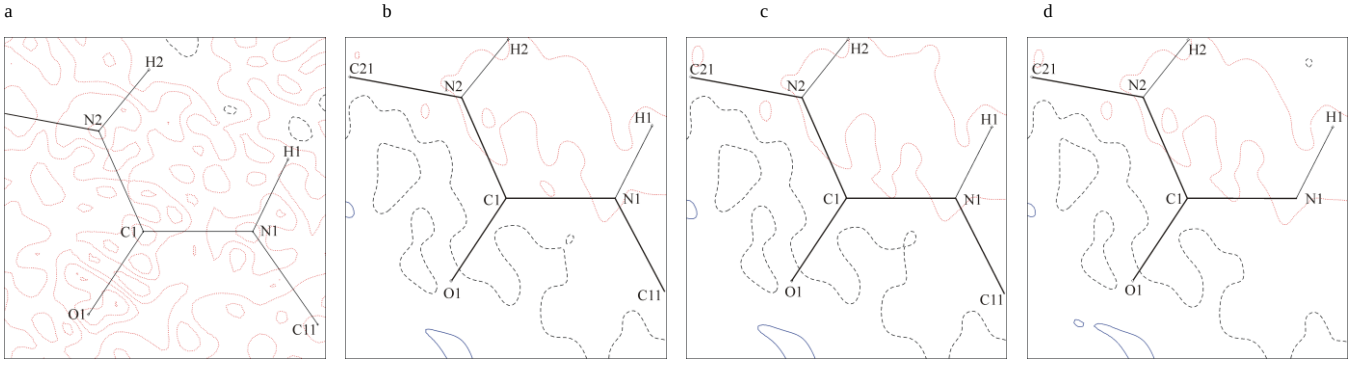

Figure S3. Residual electron density in the plane of the urea moiety for dphurea as obtained from *a*) MM, *b*) HAR (+/-), *c*) HAR and *d*) XWR. Contour intervals and colours as in Figure S1.

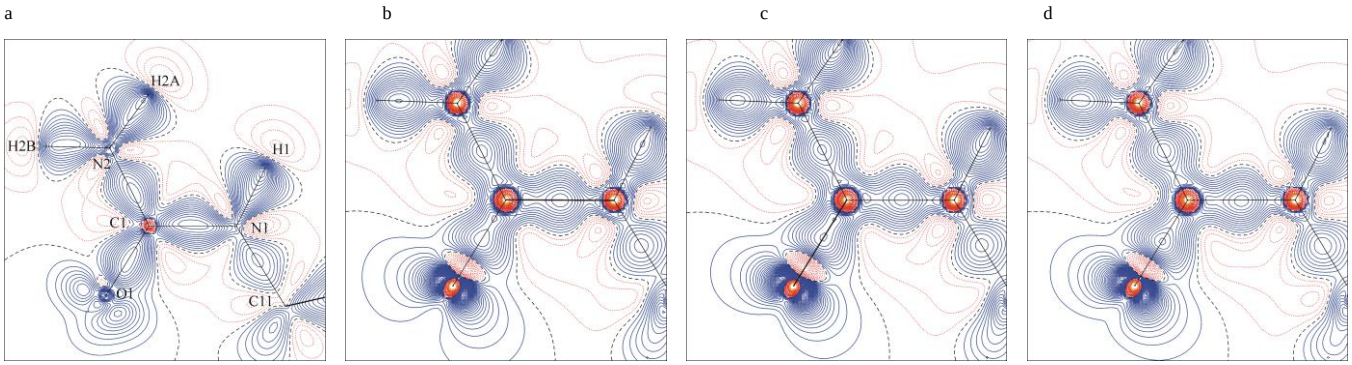

Figure S4. Static deformation density map in the plane of the urea moiety for murea as obtained from *a*) MM, *b*) HAR (+/-), *c*) HAR and *d*) XWR. Contour intervals and colours as in Figure S1.

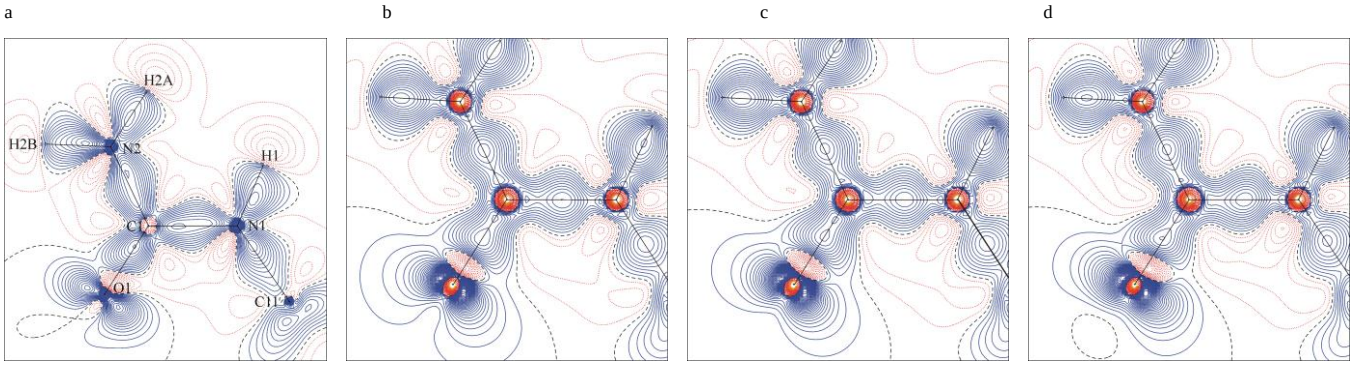

Figure S5. Static deformation density map in the plane of the urea moiety for phurea as obtained from *a*) MM, *b*) HAR (+/-), *c*) HAR and *d*) XWR. Contour intervals and colours as in Figure S1.

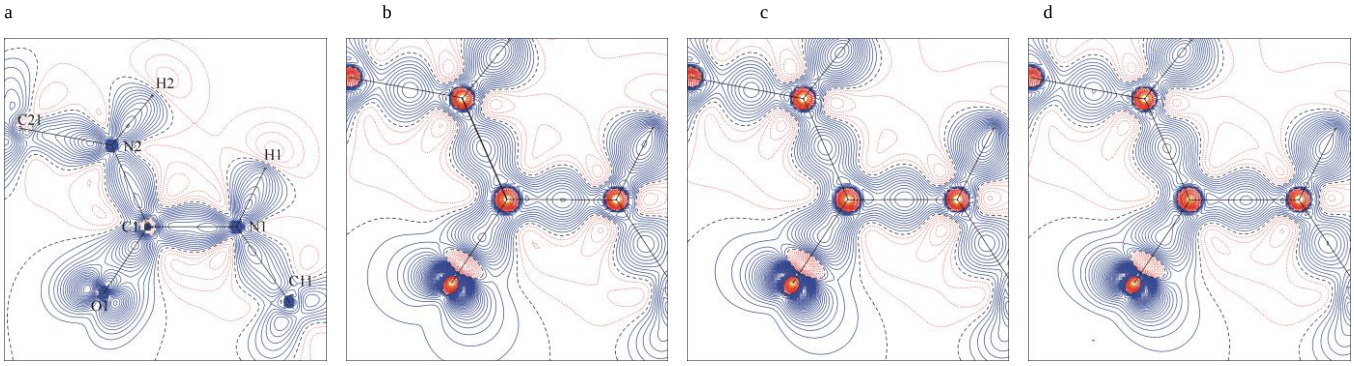

Figure S6. Static deformation density map in the plane of the urea moiety for dphurea as obtained from *a*) MM, *b*) HAR (+/-), *c*) HAR and *d*) XWR. Contour intervals and colours as in Figure S1.

Table S10. Final positional parameters [Å] and anisotropic displacement parameters [Å^2] obtained after Hirshfeld-atom refinement with a cluster of charges HAR (+/-) using the blyp/cc-pVDZ level of theory for murea.

Atom	x	y	z	U11	U22	U33	U12	U13	U23
O1	0.37465(4)	0.45320(4)	0.19599(3)	0.00672(9)	0.00674(9)	0.00482(8)	-0.00009(7)	0.00100(6)	-0.00025(6)
N1	0.20095(5)	0.34050(5)	0.40523(4)	0.0086(1)	0.0066(1)	0.00630(9)	-0.00243(8)	0.00197(8)	-0.00033(8)
N2	0.33986(4)	0.65187(5)	0.40871(4)	0.0092(1)	0.0062(1)	0.0069(1)	-0.00181(8)	0.00141(8)	-0.00128(8)
C1	0.30815(5)	0.48052(5)	0.33075(4)	0.0048(1)	0.0050(1)	0.00426(9)	-0.00022(7)	0.00013(8)	-0.00004(7)
C11	0.14253(5)	0.15871(5)	0.32754(4)	0.0091(1)	0.0070(1)	0.0103(1)	-0.00257(9)	0.00118(9)	-0.00126(9)
H1	0.149(2)	0.377(2)	0.511(1)	0.035926(0)	0.024822(0)	0.016402(0)	-0.009580(0)	0.012269(0)	-0.005538(0)
H2A	0.285(2)	0.663(2)	0.515(1)	0.043062(0)	0.027001(0)	0.017207(0)	-0.011458(0)	0.013542(0)	-0.007804(0)
H2B	0.434(2)	0.752(1)	0.362(1)	0.015665(0)	0.015168(0)	0.020317(0)	-0.003997(0)	0.000602(0)	0.002799(0)
H11A	0.081(2)	0.059(1)	0.416(1)	0.035813(0)	0.022960(0)	0.026727(0)	-0.010610(0)	0.006169(0)	0.005683(0)
H11B	0.030(2)	0.183(1)	0.240(1)	0.036825(0)	0.029026(0)	0.032880(0)	-0.004674(0)	-0.018649(0)	0.001055(0)
H11C	0.273(1)	0.087(1)	0.276(2)	0.024442(0)	0.026874(0)	0.048634(0)	-0.000754(0)	0.014289(0)	-0.013834(0)

Table S11. Final positional parameters [Å] and anisotropic displacement parameters [Å^2] obtained after Hirshfeld-atom refinement using the blyp/cc-pVDZ level of theory for murea.

Atom	x	y	z	U11	U22	U33	U12	U13	U23
O1	0.37464(4)	0.45322(4)	0.19603(3)	0.00679(9)	0.00668(9)	0.00480(8)	-0.00016(7)	0.00107(6)	-0.00029(7)
N1	0.20093(5)	0.34050(5)	0.40525(4)	0.0085(1)	0.0066(1)	0.0064(1)	-0.00241(8)	0.00188(8)	-0.00027(8)
N2	0.33989(4)	0.65190(5)	0.40872(4)	0.0091(1)	0.0062(1)	0.0069(1)	-0.00175(8)	0.00133(8)	-0.00129(8)
C1	0.30816(5)	0.48052(5)	0.33076(4)	0.0048(1)	0.0051(1)	0.0042(1)	-0.00018(7)	0.00014(8)	-0.00002(8)
C11	0.14255(5)	0.15873(5)	0.32753(4)	0.0091(1)	0.0070(1)	0.0103(1)	-0.00255(9)	0.0012(1)	-0.00126(9)
H1	0.149(2)	0.378(2)	0.509(1)	0.035022(0)	0.024730(0)	0.016648(0)	-0.009243(0)	0.012243(0)	-0.005669(0)
H2A	0.286(2)	0.664(2)	0.513(1)	0.043090(0)	0.027036(0)	0.017374(0)	-0.011506(0)	0.013770(0)	-0.007908(0)
H2B	0.432(2)	0.752(1)	0.363(1)	0.015171(0)	0.014852(0)	0.020167(0)	-0.003629(0)	0.000327(0)	0.002886(0)
H11A	0.082(2)	0.060(1)	0.416(1)	0.034666(0)	0.022755(0)	0.026559(0)	-0.010052(0)	0.005632(0)	0.005971(0)
H11B	0.031(2)	0.184(1)	0.238(1)	0.038219(0)	0.029086(0)	0.031965(0)	-0.005266(0)	-0.018770(0)	0.001713(0)
H11C	0.272(2)	0.088(1)	0.275(2)	0.025005(0)	0.027056(0)	0.049079(0)	-0.001225(0)	0.015291(0)	-0.014117(0)

Table S12. Final positional parameters [Å] and anisotropic displacement parameters [Å^2] obtained after Hirshfeld-atom refinement with a cluster of charges HAR (+/-) using the blyp/cc-pVTZ level of theory for murea.

Atom	x	y	z	U11	U22	U33	U12	U13	U23
O1	0.37469(4)	0.45320(4)	0.19596(3)	0.00673(9)	0.00682(9)	0.00473(8)	-0.00007(6)	0.00102(6)	-0.00026(6)
N1	0.20096(5)	0.34051(4)	0.40522(4)	0.0086(1)	0.00657(9)	0.00620(9)	-0.00247(8)	0.00200(8)	-0.00034(7)
N2	0.33988(4)	0.65187(4)	0.40870(4)	0.0092(1)	0.00615(9)	0.00678(9)	-0.00191(8)	0.00150(8)	-0.00134(8)
C1	0.30815(5)	0.48052(5)	0.33076(4)	0.0047(1)	0.0049(1)	0.00413(9)	-0.00025(7)	0.00015(7)	-0.00010(7)
C11	0.14255(5)	0.15871(5)	0.32754(4)	0.0089(1)	0.0069(1)	0.0103(1)	-0.00255(9)	0.00119(9)	-0.00126(9)
H1	0.149(2)	0.376(2)	0.513(1)	0.036206(0)	0.025006(0)	0.016377(0)	-0.009876(0)	0.012508(0)	-0.005574(0)
H2A	0.285(2)	0.665(2)	0.516(1)	0.039562(0)	0.026215(0)	0.016493(0)	-0.009830(0)	0.012038(0)	-0.007291(0)
H2B	0.434(2)	0.752(1)	0.362(1)	0.019249(0)	0.016179(0)	0.021272(0)	-0.005976(0)	0.002658(0)	0.001763(0)
H11A	0.082(2)	0.059(1)	0.417(1)	0.041806(0)	0.023820(0)	0.027294(0)	-0.012964(0)	0.007868(0)	0.005043(0)
H11B	0.028(2)	0.184(1)	0.240(1)	0.032980(0)	0.028778(0)	0.034833(0)	-0.002464(0)	-0.017766(0)	-0.001148(0)
H11C	0.271(1)	0.087(1)	0.274(1)	0.023133(0)	0.026525(0)	0.045412(0)	0.000426(0)	0.011228(0)	-0.013125(0)

Table S13. Final positional parameters [Å] and anisotropic displacement parameters [Å^2] obtained after Hirshfeld-atom refinement using the blyp/cc-pVTZ level of theory for murea.

Atom	x	y	z	U11	U22	U33	U12	U13	U23
O1	0.37468(4)	0.45322(4)	0.19601(3)	0.00680(9)	0.00673(9)	0.00469(8)	-0.00015(6)	0.00109(6)	-0.00031(6)
N1	0.20095(5)	0.34051(4)	0.40525(4)	0.0085(1)	0.0065(1)	0.00629(9)	-0.00245(8)	0.00191(8)	-0.00028(8)
N2	0.33991(4)	0.65190(4)	0.40871(4)	0.0091(1)	0.00613(9)	0.0068(1)	-0.00184(8)	0.00141(8)	-0.00135(8)
C1	0.30816(5)	0.48052(5)	0.33077(4)	0.0047(1)	0.0049(1)	0.00407(9)	-0.00021(7)	0.00017(7)	-0.00009(7)
C11	0.14256(5)	0.15872(5)	0.32754(4)	0.0089(1)	0.0069(1)	0.0103(1)	-0.00253(9)	0.00120(9)	-0.00126(9)
H1	0.148(2)	0.377(2)	0.510(1)	0.035344(0)	0.025009(0)	0.016498(0)	-0.009657(0)	0.012357(0)	-0.005708(0)
H2A	0.285(2)	0.665(2)	0.513(1)	0.040589(0)	0.026529(0)	0.016972(0)	-0.010418(0)	0.012840(0)	-0.007706(0)
H2B	0.432(2)	0.752(1)	0.363(1)	0.017619(0)	0.015537(0)	0.020755(0)	-0.005003(0)	0.001692(0)	0.002186(0)
H11A	0.082(2)	0.059(1)	0.417(1)	0.038806(0)	0.023419(0)	0.027025(0)	-0.011814(0)	0.006789(0)	0.005552(0)
H11B	0.029(2)	0.185(1)	0.238(1)	0.035315(0)	0.028851(0)	0.033434(0)	-0.003658(0)	-0.018223(0)	0.000112(0)
H11C	0.271(1)	0.087(1)	0.274(1)	0.024003(0)	0.026666(0)	0.047171(0)	-0.000263(0)	0.013016(0)	-0.013606(0)

Table S14. Final positional parameters [Å] and anisotropic displacement parameters [Å^2] obtained after Hirshfeld-atom refinement with a cluster of charges HAR (+/-) using the blyp/cc-pVDZ level of theory for phurea.

Atom	x	y	z	U11	U22	U33	U12	U13	U23
O1	-0.06230(3)	0.0111(3)	0.10246(1)	0.00593(3)	0.01679(6)	0.01513(5)	0.00045(4)	0.00062(3)	-0.00050(5)
N1	0.38387(3)	0.1272(3)	0.17536(1)	0.00698(4)	0.01787(7)	0.01371(5)	0.00020(4)	0.00074(3)	-0.00436(5)
N2	0.34648(3)	-0.1434(3)	0.04591(1)	0.00814(4)	0.02132(8)	0.01718(6)	-0.00086(5)	0.00206(4)	-0.00760(6)
C1	0.20828(3)	-0.0020(3)	0.10779(1)	0.00615(4)	0.01283(6)	0.01114(5)	0.00008(4)	0.00068(3)	-0.00031(5)
C11	0.28344(4)	0.2825(3)	0.24812(1)	0.00986(5)	0.01286(7)	0.01213(5)	0.00001(5)	0.00183(4)	-0.00098(5)
C12	0.06743(5)	0.4647(3)	0.22716(2)	0.01726(7)	0.01405(8)	0.01627(7)	0.00414(6)	0.00171(6)	-0.00007(6)
C13	-0.01519(6)	0.6205(3)	0.30058(2)	0.02403(9)	0.01655(9)	0.02266(9)	0.00680(8)	0.00399(7)	-0.00334(8)
C14	0.11829(6)	0.5984(3)	0.39455(2)	0.02385(9)	0.0194(1)	0.01945(8)	0.00126(8)	0.00675(7)	-0.00589(7)
C15	0.33419(6)	0.4176(3)	0.41494(2)	0.0239(1)	0.0237(1)	0.01345(7)	0.00229(8)	0.00207(6)	-0.00448(7)
C16	0.41570(5)	0.2592(3)	0.34219(2)	0.01773(7)	0.0209(1)	0.01292(6)	0.00432(7)	-0.00067(5)	-0.00286(6)
H1	0.599(1)	0.100(2)	0.1737(5)	0.011990(0)	0.051452(0)	0.037529(0)	0.001531(0)	0.001465(0)	-0.019058(0)
H2A	0.563(1)	-0.159(2)	0.0532(5)	0.013090(0)	0.051864(0)	0.042333(0)	0.001621(0)	0.002169(0)	-0.020336(0)
H2B	0.229(1)	-0.257(1)	0.0011(5)	0.021400(0)	0.033932(0)	0.030796(0)	-0.004719(0)	-0.000190(0)	-0.013100(0)
H12	-0.033(1)	0.489(1)	0.1536(3)	0.043991(0)	0.032606(0)	0.024730(0)	0.012827(0)	-0.005920(0)	0.001512(0)
H13	-0.182(2)	0.764(1)	0.2831(5)	0.052731(0)	0.038142(0)	0.049558(0)	0.027576(0)	-0.002031(0)	-0.008683(0)
H14	0.055(2)	0.723(1)	0.4521(4)	0.050508(0)	0.041585(0)	0.034923(0)	0.007072(0)	0.013153(0)	-0.017076(0)
H15	0.439(1)	0.404(2)	0.4875(4)	0.054497(0)	0.051630(0)	0.020477(0)	0.008269(0)	-0.005657(0)	-0.007879(0)
H16	0.583(1)	0.116(2)	0.3563(4)	0.039165(0)	0.045645(0)	0.032783(0)	0.022216(0)	-0.011187(0)	-0.008253(0)

Table S15. Final positional parameters [Å] and anisotropic displacement parameters [Å^2] obtained after Hirshfeld-atom refinement using the blyp/cc-pVDZ level of theory for phurea.

Atom	x	y	z	U11	U22	U33	U12	U13	U23
O1	-0.06222(3)	0.0111(3)	0.10246(1)	0.00587(3)	0.01685(6)	0.01513(5)	0.00045(4)	0.00062(3)	-0.00061(5)
N1	0.38391(3)	0.1273(3)	0.17536(1)	0.00706(4)	0.01780(7)	0.01365(5)	0.00018(4)	0.00073(3)	-0.00432(5)
N2	0.34652(3)	-0.1434(3)	0.04591(1)	0.00822(4)	0.02124(8)	0.01714(6)	-0.00084(5)	0.00208(4)	-0.00754(6)
C1	0.20831(3)	-0.0020(3)	0.10779(1)	0.00610(4)	0.01284(6)	0.01116(5)	0.00008(4)	0.00068(3)	-0.00027(5)
C11	0.28344(4)	0.2825(3)	0.24812(1)	0.00984(5)	0.01285(7)	0.01213(5)	0.00002(5)	0.00183(4)	-0.00097(5)
C12	0.06745(5)	0.4647(3)	0.22717(2)	0.01725(7)	0.01406(8)	0.01626(7)	0.00414(6)	0.00171(6)	-0.00007(6)
C13	-0.01520(6)	0.6205(3)	0.30058(2)	0.02403(9)	0.01655(9)	0.02262(9)	0.00684(8)	0.00397(7)	-0.00334(8)
C14	0.11834(6)	0.5984(3)	0.39456(2)	0.02381(9)	0.0194(1)	0.01945(8)	0.00125(8)	0.00673(7)	-0.00587(7)
C15	0.33419(6)	0.4176(3)	0.41494(2)	0.0239(1)	0.0237(1)	0.01347(7)	0.00227(8)	0.00210(6)	-0.00450(7)
C16	0.41571(5)	0.2592(3)	0.34218(2)	0.01772(7)	0.0209(1)	0.01292(6)	0.00428(7)	-0.00066(5)	-0.00287(6)
H1	0.597(1)	0.099(2)	0.1740(5)	0.012010(0)	0.051098(0)	0.037286(0)	0.001739(0)	0.001368(0)	-0.018751(0)
H2A	0.559(1)	-0.160(2)	0.0531(4)	0.013143(0)	0.051363(0)	0.042057(0)	0.001753(0)	0.002145(0)	-0.019954(0)
H2B	0.229(1)	-0.255(1)	0.0015(5)	0.021376(0)	0.033889(0)	0.030766(0)	-0.004654(0)	-0.000215(0)	-0.013026(0)
H12	-0.037(1)	0.488(1)	0.1531(3)	0.043751(0)	0.032895(0)	0.024915(0)	0.013022(0)	-0.006143(0)	0.001300(0)
H13	-0.183(2)	0.765(1)	0.2829(5)	0.052915(0)	0.038234(0)	0.049561(0)	0.027695(0)	-0.002074(0)	-0.008711(0)
H14	0.056(2)	0.722(1)	0.4526(4)	0.050531(0)	0.041655(0)	0.034740(0)	0.007032(0)	0.013110(0)	-0.017044(0)
H15	0.440(1)	0.404(2)	0.4874(4)	0.054389(0)	0.051710(0)	0.020547(0)	0.008346(0)	-0.005747(0)	-0.007949(0)
H16	0.585(1)	0.116(2)	0.3561(4)	0.039018(0)	0.045753(0)	0.032804(0)	0.022204(0)	-0.011153(0)	-0.008326(0)

Table S16. Final positional parameters [Å] and anisotropic displacement parameters [Å^2] obtained after Hirshfeld-atom refinement with a cluster of charges HAR (+/-) using the blyp/cc-pVTZ level of theory for phurea.

Atom	x	y	z	U11	U22	U33	U12	U13	U23
O1	-0.06235(3)	0.0114(2)	0.10247(1)	0.00587(3)	0.01684(6)	0.01521(5)	0.00047(4)	0.00063(3)	-0.00047(4)
N1	0.38385(3)	0.1275(2)	0.17536(1)	0.00691(4)	0.01787(7)	0.01371(5)	0.00019(4)	0.00073(3)	-0.00445(5)
N2	0.34648(3)	-0.1431(2)	0.04591(1)	0.00807(4)	0.02137(8)	0.01724(6)	-0.00086(5)	0.00207(4)	-0.00774(6)
C1	0.20830(3)	-0.0017(2)	0.10779(1)	0.00602(4)	0.01280(6)	0.01109(5)	0.00009(4)	0.00067(3)	-0.00038(5)
C11	0.28345(4)	0.2828(2)	0.24812(1)	0.00978(5)	0.01279(7)	0.01203(5)	0.00006(4)	0.00180(4)	-0.00097(5)
C12	0.06740(5)	0.4650(2)	0.22716(2)	0.01726(7)	0.01401(8)	0.01612(7)	0.00419(5)	0.00170(5)	-0.00010(6)
C13	-0.01520(6)	0.6208(2)	0.30058(2)	0.02397(9)	0.01657(9)	0.02253(9)	0.00689(8)	0.00396(7)	-0.00335(8)
C14	0.11831(6)	0.5987(3)	0.39456(2)	0.02383(9)	0.0193(1)	0.01935(8)	0.00133(8)	0.00669(7)	-0.00594(7)
C15	0.33421(6)	0.4178(2)	0.41494(2)	0.02392(9)	0.0237(1)	0.01337(7)	0.00234(8)	0.00205(6)	-0.00449(7)
C16	0.41572(5)	0.2594(2)	0.34218(2)	0.01769(7)	0.02085(9)	0.01279(6)	0.00439(6)	-0.00069(5)	-0.00289(6)
H1	0.600(1)	0.101(2)	0.1740(5)	0.011896(0)	0.051618(0)	0.037611(0)	0.001444(0)	0.001459(0)	-0.019235(0)
H2A	0.565(1)	-0.159(2)	0.0533(4)	0.013022(0)	0.052331(0)	0.042592(0)	0.001662(0)	0.002131(0)	-0.020735(0)
H2B	0.229(1)	-0.258(1)	0.0005(4)	0.021417(0)	0.034025(0)	0.030827(0)	-0.004675(0)	-0.000240(0)	-0.013262(0)
H12	-0.034(1)	0.489(1)	0.1536(3)	0.044062(0)	0.032642(0)	0.024697(0)	0.012910(0)	-0.006058(0)	0.001446(0)
H13	-0.185(1)	0.763(1)	0.2833(5)	0.052294(0)	0.038784(0)	0.049673(0)	0.027827(0)	-0.002294(0)	-0.009066(0)
H14	0.055(2)	0.723(1)	0.4525(4)	0.050525(0)	0.041783(0)	0.034782(0)	0.007178(0)	0.013120(0)	-0.017098(0)
H15	0.442(1)	0.402(1)	0.4880(4)	0.054720(0)	0.051725(0)	0.020488(0)	0.008509(0)	-0.005939(0)	-0.007770(0)
H16	0.584(1)	0.115(1)	0.3562(4)	0.039269(0)	0.045687(0)	0.032890(0)	0.022360(0)	-0.011358(0)	-0.008374(0)

Table S17. Final positional parameters [Å] and anisotropic displacement parameters [Å^2] obtained after Hirshfeld-atom refinement using the blyp/cc-pVTZ level of theory for phurea.

Atom	x	y	z	U11	U22	U33	U12	U13	U23
O1	-0.06226(3)	0.0114(2)	0.10247(1)	0.00580(3)	0.01689(6)	0.01518(5)	0.00047(4)	0.00063(3)	-0.00059(4)
N1	0.38388(3)	0.1276(2)	0.17536(1)	0.00700(4)	0.01781(7)	0.01365(5)	0.00017(4)	0.00072(3)	-0.00441(5)
N2	0.34652(3)	-0.1431(2)	0.04591(1)	0.00817(4)	0.02130(8)	0.01720(6)	-0.00083(5)	0.00208(4)	-0.00767(6)
C1	0.20833(3)	-0.0017(2)	0.10779(1)	0.00597(4)	0.01282(6)	0.01111(5)	0.00008(4)	0.00066(3)	-0.00034(5)
C11	0.28345(4)	0.2828(2)	0.24812(1)	0.00978(5)	0.01279(7)	0.01204(5)	0.00006(4)	0.00180(4)	-0.00096(5)
C12	0.06743(5)	0.4651(2)	0.22716(2)	0.01725(7)	0.01402(8)	0.01612(7)	0.00420(6)	0.00170(5)	-0.00011(6)
C13	-0.01521(6)	0.6208(2)	0.30058(2)	0.02399(9)	0.01658(9)	0.02250(9)	0.00694(8)	0.00394(7)	-0.00336(8)
C14	0.11836(6)	0.5988(3)	0.39457(2)	0.02380(9)	0.0193(1)	0.01935(8)	0.00133(8)	0.00667(7)	-0.00592(7)
C15	0.33421(6)	0.4179(2)	0.41494(2)	0.02391(9)	0.0237(1)	0.01339(7)	0.00232(8)	0.00207(6)	-0.00450(7)
C16	0.41573(5)	0.2595(2)	0.34218(2)	0.01769(7)	0.0209(1)	0.01279(6)	0.00435(7)	-0.00069(5)	-0.00289(6)
H1	0.598(1)	0.100(2)	0.1745(4)	0.011911(0)	0.051360(0)	0.037363(0)	0.001720(0)	0.001254(0)	-0.018941(0)
H2A	0.560(1)	-0.160(2)	0.0532(4)	0.013077(0)	0.051715(0)	0.042237(0)	0.001834(0)	0.002039(0)	-0.020250(0)
H2B	0.229(1)	-0.257(1)	0.0010(4)	0.021393(0)	0.033940(0)	0.030830(0)	-0.004633(0)	-0.000276(0)	-0.013185(0)
H12	-0.037(1)	0.488(1)	0.1531(3)	0.043767(0)	0.032879(0)	0.024824(0)	0.013023(0)	-0.006228(0)	0.001267(0)
H13	-0.186(1)	0.763(1)	0.2832(5)	0.052503(0)	0.038720(0)	0.049600(0)	0.027863(0)	-0.002269(0)	-0.009006(0)
H14	0.056(2)	0.723(1)	0.4528(4)	0.050606(0)	0.041740(0)	0.034678(0)	0.007106(0)	0.013047(0)	-0.017094(0)
H15	0.442(1)	0.402(2)	0.4878(4)	0.054637(0)	0.051757(0)	0.020498(0)	0.008532(0)	-0.005958(0)	-0.007787(0)
H16	0.585(1)	0.116(1)	0.3561(4)	0.039050(0)	0.045872(0)	0.032872(0)	0.022312(0)	-0.011316(0)	-0.008443(0)

Table S18. Final positional parameters [Å] and anisotropic displacement parameters [Å^2] obtained after Hirshfeld-atom refinement with a cluster of charges HAR (+/-) using the blyp/cc-pVDZ level of theory for dphurea.

Atom	x	y	z	U11	U22	U33	U12	U13	U23
O1	0.37631(1)	0.27781(2)	0.40480(7)	0.00660(4)	0.03056(7)	0.01507(5)	-0.00049(3)	0.00145(3)	0.00084(5)
N1	0.59176(2)	0.21698(2)	0.49121(7)	0.00814(4)	0.02045(6)	0.01423(5)	0.00020(3)	0.00170(3)	0.00192(4)
N2	0.59533(2)	0.29951(2)	0.31032(7)	0.00779(4)	0.02003(6)	0.01324(5)	0.00048(3)	0.00205(3)	0.00049(4)
C1	0.51205(2)	0.26614(2)	0.40308(7)	0.00672(4)	0.01685(5)	0.01263(5)	-0.00087(3)	0.00137(4)	-0.00087(4)
C11	0.53216(2)	0.17590(2)	0.59628(7)	0.01044(5)	0.01573(5)	0.01422(6)	-0.00202(4)	0.00121(4)	0.00095(4)
C12	0.42415(2)	0.24707(2)	0.65356(7)	0.01309(6)	0.01977(7)	0.01395(6)	-0.00155(5)	0.00286(5)	-0.00048(5)
C13	0.37245(3)	0.20467(3)	0.75887(7)	0.02062(9)	0.0289(1)	0.01492(8)	-0.00426(7)	0.00550(6)	0.00010(6)
C14	0.43033(3)	0.09362(3)	0.80925(7)	0.0282(1)	0.0326(1)	0.0189(1)	-0.00739(9)	0.00400(8)	0.00801(8)
C15	0.54003(3)	0.02405(3)	0.75270(7)	0.0282(1)	0.0242(1)	0.0262(1)	-0.00334(8)	0.00156(9)	0.01155(8)
C16	0.58950(3)	0.06399(2)	0.64590(7)	0.01903(8)	0.01747(7)	0.02325(9)	-0.00017(5)	0.00180(6)	0.00511(6)
C21	0.53687(2)	0.34544(2)	0.20633(7)	0.01014(5)	0.01471(5)	0.01337(5)	-0.00004(3)	0.00154(4)	-0.00061(4)
C22	0.41586(2)	0.42922(2)	0.20170(7)	0.01382(6)	0.01665(6)	0.01707(7)	0.00279(4)	0.00068(5)	-0.00031(5)
C23	0.36298(3)	0.47121(2)	0.09638(7)	0.01875(8)	0.01661(6)	0.02080(8)	0.00177(5)	-0.00215(6)	0.00294(6)
C24	0.43088(3)	0.43239(2)	-0.00433(7)	0.0256(1)	0.01992(8)	0.01717(8)	-0.00063(6)	-0.00243(7)	0.00364(6)
C25	0.55398(3)	0.35188(3)	0.00083(7)	0.0274(1)	0.0267(1)	0.01390(8)	0.00373(7)	0.00293(7)	0.00093(7)
C26	0.60697(3)	0.30813(2)	0.10538(7)	0.01863(7)	0.02303(8)	0.01418(7)	0.00482(6)	0.00396(6)	-0.00005(6)
H1	0.7009(5)	0.2063(6)	0.4790(5)	0.013946(0)	0.049747(0)	0.031697(0)	0.005287(0)	0.003401(0)	0.009238(0)
H2	0.6998(6)	0.2711(6)	0.3107(5)	0.014974(0)	0.049120(0)	0.031796(0)	0.008217(0)	0.005444(0)	0.008953(0)
H12	0.3845(6)	0.3374(6)	0.6168(5)	0.036028(0)	0.033942(0)	0.030420(0)	0.009406(0)	0.007168(0)	0.004903(0)
H13	0.2872(7)	0.2600(6)	0.8019(5)	0.042135(0)	0.060712(0)	0.033263(0)	0.011065(0)	0.017990(0)	0.003511(0)
H14	0.3936(7)	0.0610(7)	0.8936(6)	0.051027(0)	0.054688(0)	0.026444(0)	-0.009326(0)	0.009572(0)	0.012378(0)
H15	0.5891(8)	-0.0654(6)	0.7903(6)	0.059781(0)	0.036785(0)	0.036314(0)	0.005020(0)	-0.001327(0)	0.014310(0)
H16	0.6739(7)	0.0090(6)	0.6001(5)	0.043397(0)	0.040777(0)	0.035176(0)	0.016792(0)	0.007169(0)	0.006186(0)
H22	0.3637(6)	0.4587(6)	0.2794(4)	0.031377(0)	0.038691(0)	0.024422(0)	0.011452(0)	0.004541(0)	-0.001975(0)
H23	0.2667(7)	0.5349(6)	0.0939(4)	0.037168(0)	0.047240(0)	0.036652(0)	0.019496(0)	-0.004061(0)	0.004873(0)
H24	0.3870(7)	0.4632(6)	-0.0871(5)	0.048823(0)	0.044602(0)	0.023214(0)	0.003588(0)	-0.008677(0)	0.005093(0)
H25	0.6073(8)	0.3158(7)	-0.0778(6)	0.055672(0)	0.050175(0)	0.022403(0)	0.012061(0)	0.010267(0)	-0.001771(0)
H26	0.7001(6)	0.2427(6)	0.1097(5)	0.036676(0)	0.050874(0)	0.032170(0)	0.021431(0)	0.009397(0)	0.004102(0)

Table S19. Final positional parameters [Å] and anisotropic displacement parameters [Å^2] obtained after Hirshfeld-atom refinement using the blyp/cc-pVDZ level of theory for dphurea.

Atom	x	y	z	U11	U22	U33	U12	U13	U23
O1	0.37634(1)	0.27781(2)	0.40479(7)	0.00657(4)	0.03065(7)	0.01504(5)	-0.00046(4)	0.00146(3)	0.00091(5)
N1	0.59178(2)	0.21698(2)	0.49120(7)	0.00820(4)	0.02039(6)	0.01421(5)	0.00019(3)	0.00168(3)	0.00190(4)
N2	0.59534(2)	0.29951(2)	0.31030(7)	0.00785(4)	0.01998(6)	0.01321(5)	0.00045(3)	0.00205(3)	0.00048(4)
C1	0.51206(2)	0.26614(2)	0.40306(7)	0.00668(4)	0.01685(5)	0.01267(5)	-0.00085(3)	0.00137(4)	-0.00089(4)
C11	0.53215(2)	0.17591(2)	0.59628(7)	0.01042(5)	0.01573(5)	0.01424(6)	-0.00203(4)	0.00120(4)	0.00094(5)
C12	0.42415(2)	0.24706(2)	0.65355(7)	0.01309(6)	0.01976(7)	0.01394(6)	-0.00155(5)	0.00285(5)	-0.00047(5)
C13	0.37245(3)	0.20468(3)	0.75886(7)	0.02064(9)	0.0289(1)	0.01491(8)	-0.00428(7)	0.00551(6)	0.00008(7)
C14	0.43032(4)	0.09363(3)	0.80923(7)	0.0282(1)	0.0326(1)	0.0189(1)	-0.00741(9)	0.00399(8)	0.00801(9)
C15	0.54000(3)	0.02405(3)	0.75268(7)	0.0283(1)	0.0243(1)	0.0262(1)	-0.00335(8)	0.00156(9)	0.01153(9)
C16	0.58951(3)	0.06399(2)	0.64588(7)	0.01902(8)	0.01746(7)	0.02325(9)	-0.00019(5)	0.00179(6)	0.00511(6)
C21	0.53686(2)	0.34544(2)	0.20631(7)	0.01012(5)	0.01471(5)	0.01338(6)	-0.00004(4)	0.00154(4)	-0.00061(4)
C22	0.41587(2)	0.42921(2)	0.20168(7)	0.01381(6)	0.01667(6)	0.01706(7)	0.00279(4)	0.00068(5)	-0.00031(5)
C23	0.36297(3)	0.47121(2)	0.09637(7)	0.01877(8)	0.01660(6)	0.02078(8)	0.00174(5)	-0.00216(6)	0.00295(6)
C24	0.43087(3)	0.43239(2)	-0.00434(7)	0.0256(1)	0.01992(8)	0.01717(8)	-0.00063(6)	-0.00242(7)	0.00364(6)
C25	0.55399(3)	0.35188(3)	0.00081(7)	0.0274(1)	0.0267(1)	0.01392(8)	0.00372(8)	0.00293(7)	0.00093(7)
C26	0.60697(3)	0.30813(2)	0.10537(7)	0.01865(8)	0.02301(8)	0.01415(7)	0.00477(6)	0.00396(6)	-0.00007(6)
H1	0.6987(5)	0.2059(6)	0.4792(5)	0.014026(0)	0.049379(0)	0.031545(0)	0.005377(0)	0.003453(0)	0.009043(0)
H2	0.6984(6)	0.2712(6)	0.3098(5)	0.015080(0)	0.048848(0)	0.031692(0)	0.008322(0)	0.005563(0)	0.008787(0)
H12	0.3844(6)	0.3373(6)	0.6165(5)	0.035966(0)	0.034079(0)	0.030496(0)	0.009475(0)	0.007314(0)	0.005083(0)
H13	0.2884(7)	0.2601(6)	0.8017(5)	0.042228(0)	0.060466(0)	0.033355(0)	0.011080(0)	0.018138(0)	0.003649(0)
H14	0.3935(7)	0.0613(7)	0.8939(6)	0.051075(0)	0.054532(0)	0.026463(0)	-0.009357(0)	0.009655(0)	0.012349(0)
H15	0.5891(8)	-0.0658(6)	0.7898(6)	0.060033(0)	0.036407(0)	0.036209(0)	0.004958(0)	-0.001371(0)	0.014039(0)
H16	0.6737(7)	0.0096(6)	0.6006(5)	0.043328(0)	0.040686(0)	0.035036(0)	0.016673(0)	0.007093(0)	0.006048(0)
H22	0.3637(6)	0.4577(6)	0.2798(5)	0.031174(0)	0.038956(0)	0.024419(0)	0.011373(0)	0.004677(0)	-0.001762(0)
H23	0.2665(7)	0.5344(6)	0.0941(4)	0.036938(0)	0.047447(0)	0.036735(0)	0.019442(0)	-0.003955(0)	0.004990(0)
H24	0.3872(7)	0.4632(6)	-0.0867(5)	0.048744(0)	0.044325(0)	0.023261(0)	0.003516(0)	-0.008690(0)	0.005099(0)
H25	0.6068(8)	0.3160(7)	-0.0777(6)	0.055729(0)	0.049851(0)	0.022321(0)	0.011987(0)	0.010104(0)	-0.001836(0)
H26	0.7000(6)	0.2433(6)	0.1098(5)	0.036627(0)	0.050857(0)	0.032067(0)	0.021386(0)	0.009279(0)	0.004008(0)

Table S20. Final positional parameters [Å] and anisotropic displacement parameters [Å^2] obtained after Hirshfeld-atom refinement with a cluster of charges HAR (+/-) using the blyp/cc-pVTZ level of theory for dphurea.

Atom	x	y	z	U11	U22	U33	U12	U13	U23
O1	0.37628(1)	0.27780(2)	0.40473(6)	0.00654(3)	0.03057(6)	0.01514(5)	-0.00048(3)	0.00145(3)	0.00081(5)
N1	0.59176(2)	0.21699(2)	0.49113(6)	0.00805(4)	0.02049(5)	0.01419(5)	0.00021(3)	0.00169(3)	0.00197(4)
N2	0.59534(2)	0.29952(2)	0.31025(6)	0.00771(4)	0.02006(5)	0.01317(5)	0.00051(3)	0.00205(3)	0.00052(4)
C1	0.51207(2)	0.26614(2)	0.40301(6)	0.00660(4)	0.01683(5)	0.01255(5)	-0.00085(3)	0.00136(3)	-0.00084(4)
C11	0.53216(2)	0.17589(2)	0.59622(6)	0.01038(5)	0.01562(5)	0.01415(5)	-0.00197(4)	0.00124(4)	0.00095(4)
C12	0.42415(2)	0.24708(2)	0.65349(6)	0.01301(5)	0.01969(6)	0.01385(6)	-0.00150(4)	0.00289(4)	-0.00045(5)
C13	0.37244(3)	0.20468(3)	0.75880(6)	0.02059(8)	0.02884(9)	0.01486(7)	-0.00419(7)	0.00555(6)	0.00015(6)
C14	0.43032(3)	0.09361(3)	0.80919(7)	0.0282(1)	0.0324(1)	0.01881(9)	-0.00725(8)	0.00409(7)	0.00801(8)
C15	0.54001(3)	0.02402(3)	0.75261(7)	0.0282(1)	0.02417(9)	0.0262(1)	-0.00328(7)	0.00160(8)	0.01161(8)
C16	0.58952(2)	0.06398(2)	0.64582(6)	0.01897(8)	0.01736(7)	0.02318(9)	-0.00011(5)	0.00184(6)	0.00516(6)
C21	0.53689(2)	0.34544(2)	0.20625(6)	0.01006(4)	0.01465(5)	0.01325(5)	-0.00001(3)	0.00155(4)	-0.00061(4)
C22	0.41587(2)	0.42922(2)	0.20163(6)	0.01376(6)	0.01662(6)	0.01692(6)	0.00286(4)	0.00066(4)	-0.00028(5)
C23	0.36299(2)	0.47122(2)	0.09629(6)	0.01867(7)	0.01657(6)	0.02068(8)	0.00185(5)	-0.00214(6)	0.00294(5)
C24	0.43087(3)	0.43240(2)	-0.00441(6)	0.02559(9)	0.01988(7)	0.01704(8)	-0.00055(6)	-0.00243(6)	0.00365(6)
C25	0.55399(3)	0.35188(3)	0.00075(6)	0.0274(1)	0.02666(9)	0.01375(7)	0.00382(7)	0.00290(6)	0.00093(6)
C26	0.60697(2)	0.30812(2)	0.10532(6)	0.01857(7)	0.02296(7)	0.01407(6)	0.00490(5)	0.00395(5)	-0.00006(5)
H1	0.7015(5)	0.2064(6)	0.4788(5)	0.014480(0)	0.048770(0)	0.031630(0)	0.006600(0)	0.004060(0)	0.009060(0)
H2	0.7000(5)	0.2705(6)	0.3105(5)	0.015420(0)	0.048280(0)	0.031810(0)	0.009020(0)	0.005790(0)	0.008810(0)
H12	0.3845(5)	0.3374(5)	0.6164(5)	0.036370(0)	0.031810(0)	0.030560(0)	0.008460(0)	0.007420(0)	0.004290(0)
H13	0.2869(7)	0.2602(6)	0.8017(5)	0.042510(0)	0.058190(0)	0.032750(0)	0.009680(0)	0.018220(0)	0.002930(0)
H14	0.3931(7)	0.0600(7)	0.8938(5)	0.051810(0)	0.053780(0)	0.025640(0)	-0.008140(0)	0.009180(0)	0.012040(0)
H15	0.5890(8)	-0.0643(6)	0.7914(5)	0.058340(0)	0.037290(0)	0.036410(0)	0.005090(0)	-0.001180(0)	0.015080(0)
H16	0.6739(6)	0.0091(5)	0.6003(5)	0.041260(0)	0.041170(0)	0.035580(0)	0.016570(0)	0.007030(0)	0.006720(0)
H22	0.3630(6)	0.4590(5)	0.2803(4)	0.031860(0)	0.036480(0)	0.024880(0)	0.011290(0)	0.004410(0)	-0.002460(0)
H23	0.2659(6)	0.5353(5)	0.0938(4)	0.038030(0)	0.043910(0)	0.036740(0)	0.018850(0)	-0.004270(0)	0.004840(0)
H24	0.3878(7)	0.4633(6)	-0.0873(5)	0.049390(0)	0.045260(0)	0.022620(0)	0.003720(0)	-0.008120(0)	0.005030(0)
H25	0.6074(7)	0.3164(6)	-0.0778(5)	0.052930(0)	0.053030(0)	0.021950(0)	0.011090(0)	0.010590(0)	0.000020(0)
H26	0.7008(5)	0.2425(5)	0.1097(5)	0.035100(0)	0.051160(0)	0.031870(0)	0.020930(0)	0.008520(0)	0.004260(0)

Table S21. Final positional parameters [Å] and anisotropic displacement parameters [Å^2] obtained after Hirshfeld-atom refinement using the blyp/cc-pVTZ level of theory for dphurea.

Atom	x	y	z	U11	U22	U33	U12	U13	U23
O1	0.37632(1)	0.27781(2)	0.40474(6)	0.00651(3)	0.03064(7)	0.01509(5)	-0.00046(3)	0.00146(3)	0.00088(5)
N1	0.59177(2)	0.21698(2)	0.49114(6)	0.00812(4)	0.02042(6)	0.01416(5)	0.00019(3)	0.00168(3)	0.00196(4)
N2	0.59535(2)	0.29952(2)	0.31026(6)	0.00778(4)	0.02002(5)	0.01314(5)	0.00047(3)	0.00206(3)	0.00051(4)
C1	0.51208(2)	0.26614(2)	0.40301(6)	0.00656(4)	0.01683(5)	0.01259(5)	-0.00084(3)	0.00136(4)	-0.00086(4)
C11	0.53215(2)	0.17590(2)	0.59623(6)	0.01036(5)	0.01563(5)	0.01417(6)	-0.00198(4)	0.00123(4)	0.00095(4)
C12	0.42415(2)	0.24708(2)	0.65350(6)	0.01301(5)	0.01970(6)	0.01384(6)	-0.00150(5)	0.00289(4)	-0.00044(5)
C13	0.37244(3)	0.20468(3)	0.75881(6)	0.02062(8)	0.02882(9)	0.01486(7)	-0.00420(7)	0.00556(6)	0.00013(6)
C14	0.43031(3)	0.09362(3)	0.80919(7)	0.0282(1)	0.0325(1)	0.01882(9)	-0.00726(8)	0.00408(7)	0.00802(8)
C15	0.53998(3)	0.02401(3)	0.75261(7)	0.0282(1)	0.02418(9)	0.0261(1)	-0.00330(7)	0.00160(8)	0.01158(8)
C16	0.58953(3)	0.06398(2)	0.64583(7)	0.01896(8)	0.01736(7)	0.02318(9)	-0.00013(5)	0.00182(6)	0.00515(6)
C21	0.53688(2)	0.34544(2)	0.20626(6)	0.01004(4)	0.01464(5)	0.01326(5)	-0.00001(3)	0.00155(4)	-0.00061(4)
C22	0.41588(2)	0.42922(2)	0.20164(6)	0.01375(6)	0.01663(6)	0.01692(7)	0.00286(4)	0.00067(5)	-0.00028(5)
C23	0.36298(2)	0.47123(2)	0.09630(6)	0.01870(7)	0.01657(6)	0.02066(8)	0.00182(5)	-0.00215(6)	0.00295(6)
C24	0.43086(3)	0.43240(2)	-0.00440(6)	0.02556(9)	0.01988(8)	0.01705(8)	-0.00055(6)	-0.00243(6)	0.00365(6)
C25	0.55400(3)	0.35189(3)	0.00075(6)	0.0273(1)	0.02666(9)	0.01378(7)	0.00381(7)	0.00290(6)	0.00094(6)
C26	0.60698(2)	0.30812(2)	0.10533(6)	0.01859(7)	0.02294(7)	0.01405(7)	0.00485(5)	0.00394(5)	-0.00007(5)
H1	0.6996(5)	0.2061(6)	0.4791(5)	0.013876(0)	0.049861(0)	0.031493(0)	0.005342(0)	0.003397(0)	0.009210(0)
H2	0.6985(5)	0.2706(5)	0.3096(5)	0.015048(0)	0.049011(0)	0.031642(0)	0.008478(0)	0.005591(0)	0.008881(0)
H12	0.3845(5)	0.3373(5)	0.6162(5)	0.035906(0)	0.033476(0)	0.030337(0)	0.009245(0)	0.007249(0)	0.005053(0)
H13	0.2882(7)	0.2604(6)	0.8016(5)	0.042240(0)	0.059357(0)	0.033243(0)	0.011012(0)	0.018085(0)	0.003537(0)
H14	0.3933(7)	0.0603(7)	0.8940(5)	0.050971(0)	0.053936(0)	0.026514(0)	-0.009036(0)	0.009749(0)	0.012458(0)
H15	0.5889(8)	-0.0650(6)	0.7909(5)	0.059550(0)	0.036889(0)	0.036181(0)	0.005496(0)	-0.001120(0)	0.014406(0)
H16	0.6738(7)	0.0097(5)	0.6007(5)	0.042996(0)	0.041087(0)	0.035107(0)	0.017007(0)	0.007281(0)	0.006316(0)
H22	0.3628(6)	0.4581(5)	0.2806(4)	0.031087(0)	0.038754(0)	0.024348(0)	0.011342(0)	0.004757(0)	-0.001717(0)
H23	0.2659(6)	0.5349(5)	0.0940(4)	0.036896(0)	0.047459(0)	0.036664(0)	0.019561(0)	-0.003829(0)	0.005142(0)
H24	0.3880(7)	0.4635(6)	-0.0870(5)	0.048692(0)	0.044759(0)	0.023099(0)	0.003810(0)	-0.008527(0)	0.005231(0)
H25	0.6066(7)	0.3165(6)	-0.0778(5)	0.055446(0)	0.050286(0)	0.022177(0)	0.012143(0)	0.010073(0)	-0.001770(0)
H26	0.7005(6)	0.2430(5)	0.1096(5)	0.036481(0)	0.051161(0)	0.031997(0)	0.021558(0)	0.009287(0)	0.004082(0)