Electronic Supplementary Material (ESI) for CrystEngComm.


# Displacement Parameters from Density-Functional Theory and their Validation in the Experimental Charge Density of Tartaric Acid

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**Figure S3** Displacement ellipsoids and atom numbering for **1** at 100 K (90%). ADPs for H atoms were obtained from the SHADE server (A. Ø. Madsen. SHADE web server for estimation of hydrogen anisotropic displacement parameters. *J. Appl. Cryst.*, 2006, **39**, 757).

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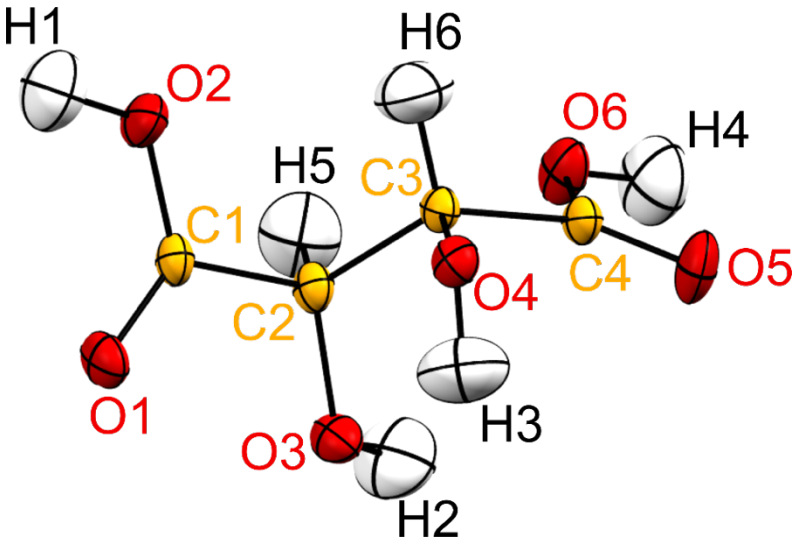



**Figure S1** Calculated displacement ellipsoids (90%) based on the harmonic approximation and atom numbering for **1** at 100 K.

**Table S1** ADPs for all atoms in **1** in the harmonic and in the quasi-harmonic approximation at 100 K (atom numbering according to Fig. S1).

Harmonic approximation

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| O1 | 0.01037 | 0.01326 | 0.005063 | –0.00025 | 0.002246 | –0.00164 |
| O2 | 0.009121 | 0.01485 | 0.007929 | –0.00117 | 0.00351 | 0.001918 |
| O3 | 0.007649 | 0.01294 | 0.007524 | –1.4E-05 | 0.002525 | –0.00212 |
| O4 | 0.008396 | 0.00843 | 0.006653 | 0.000852 | 0.002505 | –0.00063 |
| O5 | 0.017388 | 0.01156 | 0.008864 | –0.00108 | 0.006502 | 0.003125 |
| O6 | 0.015058 | 0.01282 | 0.006134 | 0.00242 | 0.0041 | 0.004064 |
| H1 | 0.020273 | 0.02332 | 0.016926 | –0.00157 | 0.00751 | 0.000822 |
| H2 | 0.019601 | 0.02846 | 0.018897 | 0.003479 | 0.00947 | –0.00292 |
| H3 | 0.014352 | 0.02352 | 0.023653 | 0.004677 | 0.001701 | 0.001917 |
| H4 | 0.02605 | 0.02516 | 0.013062 | 0.002194 | 0.007495 | 0.002656 |
| H5 | 0.02543 | 0.01655 | 0.018606 | 0.005367 | 0.004081 | 0.002247 |
| H6 | 0.011914 | 0.02423 | 0.019983 | 0.000326 | 0.002934 | 0.001594 |
| C1 | 0.008582 | 0.00745 | 0.005231 | –0.00073 | 0.002655 | –0.00045 |
| C2 | 0.008135 | 0.00761 | 0.005082 | –1.9E-05 | 0.002393 | –0.00051 |
| C3 | 0.006622 | 0.00819 | 0.004714 | –0.00031 | 0.001868 | –0.0002 |
| C4 | 0.007524 | 0.00957 | 0.004654 | –0.0004 | 0.001973 | 0.000519 |

Quasiharmonic approximation

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| O1 | 0.011445 | 0.014430 | 0.005261 | –0.000276 | 0.002399 | –0.001567 |
| O2 | 0.009930 | 0.016970 | 0.008307 | –0.001481 | 0.003712 | 0.002023 |
| O3 | 0.008335 | 0.014160 | 0.008005 | 0.000180 | 0.002675 | –0.002139 |
| O4 | 0.009167 | 0.009770 | 0.007051 | 0.000829 | 0.002720 | –0.000873 |
| O5 | 0.019697 | 0.013380 | 0.009277 | –0.000947 | 0.007135 | 0.003920 |
| O6 | 0.016416 | 0.014550 | 0.006369 | 0.002473 | 0.004346 | 0.004521 |
| H1 | 0.021215 | 0.025040 | 0.017209 | –0.001852 | 0.007821 | 0.001012 |
| H2 | 0.020461 | 0.029870 | 0.019682 | 0.003836 | 0.009681 | –0.003332 |
| H3 | 0.015149 | 0.024840 | 0.024701 | 0.004830 | 0.001870 | 0.001871 |
| H4 | 0.027362 | 0.026760 | 0.013170 | 0.002317 | 0.007600 | 0.002916 |
| H5 | 0.026437 | 0.017950 | 0.018991 | 0.005637 | 0.004133 | 0.002404 |
| H6 | 0.012587 | 0.026180 | 0.020296 | 0.000165 | 0.003031 | 0.001637 |
| C1 | 0.009401 | 0.008460 | 0.005434 | –0.000737 | 0.002834 | –0.000433 |
| C2 | 0.008825 | 0.008810 | 0.005279 | 0.000084 | 0.002535 | –0.000469 |
| C3 | 0.007274 | 0.009630 | 0.004917 | –0.000358 | 0.002041 | –0.000239 |
| C4 | 0.008359 | 0.011050 | 0.004874 | –0.000426 | 0.002192 | 0.000627 |

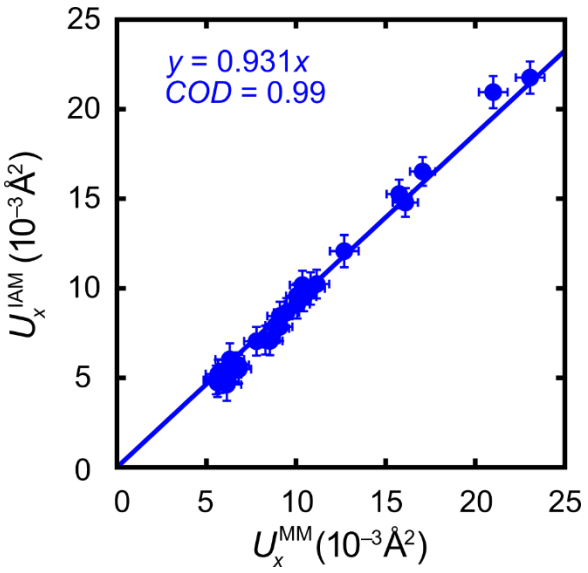



**Figure S2** Scatter plot of experimental main-axis components of displacement tensors from the independent atom model (IAM) versus experimental results from multipole refinement (MM) at 100 K for **1**. Horizontal and vertical lines correspond to 10 standard uncertainties of the experimental values.

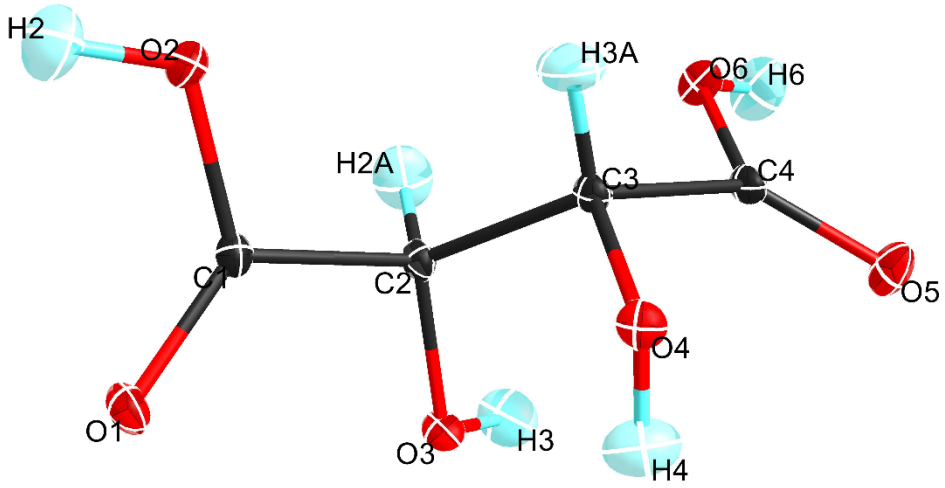



**Figure S3** Displacement ellipsoids and atom numbering for **1** at 100 K (90%). ADPs for H atoms were obtained from the SHADE server (A. Ø. Madsen. SHADE web server for estimation of hydrogen anisotropic displacement parameters. *J. Appl. Cryst.*, 2006, **39**, 757).

**Table S2** ADPs of all atoms in **1** at 100 K, H atoms with ADPs fixed to the values obtained from the SHADE server (atom numbering according to Fig. S3).

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| O1 | 0.01009(14) | 0.01437(16) | 0.00518(12) | -0.00036(13) | 0.00162(10) | -0.00159(14) |
| O2 | 0.00818(13) | 0.01546(17) | 0.00854(14) | -0.00176(12) | 0.00329(11) | 0.00177(13) |
| O3 | 0.00690(13) | 0.01397(17) | 0.00824(14) | -0.00023(12) | 0.00246(10) | -0.00226(13) |
| O4 | 0.00763(13) | 0.00848(13) | 0.00702(13) | 0.00145(11) | 0.00174(10) | -0.00040(12) |
| O5 | 0.01829(19) | 0.01317(17) | 0.00959(16) | -0.00053(14) | 0.00632(13) | 0.00596(17) |
| O6 | 0.01558(18) | 0.01423(17) | 0.00621(14) | 0.00311(13) | 0.00392(12) | 0.00515(15) |
| C1 | 0.00779(14) | 0.00854(15) | 0.00591(13) | -0.00093(11) | 0.00212(10) | -0.00043(12) |
| C2 | 0.00782(13) | 0.00785(13) | 0.00555(13) | -0.00001(11) | 0.00202(9) | -0.00053(12) |
| C3 | 0.00679(13) | 0.00817(14) | 0.00506(13) | -0.00006(11) | 0.00134(9) | -0.00014(11) |
| C4 | 0.00850(14) | 0.00984(15) | 0.00508(14) | -0.00031(12) | 0.00188(10) | 0.00106(13) |
| H2 | 0.02073 | 0.02073 | 0.02073 | 0.00000 | 0.00375 | 0.00000 |
| H2A | 0.03390 | 0.03390 | 0.03390 | 0.00000 | 0.00614 | 0.00000 |
| H3 | 0.01811 | 0.01811 | 0.01811 | 0.00000 | 0.00328 | 0.00000 |
| H3A | 0.01038 | 0.01038 | 0.01038 | 0.00000 | 0.00188 | 0.00000 |
| H4 | 0.01495 | 0.01495 | 0.01495 | 0.00000 | 0.00271 | 0.00000 |
| H6 | 0.03424 | 0.03424 | 0.03424 | 0.00000 | 0.00620 | 0.00000 |

**Table S3** Resolution & completeness statistics (cumulative and Friedel pairs averaged)

| θ | sinθ/λ | Complete | Expected | Measured | Missing |
|---|---|---|---|---|---|
| 20.82 | 0.500 | 1.000 | 328 | 328 | 0 |
| 23.01 | 0.550 | 1.000 | 437 | 437 | 0 |
| 25.24 | 0.600 | 1.000 | 554 | 554 | 0 |
| 27.51 | 0.650 | 1.000 | 697 | 697 | 0 |
| 29.84 | 0.700 | 1.000 | 864 | 864 | 0 |
| 32.21 | 0.750 | 1.000 | 1060 | 1060 | 0 |
| 34.65 | 0.800 | 1.000 | 1286 | 1286 | 0 |
| 37.17 | 0.850 | 1.000 | 1533 | 1533 | 0 |
| 39.77 | 0.900 | 1.000 | 1809 | 1809 | 0 |
| 42.47 | 0.950 | 1.000 | 2130 | 2130 | 0 |
| 45.29 | 1.000 | 1.000 | 2475 | 2475 | 0 |
| 48.27 | 1.050 | 1.000 | 2847 | 2847 | 0 |
| 51.43 | 1.100 | 0.998 | 3266 | 3261 | 5 |
| 54.52 | 1.146 | 0.978 | 3694 | 3611 | 83 |

The reported completeness refers to the actual *h,k,l* index range

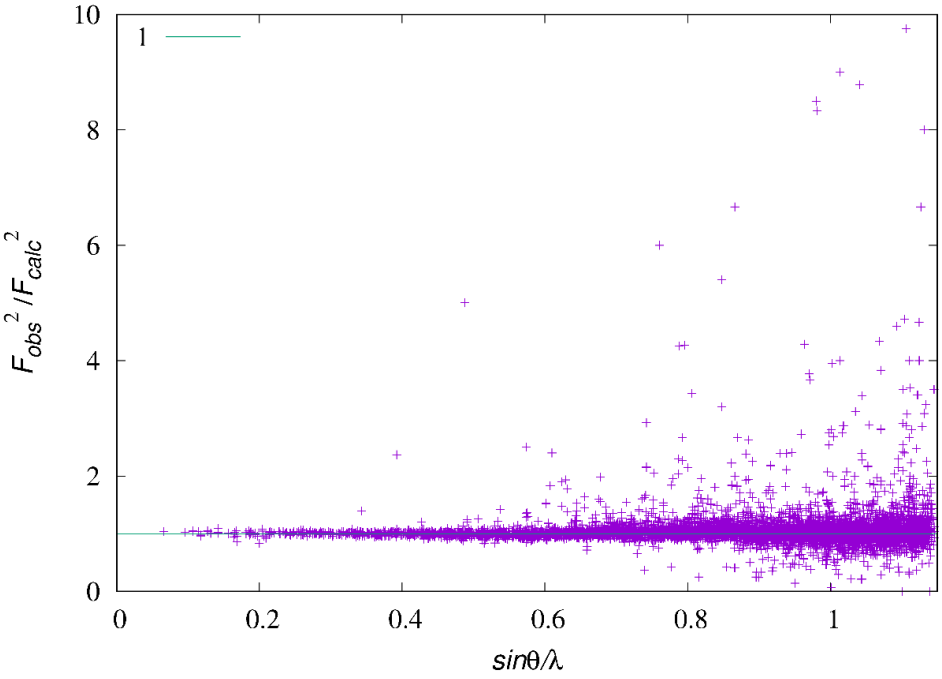
**Table S4** *R*-Value statistics as a function of resolution (in resolution shells).

| θ | sinθ/λ | # | *R*1 | w*R*2 | *S* | *R*σ | av(I/SigW) | av(I) | av(SigW) |
|---|---|---|---|---|---|---|---|---|---|
| 12.38 | 0.302 | 127 | 0.046 | 0.127 | 2.694 | 0.021 | 21.03 | 405.44 | 19.80 |
| 15.68 | 0.380 | 128 | 0.037 | 0.081 | 1.631 | 0.019 | 19.81 | 141.34 | 6.67 |
| 18.02 | 0.435 | 135 | 0.025 | 0.083 | 1.599 | 0.019 | 18.96 | 124.41 | 6.07 |
| 19.90 | 0.479 | 116 | 0.025 | 0.097 | 1.790 | 0.020 | 18.36 | 93.69 | 4.74 |
| 21.51 | 0.516 | 124 | 0.030 | 0.100 | 1.760 | 0.023 | 17.08 | 60.37 | 3.15 |
| 22.94 | 0.548 | 145 | 0.034 | 0.095 | 1.607 | 0.027 | 16.53 | 44.67 | 2.46 |
| 24.22 | 0.577 | 118 | 0.028 | 0.078 | 1.291 | 0.026 | 16.09 | 40.87 | 2.22 |
| 25.40 | 0.603 | 128 | 0.027 | 0.083 | 1.388 | 0.025 | 16.22 | 33.26 | 1.80 |
| 26.49 | 0.628 | 137 | 0.024 | 0.064 | 1.083 | 0.022 | 16.46 | 33.68 | 1.74 |
| 27.52 | 0.650 | 113 | 0.022 | 0.066 | 1.056 | 0.025 | 15.34 | 22.74 | 1.23 |
| 28.49 | 0.671 | 126 | 0.020 | 0.057 | 0.997 | 0.023 | 17.07 | 32.41 | 1.70 |
| 29.41 | 0.691 | 140 | 0.023 | 0.065 | 1.068 | 0.028 | 15.91 | 21.76 | 1.21 |
| 30.28 | 0.709 | 118 | 0.024 | 0.069 | 1.045 | 0.034 | 14.49 | 19.92 | 1.18 |
| 31.12 | 0.727 | 124 | 0.022 | 0.061 | 0.889 | 0.038 | 13.89 | 23.87 | 1.47 |
| 31.93 | 0.744 | 112 | 0.023 | 0.062 | 0.870 | 0.038 | 13.09 | 22.85 | 1.42 |
| 32.71 | 0.760 | 132 | 0.024 | 0.062 | 0.896 | 0.040 | 13.77 | 22.55 | 1.43 |
| 33.46 | 0.776 | 116 | 0.022 | 0.057 | 0.831 | 0.040 | 14.03 | 21.40 | 1.35 |
| 34.20 | 0.791 | 123 | 0.025 | 0.062 | 0.821 | 0.047 | 12.38 | 17.89 | 1.22 |
| 34.91 | 0.805 | 129 | 0.027 | 0.066 | 0.863 | 0.050 | 12.15 | 14.96 | 1.05 |
| 54.52 | 1.146 | 3756 | 0.044 | 0.101 | 0.915 | 0.083 | 7.84 | 8.11 | 0.80 |

overall $R\sigma = \Sigma(\sigma(I)) / \Sigma (I) =$ 0.0335

**Refinement**

The final MM comprised multipoles up to hexadecapoles for non-H atoms and up to bond--directed dipoles for the H (C-H) atoms, quadrupoles for the H (O-H) atoms. Positional parameters of H atoms were refined freely in a step-wise approach, and their ADPs were fixed to the results obtained from theory in the harmonic approximation.



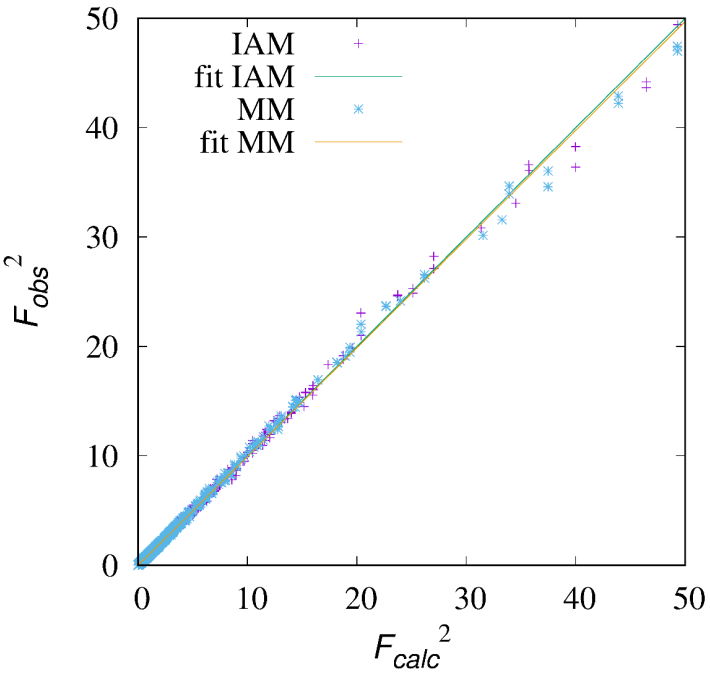




**Figure S4** Scatter plots of X-ray refinement results (MM) for **1.**

**Table S5** Monopole populations, contraction parameters κ and κ' and net atomic charges.

| Atom | Pval | κ | P00 | κ ' | Net charge |
|---|---|---|---|---|---|
| O(1) | 6.18(5) | 0.984(3) | 0.000 | 1.04(4) | -0.18(5) |
| O(2) | 6.27(5) | 0.984(3) | 0.000 | 1.04(4) | -0.27(5) |
| O(3) | 6.41(5) | 0.979(3) | 0.000 | 1.12(4) | -0.41(5) |
| O(4) | 6.34(5) | 0.979(3) | 0.000 | 1.12(4) | -0.34(5) |
| O(5) | 6.25(6) | 0.984(3) | 0.000 | 1.04(4) | -0.25(6) |
| O(6) | 6.19(5) | 0.984(3) | 0.000 | 1.04(4) | -0.19(5) |
| C(1) | 4.27(9) | 0.974(7) | 0.000 | 0.81(2) | -0.27(9) |
| C(2) | 4.23(9) | 0.979(6) | 0.000 | 0.85(2) | -0.23(9) |
| C(3) | 4.13(9) | 0.979(6) | 0.000 | 0.85(2) | -0.13(9) |
| C(4) | 4.17(9) | 0.974(7) | 0.000 | 0.81(2) | -0.17(9) |
| H(2) | 0.57(3) | 1.34(3) | 0.000 | 1.500 | +0.43(3) |
| H(3) | 0.59(3) | 1.34(3) | 0.000 | 1.500 | +0.41(3) |
| H(4) | 0.68(4) | 1.34(3) | 0.000 | 1.500 | +0.32(4) |
| H(6) | 0.59(4) | 1.34(3) | 0.000 | 1.500 | +0.41(4) |
| H(2A) | 0.56(4) | 1.34(3) | 0.000 | 1.500 | +0.44(4) |
| H(3A) | 0.57(4) | 1.34(3) | 0.000 | 1.500 | +0.43(4) |

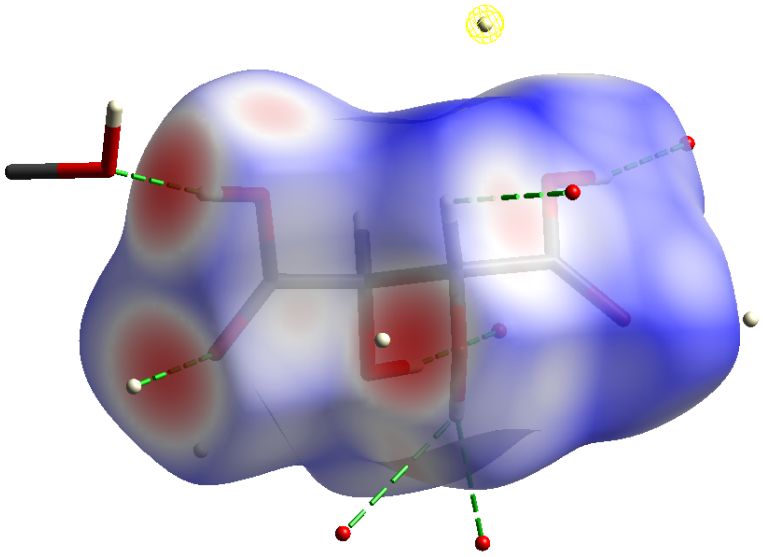


**Figure S5** H bonds in **1**; the Hirshfeld surface shows a molecule of tartaric acid. Surface colours encode the electrostatic potential (red negative, blue positive).

**Table S6** Bond distances in **1** (Å).

| | | | |
|---|---|---|---|
| O1-C1 | 1.2185(4) | O4-H4 | 0.977(7) |
| O2-C1 | 1.3131(4) | O6-H6 | 0.987(8) |
| O3-C2 | 1.3993(4) | C1-C2 | 1.5186(4) |
| O4-C3 | 1.4101(5) | C2-C3 | 1.5456(5) |
| O5-C4 | 1.2103(5) | C3-C4 | 1.5211(4) |
| O6-C4 | 1.3183(5) | C2-H2A | 1.083(10) |
| O2-H2 | 0.982(9) | C3-H3A | 1.085(9) |
| O3-H3 | 0.979(7) | | |

**Table S7** Bond angles in **1** (°).

| | | | |
|---|---|---|---|
| C1-O2-H2 | 115.4(5) | O4-C3-C4 | 112.14(3) |
| C2-O3-H3 | 107.4(4) | C2-C3-C4 | 110.59(3) |
| C3-O4-H4 | 109.7(5) | O5-C4-C3 | 124.46(3) |
| C4-O6-H6 | 113.4(5) | O6-C4-C3 | 109.80(3) |
| O1-C1-C2 | 123.47(3) | O5-C4-O6 | 125.73(3) |
| O2-C1-C2 | 111.18(3) | O3-C2-H2A | 112.5(5) |
| O1-C1-O2 | 125.31(3) | C1-C2-H2A | 108.5(5) |
| O3-C2-C1 | 108.70(2) | C3-C2-H2A | 109.2(5) |
| O3-C2-C3 | 111.08(3) | O4-C3-H3A | 106.8(5) |
| C1-C2-C3 | 106.66(3) | C2-C3-H3A | 109.9(5) |
| O4-C3-C2 | 110.99(3) | C4-C3-H3A | 106.3(4) |

**Table S8** Hydrogen bond geometry [Å, deg.] in **1**.

| D(onor) | Hydrogen | A(cceptor) | D-H | H···A | D···A | D-H···A |
|---|---|---|---|---|---|---|
| O2 | H2 | O4$^{i}$ | 0.979(9) | 1.640(9) | 2.6163(4) | 174.8(8) |
| O3 | H3 | O5$^{ii}$ | 0.980(8) | 1.836(8) | 2.8107(4) | 173.0(7) |
| O4 | H4 | O1$^{iii}$ | 0.976(7) | 1.905(8) | 2.8579(4) | 164.7(7) |
| O6 | H6 | O1$^{iv}$ | 0.982(8) | 1.712(8) | 2.6781(4) | 167.2(8) |
| C3 | H3A | O6$^{v}$ | 1.083(9) | 2.497(10) | 3.0607(5) | 111.2(7) |

Symmetry operators: *i* = 2-*x*, *y*-0.5, 1-*z*
*ii* = 1-*x*, *y*-0.5, 2-*z*
*iii* = 1-*x*, *y*+0.5, 1-*z*
*iv* = *x*, *y*, 1+*z*
*v* = 2-*x*, *y*+0.5, 2-*z*

**Table S9** Diagonal components *U* of the displacement tensors, sorted from smallest (min), medium (med) to largest (max) for theory and experiment, given in $10^{-3}$ Å$^2$. Similarity indices ($S_{12}$) are given in percent.

| | Theory | | | Experiment | | | |
|---|---|---|---|---|---|---|---|
| Atom | $U_{min}$ | $U_{med}$ | $U_{max}$ | $U_{min}$ | $U_{med}$ | $U_{max}$ | $S_{12}$ |
| O1 | 4.704 | 9.664 | 14.002 | 4.959 | 10.178 | 14.783 | 0.196 |
| O2 | 5.425 | 10.206 | 15.539 | 5.600 | 9.515 | 16.519 | 0.168 |
| O3 | 5.743 | 8.253 | 13.684 | 5.482 | 8.443 | 15.258 | 0.366 |
| O4 | 5.375 | 8.635 | 9.040 | 5.716 | 7.928 | 9.567 | 0.293 |
| O5 | 5.175 | 11.780 | 19.334 | 6.026 | 12.068 | 21.760 | 0.661 |
| O6 | 4.901 | 9.770 | 18.529 | 4.617 | 9.985 | 20.946 | 0.220 |
| C1 | 4.298 | 7.312 | 9.131 | 5.207 | 7.058 | 9.106 | 0.386 |
| C2 | 4.368 | 7.399 | 8.613 | 4.958 | 7.102 | 8.644 | 0.186 |
| C3 | 4.177 | 6.780 | 8.253 | 4.728 | 7.038 | 7.845 | 0.276 |
| C4 | 4.130 | 7.574 | 9.716 | 4.877 | 7.746 | 10.231 | 0.303 |

**Table S10** Topological properties of (3,-1) critical points for hydrogen bonds in **1**.

$d_1$ ($d_2$) is the distance from the first (second) atom to the (3, -1) critical point, $R_{ij} = d_1 + d_2$, $\rho$ is the electron density, $\nabla^2\rho$ is the Laplacian of the electron density. $G(a.u.)$ is the kinetic energy density, $V(a.u.)$ the potential energy density and $E(a.u.)$ the total energy density.

| Bond | $R_{ij}$(Å) | $d_1$(Å) | $\rho(e\cdot$Å$^{-3})$ | $\nabla^2\rho(e\cdot$Å$^{-5})$ | $G(a.u.)$ | $V(a.u.)$ | $E(a.u.)$ |
|---|---|---|---|---|---|---|---|
| H2$\cdots$O4$^{i}$ | 1.6428 | 0.5353 | 0.34(9) | 1.2(3) | 0.028(5) | –0.044(7) | –0.016(9) |
| H3$\cdots$O5$^{ii}$ | 1.8480 | 0.6242 | 0.18(9) | 0.8(2) | 0.012(5) | –0.016(6) | –0.004(8) |
| H4$\cdots$O1$^{iii}$ | 1.9086 | 0.6856 | 0.17(7) | 1.5(2) | 0.016(4) | –0.017(5) | –0.001(6) |
| H6$\cdots$O1$^{iv}$ | 1.7186 | 0.5604 | 0.26(9) | 1.1(3) | 0.020(5) | –0.029(6) | –0.008(8) |
| H3A$\cdots$O6$^{v}$ | 2.5093 | 1.1028 | 0.064(3) | 0.88(3) | 0.0073(12) | –0.0055(11) | 0.0018(16) |

i=2-x, y-0.5,1-z; ii=1-x, y-0.5,2-z; iii=1-x, y+0.5,1-z ; iv=x, y,1+z; v=2-x, y+0.5,2-z

| contact | D···A [Å] | D–H [Å] | H···A [Å] | <O2-H2···O4$^{i}$ | ρ [eÅ$^{-3}$] |
|---|---|---|---|---|---|
| O2-H2···O4$^{i}$<br>i=2-x, y-0.5,1-z | 2.6163(4) | 0.979(9) | 1.640(9) | 174.8(8) | 0.34(11) |

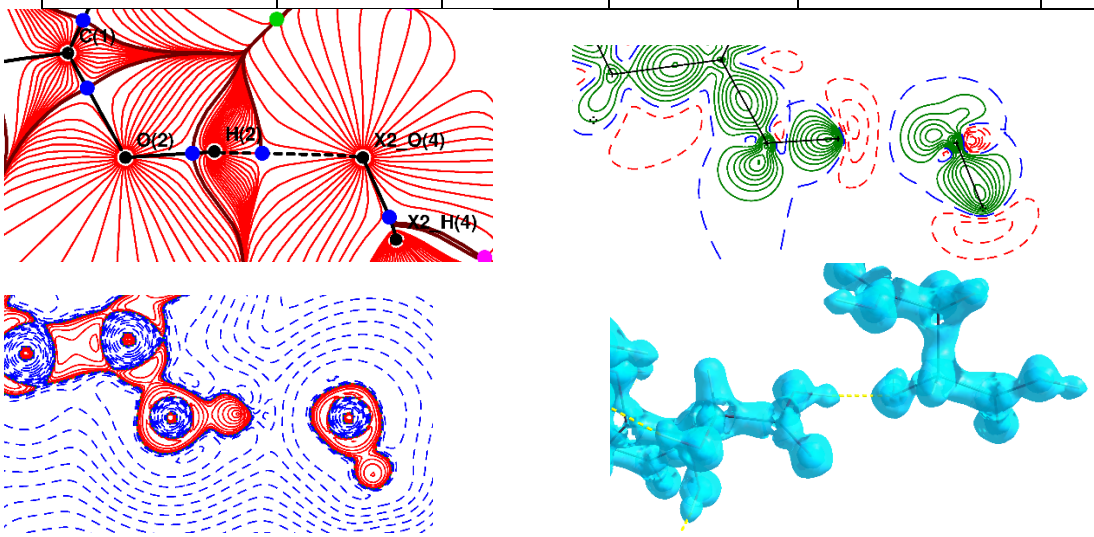



**Figure S6** Gradient trajectory plot, deformation density (contour lines at 0.1 eÅ$^{-3}$) and Laplacian (isosurface at -2 eÅ$^{-5}$) of electron density for O2–H2···O4$^{i}$.

| contact | D···A [Å] | D–H [Å] | H···A [Å] | <O2-H2···O4$^{i}$ | ρ [eÅ$^{-3}$] |
|---|---|---|---|---|---|
| O3-H3···O5$^{ii}$<br>ii=1-x, y-0.5,2-z | 2.8107(4) | 0.980(8) | 1.836(8) | 173.0(7) | 0.18(9) |

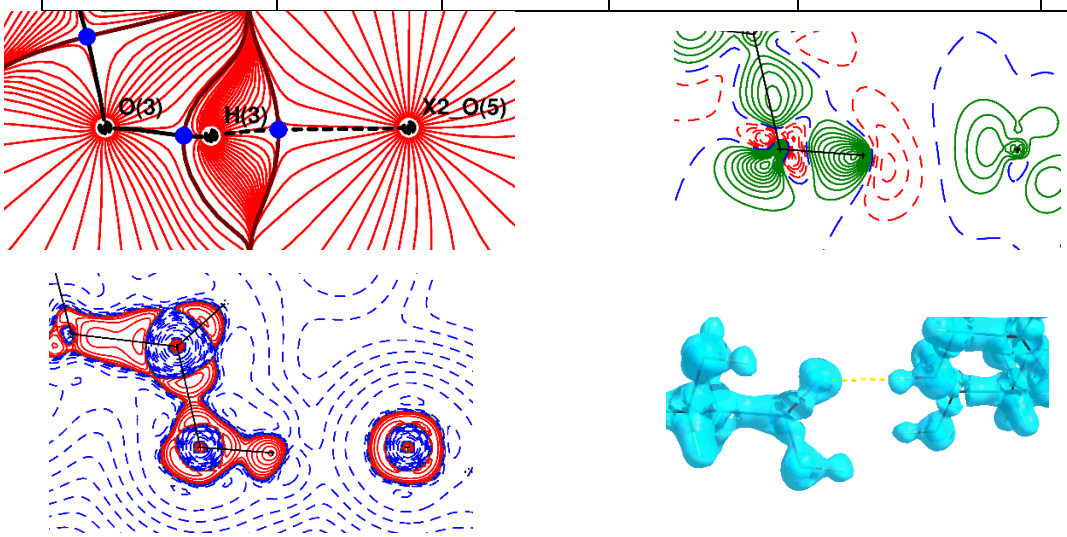



**Figure S7** Gradient trajectory plot, deformation density (contour lines at 0.1 eÅ$^{-3}$) and Laplacian (isosurface at -2 eÅ$^{-5}$) of electron density for O3–H3···O5$^{ii}$.

| contact | D···A [Å] | D–H [Å] | H···A [Å] | <O2-H2···O4$^{i}$ | ρ [eÅ$^{-3}$] |
|---|---|---|---|---|---|
| O4-H4···O1$^{iii}$<br>iii=1-x, y+0.5,1-z | 2.8579(4) | 0.976(7) | 1.905(8) | 164.7(7) | 0.17(7) |

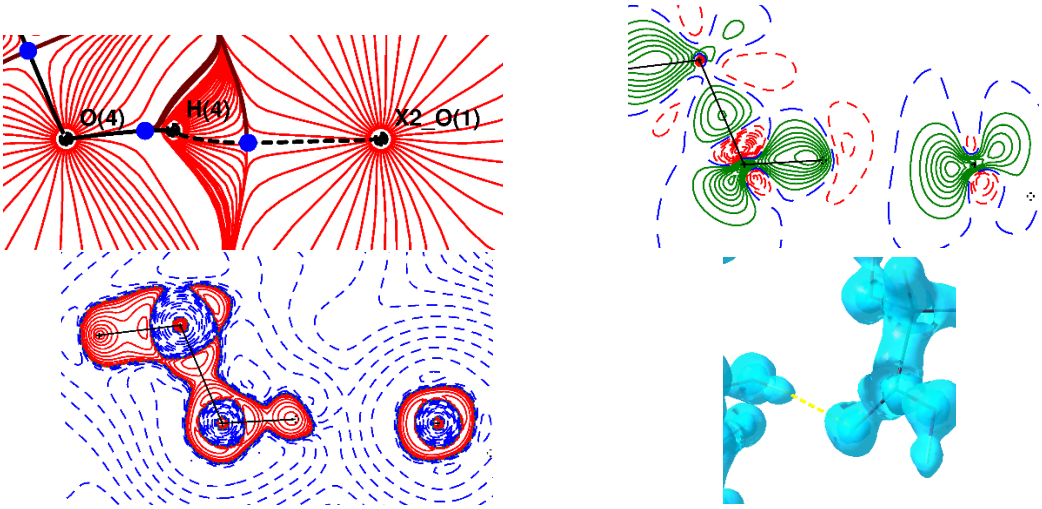



**Figure S8** Gradient trajectory plot, deformation density (contour lines at 0.1 eÅ$^{-3}$) and Laplacian (isosurface at -2 eÅ$^{-5}$) of electron density for O4–H4···O1$^{iii}$.

| contact | D···A [Å] | D–H [Å] | H···A [Å] | <O2-H2···O4$^{i}$ | ρ [eÅ$^{-3}$] |
|---|---|---|---|---|---|
| O6-H6···O1$^{iv}$<br>iv=x, y,1+z | 2.6781(4) | 0.982(8) | 1.712(8) | 167.2(8) | 0.26(10) |

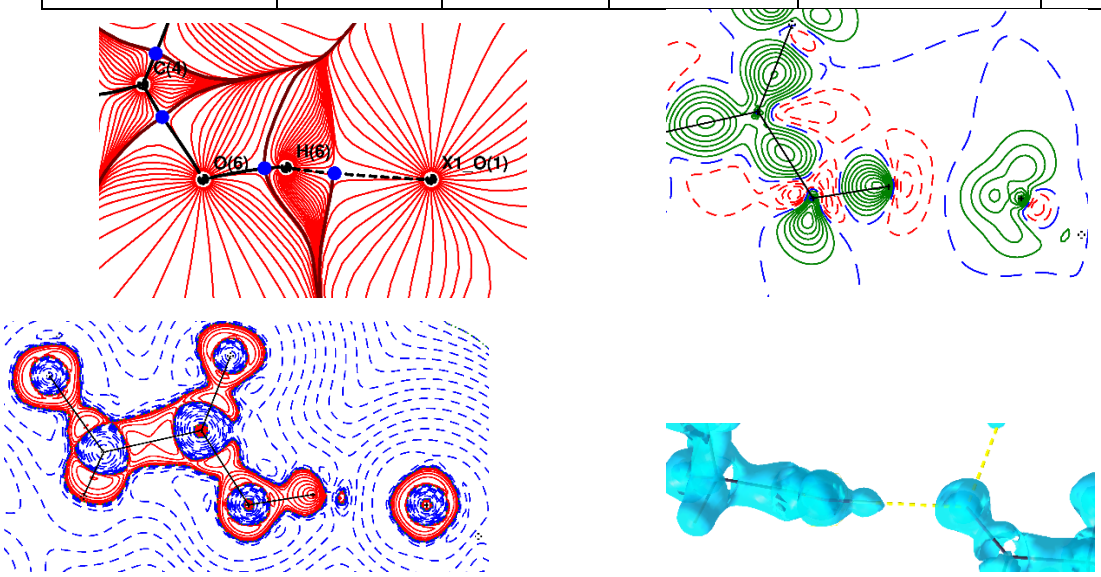



**Figure S9** Gradient trajectory plot, deformation density (contour lines at 0.1 eÅ$^{-3}$) and Laplacian (isosurface at -2 eÅ$^{-5}$) of electron density for O6–H6···O1$^{iv}$.

| contact | D···A [Å] | D–H [Å] | H···A [Å] | <O2-H2···O4$^{i}$ | ρ [eÅ$^{-3}$] |
|---|---|---|---|---|---|
| C3-H3A···O6$^{v}$<br>v=2-x, y+0.5,2-z | 3.0607(5) | 1.083(9) | 2.497(10) | 111.2(7) | 0.064(3) |

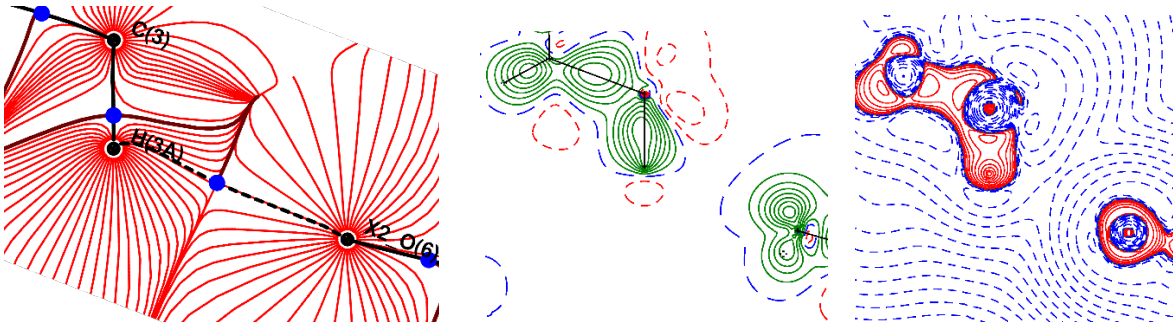



**Figure S10** Gradient trajectory plot, deformation density (contour lines at 0.1 eÅ$^{-3}$) and Laplacian (isosurface at -2 eÅ$^{-5}$) of electron density for C3–H3A···O6$^{v}$.

**Table S11** Topological properties of (3,-1) critical points for covalent bonds in **1**.

| Bond | $R_{ij}$(Å) | $d_1$(Å) | $\rho(e\cdot Å^{-3})$ | $\nabla^2\rho(e\cdot Å^{-5})$ |
|---|---|---|---|---|
| O1—C1 | 1.2182 | 0.8203 | 2.82(3) | −2.3(2) |
| O2—C1 | 1.3134 | 0.8739 | 2.46(3) | −26.5(2) |
| O2—H2 | 0.9844 | 0.7405 | 2.4(2) | −52.3(9) |
| O3—C2 | 1.4004 | 0.8552 | 2.06(3) | −21.0(2) |
| O3—H3 | 0.9850 | 0.7220 | 2.6(2) | −50.4(9) |
| O4—C3 | 1.4105 | 0.8694 | 1.96(3) | −24.7(2) |
| O4—H4 | 0.9844 | 0.7256 | 2.6(2) | −43.5(9) |
| O5—C4 | 1.2108 | 0.8124 | 2.91(4) | −6.3(3) |
| O6—C4 | 1.3187 | 0.8755 | 2.39(3) | −26.4(2) |
| O6—H6 | 0.9856 | 0.7246 | 2.5(2) | −45.5(9) |
| C1—C2 | 1.5193 | 0.8289 | 1.89(3) | −17.74(7) |
| C1—H2 | 2.0046 | 1.7607 | 2.4(2) | −52.3(9) |
| C2—C3 | 1.5474 | 0.7710 | 1.77(3) | −14.64(8) |
| C2—H2A | 1.0833 | 0.7262 | 1.9(2) | −20.9(5) |
| C3—C4 | 1.5211 | 0.7149 | 1.81(3) | −19.08(7) |
| C3—H3A | 1.0830 | 0.7378 | 2.0(2) | −21.4(5) |
| C4—H6 | 1.9875 | 1.7265 | 2.5(2) | −45.5(9) |

**Figs. S11 - S13** show the residual electron density distribution for **1**.

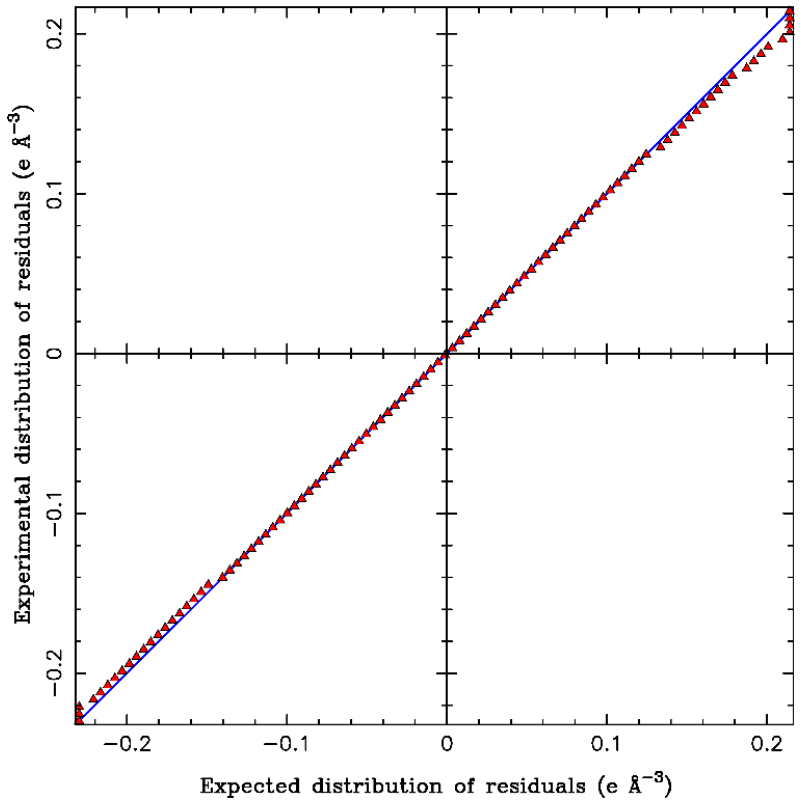



**Figure S11** Normal probability plot for residuals in the electron density in **1**.

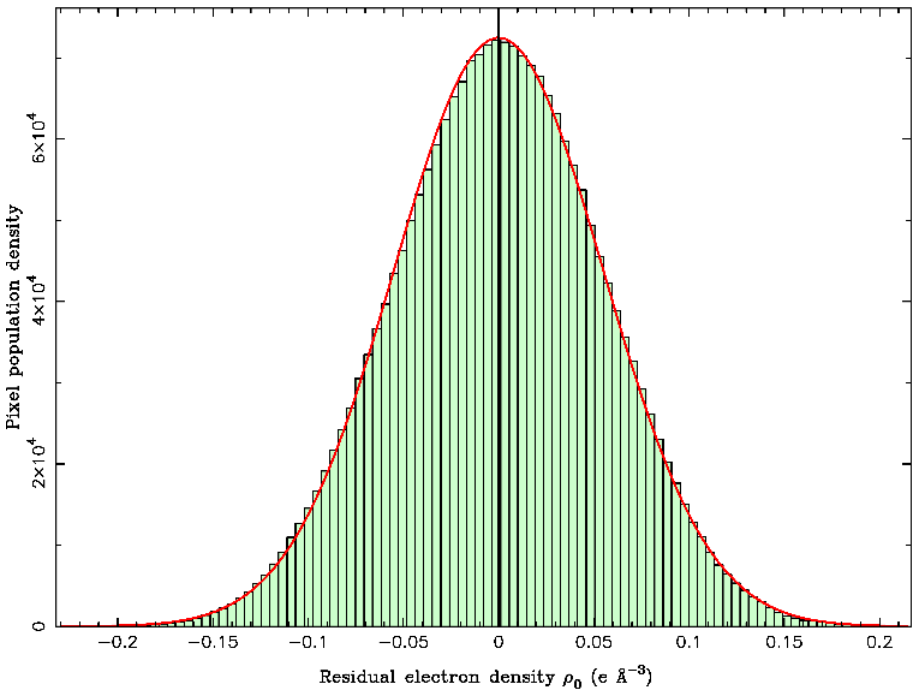



**Figure S12** Probability distribution histogram for residuals in the electron density in **1**.

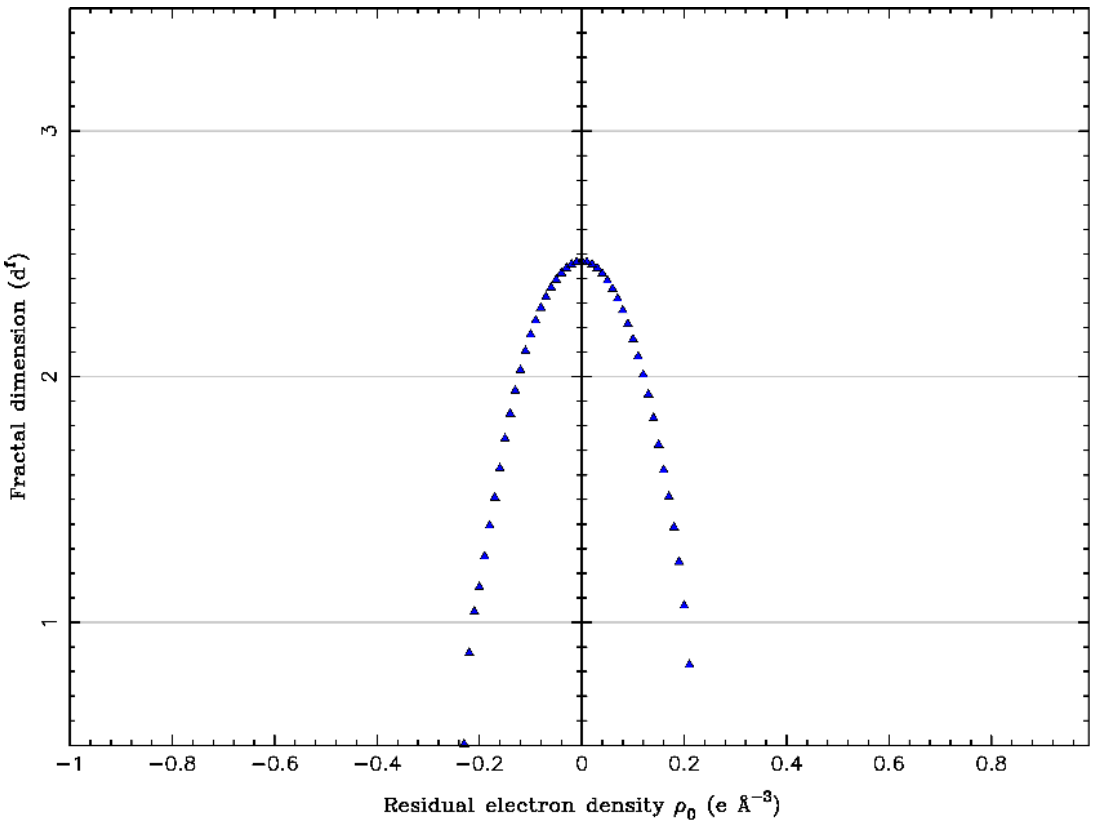



**Figure S13** Fractal dimension plot for residuals in the electron density in **1**.

**Figure S14** *PEANUT* plots of differences

ADPs (experiment, MM based) - ADPs (calculated, quasi-harmonic approximation)

Differences are scaled by a factor of 2 (top) and 4 (bottom), blue positive, red negative.