Refinements on electron diffraction data of β-glycine in MoPro: A quest for improved structure model

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Supplementary Information

Table S1. Electron diffraction scattering factors *f*(*s*) as a function of $s = \sin\theta/\lambda$, Coefficients A1 A2 A3 A4 B1 B2 B3 B4 published by Peng, (1999), in Micron. **30**, 625–648, where $f(s) = \sum_{i=1,4} A_i * \exp(-B_i * s^2)$

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CHEM H
CORE GAUS
 .0367  .1269   .2360 .1290    .5608  3.7913   13.5557  37.7229

CHEM C
CORE  GAUS
 .1361 .5482   1.2266  .5971    .3731 3.2814   13.0456 41.0202

CHEM N
CORE  GAUS
.1372 .5344   1.0862  .4547    .3287 2.6733   10.3165 32.7631

CHEM O
CORE  GAUS
 .1433  .5103   .9370  .3923   .3055  2.2683  8.2625  25.6645
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Table S2. . Electron diffraction scattering factors *f*(*s*) as a function of *s* =, $\sin\theta/\lambda$ Coefficients A1 A2 A3 A4 A5 B1 B2 B3 B4 B5 as published in the International Tables of Crystallography (Volume C ,Tables 4.2.6.8 and 6.1.1.4). Here, $f(s) = \sum_{i=1,5} A_i * \exp(-B_i * s^2)$

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CHEM H
CORE GAUS
0.0088 0.0449 0.1481 0.2356 0.0914   0.1152 1.0867 4.9755 16.5591 43.2743

CHEM C
CORE  GAUS
0.0489 0.2091 0.7537 1.142 0.3555    0.114 1.0825 5.4281 17.8811 51.1341

CHEM N
CORE  GAUS
0.0267 0.1328 0.5301 1.102 0.4215    0.0541 0.5165 2.8207 10.6297 34.3764

CHEM O
CORE  GAUS
 0.0365 0.1729 0.5805 0.8814 0.3121    0.0652 0.6184 2.9449 9.6298 28.2194
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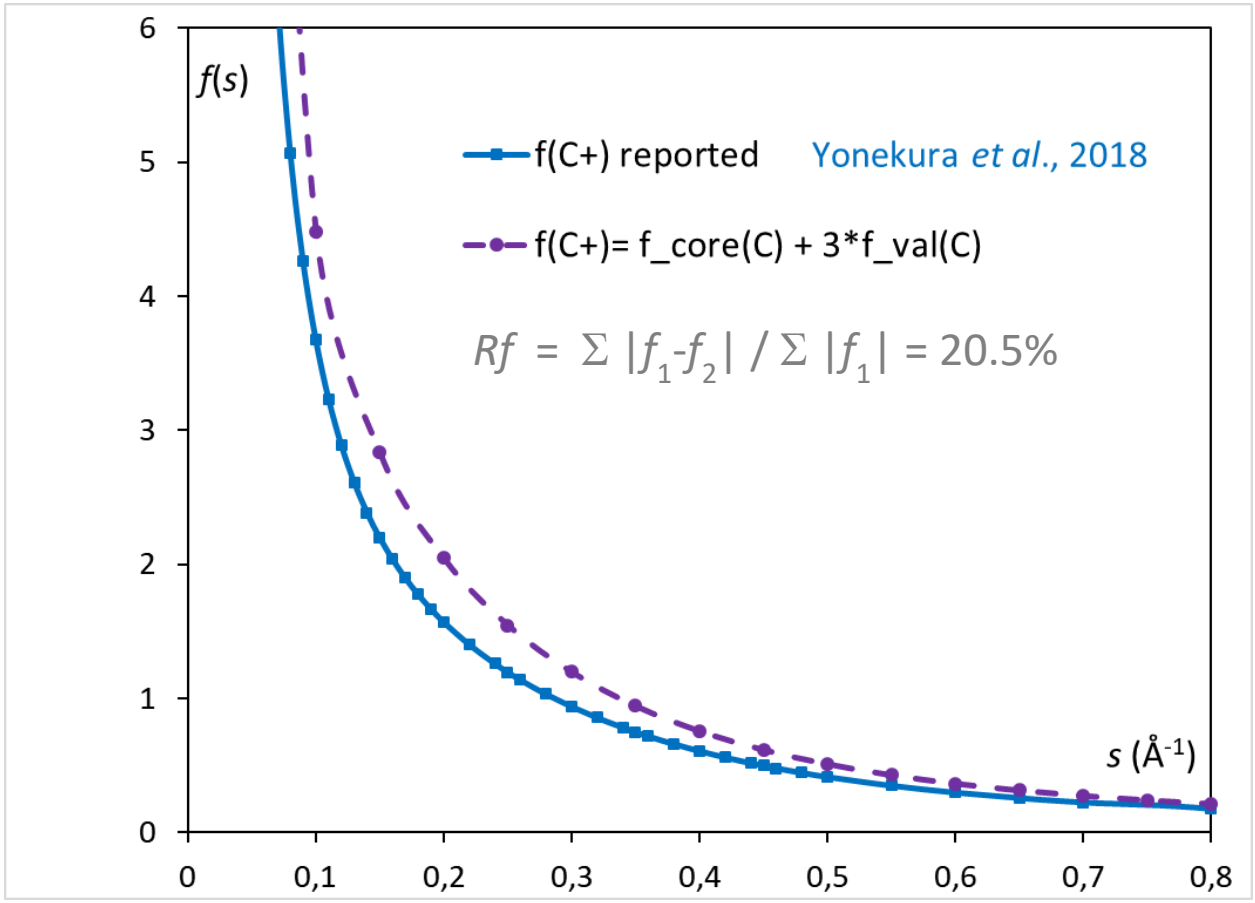
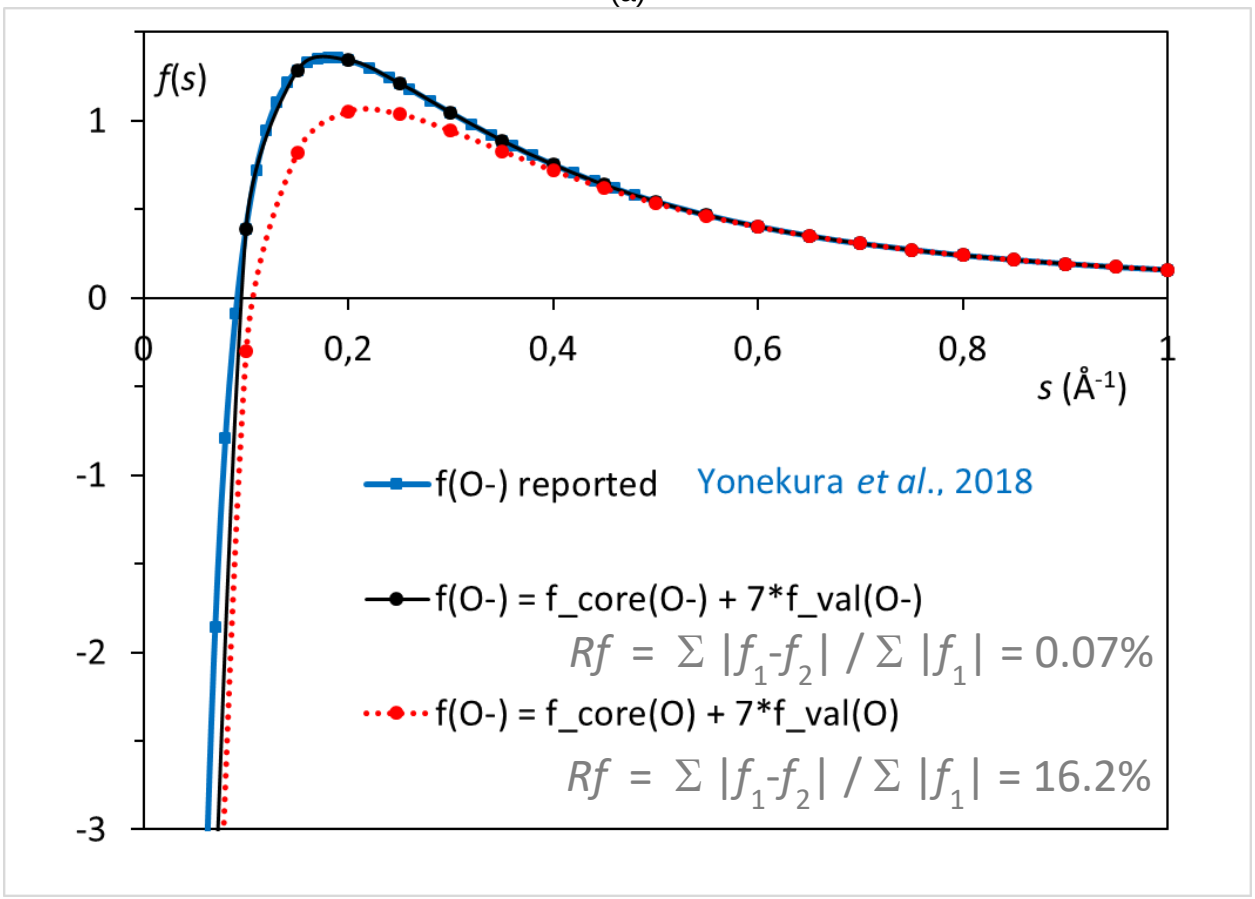
Table S3: Bond distances (Å) derived from IAM and TAAM refinement of β-Glycine

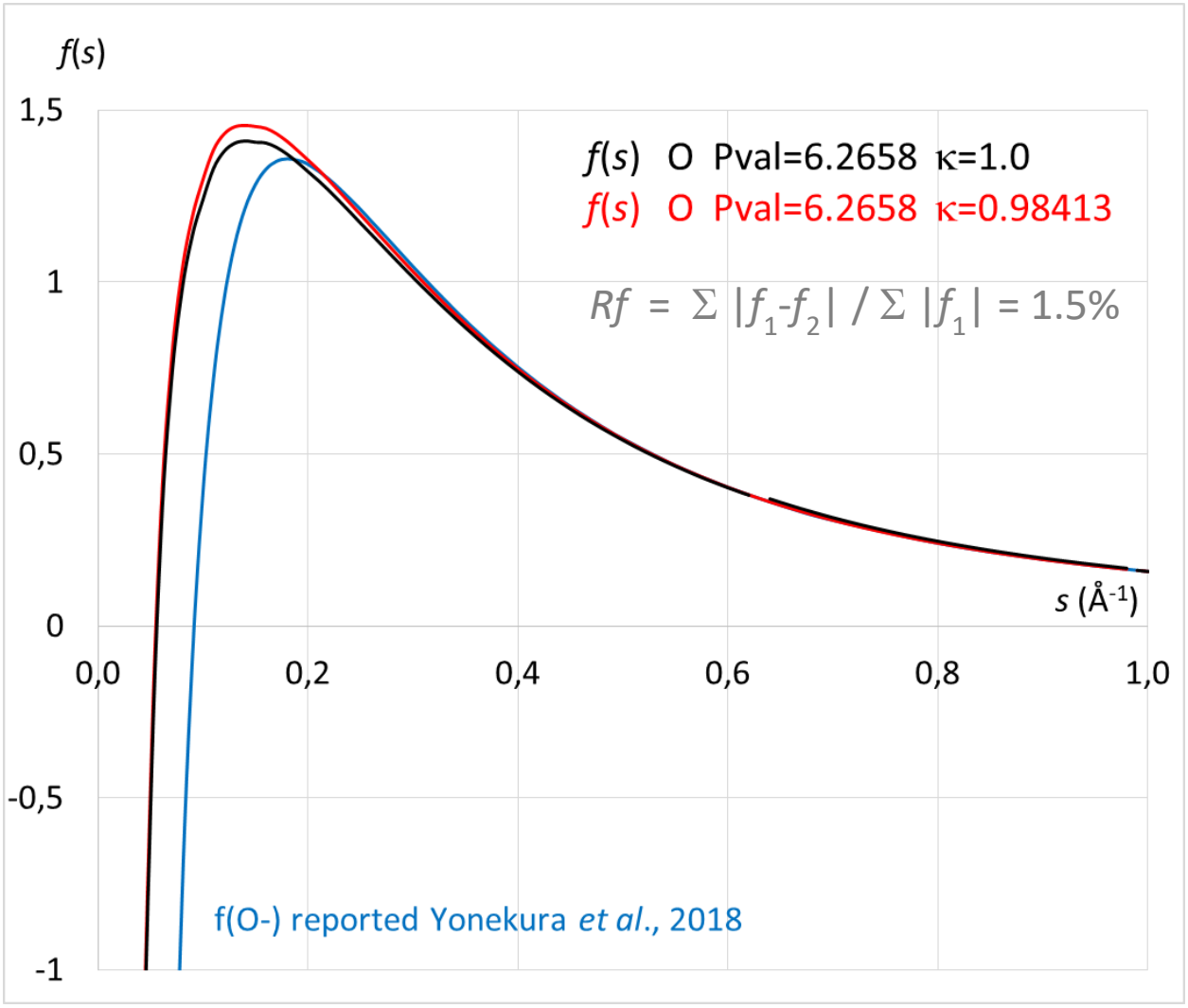
Method	Bond	IAM	IAM_Peng	IAM_IT	TAAM_ELMAM2	TAAM_UBDB
Program	Type	SHELX	MoPro	MoPro	MoPro	MoPro
1	C1-C2	1.58(6)	1.58(6)	1.58(6)	1.58(6)	1.58(9)
2	C2-O1	1.32(3)	1.32(6)	1.32(6)	1.32(8)	1.32(1)
3	C2-O2	1.32(2)	1.32(1)	1.32(1)	1.32(3)	1.32(2)
4	N1-C1	1.54(4)	1.54(7)	1.53(7)	1.54(6)	1.54(5)
5	N1-H1A	1.21(4)	1.22(4)	1.22(4)	1.19(2)	1.19(2)
6	N1-H1B	1.11(7)	1.09(6)	1.10(6)	1.07(7)	1.10(6)
7	N1-H1C	1.23(5)	1.22(3)	1.22(3)	1.18(3)	1.17(3)
8	C1-H1D	1.16(5)	1.17(4)	1.17(3)	1.14(3)	1.14(3)
9	C1-H1E	1.32(6)	1.31(5)	1.31(5)	1.20(5)	1.17(5)


f(s)
s (Å-1)
f(C+) reported
Yonekura et al., 2018
f(C+)= f_core(C) + 3*f_val(C)
Rf = Σ |f1-f2| / Σ |f1| = 20.5%

(a)

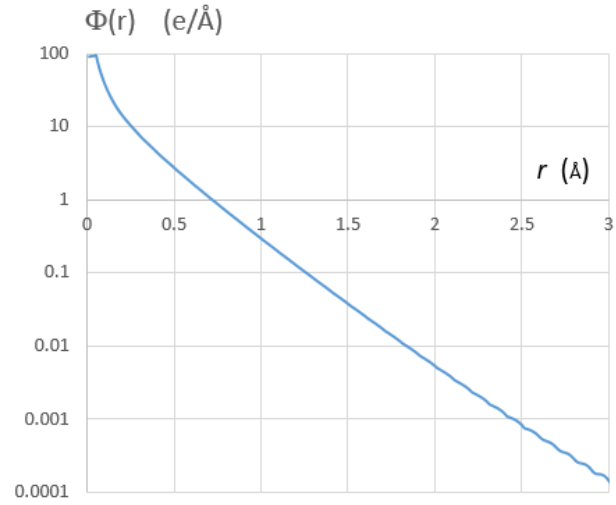

f(s)
s (Å-1)
f(O-) reported
Yonekura et al., 2018
f(O-) = f_core(O-) + 7*f_val(O-)
Rf = Σ |f1-f2| / Σ |f1| = 0.07%
f(O-) = f_core(O) + 7*f_val(O)
Rf = Σ |f1-f2| / Σ |f1| = 16.2%

(b)

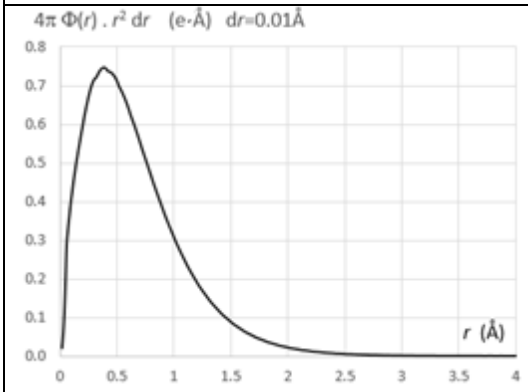


(c)

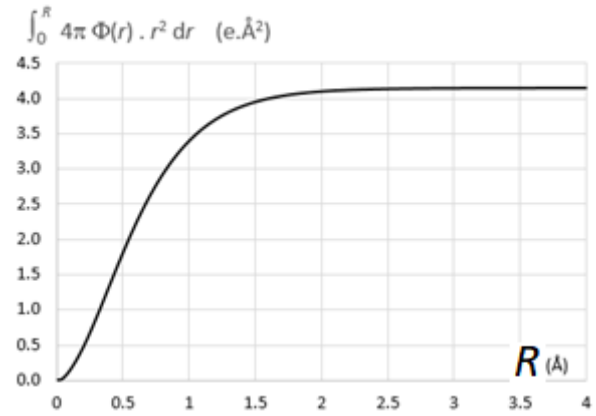
Figure S1. Comparison of *f*(*s*) electron scattering factors (Å) as a function of reciprocal resolution $s = \sin\theta/\lambda$ (Å^{-1}) for (**a**) a carbon atom with charge +1e, f(C+) and (**b**) an oxygen atom with charge -1e, f(O-) from current study and earlier reported by Yonekura *et al.*, 2018. Current *f*(*s*) were obtained by the Mott-Bethe equation on X-ray scattering factors for neutral atoms (C, O) and for ions (O-) with the valence part rescaled to reproduce desired charges of carbon and oxygen using the $f = f_{core} + P_{val}f_{val}$ approach. The reported *f*(*s*) values were computed on isolated carbon and oxygen ions (Yonekura *et al.*, 2018). The *f*(*s*) derived from neutral atoms differ from the reported ones by *R*-factor *Rf* = 20.5 and 16.2 % for (**a**) f(C+) and (**b**) f(O-), respectively. The *f*(*s*) derived from oxygen anion, f(O-) = f_{core}(O-)+7f_{val}(O-), differ from the reported one by *Rf* = 0.07%. (**c**) Electron scattering factor of the spherical part of carboxylate oxygen atom after ELMAM2 database transfer (charge -0.2658 e). For comparison, *f*(*s*) was also computed for the atom with same P_{val} valence population, but *κ* expansion contraction coefficient set to unity.



(a) Electrostatic potential as a function of distance to nucleus.



(b) Contribution, as a function of distance, to the global integration in spherical coordinates



(c) Convergence of the cubature from r=0 to r=R in spherical coordinates

Figure S2. Cubature of the electrostatic potential generated by an IAM carbon atom (neutral and spherical). The integration is done in spherical coordinates: $I_a = 4\pi \int \Phi_a(r)\ r^2\, dr$

1 e/Å corresponds to 14,40 Volts.

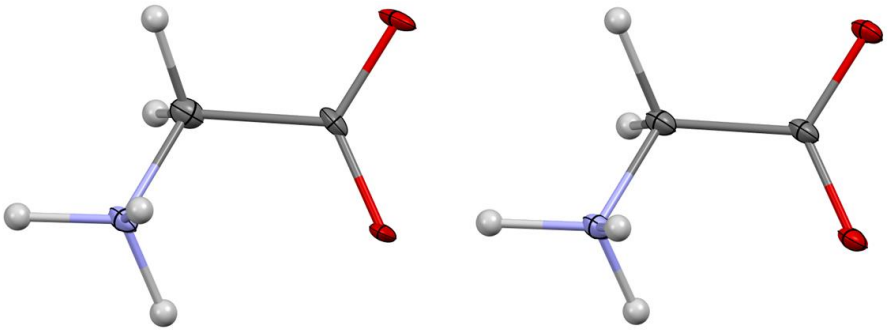
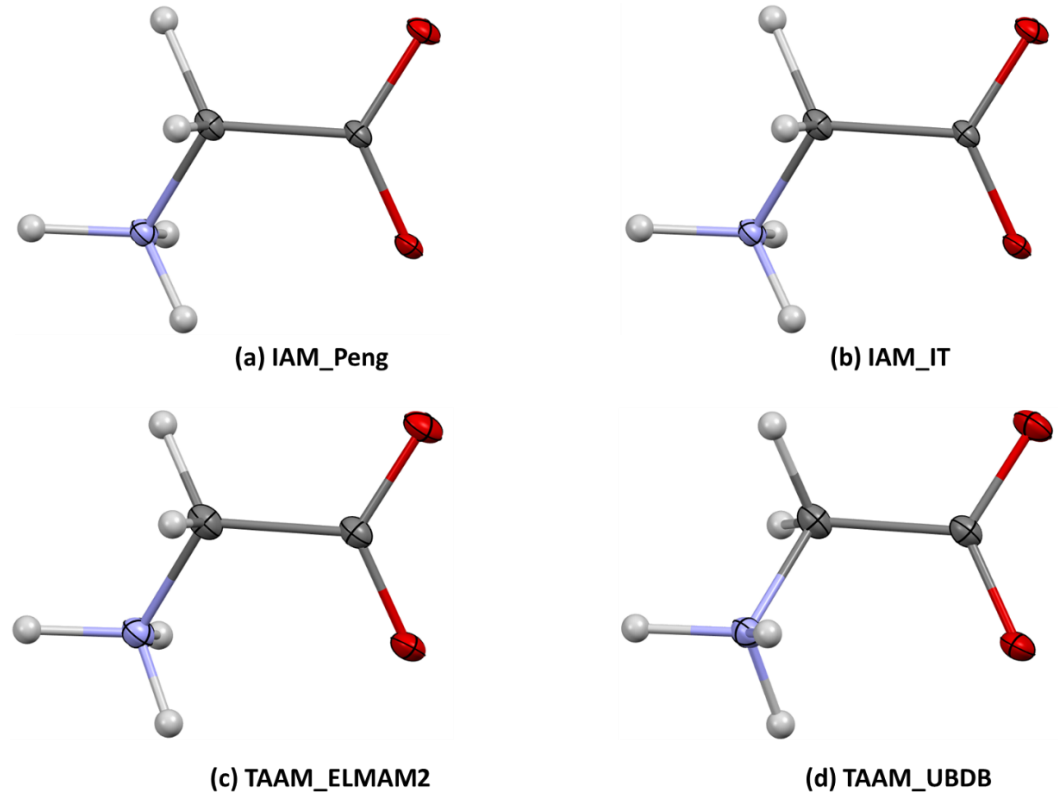


Figure S3: Thermal ellipsoid diagram of β-glycine (a) reported structure (Broadhurst *et al.*, 2020) (b) re-refined structure (Table 2) with *U*ij isotropy and rigid bond restraints in SHELX.



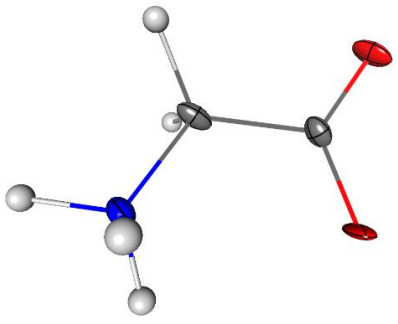


Figure S4:
Thermal ellipsoid diagram of β-glycine with spherical IAM and aspherical TAAM refinement, with MoPro. *Uij* isotropy and rigid bond restraints were applied, except for the last diagram (e).