

**MS46-1-2 CODATA, IUCr, PDBj collaboration for medical-protein crystal structure definitive versions of data files #MS46-1-2**

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**Abstract**

Envisaging a process akin to a journal's peer review we have set up an IUCr and PDBj collaboration for medical-protein crystal structure definitive versions of data files within the CODATA GOSC Case Studies (see <https://codata.org/initiatives/decadal-programme2/global-open-science-cloud/case-studies/diffraction-data/>). Quoting from our Case Study webpage "The overall reproducibility of the diffraction data and their linked molecular model is the overarching guide. The scope of this challenge, in general terms, can be judged by the fact that the FAIR movement (FAIR=Findable, Accessible, Interoperable, Reusable) did not include data quality in its criteria. In the spirit of scientific reproducibility, we introduce a term somewhere between reusability and reproducibility, namely definitive reusability." That PDBj had launched a raw diffraction images data archive XRDa <https://xrda.pdbj.org/> was pivotal as it would allow a combined evaluation of raw data, processed structure factors and derived protein molecular model. This also would lead to general community benefit beyond medical pandemic challenges, although of course very important, to the whole of macromolecular crystallography. Feedback on a PDBj deposition is made by JRH and LKB to GK and who then can decide, like a journal editor exactly what feedback is made to a depositor to PDBj for a possible reversioning of a PDBj deposition. Progress of this initiative will be described and spans covid-19 and other medically important proteins (e.g. see Brink and Helliwell (2022), Hanau and Helliwell, 2022, Helliwell 2021).

**References**

Brink, A. and Helliwell, J.R. (2022) IUCrJ 9, 180-193.

Hanau, S. and Helliwell, J.R. (2022) Acta Cryst. (2022). F78, 96–112.

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