

Looking at examples from PAIRREF publications - Maly et al 2020

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Introduction

The paper

Malý, M., Diederichs, K., Dohnálek, J. and Kolenko, P., 2020. Paired refinement under the control of PAIRREF. IUCrJ, 7(4), pp.681-692.

provides a nice set of examples that could be used for testing our programs: always more interesting to use something other people have also looked at (similar to [Fragment Binding to the Nsp3 Macrodomain of SARS-CoV-2](#) and [FragMAXapp 202106 paper](#)). The example datasets are:

Molecule	PDB	Diffraction Images	Remarks
Cysteine Dioxygenase (CDO)	3ELN PDBpeep Table -1	https://data.sbgrid.org/dataset/751/	
Endothiapepsin (EP)	4Y4G PDBpeep Table -1	https://proteindiffraction.org/project/4y4g/	
olive flounder [Paralichthys olivaceus] interferon gamma (POLI)	6F1E PDBpeep Table -1	https://doi.org/10.5281/zenodo.3369717	
Bilirubin oxidase (BO)	6I3J PDBpeep Table-1	https://proteindiffraction.org/project/6i3j/	
Thermolysine (TL)	NA	https://zenodo.org/record/49559	Low dose, high multiplicity (I03/DLS)
Lysozyme (SIM)	NA	https://data.sbgrid.org/dataset/746/	Simulated (MLFSOM) data.

Take-1

Molecule	PAIRREF resolution		autoPROC/STARANISO alldefaults			Remarks
	conservative	optimal	log	isotropic ($\langle I/\sigma \rangle > 2$)	STARANISO	
CDO	2.00	1.50	3ELN.01/summary.html	1.607	(1.487, 1.487, 1.574) 1.487	<ul style="list-style-type: none"> • beamstop definitely requires manual masking • flickering pixels? • poor image ranges (at beginning) • spike in data quality around image 180: <ul style="list-style-type: none"> • gap in time between image 180 and 181: recentering? • overloads (ADSC CCD)
EP	1.44	1.20	4y4g.01/summary.html	1.494	(1.190, 1.316, 1.611) 1.190	<ul style="list-style-type: none"> • static shadow in lower left corner of detector • damaged/flickering pixels • overloads (Pilatus) • big cusp along good diffracting direction
POLI	2.30	2.00	6F1E.01/summary.html	2.495	(2.782, 2.199, 2.086) 2.132	<ul style="list-style-type: none"> • big beamstop and holder • flickering pixels • ice • minor 2nd lattice?
BO	2.59	2.50	6i3j.01/summary.html	2.643	(2.311, 2.427, 2.560) 2.335	<ul style="list-style-type: none"> • very big beamstop and holder • split spots? • crystal-detector distance <i>just</i> about short enough

TL	1.80	1.50	thermc_5.01/summary.html	1.831	(1.785, 1.785, 1.642) 1.643	<ul style="list-style-type: none">• weak images give problems in automatic beamstop masking• flickering spots• cusp along best diffracting direction• crystal-detector distance too long
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