

Materials List for:

Fully Autonomous Characterization and Data Collection from Crystals of Biological Macromolecules

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URL: <https://www.jove.com/video/59032>

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Materials

Name	Company	Catalog Number	Comments
Beamline MASSIF-1	ESRF		
BL21DE3	New England Biolabs	C2527I	
chloramphenicol	Roth	3886.1	
Concentrators: Amicon Ultra-4 Ultracel -30K	Merck Millipore	UFC803024	
Dialyzing membrane	Spectrumlabs	132655	
DMSO	Sigma-Aldrich	D8418	
Dnase	Roche	11284932001	
DTT	Euromedex	EU0006-B	
EDTA- free protease inhibitors	Roche	4,693,159,001	
glycerol	VWR Chemicals Prolabo	14388.29T	
His-trap HP	GE healthcare	17-5247-01	
imidazole	Sigma-Aldrich	56750-500G	
IPTG	Euromedex	EU0008-B	
LB medium	Sigma-Aldrich	L3022	
lipoic acid	Sigma-Aldrich	T5625	
loop	Hampton Research	HR8-124	
lysozyme	Roche	10 837 059 001	
MonoQ 5/50 GL	GE healthcare	17-5166-01	
NaCl	Fisher Chemical	S/3160/60	
Sonicator vibra cell 75/15	SONICS		
SPINE pucks	MiTeGen	SKU: M-CSM003-0001A	
Tris base	Euromedex	26-128-3094-B	
Sodium Formate	Sigma-Aldrich	1064430500	
GCSH purification buffer	20 mM TRIS pH 8, 200 mM NaCl		
GCSH cryo-protection buffer	0.25 M Sodium Formate pH 4, 30% glycerol		
Programs:			
MxCube		Gabadinho, J. et al. MxCuBE : a synchrotron beamline control environment customized for macromolecular crystallography experiments. Journal of Synchrotron Radiation. 17 (5), 700-707, doi: 10.1107/S0909049510020005 (2010)	local development

ISPyB	ESRF	Solange Delagenière, Patrice Brechereau, Ludovic Launer, Alun W. Ashton, Ricardo Leal, Stéphanie Veyrier, José Gabadinho, Elspeth J. Gordon, Samuel D. Jones, Karl Erik Levik, Seán M. McSweeney, Stéphanie Monaco, Max Nanao, Darren Spruce, Olof Svensson, Martin A. Walsh, Gordon A. Leonard; ISPyB: an information management system for synchrotron macromolecular crystallography, <i>Bioinformatics</i> , Volume 27, Issue 22, 15 November 2011, Pages 3186-3192, https://doi.org/10.1093/bioinformatics/btr535	local development
MXCube2	ESRF	Gabadinho, J. <i>et al.</i> <i>MxCuBE</i> : a synchrotron beamline control environment customized for macromolecular crystallography experiments. <i>Journal of Synchrotron Radiation</i> . 17 (5), 700-707, doi: 10.1107/S0909049510020005 (2010). De Santis, D., Leonard, G. <i>Notiziario Neutroni e Luce di Sincrotrone</i> , Consiglio Nazionale delle Ricerche. (19), 24-226 (2014).	local development
BES workflow server		Brockhauser, S. <i>et al.</i> The use of workflows in the design and implementation of complex experiments in macromolecular crystallography. <i>Acta Crystallographica Section D Biological Crystallography</i> . 68 (8), 975-984, doi: 10.1107/S090744491201863X (2012).	
DOZOR	ESRF	Bourenkov and Popov, unpublished	local development
BLISS beamline control		Guijarro, M. <i>et al.</i> BLISS - Experiments Control for ESRF EBS Beamlines. <i>Proceedings of the 16th Int. Conf. on Accelerator and Large Experimental Control Systems</i> , ICALEPCS2017, Barcelona, Spain. doi: 10.18429/jacow-icalepcs2017-webpl05 (2018).	local development
AUTO processing of images		Monaco, S. <i>et al.</i> Automatic processing of macromolecular crystallography X-ray diffraction data at the ESRF. <i>Journal of Applied Crystallography</i> . 46 (3), 804-810, doi: 10.1107/S0021889813006195 (2013)	local development
BEST and EDNA		Incardona, M.-F., Bourenkov, G.P., Levik, K., Pieritz, R.A., Popov, A.N., Svensson, O. EDNA : a framework for plugin-based applications applied to X-ray experiment online data analysis. <i>Journal of Synchrotron Radiation</i> . 16 (6), 872-879, doi: 10.1107/S0909049509036681 (2009).	local development

CCP4		Winn, M.D. <i>et al.</i> Overview of the CCP 4 suite and current developments. <i>Acta Crystallographica Section D Biological Crystallography</i> . 67 (4), 235-242, doi: 10.1107/S0907444910045749 (2011).	
Phaser MR		McCoy, A.J., Grosse-Kunstleve, R.W., Adams, P.D., Winn, M.D., Storoni, L.C., Read, R.J. <i>Phaser</i> crystallographic software. <i>Journal of Applied Crystallography</i> . 40 (4), 658-674, doi: 10.1107/S0021889807021206 (2007).	
Coot		Emsley, P., Cowtan, K. Coot: model-building tools for molecular graphics. <i>Acta Crystallogr D Biol Crystallogr</i> . 60 , 2126-32 (2004).	
refmac5		Murshudov, G.N., Vagin, A.A., Dodson, E.J. Refinement of Macromolecular Structures by the Maximum-Likelihood Method. <i>Acta Crystallographica Section D</i> . 53 , 240--255 (1997).	
Matthews		Matthews, B.W. Solvent content of protein crystals. <i>Journal of Molecular Biology</i> . 33 (2), 491-497 (1968).	