

Materials List for

Modeling Ligands into Maps Derived from Electron Cryomicroscopy

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Materials

Name	Company	Catalog Number	Comments
CCP4-8.0	Consortium of several institutes	https://www.ccp4.ac.uk	Free for academic users and includes Coot and list of tools developed for X-ray crystallography
CCP-EM	Consortium of several institutes	https://www.ccpem.ac.uk/ download.php	Free for academic users and includes Coot, Relion and many others
Coot	Paul Emsley, LMB, Cambridge	https://www2.mrc-lmb.cam.ac.uk/ personal/pemsley/coot/	General software for model building but also available with other suites described above
DockinMap (Phenix)	Consortium of several institutes	https://phenix-online.org/ documentation/reference/ dock_in_map.html	Software inside the Phenix suite for docking model into cryoEM maps
Electron Microscopy Data Bank	Consortium of several institutes	https://www.ebi.ac.uk/emdb/	Public Repository for Electron Microscopy maps
Falcon	Thermo Fisher Scientific	https://assets.thermofisher.com/ TFS-Assets/MSD/Technical-Notes/ Falcon-3EC-Datasheet.pdf	Commercial, camera from Thermo Fisher
Phenix	Consortium of several institutes	https://phenix-online.org/download	Free for academic users and includes Coot
Protein Data Bank	Consortium of several institutes	https://rcsb.org	Public database of macromolecular structures
Pymol	Schrodinger	https://pymol.org/2/	Molecular viusalization tool. Educational version is free but comes with limitation. The full version can be obtained with a small fee.
Relion	MRC-LMB, Cambridge	https://relion.readthedocs.io/en/ release-4.0/Installation.html	Software for cryoEM image processing, also available with CCP-EM
Titan Krios	Thermo Fisher Scientific	https://www.thermofisher.com/in/ en/home/electron-microscopy/ products/transmission-electron- microscopes/krios-g4-cryo-tem.html? cid=msd_ls_xbu_xmkt_tem- krios_285811_gl_pso_gaw_tpne1c& gad_source=1&gclid=CjwKCAiA-P- rBhBEEiwAQEXhHyw5c8MKThmdA	Commercial, cryoTEM from Thermo Fisher

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		AkZesWC4FYQSwlQRk ZApkj08MfYG040DtiiuL8 RihoCebEQAvD_BwE	
UCSF Chimera	UCSF, USA	https://www.cgl.ucsf.edu/chimera/ download.html	General purpose software for display, analysis and more
UCSF Chimera X	UCSF, USA	https://www.cgl.ucsf.edu/chimerax/	General purpose software for display, analysis and more