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Libraries:

CCTBX (python/C++)	General crystallography. Computation, optimization, I/O, incl. sublibraries
Clipper (C++)	Macromolecular crystallography, I/O for CCP4 formats
CRYSML (Fortran90)	Powder diffraction, magnetism, symmetry, structures, refinement
biopython (python)	mmcif/PDB coordinates, sequences, geometry, easy extension
mmDB (C++)	Macromolecular crystallography, PDB, symmetry
CMTZLIB (C/C++)	Handling mtz (including unmerged)
CSXMLIB (C/C++ namespace)	Handling symmetry
OBJCRYST (C++)	Powder diffraction, part of Fox
Pyobjcryst (python)	Powder diffraction, part of Fox
DISCAMB (C++)	Calculates SFs for multipole models
OpenBabel (C++)	General library for file formats in chemistry
scipy (python)	Computing for all kinds
DISCUS	Tool for programming in diffuse scattering, good for teaching
API of CSD	Search functions for SMX
APIs of PDB/RCSB	Search functions for MX
MMTF-PYSPARK (python, others)	Fast PDB queries and structure file operations