

DIALS cheat sheet



Main processing commands

Input	Output	Description
<code>dials.import image_*.cbf</code>	<code>datablock.json</code>	Import images
<code>dials.find_spots datablock.json [nproc=8]</code>	<code>strong.pickle</code>	Find strong spots on sequence of images, optionally using nproc processors
<code>dials.index datablock.json strong.pickle [unit_cell=79,79,37,90,90,90] [space_group=P43212]</code>	<code>experiments.json</code> <code>indexed.pickle</code>	Autoindex results of spotfinding, optionally specifying unit cell and space group (if known)
<code>dials.refine_bravais_settings experiments.json indexed.pickle</code>	<code>bravais_settings_[n].json</code>	Refine crystal models in Bravais settings consistent with primitive unit cell
<code>dials.reindex indexed.pickle change_of_basis_op=-b,-a,-c</code>	<code>reindexed.pickle</code>	Reindex an indexed.pickle or experiment.json file with the given change of basis operator
<code>dials.refine bravais_settings_[n].json reindexed.pickle [scan_varying=true]</code>	<code>refined_experiments.json</code> <code>refined.pickle</code>	Refine the experimental models against the indexed reflections, optionally allowing the crystal model to vary with image number
<code>dials.integrate refined_experiments.json refined.pickle [nproc=8]</code>	<code>integrated_experiments.json</code> <code>integrated.pickle</code>	Integrate reflections, using the strong reflections in indexed.pickle to model the reflection profiles
<code>dials.export integrated_experiments.json integrated.pickle</code>	<code>integrated.mtz</code>	Export results of dials.integrate as mtz file suitable for input to Pointless

Utilities

<code>dials.show datablock.json</code>		Show contents of DIALS model files
<code>dials.show experiments.json</code>		
<code>dials.image_viewer datablock.json</code>		View diffraction images, optionally overlaid with reflections from spotfinding or shoeboxes from integration
<code>dials.image_viewer datablock.json strong.pickle</code>		
<code>dials.image_viewer datablock.json integrated.pickle</code>		
<code>dials.reciprocal_lattice_viewer datablock.json strong.pickle</code>		View results of spotfinding in reciprocal space
<code>dials.check_indexing_symmetry experiments.json indexed.pickle [sym_op_threshold=0.5] [grid_search_scope=3]</code>		Check indexed reflection list for presence of symmetry elements and/or perform grid search for mis-indexed origin
<code>dials.discover_better_experimental_model datablock.json strong.pickle</code>	<code>optimized_datablock.json</code>	Search for better beam centre
<code>dials.report reflections.pickle</code>	<code>dials-report.html</code>	Generate a html report from input reflections.pickle and/or experiment.json files
<code>dials.report experiments.json</code>		
<code>dials.plot_scan_varying_crystal refined_experiments.json</code>		Generate plots of scan-varying crystal orientation and unit cell

