

CellCheckCSD User Guide

1.2 Release

Copyright © 2018 Cambridge Crystallographic Data Centre

Registered Charity No 800579

Contents

1	General Information.....	1
1.1	Supported Platforms.....	1
2	Windows Version Instructions.....	2
2.1	Usage.....	2
2.2	Examples.....	2
3	Linux Version Instructions.....	3
3.1	Usage.....	3
3.2	Examples.....	3
4	Making CellCheck CSD Available Globally on Linux.....	4

1 General Information

CellCheckCSD is best used via third-party XRD data collection programs that act as an interface to it, such as Agilent's CrysAlis^{Pro}, or Bruker's APEX2. CellCheckCSD may also be used via the command line by first preparing a suitable XML input file, by using the arguments detailed below. See the example XML query files and the ReducedCellQuerySchema.txt file for details on how to construct a suitable input XML file.

1.1 Supported Platforms

CellCheckCSD 1.2 is supported on:

- Windows - Intel compatible, 32-bit executables (compatible with 32-bit and 64-bit versions of Windows) for:
 - Windows 7, 8 and 10
- Linux - Intel compatible. Both 32-bit and 64-bit versions are available for:
 - RedHat Enterprise 6 and 7
 - CentOS 6 and 7
 - Ubuntu 12, 14 and 16

Note: As we add support for newer versions of Linux, support for older versions may have to be withdrawn.

2 Windows Version Instructions

2.1 Usage

CellCheckCSD is run via the 'ccdc_searcher.bat' file located in the top directory of your installation. It is run in the following way via a DOS command prompt window from within the top directory of your installation:

```
ccdc_searcher.bat -query <XML query file path> [-results <XML  
results file path>] [-help]
```

- query : Required Argument - the full path to the XML query file to search for
- results : Optional Argument - the full path to the XML search results file to write; if not defined, will write results to 'ccdc_searcher.xml' in current directory
- help : Optional Argument - show usage and exit

2.2 Examples

```
ccdc_searcher.bat -query query1.xml  
ccdc_searcher.bat -query D:\queries\query2.xml -results  
D:\results\results2.xml
```

3 Linux Version Instructions

3.1 Usage

CellCheckCSD is run via the 'ccdc_searcher' script located in the 'bin' directory of your installation. It is run in the following way at a console from within the 'bin' subdirectory of your installation.

```
./ccdc_searcher -query <XML query file path> [-results <XML  
results file path>] [-help]
```

- query : Required Argument - the full path to the XML query file to search for
- results : Optional Argument - the full path to the XML search results file to write; if not defined, will write results to 'ccdc_searcher.xml' in current directory
- help : Optional Argument - show usage and exit

3.2 Examples

```
./ccdc_searcher -query query1.xml  
./ccdc_searcher -query /queries/query2.xml -results  
/results/results2.xml
```

4 Making CellCheck CSD Available Globally on Linux

To run CellCheckCSD from any location you will need to add the `<installdir>/bin` directory to your system `PATH`. To do so, use the commands:

```
export PATH=<installdir>/bin:$PATH
```

if using sh or bash shell, or

```
setenv PATH <installdir>/bin:$PATH
```

if using csh.

To make these changes permanent you will need to add these lines to your users' `.login` (csh) or `.profile` (sh) files. Alternatively, place the commands in a system-wide login or profile script (such as `/etc/profile`) to apply to all users.

Once done, typing

```
ccdc_searcher
```

from a command line prompt should start CellCheckCSD. `<installdir>` refers to the directory where WebCSD was installed.