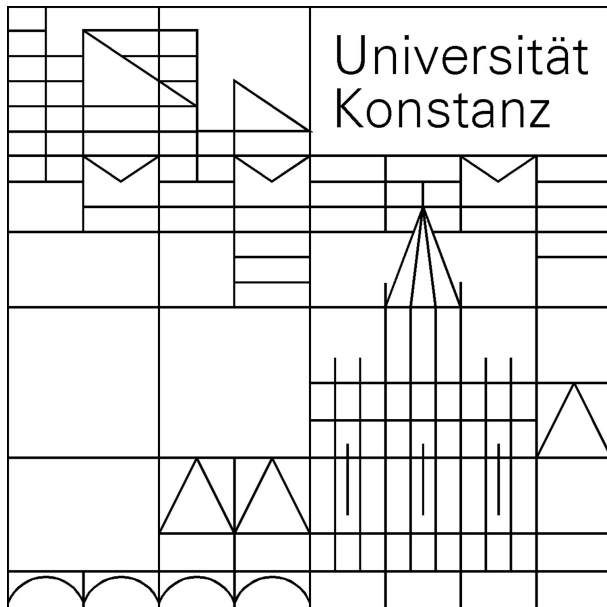


Crystallographic data processing with *XDS*, using *XDSGUI*



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The XDS program suite

Original author:
Wolfgang Kabsch
(Max-Planck-Institute
Heidelberg)

Since ~1986
I joined 2007



The XDS+ programs

- **XDS** - the main program: indexing, integrating, scaling, statistics
- *XSCALE*: - scale several XDS intensity data sets together; zero-dose extrapolation; statistics
- *XDSCONV*: convert to other programs' formats (e.g. MTZ file)

Programs independent from the XDS distribution:

- *XDS-Viewer* - inspect diagnostic images written by XDS, or (single) data frames (open source: sourceforge.net). Instead, *adxv* may be used
- *XDSSTAT* - additional statistics (not part of main distribution; download and use: see XDSwiki)
- **XDSGUI** – graphical user interface (open source: sourceforge.net) for XDS and *SHELX C/D/E* and *ARCIMBOLDO* (since latest version)
- *XDSCC12* – which data sets to re-index and merge?

Automatic processing: XDS

- beamline software (generating **XDS.INP**)
- scripts: **xia2** (CCP4), **autoPROC** (Globalphasing), *xdsme* (Soleil), *autoxds* (SSRL), *autoprocess* (CMCF), ... **generate_XDS.INP** (XDSwiki), *fast_dp* (Diamond)
- CCP4: *pointless*, *xdsconv* (type CCP4_I+F, or CCP4, or CCP4_I, or CCP4_F)
- SHELX: *shelxc* reads XDS_ASCII.HKL

Pipelines process standard data sets ok; fraction = ?

Automation is a good servant but a poor master!

Manual processing: *XDSGUI*

- problems in phasing and refinement
often due to bad / wrong data processing
- visually inspect frames; mask shadows
- optimize parameters, frame range,
resolution cutoff ..
- plots instead of tables
- interfaces to *XDS* through its files
- user – extensible / modifiable commands

Sources of information

- *XDS* main website:

<http://xds.mpimf-heidelberg.mpg.de> - complete, accurate, up-to-date documentation; download

- XDSwiki:


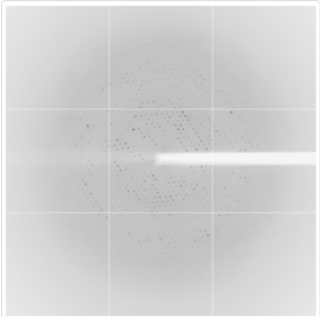
<http://strucbio.biologie.uni-konstanz.de/xdswiki> data sets; documentation; download; links to e.g.

Matthew J. Whitley's excellent tutorial given at CSHL 2018

- CCP4 bulletin board

Data used in this webinar: Nsp9 RNA binding protein of SARS CoV-2

Diffraction project datasets IDP51000_6w4b



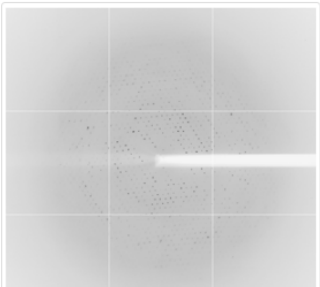
Resolution: 2.95 Å
Space group: P 61 2 2

[Download all images \(728.6 MB\)](#)
[PDB website for 6W4B](#)
[doi:10.18430/m36w4b](https://doi.org/10.18430/m36w4b)

Project details

Title	The crystal structure of Nsp9 RNA binding protein of SARS CoV-2
Authors	Tan, K., Kim, Y., Jedrzejczak, R., Maltseva, N., Endres, M., Michalska, K., Joachimiak, A., Center for Structural Genomics of Infectious Diseases (CSGID)
R / R _{free}	0.24 / 0.28
Unit cell edges [Å]	89.88 x 89.88 x 132.59
Unit cell angles [°]	90.0, 90.0, 120.0

Dataset 3-SRb4suc-2.####.img details



Number of frames	120 (1 - 120)
Distance [mm]	390.0
Oscillation width [°]	1.00
Omega [°]	-120.0
Wavelength [Å]	0.97919
Experiment Date	2020-03-06
Equipment	19-BM at APS (Advanced Photon Source)

https://proteindiffraction.org/project/IDP51000_6w4b/

References

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P.A. Karplus and K. Diederichs (2012) Linking Crystallographic Data with Model Quality. *Science* **336**, 1030-1033.

Diederichs K., "Crystallographic data and model quality" in *Nucleic Acids Crystallography* (Ed. Ennifar), Methods in Molecular Biology (Springer 2015)

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