

# 2VB1

## From XDSwiki

This reports processing of triclinic hen egg-white lysozyme data @ 0.65Å resolution (PDB id 2VB1 (<http://www.rcsb.org/pdb/explore/explore.do?structureId=2VB1>) ). Data (sweeps a to h, each comprising 60 to 360 frames of 72MB) were collected by Zbigniew Dauter at APS 19-ID and are available from here ([http://bl831.als.lbl.gov/example\\_data\\_sets/APS/19-ID/2vb1/](http://bl831.als.lbl.gov/example_data_sets/APS/19-ID/2vb1/)) . Details of data collection, processing and refinement are published (<http://journals.iucr.org/d/issues/2007/12/00/be5097/index.html>) .

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## XDS processing

1. use generate\_XDS.INP to obtain a good starting point
2. edit XDS.INP and change/add the following:

```

-----
! ORGX=3130 ORGY=3040 ! for ADSC, header values are subject to interpretation; these values from visual inspection
! the following is for masking the beamstop shadow in sweeps c-d
UNTRUSTED_RECTANGLE==0 3189 2960 3087 ! use XDS-viewer of ADXV to find the values
! the following is for sweeps e-h
UNTRUSTED_RECTANGLE=1 3160 3000 3070
TRUSTED_REGION=0 1.5 ! we want the whole detector area
ROTATION_AXIS=-1 0 0 ! at this beamline the spindle goes backwards!
SILICON=34.812736 ! account for theta-dependant absorption in the CCD's phosphor. The correction is only
! significant for hi-res data; 34.812736=32*(value for silicon as printed to CORRECT.LP if SILICON= not given)
MAXIMUM_NUMBER_OF_PROCESSORS=4 ! for fast processing on a machine with many cores (e.g. for 16 cores)
MAXIMUM_NUMBER_OF_JOBS=6 ! "overcommit" the available cores but on the whole this produces results faster
SPACE_GROUP_NUMBER=1 ! this is known
UNIT_CELL_CONSTANTS= 27.07 31.25 33.76 87.98 108.00 112.11 ! from 2vb1
FRIEDEL'S_LAW=TRUE ! we're not concerned with the anomalous signal
-----

```

Then, run "xds\_par". It completes after about 5 minutes on a fast machine, and we may inspect (at least) IDXREF.LP and CORRECT.LP (see below), and use "XDS-viewer FRAME.cbf" to get a visual impression of the integration as it applies to the last frame. By inspecting IDXREF.LP, one should make sure that everything works as it should, i.e. that a large percentage of reflections was actually indexed nicely, e.g.:

```

...
63879 OUT OF 72321 SPOTS INDEXED.
...
***** DIFFRACTION PARAMETERS USED AT START OF INTEGRATION *****
REFINED VALUES OF DIFFRACTION PARAMETERS DERIVED FROM 63879 INDEXED SPOTS
REFINED PARAMETERS:  DISTANCE BEAM AXIS CELL ORIENTATION
STANDARD DEVIATION OF SPOT POSITION (PIXELS) 0.53
STANDARD DEVIATION OF SPINDLE POSITION (DEGREES) 0.12

```

## Optimization

The main target of optimization is the asymptotic (ie. best) I/sigma (ISa) (Diederichs (2010) Acta Cryst. D 66, 733-40 (<http://dx.doi.org/10.1107/S0907444910014836>) ) as printed out by CORRECT (and XSCALE). A higher ISa should mean better data.

However: ISa also rises if more reflections are thrown out as outliers ("misfits") so it is not considered to be optimization if just WFAC1 is reduced. Please note that the default WFAC1 is 1; this should result in the rejection of about 1% of observations. If you feel that 1% is too much then just increase WFAC1, to, say, 1.5 - that should result in rejection of less than (say) 0.1%. This will slightly increase completeness, but will reduce I/sigma and ISa, and increase R-factors.

The following quantities may be tested for their influence on ISa:

- copying GXPARAM.XDS to XPARAM.XDS
- including the information from the first integration pass into XDS.INP - just do "grep \_E INTEGRATE.LP|tail -2" and get e.g.

```

BEAM_DIVERGENCE= 0.386 BEAM_DIVERGENCE_E.S.D.= 0.039
REFLECTING_RANGE= 0.669 REFLECTING_RANGE_E.S.D.= 0.096

```

copy these two lines into XDS.INP

- prevent refinement in INTEGRATE: REFINEMENT(INTEGRATE)= !

## Example: sweep e

### XDS.INP; as generated by generate\_XDS.INP

```

generate_XDS.INP ".../APS/19-ID/2vb1/p1lyso_e.0???.img"

```

Then include the changes detailed above, resulting in:

```

JOB= XYCORR INIT COLSPOT IDXREF DEFPIX INTEGRATE CORRECT
MAXIMUM_NUMBER_OF_PROCESSORS=4
MAXIMUM_NUMBER_OF_JOBS=6
ORGX= 3130 ORGY= 3040 ! check these values with adxv !
UNTRUSTED_RECTANGLE=1 3160 3000 3070 ! <xmin xmax ymin ymax> to mask shadow of beamstop; XDS-viewer to find out
DETECTOR_DISTANCE= 99.9954
OSCILLATION_RANGE= 0.500
X-RAY_WAVELENGTH= 0.6525486
NAME_TEMPLATE_OF_DATA_FRAMES=../../APS/19-ID/2vb1/p1lyso_e.0???.img
! REFERENCE_DATA_SET=xxx/XDS_ASCII.HKL ! e.g. to ensure consistent indexing
DATA_RANGE=1 360
SPOT_RANGE=1 180
! BACKGROUND_RANGE=1 10 ! rather use defaults (first 5 degree of rotation)

SPACE_GROUP_NUMBER=1 ! 0 if unknown
UNIT_CELL_CONSTANTS= 27.07 31.25 33.76 87.98 108.00 112.11 ! PDB 2vb1
INCLUDE_RESOLUTION_RANGE=50 0 ! after CORRECT, insert high resol limit; re-run CORRECT

! FRIEDEL'S_LAW=FALSE ! This acts only on the CORRECT step
! If the anom signal turns out to be, or is known to be, very low or absent,
! use FRIEDEL'S_LAW=TRUE instead (or comment out the line); re-run CORRECT

! remove the "!" in the following line:
! STRICT_ABSORPTION_CORRECTION=TRUE
! if the anomalous signal is strong: in that case, in CORRECT.LP the three
! "CHI^2-VALUE OF FIT OF CORRECTION FACTORS" values are significantly> 1, e.g. 1.5

! exclude (mask) untrusted areas of detector, e.g. beamstop shadow :
! UNTRUSTED_RECTANGLE= 1800 1950 2100 2150 ! x-min x-max y-min y-max ! repeat
! UNTRUSTED_ELLIPSE= 2034 2070 1850 2240 ! x-min x-max y-min y-max ! if needed

! parameters with changes wrt default values:
TRUSTED_REGION=0.00 1.5 ! partially use corners of detectors; 1.41421=full use
VALUE_RANGE_FOR_TRUSTED_DETECTOR_PIXELS=7000. 30000. ! often 8000 is ok
MINIMUM_ZETA=0.05 ! integrate close to the Lorentz zone; 0.15 is default
STRONG_PIXEL=6 ! COLSPOT: only use strong reflections (default is 3)
MINIMUM_NUMBER_OF_PIXELS_IN_A_SPOT=3 ! default of 6 is sometimes too high
REFINE(INTEGRATE)=CELL BEAM ORIENTATION ! AXIS DISTANCE

! parameters specifically for this detector and beamline:
DETECTOR= ADSC MINIMUM_VALID_PIXEL_VALUE= 1 OVERLOAD= 65000
SENSOR_THICKNESS=0.01 SILICON=34.812736
NX= 6144 NY= 6144 QX= 0.051294 QY= 0.051294 ! to make CORRECT happy if frames are unavailable
DIRECTION_OF_DETECTOR_X-AXIS=1 0 0
DIRECTION_OF_DETECTOR_Y-AXIS=0 1 0
INCIDENT_BEAM_DIRECTION=0 0 1
ROTATION_AXIS=-1 0 0 ! at e.g. SERCAT ID-22 this needs to be -1 0 0
FRACTION_OF_POLARIZATION=0.98 ! better value is provided by beamline staff!
POLARIZATION_PLANE_NORMAL=0 1 0

```

## CORRECT.LP 1st pass

```

STANDARD DEVIATION OF SPOT POSITION (PIXELS) 0.87
STANDARD DEVIATION OF SPINDLE POSITION (DEGREES) 0.10
CRYSTAL MOSAICITY (DEGREES) 0.126
...
a b ISa
6.630E+00 1.091E-04 37.18
...
SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION
RESOLUTION NUMBER OF REFLECTIONS COMPLETENESS R-FACTOR R-FACTOR COMPARED I/SIGMA R-meas Rmrgd-F Anomal Sig
LIMIT OBSERVED UNIQUE POSSIBLE OF DATA observed expected
1.77 9195 4841 9501 51.0% 1.5% 1.5% 8708 48.74 2.1% 1.6% 0% 0.0
1.26 29991 15327 16721 91.7% 1.5% 1.6% 29328 45.26 2.1% 1.7% 0% 0.0
1.03 38643 19731 21636 91.2% 1.7% 1.7% 37824 38.67 2.5% 2.1% 0% 0.0
0.89 46156 23404 25561 91.6% 2.3% 2.4% 45504 27.56 3.3% 3.4% 0% 0.0
0.80 51509 26034 28868 90.2% 4.0% 4.0% 50950 17.55 5.6% 7.0% 0% 0.0
0.73 55989 28253 32034 88.2% 7.0% 6.8% 55472 10.98 9.8% 13.2% 0% 0.0
0.68 59733 30115 34776 86.6% 13.1% 13.0% 59236 6.08 18.6% 26.0% 0% 0.0
0.63 35385 18436 37367 49.3% 25.6% 26.9% 33898 2.99 36.3% 52.1% 0% 0.0
0.60 8991 4972 39725 12.5% 51.2% 56.9% 8038 1.34 72.4% 105.0% 0% 0.0
total 335592 171113 246189 69.5% 2.3% 2.4% 328958 19.58 3.3% 7.4% 0% 0.0

NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES 343716
NUMBER OF REJECTED MISFITS 8112
NUMBER OF SYSTEMATIC ABSENT REFLECTIONS 0
NUMBER OF ACCEPTED OBSERVATIONS 335604
NUMBER OF UNIQUE ACCEPTED REFLECTIONS 171119

```

The number of "misfits" (rejections) is higher than expected (1 %). Either one considers the anomalous signal (of the 6 sulfurs) to be significant, or one simply increases WFAC1 from its default of 1, to (say) 1.2 .

## XDS.INP; optimized

Using the output of "grep \_E INTEGRATE.LP|tail -2" edit XDS.INP to have

```

JOB= INTEGRATE CORRECT
BEAM_DIVERGENCE= 0.428 BEAM_DIVERGENCE_E.S.D.= 0.043
REFLECTING_RANGE= 0.880 REFLECTING_RANGE_E.S.D.= 0.126
...
REFINE(INTEGRATE)= !

```

Then "cp GXPARM.XDS XPARAM.XDS", and then another round of "xds\_par". Five minutes later, we get:

## CORRECT.LP optimization pass

This looks a little bit better - less standard deviation, higher ISa, better R-factors, less misfits:

```

STANDARD DEVIATION OF SPOT POSITION (PIXELS) 0.83
STANDARD DEVIATION OF SPINDLE POSITION (DEGREES) 0.08
CRYSTAL MOSAICITY (DEGREES) 0.096

a b ISa
6.439E+00 1.076E-04 37.98
...

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION
RESOLUTION NUMBER OF REFLECTIONS COMPLETENESS R-FACTOR R-FACTOR COMPARED I/SIGMA R-meas Rmrgd-F Anomal Sig
LIMIT OBSERVED UNIQUE POSSIBLE OF DATA observed expected
1.77 9149 4817 9501 50.7% 1.5% 1.5% 8664 49.75 2.1% 1.5% 0% 0.0
1.26 30049 15348 16723 91.8% 1.5% 1.6% 29402 46.26 2.1% 1.6% 0% 0.0
1.03 38920 19863 21637 91.8% 1.7% 1.7% 38114 39.61 2.4% 2.0% 0% 0.0
0.89 46381 23508 25562 92.0% 2.2% 2.3% 45746 28.39 3.1% 3.2% 0% 0.0
0.80 51605 26071 28868 90.3% 3.8% 3.8% 51068 18.21 5.3% 6.5% 0% 0.0
0.73 56126 28314 32041 88.4% 6.6% 6.4% 55624 11.45 9.3% 12.3% 0% 0.0
0.68 59735 30093 34771 86.5% 12.6% 12.3% 59284 6.34 17.8% 24.8% 0% 0.0
0.63 35754 18620 37370 49.8% 24.1% 25.5% 34268 3.11 34.1% 48.9% 0% 0.0
0.60 9180 5075 39730 12.8% 48.6% 54.3% 8210 1.40 68.7% 100.5% 0% 0.0
total 336899 171709 246203 69.7% 2.2% 2.3% 330380 20.14 3.2% 6.9% 0% 0.0

NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES 344751
NUMBER OF REJECTED MISFITS 7842
NUMBER OF SYSTEMATIC ABSENT REFLECTIONS 0
NUMBER OF ACCEPTED OBSERVATIONS 336909
NUMBER OF UNIQUE ACCEPTED REFLECTIONS 171714

```

## further optimization

Another round of optimization again improves the R-factors and I/sigma at high resolution a bit, but it also increased the misfits back to 8200. At this point I decided to switch to FRIEDEL'S\_LAW=FALSE, and the resulting table is:

```

NOTE: Friedel pairs are treated as different reflections.

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION
RESOLUTION NUMBER OF REFLECTIONS COMPLETENESS R-FACTOR R-FACTOR COMPARED I/SIGMA R-meas Rmrgd-F Anomal Sig
LIMIT OBSERVED UNIQUE POSSIBLE OF DATA observed expected
1.77 9599 9023 19002 47.5% 1.5% 1.5% 1152 36.81 2.1% 1.6% 0% 0.0
1.26 31196 28239 33446 84.4% 1.4% 1.6% 5914 34.40 2.0% 1.6% 0% 0.0
1.03 40125 35205 43274 81.4% 1.7% 1.7% 9840 30.09 2.4% 2.0% 0% 0.0
0.89 46987 40188 51124 78.6% 2.3% 2.3% 13598 22.03 3.2% 3.4% 0% 0.0
0.80 52229 43723 57738 75.7% 3.9% 3.9% 17012 14.44 5.5% 6.6% 0% 0.0
0.73 56830 46674 64088 72.8% 7.1% 6.8% 20312 9.30 10.1% 13.2% 0% 0.0
0.68 60488 48814 69544 70.2% 13.9% 13.5% 23348 5.26 19.6% 27.1% 0% 0.0
0.63 36190 28598 74736 38.3% 28.2% 29.7% 15184 2.70 39.8% 57.3% 0% 0.0
0.60 9246 7246 79466 9.1% 57.8% 62.4% 4000 1.26 81.8% 122.0% 0% 0.0
total 342890 287710 492418 58.4% 2.8% 2.8% 110360 16.19 3.9% 9.9% 0% 0.0

NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES 345355
NUMBER OF REJECTED MISFITS 2448
NUMBER OF SYSTEMATIC ABSENT REFLECTIONS 0
NUMBER OF ACCEPTED OBSERVATIONS 342907
NUMBER OF UNIQUE ACCEPTED REFLECTIONS 287724

```

Indeed this brings the number of misfits to well below 1%, and it does make some sense.

## XSCALE results

The same strategy as shown for sweep e was used for sweeps a-d and f-h. XSCALE.INP is:

```

SPACE_GROUP_NUMBER= 1
UNIT_CELL_CONSTANTS= 27.07 31.25 33.76 87.98 108.00 112.11 ! from 2vb1 PDB entry
! cellparm for a-h gives 27.083 31.269 33.773 87.978 107.998 112.133

```

```

OUTPUT_FILE=lys-xds.ahkl
FRIEDEL'S_LAW=TRUE
RESOLUTION_SHELLS=2.91 2.06 1.68 1.45 1.30 1.19 1.10 1.03 0.97 0.92 0.88 0.84 0.81 0.78 0.75 0.73 0.71 0.69 0.67 0.65

INPUT_FILE=./a/XDS_ASCII.HKL
INCLUDE_RESOLUTION_RANGE=30 0.65
INPUT_FILE=./b/XDS_ASCII.HKL
INCLUDE_RESOLUTION_RANGE=30 0.65
INPUT_FILE=./c/XDS_ASCII.HKL
INCLUDE_RESOLUTION_RANGE=30 0.65
INPUT_FILE=./d/XDS_ASCII.HKL
INCLUDE_RESOLUTION_RANGE=30 0.65
INPUT_FILE=./e/XDS_ASCII.HKL
INCLUDE_RESOLUTION_RANGE=30 0.65
INPUT_FILE=./f/XDS_ASCII.HKL
INCLUDE_RESOLUTION_RANGE=30 0.65
INPUT_FILE=./g/XDS_ASCII.HKL
INCLUDE_RESOLUTION_RANGE=30 0.65
INPUT_FILE=./h/XDS_ASCII.HKL
INCLUDE_RESOLUTION_RANGE=30 0.65

```

## XSCALE.LP tables

The error model is adjusted by XSCALE:

a	b	ISa	ISa0	INPUT DATA SET
7.094E+00	1.294E-04	33.00	38.03	./a/XDS_ASCII.HKL
7.476E+00	1.170E-04	33.81	38.95	./b/XDS_ASCII.HKL
7.453E+00	1.598E-04	28.98	38.00	./c/XDS_ASCII.HKL
6.539E+00	1.640E-04	30.54	39.08	./d/XDS_ASCII.HKL
7.304E+00	1.342E-04	31.94	37.69	./e/XDS_ASCII.HKL
8.201E+00	1.574E-04	27.83	35.58	./f/XDS_ASCII.HKL
8.182E+00	1.759E-04	26.36	27.60	./g/XDS_ASCII.HKL
7.717E+00	3.694E-04	18.73	21.93	./h/XDS_ASCII.HKL

and there are about 1500 rejected reflections.

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION												
RESOLUTION LIMIT	NUMBER OF REFLECTIONS			COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR expected	I/SIGMA COMPARED	I/SIGMA	R-meas	Rmrgd-F	Anomal Corr	Signal to Noise
2.91	16170	2112	2147	98.4%	2.2%	2.4%	16157	78.96	2.5%	1.1%	-12%	0.7
2.06	40349	3831	3856	99.4%	2.4%	2.7%	40345	84.89	2.6%	0.9%	-9%	0.7
1.68	65329	5068	5087	99.6%	3.1%	3.2%	65321	83.77	3.3%	1.0%	0%	0.8
1.45	73373	6147	6163	99.7%	3.2%	3.5%	73371	78.02	3.4%	1.0%	2%	0.8
1.30	71196	6651	6657	99.9%	3.2%	3.5%	71196	71.07	3.4%	1.1%	4%	0.8
1.19	74542	7287	7298	99.8%	3.2%	3.4%	74534	67.06	3.3%	1.2%	5%	0.8
1.10	84918	8269	8278	99.9%	3.4%	3.7%	84891	63.24	3.6%	1.3%	7%	0.8
1.03	87890	8584	8603	99.8%	4.1%	4.4%	87855	56.26	4.4%	1.5%	5%	0.8
0.97	92917	9460	9465	99.9%	5.2%	5.6%	92894	48.90	5.5%	1.7%	4%	0.7
0.92	83994	9911	9927	99.8%	5.7%	6.3%	83969	41.67	6.0%	2.0%	6%	0.7
0.88	74100	9620	9621	100.0%	6.3%	7.1%	74082	35.74	6.7%	2.5%	4%	0.7
0.84	81322	11511	11518	99.9%	6.9%	7.7%	81300	30.43	7.3%	3.3%	1%	0.7
0.81	67539	10239	10247	99.9%	7.1%	7.7%	67518	25.96	7.7%	4.2%	2%	0.7
0.78	73980	11807	11817	99.9%	7.1%	7.3%	73951	22.34	7.7%	5.3%	2%	0.7
0.75	86111	13831	13839	99.9%	8.4%	8.6%	86076	18.77	9.2%	6.8%	2%	0.8
0.73	64554	10481	10488	99.9%	10.3%	10.4%	64525	15.73	11.3%	8.2%	3%	0.8
0.71	71891	11727	11741	99.9%	12.8%	13.0%	71844	12.95	14.0%	10.6%	3%	0.8
0.69	80168	13157	13163	100.0%	16.6%	16.9%	80065	10.16	18.2%	14.1%	2%	0.7
0.67	84431	14747	14766	99.9%	22.2%	22.7%	84231	7.44	24.4%	19.7%	3%	0.7
0.65	61031	15592	16551	94.2%	27.6%	30.6%	60165	4.36	31.8%	33.1%	1%	0.7
total	1435805	190032	191232	99.4%	3.1%	3.3%	1434290	33.42	3.3%	3.1%	3%	0.8

If two more resolution shells are added, they look like -

0.64	23276	7411	9155	81.0%	35.0%	40.6%	22324	2.90	41.7%	47.9%	3%	0.6
0.63	18044	6488	9647	67.3%	42.2%	49.7%	16630	2.22	50.7%	60.9%	-5%	0.6

So there is still useful signal beyond 0.65 Å.

Remark: The first frames of sweeps g and h show a shadow in one corner of the detector. Nothing was done by me to exclude this shadow from processing (but one should do so if the resolution should be expanded beyond 0.65 Å which the XSCALE statistics suggest to

be possible). There is however no facility in XDS to exclude bad areas of specific frames in a dataset; one would need to chop the dataset into two parts.

## Comparison of data processing: published (2006) vs XDS results

	resolution (highest resolution range)	observations	unique reflections	Multiplicity	Completeness (%)	R merge (%)	mean I/sigma
published (2006)	30-0.65Å (0.67-0.65Å)	1331953 (12764)	187165 (6353)	7.1 (2.7)	97.6 (67.3)	4.5 (18.4)	36.2 (4.2)
XDS Version Dec 06, 2010	30-0.65Å (0.67-0.65Å)	1435805 (61031)	190032 (15592)	7.5 (3.9)	99.4 (94.2)	3.1 (27.6)	33.4 (4.4)

## Data from XDS processing

I changed XSCALE.INP to have

```

!FRIEDEL'S_LAW=TRUE ! by commenting it out XSCALE will use FRIEDEL'S_LAW=FALSE
!!
!! since this is how the data were processed
RESOLUTION_SHELLS=2.91 2.06 1.68 1.45 1.30 1.19 1.10 1.03 0.97 0.92 0.88 0.84 0.80 0.76 0.73 0.70 0.67 0.65 0.64 0.63

```

and ran XSCALE again, to get a file with reflections to 0.63 Å.

Conversion to other program systems is performed with XDSCONV. XDSCONV.INP for producing a MTZ file with intensities and anomalous signal is:

```

INPUT_FILE= lys-xds.ahkl
OUTPUT_FILE=temp.hkl CCP4_I

```

After running xdscnv, I cut-and-paste the screen output:

```

!f2mtz HKLOUT temp.mtz<F2MTZ.INP
!cad HKLIN1 temp.mtz HKLOUT output_file_name.mtz<<EOF
LABIN FILE 1 ALL
!END
!EOF

```

and obtain output\_file\_name.mtz which I mv to xds-hewl-I.mtz (<ftp://turn5.biologie.uni-konstanz.de/pub/xds-datared/2vb1/xds-hewl-I.mtz>) . SFCHECK statistics for this file are here ([ftp://turn5.biologie.uni-konstanz.de/pub/xds-datared/2vb1/sfcheck\\_XXXX.pdf](ftp://turn5.biologie.uni-konstanz.de/pub/xds-datared/2vb1/sfcheck_XXXX.pdf)) .

Similarly, using OUTPUT\_FILE=temp.hkl CCP4 I obtained a file with amplitudes, xds-hewl-F.mtz (<ftp://turn5.biologie.uni-konstanz.de/pub/xds-datared/2vb1/xds-hewl-F.mtz>)

Retrieved from "<http://strucbio.biologie.uni-konstanz.de/xdswiki/index.php/2VB1>"

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