```
***** CORRECT ***** (VERSION November 3, 2014)  19-May-2015

INPUT PARAMETER VALUES
----------------------
SPACE_GROUP_NUMBER=    1 as used in the INTEGRATE step
UNIT_CELL_CONSTANTS=    36.908    78.959    78.947  89.976  89.958  90.002 as used by INTEGRATE
FRIEDEL'S_LAW=TRUE
PROFILE_FITTING= TRUE
OVERLOAD=     65000     MINPK=  75.00000    WFAC1=   1.0
INCLUDE_RESOLUTION_RANGE=    50.000     0.000
NAME_TEMPLATE_OF_DATA_FRAMES=../img/prefix_1_?????.img SMV
DATA_RANGE=       1     180
ROTATION_AXIS= -0.999999  0.000942  0.000546
OSCILLATION_RANGE=  1.000000
STARTING_ANGLE=     0.000     STARTING_FRAME=       1
X-RAY_WAVELENGTH=  0.979263
INCIDENT_BEAM_DIRECTION= -0.002920 -0.003140  1.021167
FRACTION_OF_POLARIZATION=   0.950
POLARIZATION_PLANE_NORMAL=  0.000000  1.000000  0.000000
AIR=   0.00100
DETECTOR=ADSC
SILICON=  3.704237 SENSOR_THICKNESS=  0.000000
NUMBER OF DETECTOR SEGMENTS   1
NX=  3072  NY=  3072    QX=  0.102592  QY=  0.102592
ORGX=   1539.93  ORGY=   1545.23
DETECTOR_DISTANCE=   140.310
DIRECTION_OF_DETECTOR_X-AXIS=   1.00000   0.00000   0.00000
DIRECTION_OF_DETECTOR_Y-AXIS=   0.00000   1.00000   0.00000
BEAM_DIVERGENCE_E.S.D.=   0.065
REFLECTING_RANGE_E.S.D.=   0.128
MINIMUM_ZETA=     0.050
MAXIMUM_ERROR_OF_SPOT_POSITION=   3.0
MAXIMUM_ERROR_OF_SPINDLE_POSITION=   2.0
MINIMUM_I/SIGMA=   3.0
REFLECTIONS/CORRECTION_FACTOR=      50
STRICT_ABSORPTION_CORRECTION=FALSE
CORRECTIONS= DECAY MODULATION ABSORPTION
REFERENCE_DATA_SET=


  566652 REFLECTIONS ON FILE "INTEGRATE.HKL"
       0 CORRUPTED REFLECTION RECORDS (IGNORED)
       0 MATCHING REFLECTIONS SPECIFIED IN FILE "FILTER.HKL"
       0 REFLECTIONS INCOMPLETE OR OUTSIDE IMAGE RANGE       1 ...     180
    2235 OVERLOADED REFLECTIONS (IGNORED)
     234 REFLECTIONS OUTSIDE ACCEPTED RESOLUTION RANGES
               OR TOO CLOSE TO ROTATION AXIS (IGNORED)
  564183 REFLECTIONS ACCEPTED


*******************************************************************************
```

## AUTOMATIC SPACE GROUP ASSIGNMENT

**********

XDS adopts the following approach.
(1) it looks for possible symmetries of the crystal lattice
(2) it computes a redundancy independent R-factor for all enantiomorphous
    point groups compatible with the observed lattice symmetry.
(3) it selects the group which explains the intensity data at an acceptable,
    redundancy-independent R-factor (Rmeas, Rrim) using a minimum number of
    unique reflections.

This approach does not test for the presence of screw axes. Consequently,
orthorhombic cell axes will be specified in increasing length (following
conventions), despite the possibility that different assignments for the
cell axes could become necessary for space groups P222(1) and P2(1)2(1)2
containing one or two screw axes, respectively.

The user can always override the automatic decisions by specifying the
correct space group number and unit cell constants in XDS.INP and repeating
the CORRECT step of XDS. This provides a simple way to rename orthorhombic
cell constants if screw axes are present.

In addition, the user has the option to specify in XDS.INP
(a) a reference data set or
(b) a reindexing transformation or
(c) the three basis vectors (if known from processing a previous data set
taken at the same crystal orientation in a multi-wavelength experiment).
These features of XDS are useful for resolving the issue of alternative
settings of polar or rhombohedral cells (like P4, P6, R3).

=====> Specifications provided by the user in XDS.INP:
SPACE_GROUP_NUMBER=    0 (0: unknown symmetry and unit cell)
UNIT_CELL_CONSTANTS=     0.00     0.00     0.00   0.000   0.000   0.000
UNIT_CELL_A-AXIS=     0.000     0.000     0.000 (0 0 0 : unknown)
UNIT_CELL_B-AXIS=     0.000     0.000     0.000 (0 0 0 : unknown)
UNIT_CELL_C-AXIS=     0.000     0.000     0.000 (0 0 0 : unknown)
REIDX=  0  0  0  0  0  0  0  0  0  0  0  0 (all 0 : not specified)
TEST_RESOLUTION_RANGE=   10.00    5.00 (Angstrom) for space group determination
NUMBER OF ACCEPTED REFLECTIONS FOR CALCULATING Rmeas             5566
NUMBER OF ACCEPTED UNIQUE REFLECTIONS FROM REFERENCE DATA SET       0

********** DETERMINATION OF LATTICE CHARACTER AND BRAVAIS LATTICE **********

The CHARACTER OF A LATTICE is defined by the metrical parameters of its
reduced cell as described in the INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY
Volume A, p. 746 (KLUWER ACADEMIC PUBLISHERS, DORDRECHT/BOSTON/LONDON, 1989).
Note that more than one lattice character may have the same BRAVAIS LATTICE.

A lattice character is marked "*" to indicate a lattice consistent with the
observed locations of the diffraction spots. These marked lattices must have
low values for the QUALITY OF FIT and their implicated UNIT CELL CONSTANTS
should not violate the ideal values by more than

```
MAX_CELL_AXIS_ERROR=  0.03
MAX_CELL_ANGLE_ERROR=           3.0 (Degrees)

The REINDEXING TRANSFORMATION REIDX() consists of 12 integers that relate
the original indices H,K,L from file INTEGRATE.HKL to the indices H',K',L'
with respect to the new cell.
   H'=(REIDX(1)*H+REIDX( 2)*K+REIDX( 3)*L)/IDXV+REIDX( 4)
   K'=(REIDX(5)*H+REIDX( 6)*K+REIDX( 7)*L)/IDXV+REIDX( 8)
   L'=(REIDX(9)*H+REIDX(10)*K+REIDX(11)*L)/IDXV+REIDX(12)
The value of the integer IDXV depends on the lattice type used for
specifying reflections on file INTEGRATE.HKL; IDXV is
1 for a primitive,
2 for a face or body centred,
3 for a rhombohedral,
4 for a lattice centred on all faces.
IDXV is set by XDS and cannot be input by the user.
```

| | LATTICE- CHARACTER | BRAVAIS- LATTICE | QUALITY OF FIT | UNIT CELL CONSTANTS (ANGSTROEM & DEGREES) a | b | c | alpha | beta | gamma | REINDEXING TRANSFORMATION | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| * | 31 | aP | 0.0 | 36.9 | 78.9 | 78.9 | 90.0 | 90.0 | 90.0 | 1 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 1 | 0 |
| * | 44 | aP | 0.0 | 36.9 | 78.9 | 78.9 | 90.0 | 90.0 | 90.0 | -1 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | -1 | 0 |
| * | 34 | mP | 0.2 | 36.9 | 78.9 | 78.9 | 90.0 | 90.0 | 90.0 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | -1 | 0 | 0 |
| * | 33 | mP | 0.4 | 36.9 | 78.9 | 78.9 | 90.0 | 90.0 | 90.0 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | -1 | 0 | 0 |
| * | 35 | mP | 0.4 | 78.9 | 36.9 | 78.9 | 90.0 | 90.0 | 90.0 | 0 | -1 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0 |
| * | 20 | mC | 0.5 | 111.6 | 111.6 | 36.9 | 90.0 | 90.0 | 90.0 | 0 | 1 | 1 | 0 | 0 | 1 | -1 | 0 | -1 | 0 | 0 | 0 |
| * | 32 | oP | 0.6 | 36.9 | 78.9 | 78.9 | 90.0 | 90.0 | 90.0 | -1 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | -1 | 0 |
| * | 23 | oC | 0.6 | 111.6 | 111.6 | 36.9 | 90.0 | 90.0 | 90.0 | 0 | 1 | -1 | 0 | 0 | -1 | -1 | 0 | -1 | 0 | 0 | 0 |
| * | 25 | mC | 0.6 | 111.6 | 111.6 | 36.9 | 90.0 | 90.0 | 90.0 | 0 | 1 | -1 | 0 | 0 | -1 | -1 | 0 | -1 | 0 | 0 | 0 |
| * | 21 | tP | 0.8 | 78.9 | 78.9 | 36.9 | 90.0 | 90.0 | 90.0 | 0 | 1 | 0 | 0 | 0 | 0 | -1 | 0 | -1 | 0 | 0 | 0 |
| | 39 | mC | 249.7 | 162.1 | 36.9 | 78.9 | 90.0 | 90.0 | 76.9 | 1 | -2 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0 |
| | 29 | mC | 249.8 | 36.9 | 162.1 | 78.9 | 90.0 | 90.0 | 76.9 | 1 | 0 | 0 | 0 | 1 | -2 | 0 | 0 | 0 | 0 | -1 | 0 |
| | 38 | oC | 249.8 | 36.9 | 162.1 | 78.9 | 90.0 | 90.0 | 103.1 | 1 | 0 | 0 | 0 | -1 | 2 | 0 | 0 | 0 | 0 | 1 | 0 |
| | 37 | mC | 249.9 | 162.1 | 36.9 | 78.9 | 90.0 | 90.0 | 76.9 | 1 | -2 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 0 |
| | 28 | mC | 249.9 | 36.9 | 162.1 | 78.9 | 90.0 | 90.0 | 76.9 | 1 | 0 | 0 | 0 | 1 | -2 | 0 | 0 | 0 | 0 | -1 | 0 |
| | 36 | oC | 250.0 | 36.9 | 162.1 | 78.9 | 90.0 | 90.0 | 103.1 | 1 | 0 | 0 | 0 | -1 | 2 | 0 | 0 | 0 | 0 | 1 | 0 |
| | 27 | mC | 499.7 | 162.1 | 36.9 | 111.6 | 90.0 | 133.5 | 76.9 | -1 | 2 | 0 | 0 | -1 | 0 | 0 | 0 | 0 | -1 | 1 | 0 |
| | 19 | oI | 499.9 | 36.9 | 111.6 | 117.6 | 90.0 | 71.7 | 90.0 | -1 | 0 | 0 | 0 | 0 | -1 | 1 | 0 | -1 | 1 | 1 | 0 |
| | 26 | oF | 624.5 | 36.9 | 162.1 | 162.1 | 87.0 | 103.2 | 103.1 | 1 | 0 | 0 | 0 | -1 | 2 | 0 | 0 | -1 | 0 | 2 | 0 |
| | 18 | tI | 624.7 | 111.6 | 117.6 | 36.9 | 71.7 | 90.0 | 90.0 | 0 | -1 | 1 | 0 | 1 | -1 | -1 | 0 | 1 | 0 | 0 | 0 |
| | 1 | cF | 999.0 | 117.6 | 117.6 | 117.6 | 95.7 | 95.6 | 143.4 | 1 | -1 | 1 | 0 | 1 | 1 | -1 | 0 | -1 | 1 | 1 | 0 |
| | 2 | hR | 999.0 | 87.1 | 87.1 | 117.6 | 118.4 | 61.6 | 100.3 | 1 | -1 | 0 | 0 | -1 | 0 | 1 | 0 | -1 | -1 | -1 | 0 |
| | 3 | cP | 999.0 | 36.9 | 78.9 | 78.9 | 90.0 | 90.0 | 90.0 | -1 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | -1 | 0 |
| | 5 | cI | 999.0 | 87.1 | 87.1 | 111.6 | 50.2 | 50.2 | 79.7 | -1 | 0 | -1 | 0 | -1 | 1 | 0 | 0 | 0 | 1 | -1 | 0 |
| | 4 | hR | 999.0 | 87.1 | 87.1 | 117.6 | 118.4 | 61.6 | 100.3 | -1 | -1 | 0 | 0 | 1 | 0 | -1 | 0 | 1 | -1 | 1 | 0 |
| | 6 | tI | 999.0 | 111.6 | 87.1 | 87.1 | 79.7 | 50.2 | 50.2 | 0 | 1 | -1 | 0 | -1 | 0 | -1 | 0 | -1 | 1 | 0 | 0 |
| | 7 | tI | 999.0 | 87.1 | 87.1 | 111.6 | 50.2 | 50.2 | 79.7 | -1 | 0 | -1 | 0 | -1 | 1 | 0 | 0 | 0 | 1 | -1 | 0 |
| | 8 | oI | 999.0 | 87.1 | 87.1 | 111.6 | 50.2 | 50.2 | 79.7 | 1 | -1 | 0 | 0 | 1 | 0 | 1 | 0 | 0 | -1 | 1 | 0 |
| | 9 | hR | 999.0 | 36.9 | 87.1 | 252.4 | 102.8 | 98.4 | 115.0 | 1 | 0 | 0 | 0 | -1 | 1 | 0 | 0 | -1 | -1 | 3 | 0 |
| | 10 | mC | 999.0 | 87.1 | 87.1 | 78.9 | 90.0 | 90.0 | 129.9 | 1 | 1 | 0 | 0 | 1 | -1 | 0 | 0 | 0 | 0 | -1 | 0 |
| | 11 | tP | 999.0 | 36.9 | 78.9 | 78.9 | 90.0 | 90.0 | 90.0 | -1 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | -1 | 0 |
| | 12 | hP | 999.0 | 36.9 | 78.9 | 78.9 | 90.0 | 90.0 | 90.0 | -1 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | -1 | 0 |
| | 13 | oC | 999.0 | 87.1 | 87.1 | 78.9 | 90.0 | 90.0 | 50.1 | -1 | 1 | 0 | 0 | 1 | 1 | 0 | 0 | 0 | 0 | -1 | 0 |

```
    15        tI        999.0      36.9   78.9  180.3  64.0  78.2  90.0    1  0  0  0  0  0  1  0  1 -2  1  0
    16        oF        999.0      87.1   87.1  180.3 108.0 118.9  50.1    1 -1  0  0 -1 -1  0  0 -1  1 -2  0
    14        mC        999.0      87.1   87.1   78.9  90.0  90.0  50.1   -1  1  0  0  1  1  0  0  0  0 -1  0
    17        mC        999.0      87.1   87.1   87.1  79.7 100.3  50.1   -1 -1  0  0  1 -1  0  0  1  0  1  0
    22        hP        999.0      78.9   78.9   36.9  90.0  90.0  90.0    0  1  0  0  0  0 -1  0 -1  0  0  0
    24        hR        999.0     180.3  111.6   36.9  90.0  78.2 108.0    1 -1  2  0  0 -1 -1  0  1  0  0  0
    30        mC        999.0      78.9  176.5   36.9  90.0  90.0  63.4    0  1  0  0  0  1 -2  0 -1  0  0  0
    40        oC        999.0      78.9  176.5   36.9  90.0  90.0 116.6    0 -1  0  0  0  1 -2  0  1  0  0  0
    42        oI        999.0      36.9   78.9  180.3 116.0 101.8  90.0   -1  0  0  0  0  0 -1  0  1 -2  1  0
    41        mC        999.0     176.5   78.9   36.9  90.0  90.0  63.4    0  2 -1  0  0  0 -1  0 -1  0  0  0
    43        mI        999.0      87.1  180.3   78.9 116.0 154.9  61.1   -1  1  0  0 -1  1 -2  0  0 -1  0  0

 ****** LATTICE SYMMETRY IMPLICATED BY SPACE GROUP SYMMETRY ******

BRAVAIS-            POSSIBLE SPACE-GROUPS FOR PROTEIN CRYSTALS
  TYPE                     [SPACE GROUP NUMBER,SYMBOL]
  aP      [1,P1]
  mP      [3,P2] [4,P2(1)]
 mC,mI    [5,C2]
  oP      [16,P222] [17,P222(1)] [18,P2(1)2(1)2] [19,P2(1)2(1)2(1)]
  oC      [21,C222] [20,C222(1)]
  oF      [22,F222]
  oI      [23,I222] [24,I2(1)2(1)2(1)]
  tP      [75,P4] [76,P4(1)] [77,P4(2)] [78,P4(3)] [89,P422] [90,P42(1)2]
          [91,P4(1)22] [92,P4(1)2(1)2] [93,P4(2)22] [94,P4(2)2(1)2]
          [95,P4(3)22] [96,P4(3)2(1)2]
  tI      [79,I4] [80,I4(1)] [97,I422] [98,I4(1)22]
  hP      [143,P3] [144,P3(1)] [145,P3(2)] [149,P312] [150,P321] [151,P3(1)12]
          [152,P3(1)21] [153,P3(2)12] [154,P3(2)21] [168,P6] [169,P6(1)]
          [170,P6(5)] [171,P6(2)] [172,P6(4)] [173,P6(3)] [177,P622]
          [178,P6(1)22] [179,P6(5)22] [180,P6(2)22] [181,P6(4)22] [182,P6(3)22]
  hR      [146,R3] [155,R32]
  cP      [195,P23] [198,P2(1)3] [207,P432] [208,P4(2)32] [212,P4(3)32]
          [213,P4(1)32]
  cF      [196,F23] [209,F432] [210,F4(1)32]
  cI      [197,I23] [199,I2(1)3] [211,I432] [214,I4(1)32]


 ********************* SYMMETRY OF REFLECTION INTENSITIES *********************

 Analysis of symmetry related reflections is based on strong data within a
 TEST_RESOLUTION_RANGE=   10.00    5.00 Angstrom (defined in XDS.INP).

 The symmetry test is carried out for the enantiomorphous space groups above
 (omitting those with screw axes) that conform with the observed lattice
 symmetry. The test is quantified by the redundancy independent R-factor,
 Rmeas, defined by Diederichs & Karplus, Nature Struct. Biol. 4, 269-275 (1997).

 For computation of Rmeas a minimum number of symmetry-related reflections is
 required and set by the user (in XDS.INP) as the parameter
                      MIN_RFL_Rmeas=   50

 Low values for Rmeas should be obtained if the crystal possesses the symmetry
```

elements of the tested space group. The decision whether the crystal's data
satisfy the requirements of the tested space group is based on a constant set
by the user (in XDS.INP) as the parameter
                    MAX_FAC_Rmeas=      2.
which provides an upper limit for acceptable Rmeas as a multiple of the
lowest Rmeas found for all tested space groups. If Rmeas is larger than this
upper limit, the corresponding space group symmetry is considered violated
by the observed data.

XDS will select (*) that space group that requires a minimum number of unique
reflections to account for the observed intensities at an acceptable Rmeas.

UNIQUE   = number of unique reflections
Rmeas    = redundancy independent R-factor (intensities)
COMPARED = number of reflections used for calculating Rmeas

| | SPACE-GROUP NUMBER | UNIT CELL CONSTANTS a | b | c | alpha | beta | gamma | UNIQUE | Rmeas | COMPARED | LATTICE-CHARACTER |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | 5 | 111.6 | 111.6 | 36.9 | 90.0 | 90.0 | 90.0 | 1655 | 3.8 | 3911 | 20 mC |
| | 75 | 78.9 | 78.9 | 36.9 | 90.0 | 90.0 | 90.0 | 896 | 4.6 | 4670 | 21 tP |
| * | 89 | 78.9 | 78.9 | 36.9 | 90.0 | 90.0 | 90.0 | 507 | 4.5 | 5059 | 21 tP |
| | 21 | 111.6 | 111.6 | 36.9 | 90.0 | 90.0 | 90.0 | 930 | 4.3 | 4636 | 23 oC |
| | 5 | 111.6 | 111.6 | 36.9 | 90.0 | 90.0 | 90.0 | 1656 | 4.2 | 3910 | 25 mC |
| | 1 | 36.9 | 78.9 | 78.9 | 90.0 | 90.0 | 90.0 | 3016 | 3.6 | 2550 | 31 aP |
| | 16 | 36.9 | 78.9 | 78.9 | 90.0 | 90.0 | 90.0 | 959 | 4.5 | 4607 | 32 oP |
| | 3 | 78.9 | 36.9 | 78.9 | 90.0 | 90.0 | 90.0 | 1720 | 4.3 | 3846 | 35 mP |
| | 3 | 36.9 | 78.9 | 78.9 | 90.0 | 90.0 | 90.0 | 1685 | 4.7 | 3881 | 34 mP |
| | 1 | 36.9 | 78.9 | 78.9 | 90.0 | 90.0 | 90.0 | 3016 | 3.6 | 2550 | 44 aP |

********** SELECTED SPACE GROUP AND UNIT CELL FOR THIS DATA SET **********

SPACE_GROUP_NUMBER=   89
UNIT_CELL_CONSTANTS=    78.94    78.94    36.90  90.000  90.000  90.000
UNIT_CELL_A-AXIS=   -64.886    16.823   -41.693
UNIT_CELL_B-AXIS=    38.033   -18.519   -66.653
UNIT_CELL_C-AXIS=   -11.200   -34.999     3.332
REFLECTIONS H,K,L FROM "INTEGRATE.HKL" WILL BE REINDEXED BY
H' = (  0*H +  1*K +  0*L)/ 1 +  0
K' = (  0*H +  0*K + -1*L)/ 1 +  0
L' = ( -1*H +  0*K +  0*L)/ 1 +  0

*****  8 EQUIVALENT POSITIONS IN SPACE GROUP # 89 *****

   If x',y',z' is an equivalent position to x,y,z, then
       x'=x*ML(1)+y*ML( 2)+z*ML( 3)+ML( 4)/12.0
       y'=x*ML(5)+y*ML( 6)+z*ML( 7)+ML( 8)/12.0
       z'=x*ML(9)+y*ML(10)+z*ML(11)+ML(12)/12.0

   #    1  2  3  4    5  6  7  8    9 10 11 12
   1    1  0  0  0    0  1  0  0    0  0  1  0
   2   -1  0  0  0    0 -1  0  0    0  0  1  0

```
   3   -1  0  0  0    0  1  0  0    0  0 -1  0
   4    1  0  0  0    0 -1  0  0    0  0 -1  0
   5    0 -1  0  0   -1  0  0  0    0  0 -1  0
   6    0  1  0  0    1  0  0  0    0  0 -1  0
   7    0  1  0  0   -1  0  0  0    0  0  1  0
   8    0 -1  0  0    1  0  0  0    0  0  1  0

*****************************************************************************
     MEAN DISCREPANCIES BETWEEN OBSERVED AND CALCULATED SPOT LOCATIONS
*****************************************************************************

The discrepancies in X- and Y-coordinates of the spots are depicted in the
two images DX-CORRECTIONS.cbf and DY-CORRECTIONS.cbf for inspection with
the XDS-Viewer.



*****************************************************************************
 REFINEMENT OF DIFFRACTION PARAMETERS USING ALL IMAGES
*****************************************************************************


 REFINED VALUES OF DIFFRACTION PARAMETERS DERIVED FROM 395935 INDEXED SPOTS
 REFINED PARAMETERS:   DISTANCE BEAM ORIENTATION CELL AXIS
 STANDARD DEVIATION OF SPOT    POSITION (PIXELS)     0.74
 STANDARD DEVIATION OF SPINDLE POSITION (DEGREES)    0.14
 SPACE GROUP NUMBER     89
 UNIT CELL PARAMETERS     78.977    78.977    36.914  90.000  90.000  90.000
 E.S.D. OF CELL PARAMETERS  5.1E-03 5.1E-03 8.7E-03 0.0E+00 0.0E+00 0.0E+00
 REC. CELL PARAMETERS   0.012662  0.012662  0.027090  90.000  90.000  90.000
 COORDINATES OF UNIT CELL A-AXIS   -64.921    16.823   -41.709
 COORDINATES OF UNIT CELL B-AXIS    38.045   -18.515   -66.687
 COORDINATES OF UNIT CELL C-AXIS   -11.210   -35.013     3.326
 CRYSTAL MOSAICITY (DEGREES)     0.128
 LAB COORDINATES OF ROTATION AXIS -0.999999  0.000913  0.000678
 DIRECT BEAM COORDINATES (REC. ANGSTROEM)  -0.002886 -0.003124  1.021167
 DETECTOR COORDINATES (PIXELS) OF DIRECT BEAM    1535.79   1540.87
 DETECTOR ORIGIN (PIXELS) AT                     1539.65   1545.06
 CRYSTAL TO DETECTOR DISTANCE (mm)       140.35
 LAB COORDINATES OF DETECTOR X-AXIS  1.000000  0.000000  0.000000
 LAB COORDINATES OF DETECTOR Y-AXIS  0.000000  1.000000  0.000000


 THE DATA COLLECTION STATISTICS REPORTED BELOW ASSUMES:
 SPACE_GROUP_NUMBER=   89
 UNIT_CELL_CONSTANTS=    78.98    78.98    36.91  90.000  90.000  90.000

*****************************************************************************
       MEAN INTENSITY AS FUNCTION OF SPINDLE POSITION WITHIN DATA IMAGE
*****************************************************************************

This statistics could serve as a diagnostic tool for detecting
```

shutter problems (suggested by Kay Diederichs).
Data are corrected for this effect if PATCH_SHUTTER_PROBLEM=TRUE in XDS.INP.
===> Selected : PATCH_SHUTTER_PROBLEM=FALSE

INTERVAL = Angular interval in units of the oscillation range
           covered by a data image.
NUMBER   = Number of reflections in each interval
INTENSITY= Mean intensity of the reflections in each interval
FACTOR   = Correction factor applied to intensities;
           INTENSITY(overall)/INTENSITY(interval)

| INTERVAL | | NUMBER | INTENSITY | FACTOR |
|---|---|---|---|---|
| -0.05 | 0.05 | 56404 | 4110.100 | 0.963 |
| 0.05 | 0.15 | 56105 | 4012.067 | 0.986 |
| 0.15 | 0.25 | 56411 | 3926.565 | 1.008 |
| 0.25 | 0.35 | 56086 | 3986.169 | 0.993 |
| 0.35 | 0.45 | 56415 | 3926.063 | 1.008 |
| 0.45 | 0.55 | 56647 | 3920.445 | 1.009 |
| 0.55 | 0.65 | 56642 | 3877.295 | 1.021 |
| 0.65 | 0.75 | 56541 | 3897.729 | 1.015 |
| 0.75 | 0.85 | 56190 | 3974.544 | 0.996 |
| 0.85 | 0.95 | 56742 | 3939.798 | 1.004 |
| -0.05 | 0.95 | 564183 | 3956.950 | 1.000 |

**********
CORRECTION FACTORS AS FUNCTION OF IMAGE NUMBER & RESOLUTION
**********

RECIPROCAL CORRECTION FACTORS FOR INPUT DATA SETS MERGED TO
OUTPUT FILE: XDS_ASCII.HKL

THE CALCULATIONS ASSUME FRIEDEL'S_LAW= TRUE
TOTAL NUMBER OF CORRECTION FACTORS DEFINED 660
DEGREES OF FREEDOM OF CHI^2 FIT 368398.9
CHI^2-VALUE OF FIT OF CORRECTION FACTORS 0.982
NUMBER OF CYCLES CARRIED OUT 3

CORRECTION FACTORS for visual inspection by XDS-Viewer DECAY.cbf
XMIN= 0.1 XMAX= 163.9 NXBIN= 33
YMIN= 0.00064 YMAX= 0.96824 NYBIN= 20
NUMBER OF REFLECTIONS USED FOR DETERMINING CORRECTION FACTORS 411311

**********
CORRECTION FACTORS AS FUNCTION OF X (fast) & Y(slow) IN THE DETECTOR PLANE
**********

RECIPROCAL CORRECTION FACTORS FOR INPUT DATA SETS MERGED TO
OUTPUT FILE: XDS_ASCII.HKL

THE CALCULATIONS ASSUME FRIEDEL'S_LAW= TRUE

```
TOTAL NUMBER OF CORRECTION FACTORS DEFINED     8190
DEGREES OF FREEDOM OF CHI^2 FIT            368190.8
CHI^2-VALUE OF FIT OF CORRECTION FACTORS      0.972
NUMBER OF CYCLES CARRIED OUT                     3

CORRECTION FACTORS for visual inspection by XDS-Viewer MODPIX.cbf
XMIN=     3.6 XMAX=  3068.4 NXBIN=   91
YMIN=    21.4 YMAX=  3051.7 NYBIN=   90
NUMBER OF REFLECTIONS USED FOR DETERMINING CORRECTION FACTORS     411311


*****************************************************************************
  CORRECTION FACTORS AS FUNCTION OF IMAGE NUMBER & DETECTOR SURFACE POSITION
*****************************************************************************

RECIPROCAL CORRECTION FACTORS FOR INPUT DATA SETS MERGED TO
OUTPUT FILE: XDS_ASCII.HKL

THE CALCULATIONS ASSUME         FRIEDEL'S_LAW= TRUE
TOTAL NUMBER OF CORRECTION FACTORS DEFINED      429
DEGREES OF FREEDOM OF CHI^2 FIT            368428.0
CHI^2-VALUE OF FIT OF CORRECTION FACTORS      0.965
NUMBER OF CYCLES CARRIED OUT                     3

CORRECTION FACTORS for visual inspection by XDS-Viewer ABSORP.cbf
XMIN=     0.1 XMAX=   163.9 NXBIN=   33
DETECTOR_SURFACE_POSITION=    1536    1537
DETECTOR_SURFACE_POSITION=    2057    2051
DETECTOR_SURFACE_POSITION=    1015    2051
DETECTOR_SURFACE_POSITION=    1015    1022
DETECTOR_SURFACE_POSITION=    2057    1022
DETECTOR_SURFACE_POSITION=    2714    2019
DETECTOR_SURFACE_POSITION=    2024    2701
DETECTOR_SURFACE_POSITION=    1048    2701
DETECTOR_SURFACE_POSITION=     358    2019
DETECTOR_SURFACE_POSITION=     358    1054
DETECTOR_SURFACE_POSITION=    1048     372
DETECTOR_SURFACE_POSITION=    2024     372
DETECTOR_SURFACE_POSITION=    2714    1054
NUMBER OF REFLECTIONS USED FOR DETERMINING CORRECTION FACTORS     411311


*****************************************************************************
   CORRECTION PARAMETERS FOR THE STANDARD ERROR OF REFLECTION INTENSITIES
*****************************************************************************

The variance v0(I) of the intensity I obtained from counting statistics is
replaced by v(I)=a*(v0(I)+b*I^2). The model parameters a, b are chosen to
minimize the discrepancies between v(I) and the variance estimated from
sample statistics of symmetry related reflections. This model implicates
an asymptotic limit ISa=1/SQRT(a*b) for the highest I/Sigma(I) that the
experimental setup can produce (Diederichs (2010) Acta Cryst D66, 733-740).
```

| a | b | ISa |
|---|---|---|
| 4.850E+00 | 2.087E-04 | 31.43 |

**********

STANDARD ERROR OF REFLECTION INTENSITIES AS FUNCTION OF RESOLUTION
FOR DATA SET XDS_ASCII.HKL

**********

I/Sigma = mean intensity/Sigma of a reflection in shell
Chi^2 = goodness of fit between sample variances of symmetry-related intensities and their errors (Chi^2 = 1 for perfect agreement)
R-FACTOR
observed = (SUM(ABS(I(h,i)-I(h))))/(SUM(I(h,i)))
expected = expected R-FACTOR derived from Sigma(I)

NUMBER = number of reflections in resolution shell used for calculation of R-FACTOR
ACCEPTED = number of accepted reflections
REJECTED = number of rejected reflections (MISFITS), recognized by comparison with symmetry-related reflections.

| RESOLUTION RANGE | | I/Sigma | Chi^2 | R-FACTOR observed | R-FACTOR expected | NUMBER | ACCEPTED | REJECTED |
|---|---|---|---|---|---|---|---|---|
| 39.489 | 9.845 | 27.60 | 1.23 | 2.19 | 2.35 | 444 | 449 | 105 |
| 9.845 | 7.072 | 29.39 | 0.91 | 1.86 | 2.41 | 1230 | 1231 | 55 |
| 7.072 | 5.806 | 29.49 | 0.92 | 1.94 | 2.45 | 1811 | 1813 | 49 |
| 5.806 | 5.041 | 29.88 | 0.88 | 1.91 | 2.44 | 2217 | 2217 | 53 |
| 5.041 | 4.517 | 29.29 | 0.95 | 2.00 | 2.44 | 2278 | 2281 | 63 |
| 4.517 | 4.128 | 29.61 | 0.94 | 2.00 | 2.43 | 2499 | 2501 | 46 |
| 4.128 | 3.824 | 29.49 | 0.94 | 1.91 | 2.44 | 2795 | 2803 | 66 |
| 3.824 | 3.579 | 29.45 | 0.91 | 1.95 | 2.45 | 3137 | 3138 | 97 |
| 3.579 | 3.376 | 29.41 | 0.94 | 2.01 | 2.47 | 3261 | 3261 | 116 |
| 3.376 | 3.204 | 28.86 | 0.98 | 2.04 | 2.48 | 3791 | 3794 | 108 |
| 3.204 | 3.056 | 28.40 | 0.97 | 2.07 | 2.50 | 3788 | 3789 | 110 |
| 3.056 | 2.927 | 27.26 | 1.01 | 2.10 | 2.51 | 4012 | 4012 | 120 |
| 2.927 | 2.812 | 26.77 | 1.06 | 2.25 | 2.55 | 4219 | 4220 | 105 |
| 2.812 | 2.711 | 26.36 | 1.08 | 2.29 | 2.55 | 4101 | 4101 | 123 |
| 2.711 | 2.619 | 26.33 | 1.23 | 2.58 | 2.57 | 4296 | 4297 | 178 |
| 2.619 | 2.536 | 26.02 | 1.16 | 2.56 | 2.61 | 4565 | 4565 | 116 |
| 2.536 | 2.461 | 25.76 | 1.17 | 2.54 | 2.60 | 4609 | 4609 | 122 |
| 2.461 | 2.392 | 25.26 | 1.15 | 2.50 | 2.63 | 4846 | 4846 | 129 |
| 2.392 | 2.328 | 25.05 | 1.19 | 2.56 | 2.65 | 5088 | 5088 | 150 |
| 2.328 | 2.269 | 24.88 | 1.17 | 2.56 | 2.65 | 5085 | 5085 | 149 |
| 2.269 | 2.215 | 24.03 | 1.23 | 2.65 | 2.71 | 5212 | 5212 | 161 |
| 2.215 | 2.164 | 23.62 | 1.17 | 2.70 | 2.76 | 5359 | 5359 | 108 |
| 2.164 | 2.117 | 23.83 | 1.12 | 2.64 | 2.76 | 5622 | 5622 | 114 |
| 2.117 | 2.072 | 22.70 | 1.21 | 2.77 | 2.82 | 5438 | 5438 | 162 |
| 2.072 | 2.031 | 21.67 | 1.20 | 2.97 | 2.92 | 5796 | 5796 | 163 |
| 2.031 | 1.991 | 21.49 | 1.13 | 2.93 | 2.96 | 6029 | 6029 | 117 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 1.991 | 1.954 | 21.00 | 1.13 | 3.01 | 3.04 | 5972 | 5972 | 120 |
| 1.954 | 1.919 | 20.31 | 1.13 | 3.09 | 3.11 | 6181 | 6181 | 100 |
| 1.919 | 1.886 | 19.27 | 1.19 | 3.30 | 3.22 | 6115 | 6115 | 142 |
| 1.886 | 1.854 | 18.84 | 1.09 | 3.34 | 3.36 | 6374 | 6374 | 94 |
| 1.854 | 1.824 | 18.32 | 1.09 | 3.39 | 3.45 | 6539 | 6539 | 63 |
| 1.824 | 1.795 | 16.93 | 1.06 | 3.56 | 3.65 | 6717 | 6717 | 60 |
| 1.795 | 1.768 | 17.74 | 1.06 | 3.61 | 3.63 | 6535 | 6535 | 54 |
| 1.768 | 1.742 | 16.23 | 1.08 | 3.93 | 3.94 | 6857 | 6857 | 55 |
| 1.742 | 1.717 | 15.95 | 1.06 | 3.94 | 3.99 | 6802 | 6802 | 54 |
| 1.717 | 1.693 | 15.12 | 1.07 | 4.17 | 4.21 | 7106 | 7106 | 45 |
| 1.693 | 1.670 | 14.53 | 1.00 | 4.25 | 4.39 | 6963 | 6963 | 39 |
| 1.670 | 1.648 | 14.48 | 1.02 | 4.41 | 4.49 | 7321 | 7321 | 40 |
| 1.648 | 1.626 | 14.44 | 0.99 | 4.24 | 4.42 | 7344 | 7344 | 38 |
| 1.626 | 1.606 | 14.16 | 1.02 | 4.57 | 4.68 | 7155 | 7155 | 29 |
| 1.606 | 1.586 | 12.88 | 1.04 | 5.05 | 5.06 | 7644 | 7644 | 49 |
| 1.586 | 1.567 | 12.77 | 0.96 | 4.99 | 5.20 | 7494 | 7494 | 22 |
| 1.567 | 1.549 | 11.81 | 1.01 | 5.57 | 5.67 | 7660 | 7660 | 43 |
| 1.549 | 1.531 | 11.03 | 0.99 | 5.94 | 6.08 | 7528 | 7528 | 26 |
| 1.531 | 1.514 | 11.05 | 1.05 | 6.11 | 6.09 | 8059 | 8059 | 66 |
| 1.514 | 1.498 | 10.42 | 1.02 | 6.43 | 6.44 | 7755 | 7755 | 23 |
| 1.498 | 1.482 | 10.48 | 0.97 | 6.31 | 6.49 | 7905 | 7905 | 12 |
| 1.482 | 1.466 | 9.62 | 0.99 | 7.04 | 7.18 | 7999 | 7999 | 28 |
| 1.466 | 1.451 | 9.35 | 0.99 | 7.24 | 7.36 | 8155 | 8155 | 26 |
| 1.451 | 1.437 | 9.58 | 1.00 | 7.14 | 7.25 | 8117 | 8117 | 41 |
| 1.437 | 1.423 | 8.42 | 1.00 | 8.32 | 8.38 | 8270 | 8270 | 23 |
| 1.423 | 1.409 | 7.95 | 0.96 | 8.61 | 8.90 | 8078 | 8078 | 30 |
| 1.409 | 1.396 | 8.06 | 0.95 | 8.60 | 8.88 | 8712 | 8712 | 13 |
| 1.396 | 1.383 | 7.44 | 0.96 | 9.20 | 9.48 | 8375 | 8375 | 13 |
| 1.383 | 1.370 | 7.29 | 1.02 | 9.79 | 9.80 | 8541 | 8541 | 42 |
| 1.370 | 1.358 | 6.60 | 0.97 | 10.62 | 10.88 | 8555 | 8555 | 30 |
| 1.358 | 1.346 | 6.41 | 0.96 | 10.94 | 11.25 | 8772 | 8772 | 7 |
| 1.346 | 1.334 | 6.42 | 0.99 | 11.20 | 11.31 | 8794 | 8794 | 18 |
| 1.334 | 1.323 | 6.24 | 0.94 | 11.30 | 11.65 | 8655 | 8655 | 6 |
| 1.323 | 1.312 | 5.94 | 0.95 | 11.85 | 12.27 | 8907 | 8907 | 33 |
| 1.312 | 1.301 | 5.99 | 0.96 | 11.84 | 12.13 | 8816 | 8816 | 11 |
| 1.301 | 1.290 | 5.46 | 0.98 | 13.29 | 13.44 | 9211 | 9211 | 45 |
| 1.290 | 1.280 | 5.48 | 0.98 | 13.35 | 13.46 | 8911 | 8911 | 11 |
| 1.280 | 1.270 | 5.24 | 0.95 | 13.89 | 14.20 | 8934 | 8934 | 9 |
| 1.270 | 1.260 | 4.59 | 0.96 | 16.04 | 16.42 | 9442 | 9442 | 24 |
| 1.260 | 1.251 | 4.69 | 0.98 | 15.73 | 16.00 | 9070 | 9070 | 21 |
| 1.251 | 1.241 | 4.67 | 0.95 | 15.81 | 16.16 | 9345 | 9345 | 14 |
| 1.241 | 1.232 | 4.40 | 0.93 | 16.25 | 16.86 | 9274 | 9274 | 12 |
| 1.232 | 1.223 | 4.40 | 0.98 | 16.60 | 16.91 | 9549 | 9549 | 17 |
| 1.223 | 1.215 | 4.21 | 0.94 | 17.21 | 17.81 | 9321 | 9321 | 21 |
| 1.215 | 1.206 | 4.02 | 0.96 | 18.34 | 18.76 | 9595 | 9595 | 12 |
| 1.206 | 1.198 | 4.01 | 0.92 | 17.72 | 18.49 | 8364 | 8364 | 10 |
| 1.198 | 1.189 | 3.57 | 0.89 | 19.66 | 20.92 | 7629 | 7629 | 8 |
| 1.189 | 1.181 | 3.58 | 0.88 | 19.33 | 20.74 | 7081 | 7081 | 4 |
| 1.181 | 1.173 | 3.29 | 0.89 | 21.23 | 22.41 | 6643 | 6645 | 5 |
| 1.173 | 1.166 | 3.04 | 0.87 | 22.74 | 24.41 | 6136 | 6138 | 12 |
| 1.166 | 1.158 | 3.06 | 0.85 | 22.18 | 24.07 | 5684 | 5685 | 6 |
| 1.158 | 1.151 | 2.90 | 0.83 | 23.11 | 25.34 | 5374 | 5381 | 13 |
| 1.151 | 1.143 | 2.66 | 0.85 | 25.44 | 27.55 | 5032 | 5034 | 13 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 1.143 | 1.136 | 2.54 | 0.87 | 26.80 | 28.80 | 4972 | 4974 | 7 |
| 1.136 | 1.129 | 2.51 | 0.84 | 26.50 | 28.89 | 4372 | 4378 | 7 |
| 1.129 | 1.122 | 2.44 | 0.81 | 26.73 | 29.50 | 4154 | 4160 | 10 |
| 1.122 | 1.115 | 2.25 | 0.85 | 29.26 | 31.84 | 3728 | 3735 | 3 |
| 1.115 | 1.109 | 2.09 | 0.88 | 31.96 | 34.26 | 3697 | 3706 | 7 |
| 1.109 | 1.102 | 1.91 | 0.81 | 33.30 | 37.00 | 3216 | 3224 | 1 |
| 1.102 | 1.096 | 1.95 | 0.90 | 34.25 | 36.01 | 3101 | 3115 | 4 |
| 1.096 | 1.090 | 1.81 | 0.83 | 34.71 | 38.38 | 2723 | 2738 | 5 |
| 1.090 | 1.083 | 1.62 | 0.84 | 38.71 | 42.64 | 2578 | 2608 | 5 |
| 1.083 | 1.077 | 1.50 | 0.83 | 42.06 | 46.00 | 2297 | 2324 | 5 |
| 1.077 | 1.071 | 1.35 | 0.83 | 45.65 | 49.98 | 2096 | 2134 | 8 |
| 1.071 | 1.065 | 1.28 | 0.88 | 49.65 | 52.54 | 1860 | 1899 | 3 |
| 1.065 | 1.060 | 1.21 | 0.92 | 52.01 | 54.10 | 1609 | 1661 | 4 |
| 1.060 | 1.054 | 1.08 | 0.82 | 54.66 | 59.93 | 1352 | 1413 | 6 |
| 1.054 | 1.048 | 1.07 | 0.81 | 54.19 | 59.79 | 1207 | 1275 | 13 |
| 1.048 | 1.043 | 0.94 | 0.90 | 63.34 | 65.93 | 948 | 1015 | 4 |
| 1.043 | 1.037 | 0.86 | 0.86 | 67.54 | 73.23 | 704 | 779 | 4 |
| 1.037 | 1.032 | 0.72 | 0.86 | 77.01 | 81.80 | 603 | 674 | 3 |
| 1.032 | 1.027 | 0.88 | 0.70 | 54.69 | 63.61 | 331 | 406 | 0 |
| 1.027 | 1.021 | 0.68 | 0.85 | 74.29 | 79.69 | 158 | 220 | 2 |
| 1.021 | 1.016 | 0.65 | 0.71 | 54.74 | 70.58 | 37 | 70 | 0 |
| 39.489 | 1.016 | 11.45 | 1.00 | 3.73 | 4.01 | 558638 | 559445 | 4738 |

**********
 SUMMARY OF DATA SET STATISTICS FOR VARIOUS SUBSETS OF INCLUDED DATA IMAGES
**********

Data set statistics is reported below several times, each with a different
upper limit on the number of images included. This provides the user with
the information for deciding which data images should be excluded from the
final data set because of radiation damage or other defects. If the user
decides for a subset of "good" images that differs from the specification
as given by the input parameter (see DATA_RANGE= in XDS.INP) the CORRECT-
step of XDS must be repeated with the new parameter values for DATA_RANGE=.

**********
 SUMMARY OF DATA SET STATISTICS FOR IMAGE   DATA_RANGE=       1      21
**********

         COMPLETENESS AND QUALITY OF DATA SET
         ------------------------------------

R-FACTOR
observed = (SUM(ABS(I(h,i)-I(h))))/(SUM(I(h,i)))
expected = expected R-FACTOR derived from Sigma(I)

COMPARED = number of reflections used for calculating R-FACTOR
I/SIGMA  = mean of intensity/Sigma(I) of unique reflections

(after merging symmetry-related observations)
Sigma(I) = standard deviation of reflection intensity I
estimated from sample statistics

R-meas = redundancy independent R-factor (intensities)
Diederichs & Karplus (1997), Nature Struct. Biol. 4, 269-275.

CC(1/2) = percentage of correlation between intensities from
random half-datasets. Correlation significant at
the 0.1% level is marked by an asterisk.
Karplus & Diederichs (2012), Science 336, 1030-33
Anomal = percentage of correlation between random half-sets
Corr of anomalous intensity differences. Correlation
significant at the 0.1% level is marked.
SigAno = mean anomalous difference in units of its estimated
standard deviation (|F(+)-F(-)|/Sigma). F(+), F(-)
are structure factor estimates obtained from the
merged intensity observations in each parity class.
Nano = Number of unique reflections used to calculate
Anomal_Corr & SigAno. At least two observations
for each (+ and -) parity are required.

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

| RESOLUTION LIMIT | NUMBER OF REFLECTIONS OBSERVED | UNIQUE | POSSIBLE | COMPLETENESS OF DATA | R-FACTOR observed | R-FACTOR COMPARED expected | I/SIGMA | R-meas | CC(1/2) | Anomal Corr | SigAno | Nano |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3.04 | 3323 | 1364 | 2499 | 54.6% | 1.8% | 2.1% | 2860 | 44.06 | 2.1% | 99.9* | 15 | 0.821 | 236 |
| 2.15 | 6624 | 2894 | 4242 | 68.2% | 2.1% | 2.2% | 5545 | 38.29 | 2.5% | 99.8* | 21* | 0.932 | 363 |
| 1.76 | 8679 | 3921 | 5385 | 72.8% | 2.3% | 2.5% | 7178 | 30.78 | 2.9% | 99.9* | 12 | 0.851 | 381 |
| 1.52 | 10412 | 4643 | 6314 | 73.5% | 3.3% | 3.5% | 8715 | 22.29 | 4.0% | 99.8* | 8 | 0.849 | 501 |
| 1.36 | 11576 | 5232 | 7089 | 73.8% | 5.1% | 5.3% | 9762 | 15.23 | 6.4% | 99.5* | 13 | 0.871 | 549 |
| 1.24 | 12705 | 5723 | 7842 | 73.0% | 8.5% | 8.6% | 10929 | 9.92 | 10.7% | 98.6* | 9 | 0.839 | 503 |
| 1.15 | 11098 | 5729 | 8462 | 67.7% | 11.7% | 12.0% | 8842 | 6.33 | 15.1% | 96.9* | 2 | 0.767 | 240 |
| 1.08 | 5263 | 4092 | 9086 | 45.0% | 18.6% | 19.9% | 2272 | 3.04 | 26.0% | 89.9* | 0 | 0.000 | 0 |
| 1.02 | 1513 | 1472 | 9654 | 15.2% | 41.1% | 49.0% | 82 | 1.47 | 58.2% | 83.1* | 0 | 0.000 | 0 |
| total | 71193 | 35070 | 60573 | 57.9% | 2.8% | 3.0% | 56185 | 16.61 | 3.5% | 99.9* | 11* | 0.853 | 2773 |

NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES 71854
NUMBER OF REJECTED MISFITS 657
NUMBER OF SYSTEMATIC ABSENT REFLECTIONS 0
NUMBER OF ACCEPTED OBSERVATIONS 71197
NUMBER OF UNIQUE ACCEPTED REFLECTIONS 35072

**********
SUMMARY OF DATA SET STATISTICS FOR IMAGE DATA_RANGE= 1 41
**********

COMPLETENESS AND QUALITY OF DATA SET

---

R-FACTOR
observed = (SUM(ABS(I(h,i)-I(h))))/(SUM(I(h,i)))
expected = expected R-FACTOR derived from Sigma(I)

COMPARED = number of reflections used for calculating R-FACTOR
I/SIGMA = mean of intensity/Sigma(I) of unique reflections
(after merging symmetry-related observations)
Sigma(I) = standard deviation of reflection intensity I
estimated from sample statistics

R-meas = redundancy independent R-factor (intensities)
Diederichs & Karplus (1997), Nature Struct. Biol. 4, 269-275.

CC(1/2) = percentage of correlation between intensities from
random half-datasets. Correlation significant at
the 0.1% level is marked by an asterisk.
Karplus & Diederichs (2012), Science 336, 1030-33
Anomal Corr = percentage of correlation between random half-sets
of anomalous intensity differences. Correlation
significant at the 0.1% level is marked.
SigAno = mean anomalous difference in units of its estimated
standard deviation (|F(+)-F(-)|/Sigma). F(+), F(-)
are structure factor estimates obtained from the
merged intensity observations in each parity class.
Nano = Number of unique reflections used to calculate
Anomal_Corr & SigAno. At least two observations
for each (+ and -) parity are required.

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

| RESOLUTION LIMIT | NUMBER OF REFLECTIONS OBSERVED | UNIQUE | POSSIBLE | COMPLETENESS OF DATA | R-FACTOR observed | R-FACTOR expected | COMPARED | I/SIGMA | R-meas | CC(1/2) | Anomal Corr | SigAno | Nano |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3.04 | 6609 | 1821 | 2499 | 72.9% | 1.8% | 2.2% | 6315 | 53.54 | 2.1% | 99.9* | 10 | 0.768 | 719 |
| 2.15 | 12988 | 3664 | 4242 | 86.4% | 2.2% | 2.3% | 12506 | 47.37 | 2.5% | 99.9* | 14* | 0.880 | 1511 |
| 1.76 | 17035 | 4842 | 5385 | 89.9% | 2.6% | 2.7% | 16456 | 38.15 | 3.0% | 99.9* | 8 | 0.876 | 1969 |
| 1.52 | 20287 | 5708 | 6314 | 90.4% | 3.7% | 3.8% | 19723 | 27.47 | 4.3% | 99.8* | 8 | 0.850 | 2126 |
| 1.36 | 22691 | 6408 | 7089 | 90.4% | 5.8% | 5.9% | 22155 | 18.56 | 6.8% | 99.5* | 8 | 0.861 | 2086 |
| 1.24 | 24886 | 7027 | 7842 | 89.6% | 9.5% | 9.7% | 24372 | 12.00 | 11.1% | 98.8* | 1 | 0.808 | 2058 |
| 1.15 | 21663 | 7283 | 8462 | 86.1% | 13.4% | 14.0% | 20821 | 7.37 | 16.2% | 97.1* | -1 | 0.751 | 1472 |
| 1.08 | 10276 | 5858 | 9086 | 64.5% | 20.0% | 21.4% | 8040 | 3.38 | 27.1% | 90.5* | 0 | 0.676 | 30 |
| 1.02 | 2975 | 2364 | 9654 | 24.5% | 37.2% | 40.2% | 1221 | 1.48 | 52.5% | 73.2* | 0 | 0.000 | 0 |
| total | 139410 | 44975 | 60573 | 74.2% | 3.1% | 3.3% | 131609 | 19.85 | 3.6% | 99.9* | 5 | 0.835 | 11971 |

NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES 140635
NUMBER OF REJECTED MISFITS 1220
NUMBER OF SYSTEMATIC ABSENT REFLECTIONS 0
NUMBER OF ACCEPTED OBSERVATIONS 139415
NUMBER OF UNIQUE ACCEPTED REFLECTIONS 44976

```
*****************************************************************************
 SUMMARY OF DATA SET STATISTICS FOR IMAGE   DATA_RANGE=       1      61
*****************************************************************************


         COMPLETENESS AND QUALITY OF DATA SET
         ------------------------------------

R-FACTOR
observed = (SUM(ABS(I(h,i)-I(h))))/(SUM(I(h,i)))
expected = expected R-FACTOR derived from Sigma(I)

COMPARED = number of reflections used for calculating R-FACTOR
I/SIGMA  = mean of intensity/Sigma(I) of unique reflections
           (after merging symmetry-related observations)
Sigma(I) = standard deviation of reflection intensity I
           estimated from sample statistics

R-meas   = redundancy independent R-factor (intensities)
           Diederichs & Karplus (1997), Nature Struct. Biol. 4, 269-275.

CC(1/2)  = percentage of correlation between intensities from
           random half-datasets. Correlation significant at
           the 0.1% level is marked by an asterisk.
           Karplus & Diederichs (2012), Science 336, 1030-33
Anomal   = percentage of correlation between random half-sets
 Corr      of anomalous intensity differences. Correlation
           significant at the 0.1% level is marked.
SigAno   = mean anomalous difference in units of its estimated
           standard deviation (|F(+)-F(-)|/Sigma). F(+), F(-)
           are structure factor estimates obtained from the
           merged intensity observations in each parity class.
 Nano    = Number of unique reflections used to calculate
           Anomal_Corr & SigAno. At least two observations
           for each (+ and -) parity are required.


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  CC(1/2)  Anomal  SigAno   Nano
  LIMIT     OBSERVED  UNIQUE  POSSIBLE     OF DATA   observed  expected                                        Corr

    3.04        9925    2257      2499       90.3%       1.9%      2.3%     9645   59.11      2.1%    99.9*    14*   0.829    1232
    2.15       19206    4193      4242       98.8%       2.3%      2.4%    18933   53.76      2.5%    99.9*    13*   0.910    2669
    1.76       25239    5333      5385       99.0%       2.8%      2.8%    25032   43.92      3.1%    99.9*     9    0.901    3636
    1.52       30123    6207      6314       98.3%       4.0%      4.1%    29985   31.44      4.5%    99.8*     7    0.859    4633
    1.36       33752    6945      7089       98.0%       6.6%      6.6%    33593   20.96      7.4%    99.6*     4    0.850    5419
    1.24       37096    7701      7842       98.2%      10.8%     10.8%    36950   13.39     12.1%    98.9*    -1    0.802    5845
    1.15       32187    8192      8462       96.8%      15.3%     15.7%    31677    8.12     17.6%    97.4*     1    0.791    3836
    1.08       15238    6974      9086       76.8%      23.2%     24.6%    13646    3.57     29.9%    89.8*    -1    0.698     103
    1.02        4393    3248      9654       33.6%      38.6%     42.0%     2239    1.41     54.1%    70.7*     0    0.000       0
   total      207159   51050     60573       84.3%       3.3%      3.6%   201700   22.19      3.8%    99.9*     4    0.844   27373
```

```
NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES  209471
NUMBER OF REJECTED MISFITS                            2301
NUMBER OF SYSTEMATIC ABSENT REFLECTIONS                  0
NUMBER OF ACCEPTED OBSERVATIONS                     207170
NUMBER OF UNIQUE ACCEPTED REFLECTIONS                51053


*****************************************************************************
 SUMMARY OF DATA SET STATISTICS FOR IMAGE   DATA_RANGE=       1      81
*****************************************************************************


         COMPLETENESS AND QUALITY OF DATA SET
         ------------------------------------

R-FACTOR
observed = (SUM(ABS(I(h,i)-I(h))))/(SUM(I(h,i)))
expected = expected R-FACTOR derived from Sigma(I)

COMPARED = number of reflections used for calculating R-FACTOR
I/SIGMA  = mean of intensity/Sigma(I) of unique reflections
           (after merging symmetry-related observations)
Sigma(I) = standard deviation of reflection intensity I
           estimated from sample statistics

R-meas   = redundancy independent R-factor (intensities)
           Diederichs & Karplus (1997), Nature Struct. Biol. 4, 269-275.

CC(1/2)  = percentage of correlation between intensities from
           random half-datasets. Correlation significant at
           the 0.1% level is marked by an asterisk.
           Karplus & Diederichs (2012), Science 336, 1030-33
Anomal   = percentage of correlation between random half-sets
 Corr      of anomalous intensity differences. Correlation
           significant at the 0.1% level is marked.
SigAno   = mean anomalous difference in units of its estimated
           standard deviation (|F(+)-F(-)|/Sigma). F(+), F(-)
           are structure factor estimates obtained from the
           merged intensity observations in each parity class.
 Nano    = Number of unique reflections used to calculate
           Anomal_Corr & SigAno. At least two observations
           for each (+ and -) parity are required.


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  CC(1/2)  Anomal  SigAno   Nano
  LIMIT     OBSERVED  UNIQUE  POSSIBLE     OF DATA   observed  expected                                      Corr

    3.04       13408    2389      2499       95.6%       1.8%      2.3%    13334   67.53      2.0%    99.9*    17*   0.829    1684
    2.15       25578    4235      4242       99.8%       2.3%      2.5%    25531   61.94      2.5%    99.9*    11*   0.899    3480
```

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.76 | 33621 | 5382 | 5385 | 99.9% | 2.9% | 2.9% | 33595 | 49.97 | 3.1% | 99.9* | 8 | 0.909 | 4657 |
| 1.52 | 40026 | 6314 | 6314 | 100.0% | 4.3% | 4.4% | 40010 | 35.06 | 4.7% | 99.9* | 6 | 0.873 | 5579 |
| 1.36 | 44846 | 7089 | 7089 | 100.0% | 7.2% | 7.2% | 44836 | 23.02 | 7.8% | 99.7* | 2 | 0.837 | 6379 |
| 1.24 | 49265 | 7841 | 7842 | 100.0% | 11.9% | 12.1% | 49255 | 14.59 | 13.0% | 99.2* | 0 | 0.796 | 7120 |
| 1.15 | 42768 | 8370 | 8462 | 98.9% | 17.0% | 17.6% | 42632 | 8.81 | 19.0% | 97.7* | 1 | 0.778 | 6148 |
| 1.08 | 20191 | 7772 | 9086 | 85.5% | 25.8% | 27.5% | 19035 | 3.67 | 32.1% | 89.5* | -2 | 0.723 | 1221 |
| 1.02 | 5808 | 3855 | 9654 | 39.9% | 45.5% | 48.7% | 3599 | 1.38 | 62.0% | 68.3* | -35 | 0.461 | 18 |
| total | 275511 | 53247 | 60573 | 87.9% | 3.5% | 3.7% | 271827 | 24.40 | 3.8% | 100.0* | 3 | 0.835 | 36286 |

NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES 278446
NUMBER OF REJECTED MISFITS 2916
NUMBER OF SYSTEMATIC ABSENT REFLECTIONS 0
NUMBER OF ACCEPTED OBSERVATIONS 275530
NUMBER OF UNIQUE ACCEPTED REFLECTIONS 53253

**********
SUMMARY OF DATA SET STATISTICS FOR IMAGE DATA_RANGE= 1 100
**********

COMPLETENESS AND QUALITY OF DATA SET
---

R-FACTOR
observed = (SUM(ABS(I(h,i)-I(h))))/(SUM(I(h,i)))
expected = expected R-FACTOR derived from Sigma(I)

COMPARED = number of reflections used for calculating R-FACTOR
I/SIGMA = mean of intensity/Sigma(I) of unique reflections
(after merging symmetry-related observations)
Sigma(I) = standard deviation of reflection intensity I
estimated from sample statistics

R-meas = redundancy independent R-factor (intensities)
Diederichs & Karplus (1997), Nature Struct. Biol. 4, 269-275.

CC(1/2) = percentage of correlation between intensities from
random half-datasets. Correlation significant at
the 0.1% level is marked by an asterisk.
Karplus & Diederichs (2012), Science 336, 1030-33
Anomal = percentage of correlation between random half-sets
Corr of anomalous intensity differences. Correlation
significant at the 0.1% level is marked.
SigAno = mean anomalous difference in units of its estimated
standard deviation (|F(+)-F(-)|/Sigma). F(+), F(-)
are structure factor estimates obtained from the
merged intensity observations in each parity class.
Nano = Number of unique reflections used to calculate
Anomal_Corr & SigAno. At least two observations
for each (+ and -) parity are required.

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

| RESOLUTION LIMIT | NUMBER OF REFLECTIONS OBSERVED | UNIQUE | POSSIBLE | COMPLETENESS OF DATA | R-FACTOR observed | R-FACTOR expected | COMPARED | I/SIGMA | R-meas | CC(1/2) | Anomal Corr | SigAno | Nano |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3.04 | 16728 | 2402 | 2499 | 96.1% | 1.9% | 2.4% | 16688 | 75.03 | 2.0% | 100.0* | 18* | 0.872 | 1711 |
| 2.15 | 31661 | 4240 | 4242 | 100.0% | 2.3% | 2.5% | 31648 | 68.33 | 2.5% | 100.0* | 12* | 0.924 | 3523 |
| 1.76 | 41572 | 5383 | 5385 | 100.0% | 3.0% | 3.0% | 41568 | 54.83 | 3.2% | 99.9* | 9 | 0.916 | 4692 |
| 1.52 | 49463 | 6314 | 6314 | 100.0% | 4.5% | 4.6% | 49459 | 38.17 | 4.9% | 99.9* | 6 | 0.875 | 5623 |
| 1.36 | 55412 | 7089 | 7089 | 100.0% | 7.6% | 7.7% | 55408 | 24.86 | 8.2% | 99.8* | 3 | 0.840 | 6409 |
| 1.24 | 60855 | 7842 | 7842 | 100.0% | 12.8% | 12.9% | 60848 | 15.67 | 13.7% | 99.3* | -1 | 0.797 | 7147 |
| 1.15 | 52780 | 8411 | 8462 | 99.4% | 18.2% | 19.0% | 52694 | 9.42 | 19.9% | 98.0* | 2 | 0.784 | 6916 |
| 1.08 | 24944 | 7956 | 9086 | 87.6% | 28.3% | 30.4% | 24114 | 3.85 | 33.9% | 89.9* | -1 | 0.735 | 2822 |
| 1.02 | 7153 | 4228 | 9654 | 43.8% | 49.6% | 53.0% | 5030 | 1.40 | 65.5% | 65.8* | 0 | 0.688 | 79 |
| total | 340568 | 53865 | 60573 | 88.9% | 3.6% | 3.9% | 337457 | 26.38 | 3.9% | 100.0* | 3 | 0.838 | 38922 |

NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES 343910
NUMBER OF REJECTED MISFITS 3309
NUMBER OF SYSTEMATIC ABSENT REFLECTIONS 0
NUMBER OF ACCEPTED OBSERVATIONS 340601
NUMBER OF UNIQUE ACCEPTED REFLECTIONS 53874

**********
SUMMARY OF DATA SET STATISTICS FOR IMAGE DATA_RANGE= 1 120
**********

COMPLETENESS AND QUALITY OF DATA SET

R-FACTOR
observed = (SUM(ABS(I(h,i)-I(h))))/(SUM(I(h,i)))
expected = expected R-FACTOR derived from Sigma(I)

COMPARED = number of reflections used for calculating R-FACTOR
I/SIGMA = mean of intensity/Sigma(I) of unique reflections
(after merging symmetry-related observations)
Sigma(I) = standard deviation of reflection intensity I
estimated from sample statistics

R-meas = redundancy independent R-factor (intensities)
Diederichs & Karplus (1997), Nature Struct. Biol. 4, 269-275.

CC(1/2) = percentage of correlation between intensities from
random half-datasets. Correlation significant at
the 0.1% level is marked by an asterisk.
Karplus & Diederichs (2012), Science 336, 1030-33
Anomal Corr = percentage of correlation between random half-sets
of anomalous intensity differences. Correlation

significant at the 0.1% level is marked.
SigAno = mean anomalous difference in units of its estimated standard deviation (|F(+)-F(-)|/Sigma). F(+), F(-) are structure factor estimates obtained from the merged intensity observations in each parity class.
Nano = Number of unique reflections used to calculate Anomal_Corr & SigAno. At least two observations for each (+ and -) parity are required.

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

| RESOLUTION LIMIT | NUMBER OF REFLECTIONS OBSERVED | UNIQUE | POSSIBLE | COMPLETENESS OF DATA | R-FACTOR observed | R-FACTOR expected | COMPARED | I/SIGMA | R-meas | CC(1/2) | Anomal Corr | SigAno | Nano |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3.04 | 20203 | 2410 | 2499 | 96.4% | 1.9% | 2.4% | 20170 | 81.90 | 2.1% | 100.0* | 20* | 0.904 | 1728 |
| 2.15 | 38107 | 4240 | 4242 | 100.0% | 2.4% | 2.6% | 38096 | 74.46 | 2.6% | 100.0* | 13* | 0.957 | 3536 |
| 1.76 | 50033 | 5383 | 5385 | 100.0% | 3.1% | 3.1% | 50029 | 59.52 | 3.2% | 99.9* | 12* | 0.954 | 4695 |
| 1.52 | 59407 | 6314 | 6314 | 100.0% | 4.7% | 4.7% | 59403 | 41.26 | 4.9% | 99.9* | 7 | 0.890 | 5623 |
| 1.36 | 66533 | 7089 | 7089 | 100.0% | 7.8% | 7.9% | 66530 | 26.77 | 8.3% | 99.8* | 4 | 0.851 | 6410 |
| 1.24 | 73068 | 7841 | 7842 | 100.0% | 13.2% | 13.4% | 73066 | 16.86 | 13.9% | 99.4* | 0 | 0.795 | 7151 |
| 1.15 | 63400 | 8419 | 8462 | 99.5% | 18.8% | 19.6% | 63378 | 10.14 | 20.2% | 98.3* | 0 | 0.771 | 7376 |
| 1.08 | 29926 | 7984 | 9086 | 87.9% | 29.6% | 32.0% | 29450 | 4.14 | 34.4% | 91.2* | 0 | 0.729 | 3930 |
| 1.02 | 8597 | 4308 | 9654 | 44.6% | 52.9% | 56.8% | 6964 | 1.49 | 67.8% | 65.6* | 1 | 0.685 | 384 |
| total | 409274 | 53988 | 60573 | 89.1% | 3.7% | 4.0% | 407086 | 28.54 | 4.0% | 100.0* | 4 | 0.842 | 40833 |

NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES 413103
NUMBER OF REJECTED MISFITS 3788
NUMBER OF SYSTEMATIC ABSENT REFLECTIONS 0
NUMBER OF ACCEPTED OBSERVATIONS 409315
NUMBER OF UNIQUE ACCEPTED REFLECTIONS 53998

**********
SUMMARY OF DATA SET STATISTICS FOR IMAGE DATA_RANGE= 1 140
**********

COMPLETENESS AND QUALITY OF DATA SET
---

R-FACTOR
observed = (SUM(ABS(I(h,i)-I(h))))/(SUM(I(h,i)))
expected = expected R-FACTOR derived from Sigma(I)

COMPARED = number of reflections used for calculating R-FACTOR
I/SIGMA = mean of intensity/Sigma(I) of unique reflections (after merging symmetry-related observations)
Sigma(I) = standard deviation of reflection intensity I estimated from sample statistics

R-meas = redundancy independent R-factor (intensities)

Diederichs & Karplus (1997), Nature Struct. Biol. 4, 269-275.

CC(1/2) = percentage of correlation between intensities from random half-datasets. Correlation significant at the 0.1% level is marked by an asterisk. Karplus & Diederichs (2012), Science 336, 1030-33

Anomal Corr = percentage of correlation between random half-sets of anomalous intensity differences. Correlation significant at the 0.1% level is marked.

SigAno = mean anomalous difference in units of its estimated standard deviation (|F(+)-F(-)|/Sigma). F(+), F(-) are structure factor estimates obtained from the merged intensity observations in each parity class.

Nano = Number of unique reflections used to calculate Anomal_Corr & SigAno. At least two observations for each (+ and -) parity are required.

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

| RESOLUTION LIMIT | NUMBER OF REFLECTIONS OBSERVED | UNIQUE | POSSIBLE | COMPLETENESS OF DATA | R-FACTOR observed | R-FACTOR expected | COMPARED | I/SIGMA | R-meas | CC(1/2) | Anomal Corr | SigAno | Nano |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3.04 | 23599 | 2423 | 2499 | 97.0% | 2.0% | 2.4% | 23564 | 88.25 | 2.1% | 100.0* | 25* | 0.958 | 1746 |
| 2.15 | 44536 | 4239 | 4242 | 99.9% | 2.4% | 2.6% | 44528 | 80.62 | 2.6% | 100.0* | 16* | 1.006 | 3544 |
| 1.76 | 58469 | 5384 | 5385 | 100.0% | 3.1% | 3.1% | 58466 | 64.41 | 3.3% | 100.0* | 15* | 0.988 | 4705 |
| 1.52 | 69339 | 6314 | 6314 | 100.0% | 4.7% | 4.8% | 69335 | 44.63 | 4.9% | 99.9* | 9 | 0.901 | 5626 |
| 1.36 | 77616 | 7089 | 7089 | 100.0% | 7.9% | 8.0% | 77613 | 28.95 | 8.3% | 99.8* | 5 | 0.853 | 6412 |
| 1.24 | 85227 | 7841 | 7842 | 100.0% | 13.2% | 13.4% | 85225 | 18.23 | 13.8% | 99.5* | 0 | 0.798 | 7151 |
| 1.15 | 74026 | 8419 | 8462 | 99.5% | 19.0% | 19.9% | 74011 | 10.94 | 20.1% | 98.5* | 2 | 0.776 | 7625 |
| 1.08 | 34918 | 7990 | 9086 | 87.9% | 30.1% | 32.7% | 34535 | 4.44 | 34.2% | 92.0* | 1 | 0.725 | 4537 |
| 1.02 | 10047 | 4337 | 9654 | 44.9% | 53.8% | 57.8% | 8776 | 1.60 | 67.0% | 67.4* | 4 | 0.730 | 640 |
| total | 477777 | 54036 | 60573 | 89.2% | 3.7% | 4.0% | 476053 | 30.85 | 4.0% | 100.0* | 5 | 0.853 | 41986 |

| | |
|---|---|
| NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES | 482039 |
| NUMBER OF REJECTED MISFITS | 4219 |
| NUMBER OF SYSTEMATIC ABSENT REFLECTIONS | 0 |
| NUMBER OF ACCEPTED OBSERVATIONS | 477820 |
| NUMBER OF UNIQUE ACCEPTED REFLECTIONS | 54045 |

**********

SUMMARY OF DATA SET STATISTICS FOR IMAGE DATA_RANGE= 1 160

**********

COMPLETENESS AND QUALITY OF DATA SET

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R-FACTOR
observed = (SUM(ABS(I(h,i)-I(h))))/(SUM(I(h,i)))
expected = expected R-FACTOR derived from Sigma(I)

COMPARED = number of reflections used for calculating R-FACTOR
I/SIGMA  = mean of intensity/Sigma(I) of unique reflections
           (after merging symmetry-related observations)
Sigma(I) = standard deviation of reflection intensity I
           estimated from sample statistics

R-meas   = redundancy independent R-factor (intensities)
           Diederichs & Karplus (1997), Nature Struct. Biol. 4, 269-275.

CC(1/2)  = percentage of correlation between intensities from
           random half-datasets. Correlation significant at
           the 0.1% level is marked by an asterisk.
           Karplus & Diederichs (2012), Science 336, 1030-33
Anomal   = percentage of correlation between random half-sets
 Corr      of anomalous intensity differences. Correlation
           significant at the 0.1% level is marked.
SigAno   = mean anomalous difference in units of its estimated
           standard deviation (|F(+)-F(-)|/Sigma). F(+), F(-)
           are structure factor estimates obtained from the
           merged intensity observations in each parity class.
 Nano    = Number of unique reflections used to calculate
           Anomal_Corr & SigAno. At least two observations
           for each (+ and -) parity are required.

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

| RESOLUTION LIMIT | NUMBER OF REFLECTIONS OBSERVED | UNIQUE | POSSIBLE | COMPLETENESS OF DATA | R-FACTOR observed | R-FACTOR expected | COMPARED | I/SIGMA | R-meas | CC(1/2) | Anomal Corr | SigAno | Nano |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3.04 | 27032 | 2434 | 2499 | 97.4% | 2.0% | 2.5% | 27004 | 94.67 | 2.1% | 100.0* | 29* | 1.005 | 1758 |
| 2.15 | 50985 | 4239 | 4242 | 99.9% | 2.5% | 2.6% | 50981 | 86.83 | 2.6% | 100.0* | 21* | 1.032 | 3556 |
| 1.76 | 66840 | 5384 | 5385 | 100.0% | 3.1% | 3.1% | 66840 | 69.44 | 3.2% | 100.0* | 16* | 1.020 | 4707 |
| 1.52 | 79326 | 6314 | 6314 | 100.0% | 4.6% | 4.7% | 79326 | 48.30 | 4.8% | 99.9* | 12* | 0.921 | 5626 |
| 1.36 | 88719 | 7089 | 7089 | 100.0% | 7.7% | 7.9% | 88719 | 31.41 | 8.1% | 99.8* | 4 | 0.861 | 6412 |
| 1.24 | 97481 | 7841 | 7842 | 100.0% | 12.9% | 13.2% | 97481 | 19.85 | 13.5% | 99.6* | 1 | 0.802 | 7151 |
| 1.15 | 84608 | 8419 | 8462 | 99.5% | 18.6% | 19.6% | 84599 | 11.91 | 19.7% | 98.8* | 3 | 0.777 | 7695 |
| 1.08 | 39947 | 7990 | 9086 | 87.9% | 29.9% | 32.5% | 39775 | 4.86 | 33.5% | 93.1* | 0 | 0.730 | 5570 |
| 1.02 | 11497 | 4371 | 9654 | 45.3% | 53.4% | 57.5% | 10725 | 1.74 | 65.9% | 68.4* | 2 | 0.713 | 993 |
| total | 546435 | 54081 | 60573 | 89.3% | 3.7% | 4.0% | 545450 | 33.33 | 3.9% | 100.0* | 5 | 0.861 | 43468 |

NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES  551062
NUMBER OF REJECTED MISFITS                            4584
NUMBER OF SYSTEMATIC ABSENT REFLECTIONS                  0
NUMBER OF ACCEPTED OBSERVATIONS                     546478
NUMBER OF UNIQUE ACCEPTED REFLECTIONS                54090

**********************************************************************
 STATISTICS OF SAVED DATA SET "XDS_ASCII.HKL" (DATA_RANGE=       1     180)
FILE TYPE:         XDS_ASCII      MERGE=FALSE          FRIEDEL'S_LAW=TRUE

**********

REFLECTIONS OF TYPE H,0,0  0,K,0  0,0,L OR EXPECTED TO BE ABSENT (*)

| H | K | L | RESOLUTION | INTENSITY | SIGMA | INTENSITY/SIGMA | #OBSERVED |
|---|---|---|---|---|---|---|---|
| 0 | 0 | 8 | 4.614 | 0.7361E+05 | 0.2350E+04 | 31.33 | 1 |
| 0 | 0 | 9 | 4.102 | -0.1968E+02 | 0.4141E+02 | -0.48 | 1 |
| 0 | 0 | 10 | 3.691 | 0.1230E+03 | 0.5639E+02 | 2.18 | 1 |
| 0 | 0 | 11 | 3.356 | -0.7356E+02 | 0.5851E+02 | -1.26 | 1 |
| 0 | 0 | 12 | 3.076 | 0.2228E+05 | 0.7226E+03 | 30.84 | 1 |
| 0 | 0 | 13 | 2.840 | -0.1790E+02 | 0.5949E+02 | -0.30 | 1 |
| 0 | 0 | 14 | 2.637 | 0.7811E+02 | 0.6518E+02 | 1.20 | 1 |
| 0 | 0 | 15 | 2.461 | -0.2592E+02 | 0.4060E+02 | -0.64 | 2 |
| 0 | 0 | 16 | 2.307 | 0.1708E+06 | 0.3853E+04 | 44.32 | 2 |
| 0 | 0 | 17 | 2.171 | -0.3198E+02 | 0.5485E+02 | -0.58 | 2 |
| 0 | 0 | 18 | 2.051 | -0.2976E+02 | 0.5702E+02 | -0.52 | 2 |
| 0 | 0 | 19 | 1.943 | 0.7446E+02 | 0.5368E+02 | 1.39 | 2 |
| 0 | 0 | 20 | 1.846 | 0.8714E+04 | 0.2139E+03 | 40.73 | 2 |
| 0 | 0 | 21 | 1.758 | -0.7099E+02 | 0.4920E+02 | -1.44 | 2 |
| 0 | 0 | 22 | 1.678 | 0.1030E+03 | 0.5982E+02 | 1.72 | 2 |
| 0 | 0 | 23 | 1.605 | 0.9994E+02 | 0.6638E+02 | 1.51 | 2 |
| 0 | 0 | 24 | 1.538 | 0.1180E+04 | 0.7949E+02 | 14.85 | 2 |
| 0 | 0 | 25 | 1.477 | 0.3050E+02 | 0.6789E+02 | 0.45 | 2 |
| 0 | 0 | 26 | 1.420 | 0.6007E+01 | 0.6335E+02 | 0.09 | 2 |
| 0 | 0 | 27 | 1.367 | -0.4061E+01 | 0.6536E+02 | -0.06 | 2 |
| 0 | 0 | 28 | 1.318 | 0.2548E+04 | 0.1016E+03 | 25.07 | 2 |
| 0 | 0 | 29 | 1.273 | -0.6040E+02 | 0.7801E+02 | -0.77 | 2 |
| 0 | 0 | 30 | 1.230 | 0.1556E+01 | 0.8774E+02 | 0.02 | 2 |
| 2 | 0 | 0 | 39.489 | -0.3602E+01 | 0.9342E+00 | -3.86 | 3 |
| 3 | 0 | 0 | 26.326 | 0.7301E+01 | 0.2292E+01 | 3.19 | 4 |
| 4 | 0 | 0 | 19.744 | 0.3432E+05 | 0.1097E+04 | 31.29 | 1 |
| 5 | 0 | 0 | 15.795 | 0.3027E+01 | 0.4373E+01 | 0.69 | 4 |
| 6 | 0 | 0 | 13.163 | 0.5954E+04 | 0.9628E+02 | 61.84 | 4 |
| 7 | 0 | 0 | 11.282 | -0.5694E+01 | 0.6785E+01 | -0.84 | 4 |
| 9 | 0 | 0 | 8.775 | -0.2007E+02 | 0.9036E+01 | -2.22 | 4 |
| 11 | 0 | 0 | 7.180 | -0.2971E+02 | 0.1077E+02 | -2.76 | 4 |
| 12 | 0 | 0 | 6.581 | 0.8352E+05 | 0.2664E+04 | 31.35 | 1 |
| 13 | 0 | 0 | 6.075 | -0.3640E+02 | 0.1299E+02 | -2.80 | 4 |
| 14 | 0 | 0 | 5.641 | 0.3120E+04 | 0.5493E+02 | 56.80 | 4 |
| 15 | 0 | 0 | 5.265 | -0.1380E+02 | 0.1603E+02 | -0.86 | 4 |
| 17 | 0 | 0 | 4.646 | -0.2415E+02 | 0.1946E+02 | -1.24 | 4 |
| 19 | 0 | 0 | 4.157 | -0.1062E+03 | 0.2393E+02 | -4.44 | 4 |
| 20 | 0 | 0 | 3.949 | 0.7402E+05 | 0.1184E+04 | 62.52 | 4 |
| 21 | 0 | 0 | 3.761 | -0.7724E+02 | 0.2923E+02 | -2.64 | 4 |
| 22 | 0 | 0 | 3.590 | 0.2337E+04 | 0.5128E+02 | 45.58 | 4 |
| 23 | 0 | 0 | 3.434 | 0.2737E+03 | 0.4082E+02 | 6.70 | 3 |
| 24 | 0 | 0 | 3.291 | 0.1493E+05 | 0.2455E+03 | 60.82 | 4 |
| 25 | 0 | 0 | 3.159 | -0.1427E+03 | 0.3105E+02 | -4.60 | 4 |
| 26 | 0 | 0 | 3.038 | 0.8785E+05 | 0.1405E+04 | 62.54 | 4 |
| 27 | 0 | 0 | 2.925 | -0.4403E+02 | 0.2957E+02 | -1.49 | 4 |
| 28 | 0 | 0 | 2.821 | 0.1596E+03 | 0.3492E+02 | 4.57 | 4 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 29 | 0 | 0 | 2.723 | -0.3775E+02 | 0.3709E+02 | -1.02 | 3 |
| 30 | 0 | 0 | 2.633 | 0.2309E+05 | 0.3758E+03 | 61.45 | 4 |
| 31 | 0 | 0 | 2.548 | -0.1491E+03 | 0.3508E+02 | -4.25 | 4 |
| 32 | 0 | 0 | 2.468 | 0.2378E+04 | 0.6495E+02 | 36.60 | 3 |
| 33 | 0 | 0 | 2.393 | -0.7946E+02 | 0.3559E+02 | -2.23 | 4 |
| 34 | 0 | 0 | 2.323 | 0.3269E+05 | 0.5285E+03 | 61.85 | 4 |
| 35 | 0 | 0 | 2.256 | -0.2190E+02 | 0.3709E+02 | -0.59 | 4 |
| 36 | 0 | 0 | 2.194 | 0.3120E+03 | 0.3980E+02 | 7.84 | 4 |
| 37 | 0 | 0 | 2.135 | -0.9380E+01 | 0.3744E+02 | -0.25 | 4 |
| 38 | 0 | 0 | 2.078 | 0.8514E+04 | 0.1486E+03 | 57.29 | 4 |
| 39 | 0 | 0 | 2.025 | -0.9324E+02 | 0.3416E+02 | -2.73 | 4 |
| 40 | 0 | 0 | 1.974 | 0.1704E+05 | 0.2815E+03 | 60.54 | 4 |
| 41 | 0 | 0 | 1.926 | -0.6684E+02 | 0.3585E+02 | -1.86 | 4 |
| 42 | 0 | 0 | 1.880 | 0.8117E+03 | 0.4392E+02 | 18.48 | 4 |
| 43 | 0 | 0 | 1.837 | -0.8298E+02 | 0.3932E+02 | -2.11 | 4 |
| 44 | 0 | 0 | 1.795 | 0.8554E+04 | 0.1500E+03 | 57.02 | 4 |
| 45 | 0 | 0 | 1.755 | -0.5122E+00 | 0.4094E+02 | -0.01 | 4 |
| 46 | 0 | 0 | 1.717 | 0.3103E+04 | 0.6867E+02 | 45.19 | 4 |
| 47 | 0 | 0 | 1.680 | -0.1463E+02 | 0.4231E+02 | -0.35 | 4 |
| 48 | 0 | 0 | 1.645 | 0.6151E+04 | 0.1154E+03 | 53.30 | 4 |
| 49 | 0 | 0 | 1.612 | -0.6080E+02 | 0.4453E+02 | -1.37 | 4 |
| 50 | 0 | 0 | 1.580 | 0.2183E+04 | 0.6476E+02 | 33.71 | 4 |
| 51 | 0 | 0 | 1.549 | -0.1668E+02 | 0.4376E+02 | -0.38 | 4 |
| 52 | 0 | 0 | 1.519 | 0.1384E+04 | 0.5697E+02 | 24.30 | 4 |
| 53 | 0 | 0 | 1.490 | -0.6971E+02 | 0.4411E+02 | -1.58 | 4 |
| 54 | 0 | 0 | 1.463 | 0.1060E+05 | 0.1871E+03 | 56.69 | 4 |
| 55 | 0 | 0 | 1.436 | -0.5124E+02 | 0.4730E+02 | -1.08 | 4 |
| 56 | 0 | 0 | 1.410 | 0.6853E+04 | 0.1310E+03 | 52.31 | 4 |
| 57 | 0 | 0 | 1.386 | -0.2501E+02 | 0.4847E+02 | -0.52 | 4 |
| 58 | 0 | 0 | 1.362 | 0.4307E+03 | 0.5165E+02 | 8.34 | 4 |
| 59 | 0 | 0 | 1.339 | -0.5574E+02 | 0.5184E+02 | -1.08 | 4 |
| 60 | 0 | 0 | 1.316 | 0.3193E+03 | 0.5022E+02 | 6.36 | 4 |
| 61 | 0 | 0 | 1.295 | -0.1504E+03 | 0.5655E+02 | -2.66 | 4 |
| 62 | 0 | 0 | 1.274 | 0.6526E+04 | 0.1255E+03 | 51.98 | 4 |
| 63 | 0 | 0 | 1.254 | 0.1817E+02 | 0.5824E+02 | 0.31 | 4 |
| 64 | 0 | 0 | 1.234 | 0.8310E+03 | 0.6046E+02 | 13.75 | 4 |
| 65 | 0 | 0 | 1.215 | 0.7398E+02 | 0.6063E+02 | 1.22 | 4 |
| 66 | 0 | 0 | 1.197 | 0.2604E+03 | 0.5755E+02 | 4.52 | 4 |
| 67 | 0 | 0 | 1.179 | -0.9247E+00 | 0.6380E+02 | -0.01 | 4 |
| 68 | 0 | 0 | 1.161 | -0.1625E+02 | 0.6654E+02 | -0.24 | 4 |
| 69 | 0 | 0 | 1.145 | -0.6330E+02 | 0.6373E+02 | -0.99 | 4 |
| 70 | 0 | 0 | 1.128 | 0.1065E+03 | 0.1137E+03 | 0.94 | 2 |
| 71 | 0 | 0 | 1.112 | -0.8464E+02 | 0.1007E+03 | -0.84 | 2 |

COMPLETENESS AND QUALITY OF DATA SET
---

R-FACTOR
observed = (SUM(ABS(I(h,i)-I(h))))/(SUM(I(h,i)))
expected = expected R-FACTOR derived from Sigma(I)

COMPARED = number of reflections used for calculating R-FACTOR
I/SIGMA  = mean of intensity/Sigma(I) of unique reflections

(after merging symmetry-related observations)
Sigma(I) = standard deviation of reflection intensity I
estimated from sample statistics

R-meas = redundancy independent R-factor (intensities)
Diederichs & Karplus (1997), Nature Struct. Biol. 4, 269-275.

CC(1/2) = percentage of correlation between intensities from
random half-datasets. Correlation significant at
the 0.1% level is marked by an asterisk.
Karplus & Diederichs (2012), Science 336, 1030-33
Anomal = percentage of correlation between random half-sets
Corr of anomalous intensity differences. Correlation
significant at the 0.1% level is marked.
SigAno = mean anomalous difference in units of its estimated
standard deviation (|F(+)-F(-)|/Sigma). F(+), F(-)
are structure factor estimates obtained from the
merged intensity observations in each parity class.
Nano = Number of unique reflections used to calculate
Anomal_Corr & SigAno. At least two observations
for each (+ and -) parity are required.

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

| RESOLUTION LIMIT | NUMBER OF REFLECTIONS OBSERVED | UNIQUE | POSSIBLE | COMPLETENESS OF DATA | R-FACTOR observed | R-FACTOR COMPARED expected | I/SIGMA | R-meas | CC(1/2) | Anomal Corr | SigAno | Nano |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3.04 | 27673 | 2434 | 2499 | 97.4% | 2.0% | 2.5% | 27647 | 95.91 | 2.1% | 100.0* | 31* | 1.016 | 1759 |
| 2.15 | 52200 | 4240 | 4242 | 100.0% | 2.5% | 2.6% | 52198 | 87.93 | 2.6% | 100.0* | 21* | 1.042 | 3556 |
| 1.76 | 68400 | 5384 | 5385 | 100.0% | 3.1% | 3.1% | 68400 | 70.38 | 3.2% | 100.0* | 18* | 1.024 | 4707 |
| 1.52 | 81204 | 6314 | 6314 | 100.0% | 4.6% | 4.7% | 81204 | 49.00 | 4.8% | 99.9* | 11* | 0.933 | 5626 |
| 1.36 | 90823 | 7089 | 7089 | 100.0% | 7.7% | 7.8% | 90823 | 31.91 | 8.0% | 99.9* | 5 | 0.858 | 6412 |
| 1.24 | 99789 | 7840 | 7842 | 100.0% | 12.9% | 13.1% | 99789 | 20.17 | 13.4% | 99.6* | 0 | 0.802 | 7150 |
| 1.15 | 86618 | 8419 | 8462 | 99.5% | 18.6% | 19.5% | 86609 | 12.12 | 19.5% | 98.8* | 1 | 0.773 | 7698 |
| 1.08 | 40899 | 7990 | 9086 | 87.9% | 29.8% | 32.4% | 40772 | 4.95 | 33.3% | 93.1* | 2 | 0.733 | 5746 |
| 1.02 | 11782 | 4373 | 9654 | 45.3% | 53.3% | 57.4% | 11139 | 1.78 | 65.8% | 68.2* | 2 | 0.717 | 1086 |
| total | 559388 | 54083 | 60573 | 89.3% | 3.7% | 4.0% | 558581 | 33.81 | 3.9% | 100.0* | 5 | 0.863 | 43740 |

| | |
|---|---|
| NUMBER OF REFLECTIONS IN SELECTED SUBSET OF IMAGES | 564183 |
| NUMBER OF REJECTED MISFITS | 4738 |
| NUMBER OF SYSTEMATIC ABSENT REFLECTIONS | 0 |
| NUMBER OF ACCEPTED OBSERVATIONS | 559445 |
| NUMBER OF UNIQUE ACCEPTED REFLECTIONS | 54093 |

**********
WILSON STATISTICS OF DATA SET "XDS_ASCII.HKL"
**********

Data is divided into resolution shells and a straight line
A - 2*B*SS is fitted to log<I>, where

RES    = mean resolution (Angstrom) in shell
SS     = mean of (sin(THETA)/LAMBDA)**2 in shell
<I>    = mean reflection intensity in shell
BO     = (A - log<I>)/(2*SS)
 #     = number of reflections in resolution shell

WILSON LINE (using all data) : A=  10.163 B=  11.317 CORRELATION=  0.98

| # | RES | SS | <I> | log(<I>) | BO |
|---|---|---|---|---|---|
| 829 | 5.708 | 0.008 | 2.3983E+04 | 10.085 | 5.1 |
| 1424 | 3.571 | 0.020 | 3.7261E+04 | 10.526 | -9.3 |
| 1809 | 2.787 | 0.032 | 1.5625E+04 | 9.657 | 7.9 |
| 2116 | 2.360 | 0.045 | 1.0413E+04 | 9.251 | 10.2 |
| 2359 | 2.084 | 0.058 | 7.2283E+03 | 8.886 | 11.1 |
| 2612 | 1.886 | 0.070 | 4.2438E+03 | 8.353 | 12.9 |
| 2804 | 1.736 | 0.083 | 2.7299E+03 | 7.912 | 13.6 |
| 3027 | 1.616 | 0.096 | 2.0920E+03 | 7.646 | 13.1 |
| 3177 | 1.518 | 0.108 | 1.5307E+03 | 7.333 | 13.0 |
| 3377 | 1.436 | 0.121 | 1.1592E+03 | 7.055 | 12.8 |
| 3527 | 1.366 | 0.134 | 8.9642E+02 | 6.798 | 12.6 |
| 3673 | 1.306 | 0.147 | 7.5823E+02 | 6.631 | 12.0 |
| 3832 | 1.253 | 0.159 | 6.0878E+02 | 6.411 | 11.8 |
| 4012 | 1.205 | 0.172 | 5.4225E+02 | 6.296 | 11.2 |
| 4047 | 1.163 | 0.185 | 4.5390E+02 | 6.118 | 10.9 |
| 3915 | 1.125 | 0.197 | 3.8639E+02 | 5.957 | 10.7 |
| 3530 | 1.091 | 0.210 | 3.0021E+02 | 5.704 | 10.6 |
| 2813 | 1.060 | 0.223 | 2.1307E+02 | 5.362 | 10.8 |
| 1198 | 1.034 | 0.234 | 1.5330E+02 | 5.032 | 11.0 |

HIGHER ORDER MOMENTS OF WILSON DISTRIBUTION OF  CENTRIC DATA
AS COMPARED WITH THEORETICAL VALUES. (EXPECTED: 1.00)

| # | RES | <I**2>/ 3<I>**2 | <I**3>/ 15<I>**3 | <I**4>/ 105<I>**4 |
|---|---|---|---|---|
| 292 | 5.708 | 0.575 | 0.399 | 0.254 |
| 312 | 3.571 | 0.803 | 0.555 | 0.317 |
| 327 | 2.787 | 0.867 | 0.727 | 0.559 |
| 321 | 2.360 | 0.934 | 0.883 | 0.748 |
| 320 | 2.084 | 1.189 | 1.522 | 1.964 |
| 328 | 1.886 | 0.844 | 0.703 | 0.517 |
| 324 | 1.736 | 0.886 | 0.809 | 0.648 |
| 323 | 1.616 | 0.866 | 0.746 | 0.603 |
| 321 | 1.518 | 1.113 | 1.248 | 1.383 |
| 329 | 1.436 | 0.951 | 1.126 | 1.324 |
| 320 | 1.366 | 1.010 | 1.087 | 1.159 |
| 320 | 1.306 | 1.218 | 1.193 | 1.082 |
| 323 | 1.253 | 0.847 | 0.722 | 0.558 |
| 332 | 1.205 | 0.755 | 0.725 | 0.708 |
| 294 | 1.163 | 0.960 | 0.866 | 0.708 |
| 254 | 1.125 | 1.102 | 1.082 | 0.973 |
| 187 | 1.091 | 1.140 | 0.997 | 0.746 |
| 106 | 1.060 | 1.117 | 1.087 | 0.960 |
| 30 | 1.034 | 1.711 | 1.943 | 2.030 |

| | | | | |
|---|---|---|---|---|
| 5363 | overall | 0.947 | 0.913 | 0.852 |

HIGHER ORDER MOMENTS OF WILSON DISTRIBUTION OF ACENTRIC DATA
AS COMPARED WITH THEORETICAL VALUES. (EXPECTED: 1.00)

| # | RES | <I**2>/ 2<I>**2 | <I**3>/ 6<I>**3 | <I**4>/ 24<I>**4 |
|---|---|---|---|---|
| 537 | 5.708 | 1.169 | 1.141 | 1.031 |
| 1112 | 3.571 | 0.986 | 0.902 | 0.763 |
| 1482 | 2.787 | 1.009 | 0.964 | 0.861 |
| 1795 | 2.360 | 1.007 | 0.992 | 0.967 |
| 2039 | 2.084 | 1.016 | 1.072 | 1.198 |
| 2284 | 1.886 | 1.049 | 1.090 | 1.096 |
| 2480 | 1.736 | 1.032 | 1.094 | 1.227 |
| 2704 | 1.616 | 0.979 | 0.922 | 0.839 |
| 2856 | 1.518 | 0.977 | 0.937 | 0.864 |
| 3048 | 1.436 | 0.983 | 0.936 | 0.882 |
| 3207 | 1.366 | 1.008 | 0.996 | 0.958 |
| 3353 | 1.306 | 0.976 | 0.949 | 0.906 |
| 3509 | 1.253 | 0.976 | 0.919 | 0.869 |
| 3680 | 1.205 | 1.064 | 1.114 | 1.130 |
| 3753 | 1.163 | 1.017 | 1.012 | 0.989 |
| 3661 | 1.125 | 1.017 | 1.010 | 0.988 |
| 3343 | 1.091 | 1.107 | 1.266 | 1.564 |
| 2707 | 1.060 | 1.183 | 1.265 | 1.339 |
| 1168 | 1.034 | 1.505 | 1.554 | 1.764 |
| 48718 | overall | 1.037 | 1.045 | 1.055 |

======= CUMULATIVE INTENSITY DISTRIBUTION =======

DEFINITIONS:
<I> = mean reflection intensity
Na(Z)exp = expected number of acentric reflections with I <= Z*<I>
Na(Z)obs = observed number of acentric reflections with I <= Z*<I>
Nc(Z)exp = expected number of centric reflections with I <= Z*<I>
Nc(Z)obs = observed number of centric reflections with I <= Z*<I>

Nc(Z)obs/Nc(Z)exp versus resolution and Z (0.1-1.0)

| # | RES | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1.0 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 292 | 5.708 | 1.03 | 1.10 | 1.06 | 1.03 | 1.01 | 1.03 | 1.06 | 1.08 | 1.08 | 1.10 |
| 312 | 3.571 | 1.08 | 1.06 | 1.03 | 1.06 | 1.05 | 1.03 | 1.03 | 1.01 | 1.03 | 1.01 |
| 327 | 2.787 | 1.02 | 0.99 | 1.00 | 0.97 | 0.97 | 0.98 | 0.97 | 0.99 | 1.01 | 1.03 |
| 321 | 2.360 | 1.14 | 1.05 | 1.05 | 1.03 | 1.04 | 1.05 | 1.03 | 1.04 | 1.05 | 1.03 |
| 320 | 2.084 | 1.01 | 1.06 | 1.03 | 1.08 | 1.07 | 1.06 | 1.07 | 1.05 | 1.05 | 1.04 |
| 328 | 1.886 | 0.95 | 1.01 | 1.01 | 1.01 | 0.99 | 1.00 | 1.04 | 1.04 | 1.04 | 1.03 |
| 324 | 1.736 | 1.17 | 1.12 | 1.09 | 1.10 | 1.07 | 1.04 | 1.07 | 1.07 | 1.04 | 1.06 |
| 323 | 1.616 | 0.98 | 1.07 | 1.02 | 1.00 | 0.98 | 0.99 | 0.99 | 0.97 | 0.99 | 1.00 |
| 321 | 1.518 | 0.93 | 0.89 | 0.90 | 0.91 | 0.90 | 0.91 | 0.93 | 0.96 | 0.94 | 0.95 |
| 329 | 1.436 | 1.11 | 1.13 | 1.09 | 1.09 | 1.06 | 1.09 | 1.08 | 1.07 | 1.06 | 1.06 |
| 320 | 1.366 | 0.91 | 0.95 | 1.02 | 1.06 | 1.10 | 1.09 | 1.07 | 1.07 | 1.06 | 1.07 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 320 | 1.306 | 1.02 | 0.99 | 0.97 | 0.97 | 0.98 | 0.96 | 0.93 | 0.92 | 0.93 | 0.95 |
| 323 | 1.253 | 1.06 | 0.99 | 1.03 | 1.08 | 1.06 | 1.01 | 1.01 | 1.04 | 1.05 | 1.04 |
| 332 | 1.205 | 0.96 | 1.05 | 1.10 | 1.06 | 1.09 | 1.11 | 1.14 | 1.11 | 1.11 | 1.10 |
| 294 | 1.163 | 0.93 | 0.89 | 0.94 | 0.97 | 1.03 | 1.04 | 1.02 | 1.00 | 0.99 | 0.99 |
| 254 | 1.125 | 0.90 | 0.92 | 0.93 | 0.98 | 0.95 | 0.95 | 0.94 | 0.93 | 0.93 | 0.95 |
| 187 | 1.091 | 1.12 | 0.88 | 0.83 | 0.81 | 0.88 | 0.91 | 0.94 | 0.97 | 0.99 | 0.96 |
| 106 | 1.060 | 0.99 | 0.90 | 0.93 | 0.94 | 0.94 | 0.92 | 0.96 | 0.96 | 0.98 | 1.00 |
| 30 | 1.034 | 1.88 | 1.35 | 1.20 | 1.06 | 0.96 | 1.01 | 0.95 | 0.90 | 0.86 | 0.88 |
| 5363 | overall | 1.02 | 1.01 | 1.01 | 1.02 | 1.02 | 1.02 | 1.02 | 1.02 | 1.02 | 1.02 |

Na(Z)obs/Na(Z)exp versus resolution and Z (0.1-1.0)

| # | RES | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1.0 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 537 | 5.708 | 0.88 | 0.91 | 0.94 | 0.93 | 0.91 | 0.86 | 0.85 | 0.89 | 0.91 | 0.94 |
| 1112 | 3.571 | 0.77 | 0.88 | 0.95 | 0.98 | 0.96 | 0.99 | 1.00 | 1.00 | 0.99 | 0.99 |
| 1482 | 2.787 | 1.06 | 1.02 | 1.00 | 1.03 | 1.02 | 1.01 | 1.01 | 1.01 | 1.00 | 0.99 |
| 1795 | 2.360 | 0.94 | 0.93 | 0.92 | 0.96 | 0.99 | 1.00 | 1.01 | 1.01 | 1.00 | 1.00 |
| 2039 | 2.084 | 0.95 | 1.01 | 1.02 | 1.00 | 1.02 | 1.01 | 1.02 | 1.00 | 1.01 | 1.01 |
| 2284 | 1.886 | 1.04 | 1.02 | 1.00 | 1.01 | 1.02 | 1.02 | 1.03 | 1.02 | 1.01 | 1.01 |
| 2480 | 1.736 | 0.88 | 0.96 | 0.98 | 0.99 | 0.99 | 0.98 | 0.98 | 0.98 | 0.99 | 0.99 |
| 2704 | 1.616 | 1.01 | 0.96 | 0.96 | 0.97 | 0.97 | 0.99 | 0.99 | 0.98 | 0.99 | 0.99 |
| 2856 | 1.518 | 0.98 | 1.00 | 0.98 | 1.03 | 1.03 | 1.02 | 1.01 | 1.01 | 0.99 | 1.00 |
| 3048 | 1.436 | 0.90 | 0.90 | 0.91 | 0.96 | 0.96 | 0.96 | 0.96 | 0.98 | 0.98 | 0.98 |
| 3207 | 1.366 | 1.06 | 0.98 | 0.97 | 0.98 | 0.99 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| 3353 | 1.306 | 1.17 | 1.04 | 1.03 | 1.03 | 1.01 | 1.01 | 1.00 | 1.01 | 1.00 | 0.99 |
| 3509 | 1.253 | 1.03 | 0.96 | 0.96 | 0.95 | 0.94 | 0.95 | 0.97 | 0.98 | 0.98 | 0.99 |
| 3680 | 1.205 | 1.11 | 1.02 | 0.99 | 1.00 | 1.00 | 1.00 | 1.00 | 0.99 | 1.00 | 0.99 |
| 3753 | 1.163 | 1.15 | 1.04 | 1.04 | 1.01 | 1.00 | 1.01 | 1.00 | 1.00 | 0.99 | 0.99 |
| 3661 | 1.125 | 1.31 | 1.08 | 1.02 | 1.02 | 1.00 | 0.99 | 0.99 | 0.99 | 0.99 | 0.98 |
| 3343 | 1.091 | 1.57 | 1.16 | 1.06 | 1.01 | 1.00 | 0.99 | 0.98 | 0.98 | 0.98 | 0.99 |
| 2707 | 1.060 | 2.06 | 1.32 | 1.07 | 0.99 | 0.95 | 0.95 | 0.95 | 0.93 | 0.94 | 0.95 |
| 1168 | 1.034 | 2.63 | 1.54 | 1.19 | 1.05 | 0.96 | 0.91 | 0.89 | 0.86 | 0.87 | 0.86 |
| 48718 | overall | 1.18 | 1.04 | 1.00 | 1.00 | 0.99 | 0.99 | 0.99 | 0.99 | 0.99 | 0.99 |

List of 4 reflections *NOT* obeying Wilson distribution (Z> 10.0)

| h | k | l | RES | Z | Intensity | Sigma | |
|---|---|---|---|---|---|---|---|
| 28 | 16 | 30 | 1.10 | 12.57 | 0.3774E+04 | 0.1106E+03 | "alien" |
| 32 | 28 | 5 | 1.80 | 10.98 | 0.2999E+05 | 0.2827E+03 | "alien" |
| 62 | 11 | 5 | 1.24 | 10.22 | 0.6220E+04 | 0.6805E+02 | "alien" |
| 8 | 7 | 16 | 2.20 | 10.13 | 0.7324E+05 | 0.7421E+03 | "alien" |

List of 4 reflections *NOT* obeying Wilson distribution (sorted by resolution)
Ice rings could occur at (Angstrom):
3.897,3.669,3.441, 2.671,2.249,2.072, 1.948,1.918,1.883,1.721

| h | k | l | RES | Z | Intensity | Sigma |
|---|---|---|---|---|---|---|
| 28 | 16 | 30 | 1.10 | 12.57 | 0.3774E+04 | 0.1106E+03 |

```
  62   11    5    1.24   10.22  0.6220E+04  0.6805E+02
  32   28    5    1.80   10.98  0.2999E+05  0.2827E+03
   8    7   16    2.20   10.13  0.7324E+05  0.7421E+03

NUMBER OF UNIQUE ALIEN REFLECTIONS WITH A Z-SCORE ABOVE LIMIT         0
(ALIENS ABOVE LIMIT (REJECT_ALIEN=      20.0) ARE MARKED INVALID)

NUMBER OF REFLECTION RECORDS ON OUTPUT FILE "XDS_ASCII.HKL"      564183
NUMBER OF ACCEPTED OBSERVATIONS (INCLUDING SYSTEMATIC ABSENCES)  559445
NUMBER OF REJECTED MISFITS & ALIENS (marked by -1*SIGMA(IOBS))     4738


cpu time used                 82.4 sec
elapsed wall-clock time       14.7 sec
```