<!-- CCP4 HTML LOGFILE -->
<pre>#CCP4I VERSION CCP4Interface 7.1.009
#CCP4I SCRIPT LOG aimless
#CCP4I DATE 25 Oct 2021 11:50:52
#CCP4I USER yoshihisasuzuki
#CCP4I PROJECT merge_roomtemp_GI_pf
#CCP4I JOB_ID 7
#CCP4I SCRATCH /tmp/yoshihisasuzuki
#CCP4I HOSTNAME YoshihisanoMacBook-Air.local
#CCP4I PID 36583
</pre>

 ##
 ##
 ##
 ### CCP4 7.1.009: POINTLESS   version 1.12.2 : 24/06/20##
 ##
 User: yoshihisasuzuki Run date: 25/10/2021 Run time: 11:50:52

 Please reference: Collaborative Computational Project, Number 4. 2011.
 "Overview of the CCP4 suite and current developments". Acta Cryst. D67, 235-242.
 as well as any specific reference in the program write-up.

==== Command line arguments ====
HKLOUT /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_2_mtz.tmp
XMLOUT
/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_po
intless.xml

Release Date: 24th June 2020

```
==== Input command lines ====

HKLIN                                  /Users/yoshihisasuzuki/Documents/211008suzuki01-
collection3/collection3_pointless1.mtz
HKLIN /Users/yoshihisasuzuki/Documents/211008suzuki03/collection_pointless1.mtz
## This script run with the command   ##########
#                      /Applications/ccp4-7.1/bin/pointless                      HKLOUT
"/tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_2_mtz.tmp" XMLOUT &
"/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_p
ointless.xml"
###############################################

====     End of input    ====


        ********************************************************
        *                                                      *
        *                     POINTLESS                        *
        *                       1.12.2                         *
        *                                                      *
        *   Determine Laue group from unmerged intensities     *
        *     Phil Evans MRC LMB, Cambridge                    *
        * Uses cctbx routines by Ralf Grosse-Kunstleve et al.  *
        *                                                      *
        ********************************************************


Reflection list generated from file: /Users/yoshihisasuzuki/Documents/211008suzuki01-
collection3/collection3_pointless1.mtz

Title: Untitled

   Space group from HKLIN file : I 2 2 2
```

```
   Cell:    94.08   99.32  103.13   90.00   90.00   90.00
   Resolution range in file:     41.15        1.14

Reflection             list             generated             from             file:
/Users/yoshihisasuzuki/Documents/211008suzuki03/collection_pointless1.mtz

Title: Untitled

   Space group from HKLIN file : I 2 2 2
   Cell:    94.06   99.38  103.14   90.00   90.00   90.00
   Resolution range in file:     41.16        1.14
   Batch numbers incremented by   1000
      ResolutionRange    NobsParts  Nbatches  Ndatasets
        41.16   1.14      593774    146         1

      Project: New Crystal: New Dataset: New

No possible alternative indexing

Time for reading file(s):    2.964 secs

============================================================

>*> Summary of test data read in:
   Resolution range accepted:    41.16        1.14

   Number of reflections      =        175530
   Number of observations     =       1072448
   Number of parts            =       1277349
   Number of batches in file  =           326
   Number of datasets         =             1

      Project: New Crystal: New Dataset: New
```

Run number: 1 consists of batches 1 - 180

Resolution range for run: 41.15 1.14

Phi range: -45.00 to 45.00 Time range: -45.00 to 45.00

Closest reciprocal axis to spindle: b* (angle 19.6 degrees)

Run number: 2 consists of batches 1035 - 1180

Resolution range for run: 41.15 1.14

Phi range: -28.00 to 45.00 Time range: -28.00 to 45.00

Closest reciprocal axis to spindle: c* (angle 33.6 degrees)

Dataset contains multiple unit cells and wavelengths

'deviation' is estimate of the difference of the cell (in A)
from the mean of the others
At worst this should be less the half the maximum resolution of the data

	a	b	c	alpha	beta	gamma	deviation	lambda
	94.08	99.32	103.13	90.00	90.00	90.00	0.06	0.9000
	94.06	99.38	103.14	90.00	90.00	90.00	0.06	0.9000
RMS deviation:	0.01	0.04	0.01	0.00	0.00	0.00		
Average dataset cell:	94.07	99.35	103.13	90.00	90.00	90.00		
Wavelengths:	0.89999,	0.89999						

Numbers of observations marked in the FLAG column
By default all flagged observations are rejected
Observations may be counted in more than one category

	Flagged	Accepted	Maximum	MaxAccepted
BGratio too large	0	0	1.600	0.000
PKratio too large	68457	0	148.040	0.000
Negative < 5sigma	0	0		
Gradient too large	0	0	0.335	0.000

```
   Profile-fitted overloads     300      300
   Spots on edge              22183        0
   XDS misfits (outliers)         0        0


 ===========================================================

 No alternative indexing to test

 Number of reflections  =            175530
 Number of observations =           1072448
 Number of scaled observations =        813
 Average multiplicity =                 6.1

 Resolution range in list:      41.16 ->   1.14

 Intensity normalisation for each run:
    Run   1: B-factor =   -8.3  +  -0.0092 * time  (final B  -9.1)
    Run   2: B-factor =   -8.8  +  -0.0119 * time  (final B  -9.7)

 Estimation of useful resolution for point group determination:
 -------------------------------------------------------------
 Point group correlation statistics are not reliable for very weak data,
 so a high resolution cutoff (for this purpose only) is estimated either
  from CC(1/2) using P1 (Friedel) symmetry (limit  0.60), or
  from Mean(I/sigma(I)) (limit   6.00), if there are sufficient data

 High-resolution estimate from CC(1/2):      1.56
 High-resolution estimate from <I/sig(I)>:   1.92

 High resolution limit reset to 1.56   using CC(1/2) cutoff (in P1)
```

$TABLE: Mn(I/sigI) and CC(1/2) [in P1] vs. resolution:

$GRAPHS:Resolution estimate 1.56A:0.000590296|0.772176x0|1:2,4,6,7,9:

$$

N	1/d^2	Dmid	CC(1/2)	N_CC	CCfit	Mn(I/sigI)	N	(I/sigI)/10	$$ $$
1	0.0135	8.62	0.521	312	0.999	81.91	1421	8.191	
2	0.0392	5.05	0.917	541	0.999	65.78	2691	6.578	
3	0.0649	3.93	0.967	466	0.998	57.96	2189	5.796	
4	0.0906	3.32	0.983	959	0.997	31.08	4388	3.108	
5	0.1163	2.93	0.973	2373	0.995	20.40	8806	2.040	
6	0.1420	2.65	0.972	3520	0.993	15.06	11376	1.506	
7	0.1678	2.44	0.961	5885	0.989	13.25	18399	1.325	
8	0.1935	2.27	0.951	5939	0.983	11.82	18038	1.182	
9	0.2192	2.14	0.951	7690	0.975	10.03	22756	1.003	
10	0.2449	2.02	0.939	9310	0.961	7.83	27262	0.783	
11	0.2706	1.92	0.928	4370	0.941	6.21	12744	0.621	
12	0.2964	1.84	0.895	8981	0.911	4.45	27901	0.445	
13	0.3221	1.76	0.866	8524	0.869	3.72	26001	0.372	
14	0.3478	1.70	0.817	8846	0.811	2.83	24930	0.283	
15	0.3735	1.64	0.748	11332	0.735	2.37	30294	0.237	
16	0.3992	1.58	0.646	12208	0.641	1.93	30947	0.193	
17	0.4250	1.53	0.549	12738	0.535	1.64	31085	0.164	
18	0.4507	1.49	0.459	13195	0.427	1.41	31155	0.141	
19	0.4764	1.45	0.315	13677	0.324	1.22	30210	0.122	
20	0.5021	1.41	0.208	14228	0.237	1.09	29846	0.109	
21	0.5278	1.38	0.154	14356	0.167	1.03	29078	0.103	
22	0.5536	1.34	0.094	12830	0.114	0.97	26526	0.097	
23	0.5793	1.31	0.070	12693	0.077	0.94	25665	0.094	
24	0.6050	1.29	0.044	13253	0.051	0.88	25978	0.088	
25	0.6307	1.26	0.045	14320	0.034	0.86	27124	0.086	
26	0.6564	1.23	0.034	15095	0.022	0.83	27507	0.083	
27	0.6822	1.21	0.019	15881	0.014	0.80	28390	0.080	
28	0.7079	1.19	0.031	16250	0.009	0.78	28647	0.078	
29	0.7336	1.17	0.015	16465	0.006	0.77	29237	0.077	

```
 30  0.7593    1.15    0.011   16745    0.004         0.74   29169        0.074
$$

Checking for possible twinning
L-test for twinning (acentrics only) to maximum resolution    1.563
 Neighbouring reflections for test are +- 2 on h,k,l

$TABLE: L-test for twinning, twin fraction 0.052:
$GRAPHS:Cumulative distribution of |L|, estimated fraction 0.052:N:1,2,3,4:
 $$
      |L|        N(|L|)   Untwinned     Twinned    $$ $$
     0.0000      0.0000      0.0000      0.0000
     0.0500      0.0568      0.0500      0.0749
     0.1000      0.1127      0.1000      0.1495
     0.1500      0.1686      0.1500      0.2233
     0.2000      0.2243      0.2000      0.2960
     0.2500      0.2797      0.2500      0.3672
     0.3000      0.3345      0.3000      0.4365
     0.3500      0.3897      0.3500      0.5036
     0.4000      0.4439      0.4000      0.5680
     0.4500      0.4977      0.4500      0.6294
     0.5000      0.5508      0.5000      0.6875
     0.5500      0.6033      0.5500      0.7418
     0.6000      0.6549      0.6000      0.7920
     0.6500      0.7051      0.6500      0.8377
     0.7000      0.7549      0.7000      0.8785
     0.7500      0.8030      0.7500      0.9141
     0.8000      0.8496      0.8000      0.9440
     0.8500      0.8943      0.8500      0.9679
     0.9000      0.9362      0.9000      0.9855
     0.9500      0.9736      0.9500      0.9963
     1.0000      1.0000      1.0000      1.0000
$$
```

```
      Estimated twin fraction alpha from cumulative N(|L|) plot 0.057 (+/-0.007)
   < |L| >:    0.463 (0.5 untwinned, 0.375 perfect twin)
      Estimated twin fraction alpha from < |L| >    0.052
   < L^2 >:    0.292 (0.333 untwinned, 0.2 perfect twin)
      Estimated twin fraction alpha from < L^2 >    0.048

The L-test suggests that the data are not twinned
Note that the estimate of the twin fraction from the L-test is not very accurate,
  particularly for high twin fractions. Better estimates from other tests need knowledge
of
  the point group and the twin operator, which are not available here
Also these statistics come from possibly unscaled (and unmerged) data,
 so may be inaccurate for that reason

Time for twinning test    4.973 secs

=========================================================================

Model for expectation(CC) = E(m) if symmetry is absent P(m;!S) = (1-m^k)^(1/k) with k =
2.6

Lattice symmetry == HKLIN symmetry

Unit cell (from HKLIN file) used to derive lattice symmetry with tolerance   2.0 degrees
  94.08  99.32 103.13  90.00  90.00  90.00

Tolerance (and delta) is the maximum deviation from the
 expected angle between two-fold axes in the lattice group

Lattice point group: I 2 2 2

       1 pairs rejected for E^2 too large
```

Overall CC for 20000 unrelated pairs: -0.002 N= 20000, high resolution limit   1.56

    Estimated expectation value of true correlation coefficient E(CC) = 0.723

    Estimated sd(CC) = 1.068 / Sqrt(N)

  Number of reflections omitted from ice rings: 1226

Estimated E(CC) of true correlation coefficient from identity = 0.819

****

Analysing rotational symmetry in lattice group I m m m

<!--SUMMARY_BEGIN-->

Scores for each symmetry element

Nelmt	Lklhd	Z-cc	CC	N	Rmeas	Symmetry & operator (in Lattice Cell)
1	0.920	8.61	0.86	195013	0.192	identity
2	0.911	8.10	0.81	173653	0.226 ***	2-fold l (0 0 1) {-h,-k,l}
3	0.919	8.64	0.86	309161	0.195 ***	2-fold k (0 1 0) {-h,k,-l}
4	0.906	8.05	0.81	176640	0.229 ***	2-fold h (1 0 0) {h,-k,-l}

<!--SUMMARY_END-->

Time to determine pointgroup: 7.344 secs

Acceptable Laue groups have scores above 0.19

Scores for all possible Laue groups which are sub-groups of lattice group

---

Note that correlation coefficients are from intensities approximately normalised
by resolution, so will be worse than the usual values
Rmeas is the multiplicity weighted R-factor

Lklhd is a likelihood measure, a probability used in the ranking of space groups

Z-scores are from combined scores for all symmetry elements
in the sub-group (Z+) or not in sub-group (Z-)

    NetZ = Z+ - Z-

Net Z-scores are calculated for correlation coefficients (cc)
The point-group Z-scores Zc are calculated
    as the Zcc-scores recalculated for all symmetry elements for or against,

CC- and R- are the correlation coefficients and R-factors for symmetry elements not in the group

Delta is maximum angular difference (degrees) between original cell
and cell with symmetry constraints imposed

The reindex operator converts original index scheme into the conventional
scheme for sub-group

Accepted Laue groups are marked '>'
The HKLIN Laue group is marked '=' if accepted, '-' if rejected

<!--SUMMARY_BEGIN-->

```
   Laue Group          Lklhd    NetZc   Zc+    Zc-     CC     CC-   Rmeas    R-   Delta
ReindexOperator

= 1    I m m m  ***  0.972    8.39   8.39   0.00    0.84   0.00    0.21   0.00    0.0 [h,k,l]
  2   I 1 2/m 1        0.010    0.56   8.62   8.06    0.86   0.81    0.19   0.23    0.0 [-h,-
k,l]
  3   I 1 2/m 1        0.009   -0.01   8.39   8.40    0.84   0.84    0.21   0.21    0.0 [h,l,-k]
  4   I 1 2/m 1        0.008   -0.09   8.35   8.43    0.83   0.84    0.21   0.21    0.0 [k,-h,l]
  5         P -1          0.001    0.29   8.61   8.32    0.86   0.83    0.19   0.21    0.0
[1/2h+1/2k+1/2l,1/2h-1/2k-1/2l,-1/2h+1/2k-1/2l]


<!--SUMMARY_END-->

************************************************************

Testing Lauegroups for systematic absences
------------------------------------------

No systematic absence zones to test in this lattice group

Time for systematic absence tests:    0.103 secs


Possible spacegroups:
---------------------
Indistinguishable space groups are grouped together on successive lines

'Reindex' is the operator to convert from the input hklin frame to the standard spacegroup
frame.

'TotProb' is a total probability estimate (unnormalised)
```

'SysAbsProb' is an estimate of the probability of the space group based on
the observed systematic absences.

'Conditions' are the reflection conditions (absences)

Spacegroup	TotProb	SysAbsProb	Reindex	Conditions
I 2 2 2 (23)	0.972	1.000		
I 21 21 21 (24)	0.972	1.000		

Choosing between possible best groups:

Space group	Point group	Reindex
I 2 2 2	I 2 2 2	[h,k,l]
I 21 21 21	I 2 2 2	[h,k,l]

Space group confidence (= Sqrt(Score * (Score - NextBestScore))) = 0.00

Laue group confidence (= Sqrt(Score * (Score - NextBestScore))) = 0.97

Selecting point group I 2 2 2 as multiple space groups have the same score
WARNING: You will have to determine the true space group later
The 'space group' written to output file may be missing possible screw components

<!--SUMMARY_BEGIN--> $TEXT:Result: $$ $$
Best Solution: point group I 2 2 2

```
   Reindex operator:                  [h,k,l]
   Laue group probability:            0.972
   Systematic absence probability:    1.000
   Total probability:                 0.972
   Space group confidence:            0.000
   Laue group confidence              0.967

WARNING: You will have to determine the true space group later
The 'space group' written to output file may be missing possible screw components

   Unit cell:    94.08   99.32  103.13      90.00   90.00   90.00

   41.16 to   1.56   - Resolution range used for Laue group search

   41.16 to   1.14   - Resolution range in file, used for systematic absence check

   Number of batches in file:    326

The data do not appear to be twinned, from the L-test

$$ <!--SUMMARY_END-->


HKLIN spacegroup: I 2 2 2  body-centred orthorhombic

^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^


Final point group choice has alternative indexing possibilities

Alternative indexing possibilities are marked '*' if the cells are
  too different at the maximum resolution
```

```
    CellDifference(A) ReindexOperator
 1      0.0          [h,k,l]
 2      5.1 *        [-h,l,k]

Writing unmerged data to file /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_2_mtz.tmp  in
point group I 2 2 2

   Reindexing operator          [h,k,l]

   Real space transformation    (x,y,z)

 * Title:

 Untitled

 * Base dataset:

        0 HKL_base
          HKL_base
          HKL_base

 * Number of Datasets = 1

 * Dataset ID, project/crystal/dataset names, cell dimensions, wavelength:

        1 New
          New
          New
             94.0700   99.3500  103.1350   90.0000   90.0000   90.0000
             0.89999

 * Number of Columns = 18
```

* Number of Reflections = 1277349

* Missing value set to NaN in input mtz file

* Number of Batches = 326

* Column Labels :

H K L M/ISYM BATCH I SIGI IPR SIGIPR FRACTIONCALC XDET YDET ROT WIDTH LP MPART FLAG BGPKRATIOS

* Column Types :

H H H Y B J Q J Q R R R R R I I R

* Associated datasets :

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

* Cell Dimensions : (obsolete - refer to dataset cell dimensions above)

94.0800 99.3200 103.1300 90.0000 90.0000 90.0000

* Resolution Range :

0.00059 0.77301 (41.156 - 1.137 A)

* Sort Order :

1 2 3 4 5

* Space group = 'I 2 2 2' (number 23)

(only pointgroup is fixed so far)

$TEXT:Reference: $$ Please cite $$
P.R.Evans, 'Scaling and assessment of data quality' Acta Cryst. D62, 72-82 (2006).

PDF
P.R.Evans, 'An introduction to data reduction: space-group determination, scaling and intensity statistics' Acta Cryst. D67, 282-292 (2011)

PDF
$$

```
 ##################################################################
 ##################################################################
 ##################################################################
 ### CCP4 7.1.009: AIMLESS            version 0.7.4 : 13/12/18##
 ##################################################################
 User: yoshihisasuzuki  Run date: 25/10/2021 Run time: 11:51:05


 Please reference: Collaborative Computational Project, Number 4. 2011.
 "Overview of the CCP4 suite and current developments". Acta Cryst. D67, 235-242.
 as well as any specific reference in the program write-up.

==== Command line arguments ====
HKLIN /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_2_mtz.tmp
HKLOUT /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_3_mtz.tmp
SCALES
/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7.sc
ales
ROGUES
```

/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_rogues.log
NORMPLOT
/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_normplot.xmgr
ANOMPLOT
/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_anomplot.xmgr
CORRELPLOT
/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_correlplot.xmgr
ROGUEPLOT
/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_rogueplot.xmgr
XMLOUT
/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_aimless.xml

Release Date: 13th December 2018

==== Input command lines ====

title [No title given]
resolution &
    low 41.159 &
    high 1.46
output &
    mtz MERGED
This script run with the command
/Applications/ccp4-7.1/bin/aimless   HKLIN
"/tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_2_mtz.tmp"   HKLOUT
"/tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_3_mtz.tmp"   SCALES
"/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7.s

cales" ROGUES
"/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_r
ogues.log" NORMPLOT
"/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_n
ormplot.xmgr" ANOMPLOT
"/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_a
nomplot.xmgr" CORRELPLOT &
"/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_c
orrelplot.xmgr" ROGUEPLOT
"/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_r
ogueplot.xmgr" XMLOUT
"/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_a
imless.xml"
###

==== End of input ====

```
        ********************************************************
        *                                                      *
        *                      AIMLESS                         *
        *                       0.7.4                          *
        *                                                      *
        *     Scaling & analysis of unmerged intensities       *
        *     Phil Evans MRC LMB, Cambridge                    *
        *                                                      *
        ********************************************************
```

Reading data from HKLIN filename: /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_2_mtz.tmp

Reflection list generated from file: /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_2_mtz.tmp

Title: Untitled

Space group from HKLIN file : I 2 2 2
Cell: 94.07 99.35 103.14 90.00 90.00 90.00
Resolution range in file: 41.16 1.14
Number of observation parts outside resolution limits = 662891

Time for reading HKLIN: cpu time: 1.44 secs, elapsed time: 2.0 secs

Resolution range accepted: 41.16 1.46

Number of reflections = 83670
Number of observations = 516484
Number of parts = 614458
Number of batches = 326
Number of datasets = 1

* Dataset information *
Project: New Crystal: New Dataset: New
Unit cell: 94.07 99.35 103.13 90.00 90.00 90.00
Wavelength: 0.89999
Runs: 1 2
Run number: 1 consists of batches 1 - 180
Resolution range for run: 41.16 1.46
Phi range: -45.00 to 45.00 Time range: -45.00 to 45.00
Closest reciprocal axis to spindle: b* (angle 19.6 degrees)
Run number: 2 consists of batches 1035 - 1180
Resolution range for run: 41.16 1.46
Phi range: -28.00 to 45.00 Time range: -28.00 to 45.00

Closest reciprocal axis to spindle: c* (angle 33.6 degrees)

Average unit cell: 94.07 99.35 103.13 90.00 90.00 90.00

Selection of intensity type (Isum or Ipr) will be optimised
Profile fitted value Ipr will be used for 1st scaling

Handling of partials:
MPART flags are checked
Summed partials accepted if total fraction is between 0.95 & 1.05

2496 partial sets rejected with total fraction too small
68 partial sets rejected with total fraction too large
0 partial sets rejected with gaps

Outlier rejection parameters:
In scaling:
Reflections measured 3 or more times: 6 maximum deviation from weighted mean of all other observations
Reflections measured twice: 6 maximum deviation from weighted mean
Policy for deviant reflections measured twice: KEEP
Reflections judged implausibly large will be rejected
Maximum and minimum normalised F (ie E) for acentric reflection 10.00, -5.00
Maximum and minimum normalised F (ie E) for centric reflection 13.94, -6.97

In merging:
Reflections measured 3 or more times: 6 maximum deviation from weighted mean of all other observations
Reflections measured twice: 6 maximum deviation from weighted mean
Policy for deviant reflections measured twice: KEEP
Reflections judged implausibly large will be rejected

Maximum and minimum normalised F (ie E) for acentric reflection 10.00, -5.00

Maximum and minimum normalised F (ie E) for centric reflection 13.94, -6.97

Parallisation of refinement:

Refinement stages will use a single processor

>>>> Layout of scale factors: <<<<

Run 1

Smooth scaling: 20 scales at intervals of 5 over range -45 to 45 in 18 parts

Smooth B-factors: 6 scales at intervals of 22.5 over range -45 to 45 in 4 parts

Secondary beam correction in camera frame, lmax = 4, 3

Run 2

Smooth scaling: 17 scales at intervals of 4.867 over range -28 to 45 in 15 parts

Smooth B-factors: 6 scales at intervals of 18.25 over range -28 to 45 in 4 parts

Secondary beam correction in camera frame, lmax = 4, 3

Allocation of secondary (SURFACE) scales to runs (automatic or from LINKs)

Scale set 1 used for runs 1, 2

Secondary beam parameters will be TIED to zero, ie restrained to a sphere,

with a standard deviation of 0.005, number of ties 24

Parameter variances (DIAGONAL) will be used for sigma(I) estimates

========= Initial scaling =========

The average fractional overlap = Noverlapped/Ntotal, where Noverlapped is the number of observations
with equivalent observations in a different rotation range, and Ntotal is the total number of observations

Average fractional overlap between rotation ranges for run 1
0.98 0.98 0.97 0.98 0.98 0.99 0.98 0.98 0.99 0.99
0.98 0.99 0.98 0.97 0.98 0.99 0.99 0.99

Average fractional overlap between rotation ranges for run 2
0.98 0.98 0.98 0.99 0.99 0.99 0.99 0.99 0.99 0.99
0.99 1.00 1.00 1.00 1.00

Overall fractional overlap between rotation ranges 0.99, minimum 0.97

Optimization statistics macrocycle #1

Cycle	end-this-cycle	change-from-start	change-from-last
start	-343769.566		
#1	-210221.343	133548.223	133548.223
#2	-209767.026	134002.540	454.317
#3	-209766.074	134003.492	0.952
#4	-209766.074	134003.492	0.000

Initial scales for run 1
0.838 1.045 1.095 1.158 1.277 0.960 1.219 1.154 1.182 1.103
1.470 1.084 0.914 1.331 1.304 1.141 1.378 1.363

```
Initial scales for run     2
     1.069       0.693       0.661       0.712       0.733       0.775       0.777       0.788
0.803      0.918
     0.896      1.011      1.146      1.329      1.484

Time for initial scaling: cpu time: 0.34 secs, elapsed time: 1.0 secs

Sufficient rotation ranges are above the minimum threshold for fractional overlap between
rotation ranges =  0.05

========= First round scaling =========

First scaling:    12081 reflections selected from     83675 with I/sd >  17.00, using
every   3'th reflection above that limit

   Optimization statistics macrocycle #1
   Cycle  end-this-cycle  change-from-start  change-from-last
   start    -167966.050
   #1        -67385.116    100580.934         100580.934
   #2        -62469.463    105496.587           4915.653

   ---ITERATION LIMIT OF MACROCYCLE---


Number of outliers within I+ || I- sets:    3172,  between I+ & I-       0, on |E|max
0

Time for 1st scaling: cpu time: 4.26 secs, elapsed time: 4.0 secs


========= Optimising selection of intensity estimate =========
```

The input HKLIN file contains two estimates of intensity,
a summation integration value Isum and a profile-fitted value Ipr
The optimisation here chooses the value which gives the smallest overall Rmeas:
either Ipr, Isum or a combination of the two based on the Iraw value, where
Iraw is the Isum value back-corrected for Lorentz and Polarisation

Mean Iraw for all data: 363.3

Rmeas also printed for inner and outer resolution ranges

Intensity type	Rmeas	Inner	Outer
Resolution range (A)	All	41.2-7.85	1.48-1.46
Summation intensities	0.1605	0.1069	1.0450
Profile intensities	0.1441	0.1153	0.7652
Combined intensities Imid = 291	0.1372	0.1069	0.7655
Combined intensities Imid = 436	0.1373	0.1069	0.7653

Best value:

Combined intensities Imid = 291	0.1372	0.1069	0.7655

Combined intensities will be used:
  weighted mean of profile-fitted (Ipr) & summation (Isum) intensities
    I = w * Ipr + (1-w) * Isum
    w = 1/(1+(Iraw/290.6)^3)

Time for optimisation of intensity type selection: cpu time: 0.60 secs, elapsed time: 1.0 secs

First rough optimisation and analysis of standard deviations
==========

Weighting scheme for averages: variance weights

All runs have fulls & partials

For all runs,
slopes (full, partial) of central part of normal probability plot = 1.12, 1.13
  Correction applied to parameters for fulls and partials

SD correction parameters after normal probability correction

		Fulls				Partials			
Run		SdFac	SdB	SdAdd	ISa	SdFac	SdB	SdAdd	ISa
AllRuns	Fulls & partials	1.12	0.00	0.0200	44.8	1.13	0.00	0.0200	44.4

I+ and I- will be kept separate in SD optimisation

For SD optimisation, number of outliers within I+ || I- sets: 609, between I+ & I-
0, on |E|max 0

  53845 reflections selected for SD optimisation out of 83675 in file

Damping factor: 0.050
No restraints on SD correction parameters
Cycle 1 residual 0.81420
Cycle 2 residual 0.20470
Cycle 3 residual 0.06558
Cycle 4 residual 0.02845
Cycle 5 residual 0.01469
Cycle 6 residual 0.01005

SD correction parameters after optimisation

		Fulls				Partials			
Run		SdFac	SdB	SdAdd	ISa	SdFac	SdB	SdAdd	ISa
AllRuns	Fulls & partials	1.13	0.00	0.1133	7.8	0.82	0.00	0.0806	15.1

Time for SD optimisation = cpu time: 8.55 secs, elapsed time: 8.0 secs

Number of outliers within I+ || I- sets: 588, between I+ & I- 0, on |E|max 0

========= Main scaling =========

Main scaling: 38205 reflections selected from 83675 with |E^2| > 0.80 and |E^2| < 5.00

Optimization statistics macrocycle #1

Cycle end-this-cycle change-from-start change-from-last

start -78860.697

neg scale -0.00519484 1.66539 -1.24995

neg scale -0.00589145 1.59479 -1.21361

neg scale -0.0418681 1.65277 -1.25804

neg scale -0.0103718 1.64535 -1.23962

neg scale -0.0376837 1.68916 -1.28351

neg scale -0.00727841 1.66709 -1.25205

neg scale -0.00161682 1.74041 -1.31767

neg scale -0.0224111 1.58937 -1.21807

neg scale -0.010344 1.62535 -1.22881

neg scale -0.0311172 1.72021 -1.31074

neg scale -0.0196139 1.69807 -1.28231

neg scale -0.0172422 1.71274 -1.29511

neg scale -0.0108184 1.72742 -1.3074

neg scale -0.0231972 1.55514 -1.20755

neg scale -0.0388103 1.58395 -1.22256

neg scale -0.0680452 1.59851 -1.24015

neg scale -0.0420531 1.61279 -1.23584

neg scale -0.0294727 1.61992 -1.23404

neg scale -0.0483754 1.63448 -1.24976

neg scale -0.070466 1.70754 -1.31905
neg scale -0.0617835 1.72221 -1.33121
neg scale -0.0167834 1.62707 -1.23235
neg scale -0.0412052 1.72944 -1.32772
neg scale -0.0279323 1.74416 -1.33918
neg scale -0.0314665 1.66337 -1.26046
neg scale -0.0380276 1.67798 -1.2744
neg scale -0.0398968 1.69262 -1.28768
neg scale -0.00679386 1.75139 -1.33575
neg scale -0.016481 1.67054 -1.25865
neg scale -0.0215013 1.68517 -1.2722
neg scale -0.00145404 1.67772 -1.25696
neg scale -0.00666786 1.52086 -1.19417
neg scale -0.0466672 1.54256 -1.21338
neg scale -0.0376414 1.54971 -1.21166
neg scale -0.0763468 1.56425 -1.23081
neg scale -0.0201741 1.56399 -1.20883
neg scale -0.0550036 1.57855 -1.22706
neg scale -0.110584 1.62932 -1.27448
neg scale -0.12203 1.64389 -1.28942
neg scale -0.111988 1.68025 -1.31416
neg scale -0.0940345 1.67281 -1.29796
neg scale -0.0938212 1.68741 -1.31117
neg scale -0.0892375 1.70207 -1.32382
neg scale -0.0680826 1.73144 -1.34757
neg scale -0.00976649 1.77574 -1.3797
neg scale -0.0607262 1.72395 -1.33275
neg scale -0.0105949 1.7682 -1.36574
neg scale -0.0373511 1.66509 -1.26438
neg scale -0.0425048 1.6797 -1.27795
neg scale -0.0433121 1.69432 -1.29097
neg scale -0.00658323 1.75313 -1.33816
neg scale -0.0270006 1.68685 -1.27626

neg scale -0.0221158 1.71617 -1.30131
neg scale -0.00180802 1.7456 -1.32453
neg scale -0.00996992 1.70871 -1.2873
neg scale -0.0252891 1.50827 -1.19922
neg scale -0.0192239 1.51543 -1.19797
neg scale -0.0520204 1.54429 -1.21584
neg scale -0.0904209 1.55883 -1.23476
neg scale -0.0617418 1.58024 -1.23036
neg scale -0.0888901 1.59479 -1.24722
neg scale -0.110694 1.60933 -1.26339
neg scale -0.0522208 1.58739 -1.22919
neg scale -0.126146 1.68943 -1.33152
neg scale -0.106937 1.71872 -1.35567
neg scale -0.0139871 1.57999 -1.21145
neg scale -0.0992675 1.6382 -1.27481
neg scale -0.0708921 1.74065 -1.36352
neg scale -0.0948463 1.68914 -1.31343
neg scale -0.0668926 1.73315 -1.34923
neg scale -0.0775729 1.69633 -1.31115
neg scale -0.0609591 1.72566 -1.3351
neg scale -0.0154687 1.61595 -1.22639
neg scale -0.0630331 1.67424 -1.28358
neg scale -0.0637944 1.68887 -1.29657
neg scale -0.0528649 1.7182 -1.32098
neg scale -0.0481783 1.68141 -1.28214
neg scale -0.0317289 1.70322 -1.29335
neg scale -0.0269053 1.51716 -1.20107
neg scale -0.0221888 1.52432 -1.20049
neg scale -0.0174286 1.53145 -1.20001
neg scale -0.0594748 1.54601 -1.21912
neg scale -0.0956633 1.56055 -1.23739
neg scale -0.126216 1.57509 -1.25491
neg scale -0.151097 1.58963 -1.27167

neg scale -0.0128893 1.53859 -1.19976
neg scale -0.115798 1.58224 -1.2533
neg scale -0.139146 1.59678 -1.26972
neg scale -0.0784624 1.57482 -1.23516
neg scale -0.161594 1.67678 -1.33893
neg scale -0.11557 1.61105 -1.26643
neg scale -0.130605 1.62561 -1.28149
neg scale -0.143812 1.68396 -1.33604
neg scale -0.136306 1.69858 -1.34835
neg scale -0.0909643 1.74266 -1.3824
neg scale -0.117498 1.63276 -1.27982
neg scale -0.126432 1.64731 -1.29403
neg scale -0.126104 1.69113 -1.33335
neg scale -0.105424 1.72046 -1.35711
neg scale -0.0531558 1.59623 -1.23308
neg scale -0.0921501 1.62535 -1.26382
neg scale -0.104457 1.63989 -1.27833
neg scale -0.11387 1.68368 -1.31853
neg scale -0.108401 1.69833 -1.33089
neg scale -0.0970933 1.69087 -1.31641
neg scale -0.0805944 1.72019 -1.34037
neg scale -0.0840204 1.68341 -1.30214
neg scale -0.0806316 1.69803 -1.31458
neg scale -0.00599583 1.6031 -1.21695
neg scale -0.027801 1.61765 -1.23225
neg scale -0.0448301 1.63222 -1.24696
neg scale -0.0573073 1.6468 -1.26114
neg scale -0.069104 1.67595 -1.28799
neg scale -0.0192328 1.6248 -1.23221
neg scale -0.0547873 1.68315 -1.2869
neg scale -0.0531482 1.69777 -1.29938
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neg scale -0.208409 1.61842 -1.31485
neg scale -0.213955 1.633 -1.32844
neg scale -0.215315 1.64757 -1.34166
neg scale -0.212376 1.66214 -1.35435
neg scale -0.156173 1.58193 -1.27051
neg scale -0.18796 1.611 -1.29992
neg scale -0.201367 1.6547 -1.34019
neg scale -0.127555 1.57452 -1.25526

neg scale -0.185197 1.63271 -1.31296
neg scale -0.11585 1.58878 -1.25602
neg scale -0.13409 1.60334 -1.2707
neg scale -0.147714 1.61789 -1.28484
neg scale -0.0891296 1.58136 -1.24188
neg scale -0.00154306 1.55911 -1.20041
neg scale -0.0917944 1.4469 -1.2211
neg scale -0.0310023 1.43943 -1.19874
neg scale -0.147402 1.46873 -1.24254
neg scale -0.0338464 1.44663 -1.19947
neg scale -0.0927281 1.46129 -1.22123
neg scale -0.192356 1.49053 -1.26211
neg scale -0.0931929 1.46845 -1.22152
neg scale -0.143807 1.48308 -1.24184
neg scale -0.1886 1.49767 -1.26138
neg scale -0.0389558 1.46102 -1.20113
neg scale -0.14195 1.49025 -1.2417
neg scale -0.0412206 1.4682 -1.20206
neg scale -0.0934942 1.4828 -1.22229
neg scale -0.140014 1.49742 -1.24168
neg scale -0.245453 1.5411 -1.29532
neg scale -0.269466 1.55564 -1.31179
neg scale -0.0749801 1.3324 -1.23757
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neg scale -0.237934 1.54824 -1.2942
neg scale -0.260476 1.56279 -1.31036
neg scale -0.277728 1.57733 -1.32585
neg scale -0.267267 1.58447 -1.32429
neg scale -0.278219 1.59899 -1.33892
neg scale -0.133341 1.51885 -1.24223
neg scale -0.222848 1.56253 -1.29248
neg scale -0.271299 1.6207 -1.35106
neg scale -0.267861 1.64981 -1.37717

neg scale -0.259903 1.66439 -1.38951
neg scale -0.0486723 1.49688 -1.20658
neg scale -0.164119 1.54054 -1.25964
neg scale -0.246181 1.59873 -1.32165
neg scale -0.258226 1.62782 -1.34931
neg scale -0.257536 1.64239 -1.36237
neg scale -0.252693 1.65695 -1.37499
neg scale -0.0916635 1.5186 -1.22582
neg scale -0.159638 1.54768 -1.25977
neg scale -0.24324 1.64955 -1.36058
neg scale -0.0729461 1.29025 -1.25572
neg scale -0.214357 1.59846 -1.30549
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neg scale -0.0661071 1.42375 -1.21296
neg scale -0.298834 1.43574 -1.30786
neg scale -0.419779 1.44375 -1.3699

neg scale -0.333672 1.42911 -1.32523
neg scale -0.248336 1.30279 -1.3311
neg scale -0.111925 1.27245 -1.28368
neg scale -0.0705391 1.40644 -1.21676
neg scale -0.365419 1.42247 -1.3423
neg scale -0.260225 1.31019 -1.33256
neg scale -0.0529083 1.26471 -1.26164
neg scale -0.336798 1.33993 -1.35632
neg scale -0.0501001 1.7195 -1.32089
neg scale -0.0505243 1.68772 -1.28872
neg scale -0.046258 1.67712 -1.2777
neg scale -0.103281 1.6811 -1.31025
neg scale -0.100165 1.67054 -1.29917
neg scale -0.146624 1.65342 -1.30896
neg scale -0.064923 1.62835 -1.25352
neg scale -0.0506726 1.61783 -1.24188
neg scale -0.23651 1.62974 -1.33835
neg scale -0.172025 1.61523 -1.29477
neg scale -0.0908059 1.60074 -1.25067
neg scale -0.209506 1.59817 -1.30296
neg scale -0.195573 1.58763 -1.29087
neg scale -0.256444 1.5916 -1.32272
neg scale -0.243622 1.58109 -1.3106
neg scale -0.140035 1.5561 -1.25413
neg scale -0.257656 1.55351 -1.30529
neg scale -0.368279 1.56141 -1.36777
neg scale -0.00922732 1.5311 -1.1969
neg scale -0.16845 1.53902 -1.26105
neg scale -0.0642588 1.52452 -1.21635
neg scale -0.116946 1.51797 -1.23557
neg scale -0.363834 1.52331 -1.34867
neg scale -0.0573961 1.49688 -1.20984
neg scale -0.138822 1.50086 -1.24163

neg scale -0.283694 1.50878 -1.30474
neg scale -0.0246489 1.48631 -1.19681
neg scale -0.0762158 1.47975 -1.21555
neg scale -0.232486 1.4877 -1.27875
neg scale -0.362125 1.49565 -1.341
neg scale -0.12528 1.47315 -1.23401
neg scale -0.27505 1.48108 -1.29691
neg scale -0.456404 1.47589 -1.39337
neg scale -0.183144 1.44939 -1.2569
neg scale -0.295884 1.44673 -1.30574
neg scale -0.147604 1.26705 -1.30457
neg scale -0.154458 1.42152 -1.24741
neg scale -0.0164837 1.7199 -1.30221
neg scale -0.0175106 1.70928 -1.2918
neg scale -0.0675371 1.71328 -1.32386
neg scale -0.0164451 1.69868 -1.28127
neg scale -0.069828 1.70268 -1.31342
neg scale -0.0132016 1.68809 -1.27057
neg scale -0.0483655 1.64982 -1.25905
neg scale -0.0376865 1.63927 -1.24788
neg scale -0.203466 1.63012 -1.32059
neg scale -0.253212 1.63408 -1.35181
neg scale -0.0667484 1.61168 -1.24564
neg scale -0.0502511 1.60115 -1.23397
neg scale -0.0876041 1.58407 -1.24229
neg scale -0.2777 1.59597 -1.33666
neg scale -0.14096 1.57751 -1.26211
neg scale -0.17298 1.56044 -1.26951
neg scale -0.152151 1.54993 -1.2573
neg scale -0.0508912 1.53543 -1.21341
neg scale -0.325426 1.55128 -1.33842
neg scale -0.247964 1.53679 -1.29516
neg scale -0.0769128 1.51834 -1.2201

neg scale -0.349333 1.5342 -1.34447
neg scale -0.271006 1.5197 -1.30121
neg scale -0.0994519 1.50123 -1.22629
neg scale -0.176703 1.5052 -1.25751
neg scale -0.248167 1.50917 -1.28865
neg scale -0.312634 1.51313 -1.31947
neg scale -0.369776 1.51711 -1.35005
neg scale -0.148632 1.49467 -1.2448
neg scale -0.266194 1.49205 -1.29406
neg scale -0.0863907 1.47355 -1.2191
neg scale -0.133996 1.46695 -1.23722
neg scale -0.210261 1.47093 -1.26816
neg scale -0.280688 1.47491 -1.29901
neg scale -0.448504 1.48685 -1.3898
neg scale -0.319016 1.46832 -1.31655
neg scale -0.189076 1.44314 -1.25959
neg scale -0.261834 1.44714 -1.29033
neg scale -0.107715 1.2463 -1.30041
neg scale -0.0737764 1.42853 -1.21541
neg scale -0.229695 1.43654 -1.277
neg scale -0.124671 1.25383 -1.30302
neg scale -0.0481506 1.23847 -1.27741
neg scale -0.066723 1.24602 -1.28065
neg scale -0.22415 1.28405 -1.33144
neg scale -0.15729 1.26886 -1.30809
neg scale -0.285155 1.29921 -1.3538
neg scale -0.0848741 1.25357 -1.28381
neg scale -0.0317166 1.68188 -1.27447
neg scale -0.00963347 1.65022 -1.24219
neg scale -0.0656864 1.64362 -1.26291
neg scale -0.0419595 1.62258 -1.2406
neg scale -0.109101 1.62651 -1.27212
neg scale -0.169288 1.63049 -1.3033

neg scale -0.00998995 1.60152 -1.21789
neg scale -0.149125 1.60945 -1.2807
neg scale -0.135799 1.59893 -1.26928
neg scale -0.186031 1.59237 -1.28878
neg scale -0.335914 1.59373 -1.36906
neg scale -0.0050749 1.56342 -1.20292
neg scale -0.219583 1.57529 -1.29631
neg scale -0.366103 1.57666 -1.37591
neg scale -0.113499 1.55031 -1.24155
neg scale -0.184902 1.55427 -1.27258
neg scale -0.0372174 1.51873 -1.20516
neg scale -0.116193 1.5227 -1.23614
neg scale -0.257411 1.53061 -1.29773
neg scale -0.0893674 1.51216 -1.22389
neg scale -0.0800444 1.48449 -1.21729
neg scale -0.230971 1.49246 -1.27862
neg scale -0.0477538 1.47394 -1.20465
neg scale -0.203514 1.48188 -1.26597
neg scale -0.0962511 1.46734 -1.22266
neg scale -0.217259 1.46472 -1.27091
neg scale -0.156317 1.24839 -1.32383
neg scale -0.172452 1.25594 -1.32605
neg scale -0.100062 1.24058 -1.30116
neg scale -0.0542054 1.69683 -1.29903
neg scale -0.0531816 1.68625 -1.28877
neg scale -0.0499516 1.67568 -1.27834
neg scale -0.151243 1.68366 -1.34016
neg scale -0.0374432 1.65457 -1.25722
neg scale -0.239251 1.65992 -1.3693
neg scale -0.19507 1.64541 -1.32826
neg scale -0.190548 1.63488 -1.31736
neg scale -0.0272499 1.59537 -1.22229
neg scale -0.0821311 1.5888 -1.24191

neg scale -0.150181 1.59276 -1.27271

neg scale -0.211737 1.59671 -1.30324

neg scale -0.199259 1.58619 -1.29189

neg scale -0.12673 1.54413 -1.24522

neg scale -0.366414 1.55999 -1.36585

neg scale -0.407982 1.56395 -1.39529

neg scale -0.103466 1.53362 -1.23337

neg scale -0.302552 1.5455 -1.32424

neg scale -0.355384 1.54946 -1.35409

neg scale -0.39072 1.54291 -1.37189

neg scale -0.022005 1.50202 -1.19726

neg scale -0.345995 1.51132 -1.33583

neg scale -0.304136 1.49024 -1.31132

neg scale -0.0149088 1.72909 -1.31168

neg scale -0.0208077 1.70784 -1.29211

neg scale -0.109134 1.71583 -1.35312

neg scale -0.0207103 1.69724 -1.28212

neg scale -0.115258 1.70522 -1.34323

neg scale -0.0724439 1.69062 -1.30275

neg scale -0.00855768 1.66552 -1.25155

neg scale -0.205889 1.68142 -1.37293

neg scale -0.000391912 1.65497 -1.24109

neg scale -0.0628925 1.65894 -1.2719

neg scale -0.168097 1.6669 -1.33267

neg scale -0.210126 1.67086 -1.36268

neg scale -0.0555312 1.6484 -1.26137

neg scale -0.114478 1.65236 -1.29188

neg scale -0.253027 1.65373 -1.3715

neg scale -0.290906 1.64714 -1.39048

neg scale -0.0213183 1.61679 -1.22918

neg scale -0.292959 1.63661 -1.37982

neg scale -0.0759919 1.61022 -1.24885

neg scale -0.128196 1.60368 -1.26825

neg scale -0.14872 1.57608 -1.26487
neg scale -0.389959 1.57484 -1.39049
neg scale -0.161092 1.5485 -1.26061
neg scale -0.338468 1.56035 -1.34979
neg scale -0.0659897 1.53399 -1.21888
neg scale -0.0404629 1.52349 -1.20717
neg scale -0.34998 1.53276 -1.34431
neg scale -0.0643781 1.50639 -1.21356
neg scale -0.140301 1.51034 -1.24356
neg scale -0.275677 1.51829 -1.30305
neg scale -0.00514476 1.48528 -1.18962
neg scale -0.0551976 1.74816 -1.36436
neg scale -0.0816833 1.71623 -1.33599
neg scale -0.13232 1.699 -1.34633
neg scale -0.0338432 1.66988 -1.26622
neg scale -0.214698 1.68581 -1.38544
neg scale -0.0277072 1.65932 -1.25598
neg scale -0.0860998 1.6633 -1.28625
neg scale -0.13794 1.66726 -1.3162
neg scale -0.220921 1.67522 -1.37542
neg scale -0.0197555 1.64878 -1.24572
neg scale -0.0807966 1.65276 -1.27595
neg scale -0.224944 1.66466 -1.36524
neg scale -0.0734509 1.64222 -1.26554
neg scale -0.263745 1.65809 -1.38417
neg scale -0.178957 1.63959 -1.31489
neg scale -0.22644 1.64357 -1.34451
neg scale -0.267518 1.63699 -1.36337
neg scale -0.165588 1.61855 -1.2937
neg scale -0.0242781 1.6001 -1.22301
neg scale -0.0926687 1.60407 -1.25301
neg scale -0.155628 1.60802 -1.28291
neg scale -0.00707383 1.58956 -1.21212

neg scale -0.0780089 1.59353 -1.24216
neg scale -0.143485 1.5975 -1.27199
neg scale -0.23766 1.58438 -1.30934
neg scale -0.290114 1.58833 -1.33866
neg scale -0.022112 1.562 -1.20901
neg scale -0.329215 1.58177 -1.35669
neg scale -0.210063 1.56337 -1.28698
neg scale -0.0529179 1.54492 -1.21633
neg scale -0.193047 1.55283 -1.27565
neg scale -0.0291926 1.53441 -1.20499
neg scale -0.00360948 1.52386 -1.19354
neg scale -0.280957 1.53972 -1.31156
neg scale -0.129643 1.52126 -1.2412
neg scale -0.199173 1.52523 -1.27065
neg scale -0.0280188 1.50676 -1.20003
neg scale -0.176661 1.51468 -1.25906
neg scale -0.0490789 1.48963 -1.20607
neg scale -0.00712687 1.71261 -1.28963
neg scale -0.00807204 1.70201 -1.28006
neg scale -0.135581 1.71398 -1.36879
neg scale -0.00709384 1.69142 -1.27037
neg scale -0.0591443 1.69538 -1.30025
neg scale -0.104523 1.69939 -1.32979
neg scale -0.0528013 1.66371 -1.27059
neg scale -0.154868 1.67162 -1.32973
neg scale -0.195855 1.67562 -1.35895
neg scale -0.103824 1.65711 -1.29021
neg scale -0.154529 1.66107 -1.31966
neg scale -0.198626 1.66506 -1.34893
neg scale -0.0387775 1.64259 -1.2503
neg scale -0.147765 1.64 -1.29929
neg scale -0.188644 1.6229 -1.30782
neg scale -0.233304 1.61633 -1.32643

neg scale -0.217163 1.59529 -1.3051

neg scale -0.260876 1.58872 -1.32336

neg scale -0.0390568 1.55583 -1.21379

neg scale -0.0169029 1.54532 -1.20275

neg scale -0.0903469 1.54926 -1.23202

neg scale -0.0722637 1.71037 -1.32328

neg scale -0.0280521 1.69579 -1.28453

neg scale -0.0777779 1.67862 -1.29464

neg scale -0.0756531 1.66806 -1.28485

neg scale -0.115974 1.64038 -1.28409

neg scale -0.0222712 1.60483 -1.22419

neg scale -0.0882962 1.60878 -1.2534

neg scale -0.148839 1.61275 -1.2824

neg scale -0.00687885 1.59432 -1.21382

neg scale -0.00365284 1.55622 -1.20044

neg scale -0.0757957 1.56019 -1.22935

neg scale -0.0017462 1.61574 -1.22072

neg scale -0.0546187 1.60917 -1.23936

neg scale -0.0409788 1.59868 -1.22915

#1	-57790.163	21070.534	21070.534

neg scale -0.00198414 1.53274 -1.38533

neg scale -0.00191674 1.5544 -1.39861

neg scale -0.00342168 1.49844 -1.3747

neg scale -0.00674714 1.49299 -1.37728

neg scale -0.0166612 1.50757 -1.39288

neg scale -0.00481881 1.50015 -1.37667

neg scale -0.00266003 1.50731 -1.37614

neg scale -0.0112489 1.48037 -1.38049

neg scale -0.0222034 1.49498 -1.3963

neg scale -0.0265482 1.48237 -1.39948

neg scale -0.00188367 1.43274 -1.37267

neg scale -0.0142245 1.45433 -1.38343

neg scale -0.00108452 1.44375 -1.3699

neg scale -0.022375 1.47589 -1.39337

neg scale -0.0183496 1.48685 -1.3898

#2 -63737.192 15123.505 -5947.029

$TEXT:Warning:$$ $$

WARNING: 1457 observations had a negative secondary scale, so parameters were scaled down

$$

Scale parameters:

Run 1

Primary scales and number of observations

Scales:	0.936	1.000	1.058	1.164	1.243	1.255	1.288	1.299	1.327	1.327
Sd:	0.012	0.005	0.004	0.004	0.004	0.004	0.004	0.004	0.004	0.004
Nobs:	5524	11161	16718	16861	16792	16779	16726	16822	16780	16860

Scales:	1.317	1.360	1.365	1.363	1.404	1.379	1.303	1.185	1.077	1.136
Sd:	0.004	0.005	0.005	0.005	0.005	0.006	0.006	0.005	0.006	0.018
Nobs:	16745	16618	16159	15820	15755	15380	15012	14289	9429	4587

Relative B-factors and number of observations

B-factors:	-4.949	-0.878	-1.738	-2.038	0.000	-7.056
Sd:	0.114	0.036	0.029	0.031	0.042	0.138
Nobs:	25180	50277	74734	71759	46662	22205

Run 2

Primary scales and number of observations

Scales:	2.001	1.478	1.277	1.095	1.137	1.107	1.108	1.109	1.142	1.151
Sd:	0.039	0.008	0.004	0.003	0.003	0.003	0.003	0.003	0.003	0.004
Nobs:	5440	10828	16064	15790	15352	15112	14796	14722	14667	14546

Scales:	1.138	1.088	1.083	1.035	1.010	0.943	0.999
Sd:	0.004	0.004	0.004	0.004	0.004	0.005	0.017
Nobs:	14387	14112	14158	14243	14397	9622	4820

Relative B-factors and number of observations

B-factors:	-3.760	-0.901	-1.570	-1.025	-2.158	-10.657
Sd:	0.141	0.034	0.026	0.031	0.041	0.149
Nobs:	19974	38465	56429	54378	35887	17923

Secondary scales

Scale set 1 used for runs 1, 2

Coefficient(Sd):	0.0193(21)	0.0439(18)	-0.0053(19)	0.0716(17)	0.0173(16)	0.0071(19)
Coefficient(Sd):	0.0091(19)	0.0154(20)	0.0228(15)	-0.0426(15)	0.0302(17)	0.0077(16)
Coefficient(Sd):	-0.0181(19)	-0.0335(19)	0.0143(16)	-0.0585(8)	0.0020(9)	-0.0109(10)
Coefficient(Sd):	-0.0124(9)	-0.0478(13)	-0.0060(12)	-0.0035(15)	-0.0139(15)	-0.0183(13)

Time for main scaling: cpu time: 11.84 secs, elapsed time: 12.0 secs

Secondary scale corrections, in goniometer frame (SECONDARY)

Calculated for polar angles of theta (colatitude from 0 at N pole, 180 at S pole) and phi (longitude)
Printed only for angular ranges containing data

Range of secondary corrections: 0.880 - 1.832

Secondary scale number 1

Theta	0	10	20	30	40	50	60	70	80	90	100	110	120	130	140	150	160	170
Phi																		
0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
10	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
20	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
30	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
40	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
50	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
60	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
70	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

80	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
90	-	-	-	-	-	-	-	-	1.13	1.15	-	-	-	-	-	-	-	-
100	-	-	-	-	-	-	1.02	1.07	1.11	1.12	1.08	1.02	-	-	-	-	-	-
110	-	-	-	-	-	0.99	1.01	1.04	1.06	1.06	1.03	0.97	0.93	-	-	-	-	-
120	-	-	-	-	-	0.99	1.00	1.01	1.02	1.00	0.97	0.93	0.90	-	-	-	-	-
130	-	-	-	-	-	0.99	0.99	0.99	0.99	0.97	0.94	0.92	0.90	-	-	-	-	-
140	-	-	-	-	-	1.00	1.00	1.00	0.99	0.97	0.95	0.93	0.92	-	-	-	-	-
150	-	-	-	-	-	1.01	1.02	1.02	1.01	1.00	0.99	0.97	0.97	-	-	-	-	-
160	-	-	-	-	-	1.02	1.03	1.04	1.04	1.04	1.03	1.03	1.02	-	-	-	-	-
170	-	-	-	-	-	1.02	1.03	1.05	1.06	1.07	1.07	1.07	1.06	-	-	-	-	-
180	-	-	-	-	-	1.00	1.01	1.03	1.04	1.06	1.06	1.07	1.06	-	-	-	-	-
190	-	-	-	-	-	0.97	0.98	0.99	1.00	1.01	1.02	1.03	1.03	-	-	-	-	-
200	-	-	-	-	-	0.94	0.94	0.94	0.95	0.95	0.96	0.97	0.98	-	-	-	-	-
210	-	-	-	-	-	0.92	0.92	0.92	0.92	0.91	0.91	0.92	0.93	-	-	-	-	-
220	-	-	-	-	-	0.93	0.93	0.94	0.93	0.92	0.91	0.90	0.90	-	-	-	-	-
230	-	-	-	-	-	0.95	0.98	1.00	1.01	0.99	0.95	0.92	0.90	-	-	-	-	-
240	-	-	-	-	-	1.00	1.07	1.13	1.16	1.13	1.06	0.98	0.92	-	-	-	-	-

```
-    -
  250    -    -    -    -    -    - 1.19 1.32 1.39 1.35 1.22 1.08   -    -    -    -
-    -
  260    -    -    -    -    -    -    -    - 1.67 1.62   -    -    -    -    -    -
-    -
  270    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -
-    -
  280    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -
-    -
  290    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -
-    -
  300    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -
-    -
  310    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -
-    -
  320    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -
-    -
  330    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -
-    -
  340    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -
-    -
  350    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -    -
-    -
```

$TABLE: Histogram of secondary corrections:

$GRAPHS:Histogram of secondary corrections:N:2,3:

$$

N	SecScale	Number	$$ $$
1	0.70	1492	
2	0.72	1732	
3	0.74	1971	
4	0.76	2183	

```
    5       0.78      2365
    6       0.80      2564
    7       0.82      2717
    8       0.84      2886
    9       0.86      3112
   10       0.88      3352
   11       0.90      3787
   12       0.92      4551
   13       0.94      5210
   14       0.96      6075
   15       0.98      6904
   16       1.00      8372
   17       1.02     13525
   18       1.04     23469
   19       1.06     44078
   20       1.08     75560
   21       1.10    123617
   22       1.12     79383
   23       1.14     13268
$$

Optimisation and analysis of standard deviations
================================================

Weighting scheme for averages: variance weights

All runs have fulls & partials

For all runs,
slopes (full, partial) of central part of normal probability plot =   0.86,   1.18
  Correction applied to parameters for fulls and partials

SD correction parameters after normal probability correction
```

		Fulls				Partials			
Run		SdFac	SdB	SdAdd	ISa	SdFac	SdB	SdAdd	ISa
AllRuns	Fulls & partials	0.97	0.00	0.1133	9.1	0.97	0.00	0.0806	12.8

I+ and I- will be kept separate in SD optimisation

For SD optimisation, number of outliers within I+ || I- sets: 75, between I+ & I- 0, on |E|max 0

54237 reflections selected for SD optimisation out of 83675 in file

Damping factor: 0.050

Restraints on SD correction parameters (target (+-SD)): SdB 0.0 (+-10.0)

Cycle 1 residual 0.01013 (main residual 0.01013 restraint residual 0.00000)

Cycle 2 residual 0.00463 (main residual 0.00462 restraint residual 0.00002)

Cycle 3 residual 0.00411 (main residual 0.00409 restraint residual 0.00001)

Cycle 4 residual 0.00383 (main residual 0.00383 restraint residual 0.00000)

Cycle 5 residual 0.00369 (main residual 0.00369 restraint residual 0.00000)

Cycle 6 residual 0.00358 (main residual 0.00357 restraint residual 0.00000)

SD correction parameters after optimisation

		Fulls				Partials			
Run		SdFac	SdB	SdAdd	ISa	SdFac	SdB	SdAdd	ISa
AllRuns	Fulls & partials	0.80	0.20	0.1679	7.4	0.80	-0.25	0.0858	14.5

Time for SD optimisation = cpu time: 8.86 secs, elapsed time: 9.0 secs

Normal probability analysis of anomalous differences

==========

All data			Data within expected delta 0.90		
Slope	Intercept	Number	Slope	Intercept	Number
1.04	-0.07	70065	0.92	-0.05	44273

Outlier rejection limits for I+ v I-

have been adjusted by a factor 3.70 * 0.92

Reflections measured 3 or more times: 30.8 maximum deviation from weighted mean of all other observations

Reflections measured twice: 30.8 maximum deviation from weighted mean

Policy for deviant reflections measured twice: KEEP

The anomalous signal appears to be weak so anomalous flag was left OFF

Outlier analysis

==========

Test for Emax

Number of rejected outliers within I+ || I- sets: 583, between I+ & I- 0, on |E|max 0

****

* Final statistics *

****

Numbers of observations marked in the FLAG column

By default all flagged observations are rejected

Observations may be counted in more than one category

	Flagged	Accepted	Maximum	MaxAccepted
BGratio too large	0	0	1.600	0.000
PKratio too large	68455	0	148.040	0.000
Negative < 5sigma	0	0		
Gradient too large	0	0	0.244	0.000
Profile-fitted overloads	299	0		
Spots on edge	10547	0		

XDS misfits (outliers) 0 0

****
* Merging statistics for dataset New/New/New *
****

Analysis by Batch is in groups of batches, group width 1.00 degrees, 2 batches/group

Time for determination of anisotropic axes: cpu time: 2.01 secs, elapsed time: 2.0 secs
Multiplicity 6.2 is above threshold 1.5 so deviant reflections measured twice are REJECTED in SD and Chi^2 analysis

Accepted data:

Number of unique reflections	80454
Number of observations	436606
Number of fully-recorded observations	344316
Number of partially-recorded observations	92290
Number of scaled partial observations	0
Number of rejected outliers	583
Number of observations rejected on Emax limit	0

Scale factors analysed by Batch for each dataset
==========

Note that Ok below is calculated for the centre of each rotation range,
at theta = 0 (for the B-factor)
Mn(k) is average applied scale, including any input scale
Ok is the scale calculated excluding any input scale
Analysis by Batch is in groups of batches, group width 1.00 degrees, 2 batches/group

Bdecay comes from a straight line fit to the B-factors within each run

For run number 1, slope of B (A^2/degree) 0.001

For run number 2, slope of B (A^2/degree) -0.007

$TABLE: === Scales v rotation range, New:

$GRAPHS:Mn(k) & Ok (theta=0) v. batch:N:1,5,6:

:Relative Bfactor & Decay v. batch:A:1,8,9:

$$

N	Run	Phi	Batch	Mn(k)	Ok	Number	Bfactor	Bdecay	$$ $$
1	1	-44.75	1	1.4681	0.9713	2571	-2.8573	-1.7279	
3	1	-43.75	3	1.4367	0.9847	2725	-2.6727	-1.7249	
5	1	-42.75	5	1.4119	0.9961	2673	-2.4923	-1.7219	
7	1	-41.75	7	1.3866	1.0065	2627	-2.3189	-1.7189	
9	1	-40.75	9	1.3621	1.0179	2638	-2.1552	-1.7160	
11	1	-39.75	11	1.3476	1.0326	2667	-2.0031	-1.7130	
13	1	-38.75	13	1.3336	1.0458	2664	-1.8642	-1.7100	
15	1	-37.75	15	1.3202	1.0586	2625	-1.7395	-1.7070	
17	1	-36.75	17	1.3163	1.0727	2636	-1.6295	-1.7041	
19	1	-35.75	19	1.3180	1.0912	2606	-1.5342	-1.7011	
21	1	-34.75	21	1.3252	1.1154	2626	-1.4534	-1.6981	
23	1	-33.75	23	1.3381	1.1374	2580	-1.3866	-1.6952	
25	1	-32.75	25	1.3411	1.1557	2657	-1.3330	-1.6922	
27	1	-31.75	27	1.3510	1.1714	2607	-1.2920	-1.6892	
29	1	-30.75	29	1.3567	1.1877	2650	-1.2625	-1.6862	
31	1	-29.75	31	1.3760	1.2068	2629	-1.2438	-1.6833	
33	1	-28.75	33	1.3854	1.2222	2615	-1.2349	-1.6803	
35	1	-27.75	35	1.3962	1.2334	2625	-1.2348	-1.6773	
37	1	-26.75	37	1.4012	1.2406	2618	-1.2426	-1.6743	
39	1	-25.75	39	1.4080	1.2453	2681	-1.2572	-1.6714	
41	1	-24.75	41	1.4103	1.2498	2561	-1.2776	-1.6684	
43	1	-23.75	43	1.4215	1.2527	2680	-1.3026	-1.6654	

45	1	-22.75	45	1.4304	1.2559	2562	-1.3311	-1.6625
47	1	-21.75	47	1.4338	1.2599	2689	-1.3446	-1.6595
49	1	-20.75	49	1.4495	1.2656	2611	-1.3846	-1.6565
51	1	-19.75	51	1.4610	1.2730	2731	-1.4239	-1.6535
53	1	-18.75	53	1.4776	1.2795	2609	-1.4618	-1.6506
55	1	-17.75	55	1.4859	1.2844	2649	-1.4980	-1.6476
57	1	-16.75	57	1.4984	1.2880	2668	-1.5321	-1.6446
59	1	-15.75	59	1.5096	1.2910	2584	-1.5639	-1.6416
61	1	-14.75	61	1.5153	1.2944	2674	-1.5935	-1.6387
63	1	-13.75	63	1.5242	1.2971	2680	-1.6208	-1.6357
65	1	-12.75	65	1.5345	1.3000	2639	-1.6461	-1.6327
67	1	-11.75	67	1.5428	1.3035	2681	-1.6694	-1.6298
69	1	-10.75	69	1.5516	1.3084	2609	-1.6911	-1.6268
71	1	-9.75	71	1.5630	1.3145	2631	-1.7115	-1.6238
73	1	-8.75	73	1.5688	1.3198	2705	-1.7307	-1.6208
75	1	-7.75	75	1.5816	1.3235	2667	-1.7491	-1.6179
77	1	-6.75	77	1.5871	1.3255	2657	-1.7669	-1.6149
79	1	-5.75	79	1.5923	1.3265	2657	-1.7842	-1.6119
81	1	-4.75	81	1.5967	1.3270	2706	-1.8013	-1.6089
83	1	-3.75	83	1.6008	1.3267	2672	-1.8182	-1.6060
85	1	-2.75	85	1.6053	1.3262	2647	-1.8349	-1.6030
87	1	-1.75	87	1.6044	1.3253	2731	-1.8514	-1.6000
89	1	-0.75	89	1.6101	1.3237	2625	-1.8677	-1.5971
91	1	0.25	91	1.6143	1.3221	2675	-1.8745	-1.5941
93	1	1.25	93	1.6145	1.3212	2666	-1.8828	-1.5911
95	1	2.25	95	1.6163	1.3220	2698	-1.8894	-1.5881
97	1	3.25	97	1.6261	1.3254	2708	-1.8939	-1.5852
99	1	4.25	99	1.6420	1.3319	2649	-1.8958	-1.5822
101	1	5.25	101	1.6490	1.3407	2677	-1.8946	-1.5792
103	1	6.25	103	1.6622	1.3490	2737	-1.8899	-1.5762
105	1	7.25	105	1.6650	1.3549	2662	-1.8812	-1.5733
107	1	8.25	107	1.6744	1.3586	2688	-1.8680	-1.5703
109	1	9.25	109	1.6724	1.3610	2717	-1.8498	-1.5673

111	1	10.25	111	1.6769	1.3629	2657	−1.8262	−1.5644
113	1	11.25	113	1.6698	1.3639	2679	−1.7968	−1.5614
115	1	12.25	115	1.6630	1.3645	2725	−1.7610	−1.5584
117	1	13.25	117	1.6601	1.3646	2640	−1.7186	−1.5554
119	1	14.25	119	1.6492	1.3644	2746	−1.6693	−1.5525
121	1	15.25	121	1.6406	1.3644	2649	−1.6128	−1.5495
123	1	16.25	123	1.6293	1.3647	2766	−1.5492	−1.5465
125	1	17.25	125	1.6181	1.3664	2667	−1.4787	−1.5435
127	1	18.25	127	1.6107	1.3702	2708	−1.4017	−1.5406
129	1	19.25	129	1.6028	1.3767	2640	−1.3191	−1.5376
131	1	20.25	131	1.5980	1.3851	2698	−1.2317	−1.5346
133	1	21.25	133	1.5900	1.3924	2751	−1.1410	−1.5317
135	1	22.25	135	1.5833	1.3965	2628	−1.0482	−1.5287
137	1	23.25	137	1.5779	1.3970	2643	−1.0121	−1.5257
139	1	24.25	139	1.5639	1.3943	2694	−0.9406	−1.5227
141	1	25.25	141	1.5505	1.3888	2709	−0.8768	−1.5198
143	1	26.25	143	1.5392	1.3823	2631	−0.8230	−1.5168
145	1	27.25	145	1.5317	1.3750	2635	−0.7815	−1.5138
147	1	28.25	147	1.5199	1.3654	2673	−0.7542	−1.5108
149	1	29.25	149	1.5136	1.3519	2687	−0.7431	−1.5079
151	1	30.25	151	1.5034	1.3339	2687	−0.7499	−1.5049
153	1	31.25	153	1.5017	1.3170	2678	−0.7764	−1.5019
155	1	32.25	155	1.5059	1.3010	2600	−0.8239	−1.4990
157	1	33.25	157	1.5130	1.2833	2675	−0.8939	−1.4960
159	1	34.25	159	1.5239	1.2610	2654	−0.9879	−1.4930
161	1	35.25	161	1.5268	1.2331	2689	−1.1068	−1.4900
163	1	36.25	163	1.5461	1.2090	2647	−1.2518	−1.4871
165	1	37.25	165	1.5788	1.1886	2643	−1.4232	−1.4841
167	1	38.25	167	1.6190	1.1693	2675	−1.6213	−1.4811
169	1	39.25	169	1.6542	1.1475	2604	−1.8454	−1.4781
171	1	40.25	171	1.7044	1.1232	2648	−2.0940	−1.4752
173	1	41.25	173	1.7691	1.1049	2664	−2.3651	−1.4722
175	1	42.25	175	1.8513	1.0945	2672	−2.6552	−1.4692

177	1	43.25	177	1.9627	1.0930	2648	−2.9604	−1.4663
179	1	44.25	179	2.0960	1.0989	2635	−3.2757	−1.4633
181	2	−27.75	1035	2.1656	1.6683	2683	−2.2839	−0.7625
183	2	−26.75	1037	1.9926	1.5728	2723	−2.1248	−0.7925
185	2	−25.75	1039	1.8535	1.5045	2770	−1.9711	−0.8225
187	2	−24.75	1041	1.7455	1.4524	2781	−1.8265	−0.8525
189	2	−23.75	1043	1.6503	1.4034	2821	−1.6939	−0.8825
191	2	−22.75	1045	1.5608	1.3501	2766	−1.5756	−0.9125
193	2	−21.75	1047	1.4898	1.3090	2796	−1.4726	−0.9425
195	2	−20.75	1049	1.4284	1.2744	2817	−1.3856	−0.9725
197	2	−19.75	1051	1.3721	1.2399	2809	−1.3144	−1.0024
199	2	−18.75	1053	1.3113	1.2004	2847	−1.2584	−1.0324
201	2	−17.75	1055	1.2611	1.1593	2804	−1.2166	−1.0624
203	2	−16.75	1057	1.2288	1.1302	2777	−1.1882	−1.0924
205	2	−15.75	1059	1.2130	1.1145	2762	−1.1718	−1.1224
207	2	−14.75	1061	1.2055	1.1104	2837	−1.1664	−1.1524
209	2	−13.75	1063	1.2125	1.1143	2751	−1.1707	−1.1824
211	2	−12.75	1065	1.2257	1.1211	2774	−1.1833	−1.2124
213	2	−11.75	1067	1.2292	1.1275	2816	−1.2028	−1.2424
215	2	−10.75	1069	1.2378	1.1299	2736	−1.2276	−1.2724
217	2	−9.75	1071	1.2385	1.1282	2723	−1.2334	−1.3023
219	2	−8.75	1073	1.2349	1.1233	2807	−1.2696	−1.3323
221	2	−7.75	1075	1.2368	1.1173	2773	−1.3043	−1.3623
223	2	−6.75	1077	1.2367	1.1125	2768	−1.3366	−1.3923
225	2	−5.75	1079	1.2410	1.1097	2735	−1.3656	−1.4223
227	2	−4.75	1081	1.2439	1.1084	2790	−1.3906	−1.4523
229	2	−3.75	1083	1.2478	1.1079	2740	−1.4113	−1.4823
231	2	−2.75	1085	1.2512	1.1077	2729	−1.4272	−1.5123
233	2	−1.75	1087	1.2526	1.1078	2820	−1.4381	−1.5423
235	2	−0.75	1089	1.2562	1.1079	2709	−1.4441	−1.5723
237	2	0.25	1091	1.2596	1.1080	2686	−1.4451	−1.6023
239	2	1.25	1093	1.2606	1.1085	2768	−1.4412	−1.6322
241	2	2.25	1095	1.2580	1.1093	2716	−1.4326	−1.6622

243	2	3.25	1097	1.2625	1.1110	2624	−1.4194	−1.6922
245	2	4.25	1099	1.2624	1.1141	2739	−1.4020	−1.7222
247	2	5.25	1101	1.2684	1.1194	2710	−1.3808	−1.7522
249	2	6.25	1103	1.2760	1.1267	2743	−1.3565	−1.7822
251	2	7.25	1105	1.2769	1.1335	2696	−1.3297	−1.8122
253	2	8.25	1107	1.2819	1.1386	2642	−1.3012	−1.8422
255	2	9.25	1109	1.2838	1.1420	2656	−1.2840	−1.8722
257	2	10.25	1111	1.2848	1.1447	2631	−1.2581	−1.9022
259	2	11.25	1113	1.2835	1.1472	2700	−1.2348	−1.9321
261	2	12.25	1115	1.2862	1.1486	2721	−1.2151	−1.9621
263	2	13.25	1117	1.2884	1.1489	2660	−1.1997	−1.9921
265	2	14.25	1119	1.2908	1.1481	2664	−1.1893	−2.0221
267	2	15.25	1121	1.2928	1.1460	2665	−1.1845	−2.0521
269	2	16.25	1123	1.2889	1.1426	2666	−1.1857	−2.0821
271	2	17.25	1125	1.2920	1.1387	2662	−1.1934	−2.1121
273	2	18.25	1127	1.2980	1.1340	2591	−1.2078	−2.1421
275	2	19.25	1129	1.2984	1.1271	2691	−1.2293	−2.1721
277	2	20.25	1131	1.2982	1.1175	2669	−1.2579	−2.2021
279	2	21.25	1133	1.2979	1.1064	2585	−1.2936	−2.2321
281	2	22.25	1135	1.3034	1.0978	2687	−1.3362	−2.2620
283	2	23.25	1137	1.3159	1.0922	2677	−1.3852	−2.2920
285	2	24.25	1139	1.3298	1.0888	2657	−1.4397	−2.3220
287	2	25.25	1141	1.3467	1.0866	2588	−1.4985	−2.3520
289	2	26.25	1143	1.3748	1.0839	2644	−1.5601	−2.3820
291	2	27.25	1145	1.4052	1.0812	2595	−1.7124	−2.4120
293	2	28.25	1147	1.4282	1.0769	2702	−1.8076	−2.4420
295	2	29.25	1149	1.4540	1.0699	2597	−1.9104	−2.4720
297	2	30.25	1151	1.4721	1.0603	2628	−2.0216	−2.5020
299	2	31.25	1153	1.5039	1.0495	2631	−2.1429	−2.5320
301	2	32.25	1155	1.5316	1.0411	2608	−2.2766	−2.5619
303	2	33.25	1157	1.5771	1.0347	2627	−2.4256	−2.5919
305	2	34.25	1159	1.6235	1.0288	2627	−2.5936	−2.6219
307	2	35.25	1161	1.6731	1.0228	2682	−2.7848	−2.6519

309	2	36.25	1163	1.7425	1.0151	2621	-3.0034	-2.6819
311	2	37.25	1165	1.8170	1.0082	2635	-3.2537	-2.7119
313	2	38.25	1167	1.9018	0.9998	2641	-3.5393	-2.7419
315	2	39.25	1169	2.0080	0.9880	2628	-3.8629	-2.7719
317	2	40.25	1171	2.1194	0.9736	2651	-4.2253	-2.8019
319	2	41.25	1173	2.2442	0.9618	2703	-4.6253	-2.8319
321	2	42.25	1175	2.4406	0.9554	2645	-5.0590	-2.8618
323	2	43.25	1177	2.6846	0.9559	2614	-5.5197	-2.8918
325	2	44.25	1179	2.9506	0.9626	2602	-5.9985	-2.9218

$$

N	Run	Phi	Batch	Mn(k)	Ok	Number	Bfactor	Bdecay

Agreement between batches

==========

Rmerge in this table is the difference from Mn(Imean),
but in later tables Rmerge is the difference from Mn(I+),Mn(I-)

Mean Chi^2 values are calculated for all data, and also
excluding observations with large deviations >5sd, including for reflections measured only twice (Chi^2c)

SmRmerge and SmMaxRes in table are smoothed over 5 batch groups

$TABLE: Analysis against all Batches for all runs, New:

$GRAPHS:Rmerge v Batch for all runs:N:1,15,6:

:Filtered Mean(Chi^2)(<5sd) v Batch:N:1,14:

:Mean(Chi^2), Mean(Chi^2)(<5sd) v Batch:N:1,13,14:

:Cumulative %completeness & Anom%cmpl v Batch:N:1,10,9:

:Maximum resolution limit, I/sigma > 1.0:A:1,16,11:

:Imean & RMS Scatter:N:1,3,4:

:Imean/RMS scatter:N:1,5:

:Number of rejects:N:1,8:

:Cumulative multiplicity:N:1,12:

$$

N	Batch	Mn(I)	RMSdev	I/rms	Rmerge	Number	Nrej	Cm%poss	AnoCmp	MaxRes
CMlplc	Chi^2	Chi^2c	SmRmerge	SmMaxRes	$$	$$				
1	1	77.8	19.1	4.07	0.146	4992	2	3.0	0.0	1.46
0.03	1.41	1.36	0.129	1.46						
3	3	84.0	15.4	5.47	0.130	5288	3	6.2	0.1	1.46
0.06	1.19	1.17	0.129	1.46						
5	5	86.8	14.9	5.84	0.116	5169	0	9.1	0.2	1.46
0.10	0.99	0.98	0.129	1.46						
7	7	76.2	38.1	2.00	0.130	5104	2	11.9	0.5	1.46
0.13	15.11	0.95	0.123	1.46						
9	9	85.2	22.7	3.76	0.122	5086	1	14.5	0.8	1.46
0.16	1.11	0.90	0.116	1.46						
11	11	76.6	15.0	5.10	0.115	5148	2	17.1	1.3	1.46
0.19	0.85	0.85	0.114	1.46						
13	13	78.6	12.0	6.53	0.099	5133	1	19.6	1.7	1.46
0.22	0.75	0.75	0.109	1.46						
15	15	77.2	14.6	5.31	0.105	5079	0	21.9	2.3	1.46
0.25	0.79	0.79	0.106	1.46						
17	17	74.3	12.1	6.16	0.105	5070	1	24.1	2.8	1.46
0.29	0.77	0.76	0.103	1.46						
19	19	81.0	30.9	2.62	0.104	5018	2	26.2	3.5	1.46
0.32	2.70	0.72	0.105	1.46						
21	21	71.7	21.2	3.38	0.104	5086	2	28.2	4.1	1.46
0.35	0.86	0.76	0.106	1.46						
23	23	72.2	11.0	6.57	0.107	4963	3	30.1	4.7	1.46
0.38	0.75	0.74	0.105	1.46						
25	25	72.7	12.1	6.03	0.107	5125	1	32.0	5.3	1.46
0.41	0.78	0.78	0.103	1.46						
27	27	79.0	12.4	6.37	0.102	5009	1	33.7	5.8	1.46
0.45	0.75	0.73	0.103	1.46						

29	29	84.6	12.3	6.87	0.097	5070	3	35.4	6.3	1.46
0.48	0.75	0.74	0.104	1.46						
31	31	76.3	11.8	6.45	0.104	5046	0	37.0	6.8	1.46
0.51	0.78	0.77	0.102	1.46						
33	33	77.0	11.1	6.95	0.107	4999	3	38.6	7.2	1.46
0.54	0.69	0.69	0.103	1.46						
35	35	81.1	12.2	6.64	0.100	5030	8	40.1	7.7	1.46
0.57	0.74	0.73	0.105	1.46						
37	37	75.3	11.6	6.49	0.110	4988	3	41.6	8.2	1.46
0.61	0.74	0.73	0.105	1.46						
39	39	78.3	12.3	6.39	0.106	5111	4	43.1	8.7	1.46
0.64	0.73	0.73	0.105	1.46						
41	41	81.0	10.8	7.50	0.101	4842	3	44.5	9.3	1.46
0.67	0.71	0.71	0.106	1.46						
43	43	78.6	13.3	5.89	0.109	5096	1	45.9	9.9	1.46
0.70	0.71	0.71	0.108	1.46						
45	45	77.9	11.7	6.64	0.105	4882	2	47.2	10.5	1.48
0.73	0.70	0.69	0.109	1.46						
47	47	83.3	35.8	2.33	0.119	5126	2	48.6	11.2	1.46
0.77	1.00	0.75	0.111	1.46						
49	49	75.4	11.8	6.40	0.112	5037	1	49.9	11.9	1.48
0.80	0.76	0.75	0.113	1.47						
51	51	76.5	13.1	5.85	0.111	5253	3	51.3	12.7	1.47
0.83	0.80	0.79	0.115	1.46						
53	53	71.3	11.3	6.31	0.117	5040	2	52.5	13.5	1.46
0.86	0.77	0.77	0.114	1.46						
55	55	77.7	14.0	5.54	0.114	5158	2	53.8	14.3	1.46
0.90	0.79	0.78	0.115	1.46						
57	57	77.9	16.3	4.77	0.117	5194	3	55.1	15.2	1.46
0.93	0.89	0.83	0.115	1.46						
59	59	80.7	12.7	6.36	0.114	4985	2	56.3	16.2	1.46
0.96	0.84	0.83	0.115	1.46						
61	61	83.9	13.2	6.36	0.114	5116	2	57.5	17.1	1.46

0.99	0.82	0.81	0.116	1.46						
63	63	77.7	14.5	5.36	0.116	5142	3	58.8	18.2	1.46
1.02	0.81	0.80	0.116	1.46						
65	65	76.0	12.4	6.14	0.119	5055	3	59.9	19.2	1.46
1.06	0.80	0.80	0.115	1.46						
67	67	81.6	14.1	5.79	0.116	5091	3	61.1	20.3	1.48
1.09	0.77	0.76	0.115	1.46						
69	69	88.2	17.0	5.18	0.109	4952	0	62.2	21.4	1.46
1.12	0.81	0.81	0.114	1.46						
71	71	86.2	16.8	5.12	0.113	4997	2	63.3	22.5	1.47
1.15	0.77	0.77	0.115	1.48						
73	73	84.3	15.2	5.55	0.112	5126	4	64.4	23.7	1.46
1.19	0.79	0.79	0.117	1.48						
75	75	83.3	15.0	5.55	0.122	5048	0	65.5	24.8	1.49
1.22	0.84	0.83	0.119	1.48						
77	77	71.2	12.2	5.82	0.129	5067	1	66.6	26.0	1.48
1.25	0.80	0.80	0.122	1.48						
79	79	89.8	31.0	2.89	0.120	5043	5	67.7	27.1	1.48
1.28	1.17	0.79	0.124	1.48						
81	81	72.3	13.1	5.51	0.126	5170	1	68.7	28.3	1.49
1.32	0.82	0.81	0.122	1.47						
83	83	81.2	18.5	4.39	0.123	5086	0	69.7	29.5	1.46
1.35	0.79	0.79	0.119	1.47						
85	85	82.9	13.5	6.13	0.112	5068	3	70.8	30.6	1.46
1.38	0.78	0.76	0.119	1.48						
87	87	81.9	11.4	7.16	0.114	5201	0	71.8	31.9	1.48
1.42	0.74	0.74	0.116	1.46						
89	89	74.2	12.1	6.11	0.120	5030	2	72.8	33.0	1.49
1.45	0.78	0.78	0.115	1.46						
91	91	77.4	11.5	6.75	0.112	5139	0	73.7	34.2	1.46
1.48	0.82	0.82	0.115	1.46						
93	93	73.4	12.1	6.06	0.118	5130	2	74.7	35.3	1.46
1.51	0.78	0.78	0.116	1.46						

95	95	86.1	12.1	7.13	0.113	5156	2	75.7	36.5	1.47
1.55	0.80	0.80	0.114	1.46						
97	97	83.9	13.5	6.23	0.116	5228	4	76.6	37.7	1.46
1.58	0.82	0.80	0.116	1.46						
99	99	80.4	13.2	6.10	0.113	5088	0	77.5	38.9	1.47
1.61	0.79	0.78	0.116	1.47						
101	101	77.6	12.0	6.47	0.119	5152	3	78.3	40.1	1.46
1.64	0.79	0.79	0.116	1.48						
103	103	83.1	21.1	3.93	0.119	5257	1	79.2	41.3	1.48
1.68	13.82	0.74	0.118	1.48						
105	105	86.6	14.9	5.80	0.116	5132	0	80.0	42.5	1.50
1.71	0.77	0.76	0.121	1.48						
107	107	80.0	14.2	5.62	0.125	5180	2	80.8	43.7	1.46
1.74	0.82	0.82	0.124	1.49						
109	109	76.7	13.5	5.68	0.126	5245	1	81.6	44.9	1.48
1.78	0.81	0.80	0.125	1.48						
111	111	67.8	12.1	5.59	0.133	5149	2	82.3	46.2	1.49
1.81	0.81	0.81	0.127	1.48						
113	113	76.5	13.3	5.77	0.126	5191	1	83.1	47.3	1.48
1.84	0.81	0.80	0.126	1.49						
115	115	76.5	14.2	5.40	0.125	5277	0	83.7	48.6	1.48
1.87	0.76	0.75	0.126	1.49						
117	117	79.4	13.0	6.11	0.118	5126	0	84.4	49.8	1.48
1.91	0.75	0.74	0.125	1.48						
119	119	76.8	12.2	6.29	0.130	5315	1	85.0	51.0	1.49
1.94	0.79	0.78	0.123	1.48						
121	121	78.7	12.1	6.49	0.125	5114	1	85.6	52.2	1.48
1.97	0.81	0.81	0.122	1.48						
123	123	83.0	14.4	5.77	0.120	5363	3	86.2	53.4	1.48
2.01	0.80	0.80	0.123	1.48						
125	125	82.7	12.2	6.79	0.116	5143	0	86.8	54.6	1.47
2.04	0.76	0.76	0.121	1.48						
127	127	79.8	22.9	3.48	0.124	5218	1	87.2	55.7	1.49

2.07	0.79	0.78	0.120	1.48						
129	129	74.1	13.2	5.63	0.121	5092	1	87.7	56.8	1.46
2.10	0.75	0.75	0.121	1.49						
131	131	71.6	11.9	5.99	0.122	5186	1	88.0	57.8	1.49
2.14	0.78	0.78	0.124	1.49						
133	133	76.3	12.8	5.97	0.123	5319	3	88.4	58.7	1.48
2.17	0.82	0.81	0.123	1.48						
135	135	71.2	11.8	6.04	0.132	5044	0	88.8	59.4	1.46
2.20	0.80	0.80	0.123	1.48						
137	137	76.8	13.1	5.87	0.117	5102	3	89.1	60.1	1.48
2.23	0.80	0.80	0.124	1.48						
139	139	76.1	12.1	6.31	0.125	5192	3	89.4	60.8	1.50
2.27	0.83	0.83	0.125	1.48						
141	141	74.0	15.9	4.65	0.125	5235	3	89.6	61.4	1.49
2.30	0.84	0.84	0.122	1.48						
143	143	70.0	13.1	5.34	0.126	5092	0	89.9	62.0	1.48
2.33	0.80	0.80	0.122	1.48						
145	145	73.4	13.4	5.48	0.117	5115	0	90.1	62.5	1.49
2.36	0.77	0.77	0.121	1.48						
147	147	84.2	14.9	5.67	0.116	5153	1	90.4	63.1	1.46
2.39	0.82	0.81	0.120	1.48						
149	149	76.0	14.5	5.23	0.123	5216	0	90.6	63.6	1.46
2.43	0.86	0.85	0.120	1.48						
151	151	84.8	17.5	4.84	0.119	5197	1	90.8	64.1	1.48
2.46	0.84	0.81	0.122	1.46						
153	153	70.4	12.5	5.62	0.128	5193	1	91.0	64.7	1.46
2.49	0.87	0.85	0.125	1.47						
155	155	71.1	14.1	5.05	0.125	5073	0	91.1	65.2	1.46
2.52	0.86	0.85	0.128	1.48						
157	157	74.8	15.3	4.88	0.131	5210	2	91.3	65.8	1.48
2.55	0.92	0.91	0.134	1.48						
159	159	67.3	14.8	4.54	0.139	5158	0	91.4	66.3	1.48
2.59	0.93	0.92	0.136	1.48						

161	161	64.5	15.1	4.27	0.146	5254	1	91.5	66.9	1.49
2.62	0.94	0.93	0.141	1.48						
163	163	66.0	15.1	4.36	0.140	5176	1	91.6	67.5	1.48
2.65	0.97	0.96	0.142	1.48						
165	165	63.7	17.2	3.69	0.148	5156	0	91.7	68.1	1.46
2.68	1.00	0.99	0.144	1.48						
167	167	68.5	17.3	3.96	0.139	5239	4	91.8	68.7	1.48
2.72	1.06	1.03	0.147	1.48						
169	169	68.0	17.5	3.89	0.146	5097	0	91.9	69.3	1.48
2.75	1.05	1.04	0.150	1.49						
171	171	63.2	18.3	3.45	0.164	5173	0	91.9	69.9	1.50
2.78	1.11	1.09	0.152	1.50						
173	173	69.1	27.6	2.51	0.157	5219	1	92.0	70.5	1.53
2.81	1.26	1.07	0.158	1.51						
175	175	65.0	18.0	3.62	0.155	5242	2	92.0	71.1	1.50
2.84	1.19	1.15	0.166	1.52						
177	177	64.4	21.5	3.00	0.170	5204	3	92.1	71.7	1.55
2.88	1.40	1.30	0.166	1.52						
179	179	64.7	18.9	3.43	0.183	5175	0	92.2	72.3	1.53
2.91	1.49	1.41	0.166	1.52						
181	1035	77.1	23.2	3.32	0.195	5242	3	92.3	72.6	1.57
2.94	0.99	0.98	0.151	1.54						
183	1037	79.0	19.6	4.02	0.175	5326	0	92.3	72.8	1.54
2.97	0.94	0.91	0.151	1.54						
185	1039	90.0	17.5	5.13	0.146	5367	1	92.5	73.1	1.54
3.01	0.87	0.84	0.151	1.54						
187	1041	99.1	17.0	5.84	0.130	5390	0	92.6	73.4	1.50
3.04	0.83	0.82	0.135	1.53						
189	1043	104.6	15.9	6.60	0.121	5472	2	92.7	73.7	1.51
3.08	0.84	0.83	0.123	1.52						
191	1045	100.8	15.6	6.45	0.113	5375	2	92.9	74.1	1.50
3.11	0.81	0.80	0.115	1.50						
193	1047	104.8	16.7	6.28	0.111	5416	0	93.0	74.5	1.53

3.14	0.85	0.80	0.109	1.49						
195	1049	106.6	17.1	6.25	0.102	5473	0	93.1	74.9	1.49
3.18	0.84	0.81	0.104	1.49						
197	1051	112.7	16.0	7.02	0.097	5440	1	93.3	75.4	1.46
3.21	0.85	0.85	0.100	1.48						
199	1053	112.2	19.0	5.91	0.097	5498	1	93.4	75.9	1.48
3.25	0.89	0.88	0.095	1.48						
201	1055	107.1	31.7	3.38	0.093	5446	0	93.5	76.3	1.48
3.28	1.26	0.86	0.094	1.48						
203	1057	107.2	15.4	6.96	0.087	5396	0	93.7	76.9	1.50
3.31	0.83	0.82	0.092	1.48						
205	1059	95.0	21.2	4.48	0.095	5389	0	93.8	77.4	1.48
3.35	0.86	0.83	0.092	1.48						
207	1061	107.3	13.5	7.93	0.087	5475	3	93.9	78.0	1.46
3.38	0.83	0.82	0.092	1.48						
209	1063	100.2	15.6	6.42	0.096	5349	2	94.1	78.5	1.48
3.42	0.88	0.85	0.095	1.48						
211	1065	105.3	20.8	5.06	0.096	5413	1	94.2	79.1	1.49
3.45	0.90	0.84	0.095	1.48						
213	1067	100.9	22.4	4.51	0.099	5447	2	94.3	79.8	1.48
3.48	1.92	0.82	0.097	1.48						
215	1069	102.4	16.6	6.17	0.095	5335	2	94.5	80.4	1.48
3.52	0.81	0.81	0.097	1.48						
217	1071	95.9	13.6	7.07	0.096	5297	3	94.5	81.1	1.48
3.55	0.78	0.78	0.097	1.48						
219	1073	94.4	14.2	6.64	0.097	5462	0	94.6	81.8	1.48
3.58	0.80	0.77	0.096	1.48						
221	1075	99.2	15.0	6.62	0.097	5383	1	94.7	82.5	1.48
3.62	0.79	0.78	0.096	1.48						
223	1077	93.7	12.0	7.80	0.093	5386	1	94.8	83.2	1.46
3.65	0.74	0.74	0.095	1.48						
225	1079	90.0	14.0	6.44	0.095	5311	0	94.9	83.9	1.48
3.69	0.78	0.77	0.095	1.48						

227	1081	84.8	12.4	6.86	0.095	5450	0	94.9	84.3	1.49
3.72	0.76	0.75	0.093	1.47						
229	1083	89.1	16.6	5.37	0.094	5341	2	95.0	84.8	1.46
3.75	0.79	0.78	0.093	1.46						
231	1085	97.8	14.3	6.84	0.089	5311	0	95.1	85.1	1.46
3.79	0.78	0.77	0.094	1.46						
233	1087	93.7	16.2	5.79	0.093	5500	0	95.2	85.4	1.46
3.82	0.81	0.76	0.096	1.46						
235	1089	83.2	13.0	6.41	0.101	5298	0	95.2	85.6	1.46
3.85	0.79	0.78	0.098	1.46						
237	1091	86.7	37.5	2.31	0.104	5239	0	95.3	85.8	1.46
3.89	11.57	0.75	0.099	1.46						
239	1093	81.5	21.7	3.75	0.104	5414	1	95.4	85.9	1.46
3.92	0.94	0.73	0.102	1.46						
241	1095	85.5	12.6	6.76	0.096	5313	0	95.4	86.0	1.46
3.95	0.75	0.75	0.102	1.46						
243	1097	74.8	11.8	6.36	0.105	5132	0	95.5	86.1	1.46
3.98	0.73	0.73	0.099	1.46						
245	1099	81.2	11.8	6.86	0.100	5341	0	95.5	86.3	1.48
4.02	0.75	0.74	0.098	1.47						
247	1101	88.2	14.6	6.02	0.093	5304	2	95.6	86.4	1.48
4.05	0.74	0.74	0.100	1.47						
249	1103	83.3	12.7	6.53	0.096	5365	0	95.6	86.5	1.47
4.08	0.76	0.74	0.100	1.47						
251	1105	76.7	11.6	6.62	0.107	5275	1	95.7	86.6	1.46
4.12	0.77	0.76	0.100	1.46						
253	1107	76.3	12.1	6.30	0.105	5170	2	95.7	86.7	1.46
4.15	0.73	0.73	0.103	1.46						
255	1109	78.1	12.3	6.36	0.104	5195	2	95.8	86.9	1.46
4.18	0.76	0.76	0.105	1.46						
257	1111	73.2	10.4	7.04	0.105	5149	0	95.8	87.0	1.46
4.21	0.74	0.74	0.104	1.46						
259	1113	79.0	11.8	6.71	0.106	5285	1	95.9	87.1	1.46

4.25 0.79 0.79 0.106 1.46
261 1115 88.0 13.8 6.38 0.101 5343 1 95.9 87.2 1.46
4.28 0.77 0.76 0.107 1.46
263 1117 78.2 29.0 2.70 0.114 5235 3 95.9 87.3 1.46
4.31 1.22 0.72 0.108 1.46
265 1119 72.4 20.0 3.62 0.112 5242 0 95.9 87.4 1.46
4.34 6.89 0.75 0.108 1.46
267 1121 68.8 12.4 5.55 0.108 5259 1 96.0 87.5 1.46
4.38 0.75 0.75 0.109 1.46
269 1123 73.7 13.0 5.65 0.107 5257 1 96.0 87.6 1.48
4.41 0.76 0.76 0.109 1.46
271 1125 77.3 13.5 5.74 0.104 5234 0 96.0 87.8 1.46
4.44 0.73 0.73 0.108 1.46
273 1127 69.7 15.7 4.43 0.112 5110 2 96.0 87.9 1.48
4.47 0.73 0.73 0.109 1.46
275 1129 70.3 12.1 5.80 0.110 5305 1 96.1 88.0 1.46
4.50 0.72 0.72 0.113 1.46
277 1131 71.0 14.6 4.87 0.114 5258 1 96.1 88.1 1.46
4.54 0.76 0.76 0.115 1.46
279 1133 64.0 23.5 2.73 0.124 5098 1 96.1 88.1 1.49
4.57 1.23 0.75 0.117 1.46
281 1135 74.2 28.1 2.64 0.116 5278 2 96.1 88.2 1.48
4.60 0.96 0.77 0.118 1.46
283 1137 61.6 11.4 5.41 0.124 5269 1 96.1 88.3 1.47
4.63 0.78 0.78 0.121 1.47
285 1139 70.2 12.6 5.56 0.112 5249 0 96.1 88.4 1.46
4.67 0.78 0.77 0.121 1.46
287 1141 60.9 14.6 4.18 0.129 5133 1 96.2 88.4 1.46
4.70 0.86 0.84 0.123 1.46
289 1143 59.6 12.6 4.74 0.127 5235 0 96.2 88.5 1.46
4.73 0.83 0.82 0.124 1.46
291 1145 64.7 21.9 2.95 0.126 5143 2 96.2 88.5 1.49
4.76 0.84 0.83 0.126 1.46

293	1147	65.6	13.6	4.83	0.124	5343	2	96.2	88.6	1.46
4.79	0.86	0.84	0.126	1.46						
295	1149	66.6	14.0	4.78	0.125	5129	1	96.2	88.6	1.46
4.82	0.88	0.87	0.128	1.46						
297	1151	66.1	16.4	4.04	0.126	5215	2	96.2	88.7	1.46
4.86	0.92	0.91	0.131	1.46						
299	1153	57.9	14.8	3.91	0.142	5216	1	96.2	88.7	1.48
4.89	0.95	0.94	0.136	1.46						
301	1155	63.5	15.9	4.00	0.138	5171	1	96.2	88.8	1.46
4.92	1.05	1.04	0.144	1.48						
303	1157	60.2	14.2	4.25	0.153	5199	4	96.2	88.8	1.48
4.95	1.12	1.11	0.151	1.48						
305	1159	64.1	17.1	3.74	0.162	5187	1	96.3	88.8	1.49
4.98	1.24	1.24	0.159	1.48						
307	1161	65.4	18.1	3.60	0.159	5314	2	96.3	88.9	1.48
5.02	1.33	1.32	0.169	1.48						
309	1163	63.5	21.4	2.97	0.182	5189	2	96.3	88.9	1.46
5.05	1.53	1.49	0.180	1.48						
311	1165	62.2	21.5	2.89	0.190	5221	2	96.3	89.0	1.46
5.08	1.54	1.51	0.194	1.48						
313	1167	63.7	28.6	2.23	0.208	5218	4	96.3	89.0	1.49
5.11	1.88	1.79	0.211	1.48						
315	1169	58.4	38.2	1.53	0.230	5216	0	96.3	89.1	1.49
5.14	2.20	1.89	0.229	1.49						
317	1171	60.7	26.2	2.32	0.247	5250	3	96.3	89.1	1.49
5.18	2.18	2.10	0.252	1.49						
319	1173	64.4	33.9	1.90	0.271	5348	2	96.3	89.2	1.49
5.21	2.49	2.36	0.276	1.50						
321	1175	66.0	33.1	1.99	0.300	5232	2	96.3	89.2	1.51
5.24	2.88	2.72	0.306	1.50						
323	1177	69.0	36.2	1.90	0.329	5167	3	96.4	89.3	1.51
5.27	3.13	2.91	0.306	1.50						
325	1179	65.4	39.5	1.66	0.387	5153	2	96.4	89.3	1.50

5.31 3.44 3.18 0.306 1.50
$$
N Batch Mn(I) RMSdev I/rms Rmerge Number Nrej Cm%poss AnoCmp MaxRes CMlplc Chi^2 Chi^2c SmRmerge SmMaxRes

Correlation coefficients for anomalous differences & Imean between random half-datasets (CC1/2)

==========

CC(1/2) values (for Imean and anomalous differences) are calculated by splitting the data randomly in half
CC(1/2)v for Imean is calculated from variances, see Assmann, Brehm & Diederichs(2016),J.Appl.Cryst.49,1021-1028)
The RMS Correlation Ratio (RCR) is calculated from a scatter plot of pairs of DeltaI(anom)
from the two subsets (halves) by comparing the RMS value (excluding extremes) projected on the line
with slope = 1 ('correlation') with the RMS value perpendicular to this ('error').
This ratio will be > 1 if there is a significant anomalous signal

Rsplit = (1/Sqrt(2)) Sum (|I1 - I2|)/0.5*Sum(I1 + I2) where I1,I2 are the half-dataset intensities as for CC(1/2)
Note that internal R-factors of any sort are deprecated as metrics for assessment of effective resolution

Estimates of maximum resolution for intensities and anomalous differences,
based on the point at which CC(1/2) falls below a threshold

Curve fitting as suggested by Ed Pozharski to a tanh function
of the form (1/2)(1 - tanh(z)) where z = (s - d0)/r,
s = 1/d^2, d0 is the value of s at the half-falloff value, and r controls the

steepness of falloff

Estimate of resolution limit for intensities:
Threshold (see ANALYSIS keyword): 0.30
Resolution limit determined from a curve fit to the function (1/2)(1 - tanh((s - d0)/r)),
after rejecting 2 bins
All scores are above the threshold, ie data extends to the maximum resolution of 1.46A

Estimate of resolution limit for significant anomalous differences:
Threshold (see ANALYSIS keyword): 0.15
Resolution limit determined from a linear fit
All scores are below the threshold, ie there is no apparent anomalous signal from CCanom

$TABLE: Correlations CC(1/2) within dataset, New:
$GRAPHS: CC(1/2) v resolution, max resolution 1.46, anom 0.00:0|0.469156x-0.387886|1:2,4,7,9,11,12:
: RMS anomalous correlation ratio :0|0.469156x0|2.15678:2,6:
: Rsplit :0|0.469156x0|0.444387:2,9:
 $$
  N 1/d^2 Dmid CCanom Nanom RCRanom CC1/2 NCC1/2 CC1/2v Rsplit CCfit CCanomfit $$ $$
  1 0.0078 11.31 0.649 18 2.157 0.876 208 0.927 0.132 1.000 -0.065
  2 0.0235 6.53 0.212 60 1.227 0.970 421 0.972 0.077 0.999 -0.062
  3 0.0391 5.06 -0.136 96 0.880 0.987 567 0.987 0.060 0.999 -0.060
  4 0.0547 4.27 -0.057 99 0.945 0.990 616 0.992 0.051 0.999 -0.058
  5 0.0704 3.77 -0.131 147 0.881 0.993 732 0.994 0.049 0.999 -0.056
  6 0.0860 3.41 -0.388 188 0.672 0.995 825 0.996 0.048

0.999 −0.053

7 0.1017 3.14 0.116 314 1.121 0.992 1077 0.995 0.057
0.998 −0.051

8 0.1173 2.92 −0.150 562 0.862 0.992 1449 0.996 0.058
0.998 −0.049

9 0.1329 2.74 −0.007 843 0.993 0.991 1739 0.994 0.060
0.997 −0.047

10 0.1486 2.59 0.074 1179 1.077 0.989 2026 0.992 0.061
0.996 −0.045

11 0.1642 2.47 −0.089 1456 0.915 0.988 2283 0.992 0.060
0.996 −0.042

12 0.1798 2.36 −0.024 1662 0.976 0.987 2415 0.990 0.063
0.995 −0.040

13 0.1955 2.26 −0.070 1986 0.932 0.986 2602 0.990 0.064
0.993 −0.038

14 0.2111 2.18 −0.045 2205 0.956 0.986 2714 0.989 0.066
0.992 −0.036

15 0.2268 2.10 −0.009 2470 0.991 0.983 2900 0.986 0.068
0.990 −0.033

16 0.2424 2.03 −0.035 2570 0.966 0.988 2955 0.990 0.069
0.987 −0.031

17 0.2580 1.97 −0.050 2692 0.952 0.986 3083 0.988 0.077
0.984 −0.029

18 0.2737 1.91 −0.007 2808 0.994 0.985 3166 0.985 0.085
0.980 −0.027

19 0.2893 1.86 −0.021 2458 0.979 0.977 3175 0.979 0.107
0.975 −0.025

20 0.3050 1.81 −0.012 2535 0.988 0.970 3256 0.973 0.122
0.969 −0.022

21 0.3206 1.77 −0.037 2314 0.964 0.961 3350 0.966 0.139
0.962 −0.020

22 0.3362 1.72 0.015 2432 1.015 0.951 3471 0.955 0.158
0.953 −0.018

```
 23   0.3519     1.69  -0.004       2794       0.996     0.948       3564     0.952      0.179
0.942     -0.016
 24   0.3675     1.65  -0.040       2940       0.961     0.937       3655     0.942      0.199
0.929     -0.013
 25   0.3831     1.62  -0.016       3115       0.985     0.924       3760     0.929      0.222
0.913     -0.011
 26   0.3988     1.58   0.046       3211       1.047     0.894       3780     0.900      0.263
0.894     -0.009
 27   0.4144     1.55  -0.004       3353       0.996     0.865       3897     0.876      0.298
0.872     -0.007
 28   0.4301     1.52  -0.004       3488       0.996     0.836       3968     0.848      0.329
0.845     -0.005
 29   0.4457     1.50   0.013       3553       1.013     0.818       4025     0.828      0.359
0.814     -0.002
 30   0.4613     1.47  -0.049       3633       0.953     0.738       4103     0.760      0.444
0.779     -0.000
$$
Overall:            -0.026     57181      0.974    0.989     75782    0.955     0.082
                    CCanom       Nanom     RCRanom     CC1/2     NCC1/2    CC1/2v     Rsplit
CCfit CCanomfit



Analysis of anisotropy of data
==============================

Mn(I/sd) and half-dataset correlation coefficients CC(1/2) are analysed by resolution
within an maxangle of 20 degrees of principal axes of anisotropy
weighted according to angle, w = [cos(angle) - cos(maxangle)]/[1 - cos(maxangle)],
   Principal axes are along a*, b*, c*

Eigenvalues of [B](orth) along principal axes :    0.810   -2.296    1.486
Difference between maximum and minimum anisotropic B (= 8 pi^2 U)     3.8
```

Estimated maximum resolution limits, a*: 1.46, b*: 1.46, c*: 1.46
Columns 'CCft' are values from curve-fitting as for overall analysis

$TABLE: Anisotropy analysis of CC(1/2) and I/sd, New:
$GRAPHS: Anisotropic CC(1/2) v resolution:0|0.469156x0|1:2,4,5,6,13,14,15:
: Anisotropic Mn(I/sd) v resolution:0|0.469156x0|20.5826:2,7,8,9:
: Projected CC(1/2) v resolution:0|0.469156x0|1:2,10,11,12:
$$

N	1/d^2	Dmid	CC:a*	CC:b*	CC:c*	I/sd:a*	I/sd:b*	I/sd:c*	CCp1	CCp2	CCp3	CCft:a*	CCft:b*	CCft:c*	$$ $$
1	0.0078	11.31	0.798	0.798	0.798	19.60	19.60	19.60	0.985	0.983	0.982	0.999	1.000	0.999	
2	0.0235	6.53	0.999	0.780	0.999	13.14	18.81	11.39	0.994	0.993	0.995	0.999	1.000	0.999	
3	0.0391	5.06	1.000	0.968	0.998	12.08	19.25	12.91	0.994	0.989	0.995	0.998	1.000	0.998	
4	0.0547	4.27	0.994	0.994	0.998	13.15	18.45	12.81	0.995	0.995	0.995	0.998	1.000	0.998	
5	0.0704	3.77	0.975	0.993	0.995	13.72	17.97	11.64	0.990	0.994	0.995	0.998	1.000	0.998	
6	0.0860	3.41	0.989	0.997	0.978	12.10	16.74	9.97	0.989	0.991	0.994	0.997	0.999	0.997	
7	0.1017	3.14	0.977	0.992	0.984	9.72	16.08	10.10	0.987	0.988	0.993	0.996	0.999	0.997	
8	0.1173	2.92	0.973	0.994	0.995	10.78	18.91	10.38	0.982	0.992	0.989	0.995	0.999	0.996	
9	0.1329	2.74	0.976	0.995	0.983	10.82	20.58	10.90	0.985	0.993	0.991	0.994	0.999	0.996	
10	0.1486	2.59	0.984	0.995	0.984	11.93	20.22	10.52	0.985	0.991	0.991	0.993	0.998	0.995	
11	0.1642	2.47	0.974	0.994	0.993	12.58	19.52	10.56	0.986	0.991					

0.991 0.991 0.998 0.994

12 0.1798 2.36 0.983 0.994 0.983 11.36 18.15 11.14 0.983 0.989 0.989 0.989 0.997 0.992

13 0.1955 2.26 0.986 0.985 0.986 10.89 18.34 11.40 0.985 0.988 0.986 0.987 0.996 0.991

14 0.2111 2.18 0.978 0.995 0.983 11.75 18.60 12.04 0.984 0.991 0.983 0.984 0.995 0.989

15 0.2268 2.10 0.988 0.992 0.976 10.62 16.90 11.47 0.977 0.984 0.985 0.980 0.994 0.987

16 0.2424 2.03 0.987 0.992 0.985 9.75 15.89 10.90 0.973 0.980 0.978 0.975 0.992 0.985

17 0.2580 1.97 0.982 0.991 0.984 8.39 15.11 10.96 0.956 0.977 0.975 0.970 0.990 0.982

18 0.2737 1.91 0.975 0.992 0.986 8.14 13.70 10.21 0.948 0.956 0.948 0.963 0.987 0.979

19 0.2893 1.86 0.972 0.970 0.965 6.56 8.74 7.39 0.954 0.939 0.948 0.954 0.983 0.974

20 0.3050 1.81 0.965 0.971 0.937 6.33 8.21 7.57 0.916 0.931 0.942 0.944 0.978 0.970

21 0.3206 1.77 0.963 0.975 0.947 5.11 8.44 7.37 0.923 0.925 0.930 0.931 0.972 0.964

22 0.3362 1.72 0.901 0.946 0.958 3.50 7.20 7.02 0.871 0.907 0.927 0.916 0.965 0.958

23 0.3519 1.69 0.905 0.958 0.940 3.85 6.55 7.03 0.827 0.888 0.907 0.898 0.955 0.950

24 0.3675 1.65 0.838 0.966 0.942 3.70 6.19 6.75 0.763 0.926 0.916 0.877 0.943 0.941

25 0.3831 1.62 0.832 0.944 0.946 3.52 5.70 6.70 0.718 0.868 0.885 0.852 0.928 0.930

26 0.3988 1.58 0.740 0.882 0.906 2.66 3.85 5.68 0.709 0.888 0.862 0.823 0.909 0.918

27 0.4144 1.55 0.774 0.913 0.889 2.63 3.87 4.65 0.720 0.802 0.870 0.789 0.885 0.904

28 0.4301 1.52 0.780 0.847 0.924 2.64 3.61 4.93 0.824 0.793 0.925 0.751 0.857 0.887

29 0.4457 1.50 0.813 0.817 0.901 2.37 3.12 4.32 0.446 0.700 0.884 0.709 0.823 0.868

30 0.4613 1.47 0.585 0.685 0.823 1.90 2.32 3.23 0.705 0.706 0.895 0.663 0.783 0.847

$$

Overall: 0.976 0.976 0.966 7.64 11.64 8.92 0.989 0.989 0.989 0.0 0.0 0.0

CC:a* CC:b* CC:c* I/sd:a* I/sd:b* I/sd:c* CCp1 CCp2 CCp3 CCft:a* CCft:b* CCft:c*

Cumulative CC(1/2) analysed by Batch for each dataset

==========

Analysis by Batch is in groups of batches, group width 1.00 degrees, 2 batches/group

$TABLE: Cumulative CC(1/2) in resolution ranges vs. Batch:

$GRAPHS:Cumulative CC(1/2):N:1,4,5,6,7:

$$

N	Run	Batch	3.26-2.31	2.31-1.88	1.88-1.63	1.63-1.46	$$ $$
1	1	1	-	-	-	-	
3	1	3	0.82	0.98	0.91	0.82	
5	1	5	0.82	0.98	0.91	0.69	
7	1	7	0.99	0.98	0.92	0.79	
9	1	9	0.82	0.97	0.88	0.73	
11	1	11	0.97	0.96	0.87	0.80	
13	1	13	0.99	0.98	0.92	0.71	
15	1	15	0.99	0.97	0.91	0.76	
17	1	17	0.99	0.98	0.90	0.75	
19	1	19	0.99	0.98	0.90	0.74	

21	1	21	0.99	0.97	0.91	0.74
23	1	23	0.99	0.98	0.91	0.73
25	1	25	0.99	0.98	0.93	0.74
27	1	27	0.99	0.98	0.93	0.79
29	1	29	0.99	0.98	0.93	0.74
31	1	31	0.99	0.98	0.93	0.68
33	1	33	0.99	0.98	0.95	0.77
35	1	35	1.00	0.98	0.93	0.75
37	1	37	0.99	0.98	0.94	0.82
39	1	39	0.99	0.98	0.93	0.81
41	1	41	0.99	0.98	0.94	0.78
43	1	43	0.99	0.98	0.94	0.81
45	1	45	0.99	0.99	0.92	0.76
47	1	47	0.99	0.98	0.93	0.79
49	1	49	0.99	0.98	0.94	0.77
51	1	51	0.99	0.98	0.95	0.73
53	1	53	0.99	0.98	0.94	0.73
55	1	55	0.99	0.98	0.93	0.77
57	1	57	0.99	0.98	0.92	0.80
59	1	59	1.00	0.98	0.94	0.75
61	1	61	0.99	0.98	0.93	0.75
63	1	63	0.99	0.99	0.94	0.76
65	1	65	0.99	0.99	0.93	0.76
67	1	67	0.99	0.98	0.93	0.73
69	1	69	0.99	0.98	0.93	0.73
71	1	71	0.99	0.98	0.93	0.80
73	1	73	0.99	0.98	0.94	0.76
75	1	75	0.99	0.98	0.93	0.72
77	1	77	0.99	0.98	0.94	0.78
79	1	79	0.99	0.99	0.95	0.73
81	1	81	0.99	0.98	0.93	0.72
83	1	83	0.99	0.99	0.93	0.77
85	1	85	0.99	0.98	0.93	0.75

87	1	87	0.99	0.98	0.94	0.80
89	1	89	0.99	0.99	0.94	0.74
91	1	91	0.99	0.99	0.94	0.78
93	1	93	0.99	0.99	0.95	0.78
95	1	95	0.99	0.98	0.94	0.77
97	1	97	0.99	0.99	0.93	0.73
99	1	99	0.99	0.98	0.93	0.76
101	1	101	0.99	0.98	0.95	0.79
103	1	103	0.99	0.99	0.95	0.70
105	1	105	0.99	0.99	0.93	0.74
107	1	107	0.99	0.98	0.94	0.77
109	1	109	0.99	0.99	0.93	0.72
111	1	111	0.99	0.99	0.93	0.69
113	1	113	0.99	0.98	0.95	0.75
115	1	115	0.99	0.99	0.95	0.74
117	1	117	0.99	0.99	0.95	0.77
119	1	119	0.99	0.99	0.92	0.72
121	1	121	0.99	0.99	0.94	0.72
123	1	123	0.99	0.98	0.94	0.71
125	1	125	0.99	0.99	0.93	0.74
127	1	127	0.99	0.99	0.92	0.71
129	1	129	0.99	0.99	0.92	0.75
131	1	131	0.99	0.99	0.93	0.74
133	1	133	0.99	0.98	0.94	0.72
135	1	135	0.99	0.98	0.94	0.78
137	1	137	0.99	0.99	0.95	0.76
139	1	139	0.99	0.98	0.93	0.74
141	1	141	0.99	0.98	0.94	0.73
143	1	143	0.99	0.98	0.93	0.72
145	1	145	0.99	0.98	0.95	0.73
147	1	147	0.99	0.99	0.95	0.77
149	1	149	0.99	0.99	0.94	0.77
151	1	151	0.99	0.99	0.94	0.75

153	1	153	0.99	0.98	0.95	0.75
155	1	155	0.99	0.98	0.95	0.75
157	1	157	0.99	0.98	0.94	0.75
159	1	159	0.99	0.98	0.93	0.75
161	1	161	0.99	0.98	0.94	0.76
163	1	163	0.98	0.98	0.93	0.78
165	1	165	0.99	0.98	0.94	0.72
167	1	167	0.97	0.98	0.95	0.76
169	1	169	0.98	0.98	0.94	0.79
171	1	171	0.98	0.98	0.94	0.75
173	1	173	0.98	0.98	0.94	0.77
175	1	175	0.97	0.98	0.94	0.75
177	1	177	0.97	0.98	0.94	0.69
179	1	179	0.98	0.98	0.93	0.72
181	2	1035	0.99	0.98	0.95	0.77
183	2	1037	0.98	0.98	0.95	0.79
185	2	1039	0.99	0.99	0.95	0.77
187	2	1041	0.99	0.99	0.95	0.80
189	2	1043	0.99	0.99	0.95	0.78
191	2	1045	0.99	0.99	0.96	0.78
193	2	1047	0.99	0.99	0.96	0.81
195	2	1049	0.99	0.99	0.95	0.79
197	2	1051	1.00	0.99	0.96	0.83
199	2	1053	1.00	0.99	0.96	0.84
201	2	1055	1.00	0.99	0.96	0.79
203	2	1057	1.00	0.99	0.95	0.81
205	2	1059	0.99	0.99	0.97	0.81
207	2	1061	1.00	0.99	0.96	0.82
209	2	1063	0.99	0.99	0.97	0.81
211	2	1065	0.99	0.99	0.96	0.84
213	2	1067	1.00	0.99	0.96	0.84
215	2	1069	0.99	0.99	0.96	0.85
217	2	1071	0.99	0.99	0.96	0.82

219	2	1073	0.99	0.99	0.96	0.85
221	2	1075	0.99	0.99	0.96	0.84
223	2	1077	0.99	0.99	0.96	0.86
225	2	1079	0.99	0.99	0.96	0.84
227	2	1081	1.00	0.99	0.96	0.83
229	2	1083	0.99	0.99	0.96	0.83
231	2	1085	0.99	0.99	0.97	0.82
233	2	1087	0.99	0.99	0.97	0.87
235	2	1089	0.99	0.99	0.96	0.84
237	2	1091	0.99	0.99	0.96	0.86
239	2	1093	0.99	0.99	0.96	0.80
241	2	1095	0.99	0.99	0.97	0.82
243	2	1097	0.99	0.99	0.97	0.85
245	2	1099	0.99	0.99	0.96	0.83
247	2	1101	0.99	0.99	0.97	0.85
249	2	1103	0.99	0.99	0.96	0.84
251	2	1105	0.99	0.99	0.97	0.82
253	2	1107	0.99	0.99	0.97	0.85
255	2	1109	0.99	0.99	0.97	0.79
257	2	1111	1.00	0.99	0.97	0.84
259	2	1113	0.99	0.99	0.96	0.85
261	2	1115	0.99	0.99	0.98	0.86
263	2	1117	0.99	0.99	0.97	0.84
265	2	1119	0.99	0.99	0.97	0.87
267	2	1121	1.00	0.99	0.98	0.84
269	2	1123	1.00	0.99	0.97	0.87
271	2	1125	1.00	0.99	0.98	0.88
273	2	1127	1.00	0.99	0.97	0.89
275	2	1129	0.99	0.99	0.98	0.89
277	2	1131	1.00	0.99	0.97	0.87
279	2	1133	0.99	0.99	0.98	0.86
281	2	1135	0.99	0.99	0.96	0.88
283	2	1137	0.99	0.99	0.97	0.88

285	2	1139	0.99	0.99	0.98	0.89
287	2	1141	0.99	0.99	0.98	0.89
289	2	1143	0.99	0.99	0.97	0.87
291	2	1145	0.99	0.99	0.97	0.86
293	2	1147	0.99	0.99	0.97	0.87
295	2	1149	0.99	0.99	0.97	0.90
297	2	1151	0.99	0.99	0.97	0.87
299	2	1153	0.99	0.99	0.97	0.90
301	2	1155	0.99	0.99	0.97	0.87
303	2	1157	0.99	0.99	0.97	0.86
305	2	1159	0.99	0.99	0.97	0.90
307	2	1161	0.99	0.99	0.97	0.89
309	2	1163	0.99	0.99	0.97	0.87
311	2	1165	0.99	0.99	0.96	0.87
313	2	1167	0.99	0.99	0.96	0.85
315	2	1169	0.99	0.99	0.96	0.87
317	2	1171	0.99	0.99	0.97	0.86
319	2	1173	0.98	0.97	0.96	0.86
321	2	1175	0.98	0.98	0.95	0.87
323	2	1177	0.97	0.97	0.95	0.85
325	2	1179	0.98	0.97	0.95	0.84

$$

N	Run	Batch	3.26-2.31	2.31-1.88	1.88-1.63	1.63-1.46

Analysis by 4sinTheta/Lambda^2 bins (all statistics use Mn(I+),Mn(I-)etc)

==========

Rmrg :- conventional Rmerge = Sum(|Ihl - < Ih >|)/Sum(< Ih >)

Rcum :- Rmrg up to this range

Rfull :- Rmrg for fully-recorded observations only

Rmeas :- multiplicity-independent R = Sum(Sqrt(N/(N-1))(|Ihl - < Ih >|))/Sum(< Ih >)

Rpim :- Precision-indicating R = Sum(Sqrt(1/(N-1))(|Ihl - < Ih >|))/Sum(< Ih >)

Nmeas :- Number of observations used in statistics
AvI :- unmerged Ihl averaged in bin < Ihl >
RMSdev :- rms scatter of observations from mean < Ih >
I/RMS :- < Ihl > / rms scatter = Av_I/RMSdev
sd :- average standard deviation derived from experimental SDs, after
application of SdFac SdB SdAdd 'correction' terms
Mn(I/sd):- average < merged< Ih >/sd(< Ih >) > ~= signal/noise
Frcbias :- partial bias = Mean(Mn(If) - Ip)/Mean(Mn(I))
for mixed sets only (If is a full if present, else the
partial with the smallest number of parts)
Chi^2 :- mean goodness of fit, all data
Chi^2c :- mean goodness of fit, excluding large differences

All statistics in this table are relative to the overall mean I+/- (anomalous off)
Mean Chi^2 values are calculated for all data, and also
excluding observations with large deviations >5sd, including for reflections measured only twice

$TABLE: Analysis against resolution, New:
$GRAPHS:I/sigma, Mean Mn(I)/sd(Mn(I)):0|0.469156x0|19.6041:2,13,14:
:Filtered Mean(Chi^2)(<5sd) v Resolution:N:2,17:
:Mean(Chi^2), Mean(Chi^2)(<5sd) v Resolution:N:2,16,17:
:Rmerge, Rfull, Rmeas, Rpim v Resolution:0|0.469156x0|0.812081:2,4,5,7,8:
:Average I, RMSdeviation and Sd:0|0.469156x0|869.162:2,10,11,12:
:Fractional bias:0|0.469156x-0.0821763|0.312209:2,15:
$$

N	1/d^2	Dmid	Rmrg	Rfull	Rcum	Rmeas	Rpim	Nmeas	AvI	RMSdev	sd	I/RMS	Mn(I/sd)	FrcBias	Chi^2	Chi^2c	$$	$$
1	0.0078	11.31	0.094	0.075	0.094	0.127	0.085	563	814	207	55	3.9	19.6	0.312	230.18	1.38		
2	0.0235	6.53	0.060	0.085	0.073	0.077	0.048	1260	520	85	37	6.1	18.3	0.083	46.06	1.21		

3	0.0391	5.06	0.049	0.080	0.060	0.063	0.039	1716	757	79	54
9.5	18.0	-0.015	1.90	1.06							
4	0.0547	4.27	0.044	0.081	0.053	0.056	0.034	1908	869	71	63
12.2	18.1	-0.015	1.04	0.97							
5	0.0704	3.77	0.041	0.088	0.050	0.053	0.032	2341	735	54	54
13.5	17.6	-0.029	1.03	0.89							
6	0.0860	3.41	0.045	0.089	0.049	0.057	0.034	2836	443	33	35
13.4	16.4	-0.029	0.93	0.87							
7	0.1017	3.14	0.052	0.086	0.049	0.065	0.038	3793	278	24	24
11.7	15.6	-0.028	0.87	0.85							
8	0.1173	2.92	0.059	0.084	0.051	0.072	0.039	5759	204	18	21
11.3	15.9	-0.023	0.82	0.78							
9	0.1329	2.74	0.068	0.087	0.053	0.080	0.041	7764	172	18	19
9.6	16.0	-0.036	0.84	0.81							
10	0.1486	2.59	0.073	0.088	0.055	0.084	0.041	9993	151	17	19
9.0	15.7	-0.027	0.80	0.77							
11	0.1642	2.47	0.077	0.090	0.058	0.088	0.041	11932	145	18	19
8.3	15.8	-0.031	0.80	0.78							
12	0.1798	2.36	0.082	0.093	0.061	0.093	0.042	13222	140	18	19
7.8	15.5	-0.030	0.82	0.81							
13	0.1955	2.26	0.085	0.094	0.064	0.095	0.041	15100	133	18	19
7.4	15.5	-0.023	0.80	0.79							
14	0.2111	2.18	0.091	0.097	0.067	0.101	0.042	16460	125	18	18
6.8	15.4	-0.027	0.83	0.82							
15	0.2268	2.10	0.099	0.105	0.070	0.109	0.045	18075	106	18	16
6.1	14.4	-0.026	0.85	0.83							
16	0.2424	2.03	0.108	0.113	0.073	0.118	0.047	18809	91	15	15
5.9	13.5	-0.018	0.86	0.85							
17	0.2580	1.97	0.121	0.125	0.076	0.132	0.052	19856	78	15	14
5.4	12.6	-0.019	0.91	0.90							
18	0.2737	1.91	0.136	0.140	0.079	0.148	0.058	20437	65	13	13
4.9	11.5	-0.023	0.95	0.94							
19	0.2893	1.86	0.162	0.163	0.082	0.178	0.072	18659	51	13	11

4.0 9.3 -0.027 0.95 0.93

20 0.3050 1.81 0.183 0.185 0.085 0.202 0.082 18799 43 12 11
3.7 8.4 -0.019 0.99 0.96

21 0.3206 1.77 0.196 0.199 0.088 0.217 0.091 18430 38 11 10
3.6 7.7 -0.018 0.96 0.94

22 0.3362 1.72 0.229 0.229 0.091 0.253 0.106 19010 32 10 10
3.2 6.9 -0.017 0.94 0.92

23 0.3519 1.69 0.273 0.273 0.095 0.301 0.124 20580 26 10 10
2.7 6.1 -0.033 0.95 0.94

24 0.3675 1.65 0.310 0.310 0.098 0.341 0.139 21426 24 10 10
2.4 5.6 -0.020 0.96 0.93

25 0.3831 1.62 0.357 0.350 0.102 0.392 0.159 22399 20 10 10
2.1 4.9 -0.044 0.92 0.91

26 0.3988 1.58 0.421 0.422 0.106 0.463 0.187 22809 17 9 10
1.8 4.3 -0.007 0.95 0.94

27 0.4144 1.55 0.482 0.473 0.110 0.529 0.213 23657 15 9 10
1.6 3.8 -0.058 0.91 0.90

28 0.4301 1.52 0.547 0.536 0.115 0.599 0.241 24248 13 9 10
1.4 3.4 -0.021 0.90 0.89

29 0.4457 1.50 0.608 0.593 0.119 0.666 0.267 24777 12 9 10
1.3 3.1 -0.082 0.87 0.86

30 0.4613 1.47 0.742 0.722 0.124 0.812 0.325 25334 10 9 10
1.1 2.5 -0.073 0.85 0.84

$$

Overall: 0.124 0.157 0.124 0.139 0.061 431952 79 18 14
4.4 9.7 -0.025 1.79 0.89

N 1/d^2 Dmid Rmrg Rfull Rcum Rmeas Rpim Nmeas AvI RMSdev sd
I/RMS Mn(I/sd) FrcBias Chi^2 Chi^2c

By 4sinTheta/Lambda^2 bins (statistics with and without anomalous)

==========

Statistics labelled 'Ov' are relative to the overall mean I+/-, ignoring anomalous
Other statistics are with either I+ or I- sets, for acentrics, ie with anomalous

$TABLE: Analysis against resolution, with & without anomalous (Ov), New:
$GRAPHS:Rmerge, Rmeas, Rpim v Resolution:0|0.469156x0|0.812081:2,4,5,8,9,10,11:
$$

N	1/d^2	Dmid	Rmrg	RmrgOv	Rcum	RcumOv	Rmeas	RmeasOv	Rpim	RpimOv	Nmeas
1	0.0078	11.31	0.101	0.094	0.101	0.094	0.141	0.127	0.098	0.085	563
2	0.0235	6.53	0.054	0.060	0.071	0.073	0.074	0.077	0.049	0.048	1260
3	0.0391	5.06	0.046	0.049	0.057	0.060	0.063	0.063	0.042	0.039	1716
4	0.0547	4.27	0.042	0.044	0.051	0.053	0.056	0.056	0.037	0.034	1908
5	0.0704	3.77	0.039	0.041	0.047	0.050	0.053	0.053	0.035	0.032	2341
6	0.0860	3.41	0.045	0.045	0.047	0.049	0.060	0.057	0.039	0.034	2836
7	0.1017	3.14	0.053	0.052	0.048	0.049	0.071	0.065	0.046	0.038	3793
8	0.1173	2.92	0.059	0.059	0.049	0.051	0.077	0.072	0.049	0.039	5759
9	0.1329	2.74	0.065	0.068	0.052	0.053	0.083	0.080	0.051	0.041	7764
10	0.1486	2.59	0.069	0.073	0.055	0.055	0.087	0.084	0.052	0.041	9993
11	0.1642	2.47	0.073	0.077	0.058	0.058	0.091	0.088	0.053	0.041	11932
12	0.1798	2.36	0.077	0.082	0.061	0.061	0.096	0.093	0.055	0.042	

13222

13 0.1955 2.26 0.080 0.085 0.063 0.064 0.098 0.095 0.056 0.041
15100

14 0.2111 2.18 0.086 0.091 0.066 0.067 0.104 0.101 0.058 0.042
16460

15 0.2268 2.10 0.092 0.099 0.069 0.070 0.112 0.109 0.061 0.045
18075

16 0.2424 2.03 0.100 0.108 0.072 0.073 0.120 0.118 0.065 0.047
18809

17 0.2580 1.97 0.112 0.121 0.075 0.076 0.134 0.132 0.072 0.052
19856

18 0.2737 1.91 0.125 0.136 0.079 0.079 0.150 0.148 0.081 0.058
20437

19 0.2893 1.86 0.152 0.162 0.082 0.082 0.182 0.178 0.098 0.072
18659

20 0.3050 1.81 0.169 0.183 0.085 0.085 0.204 0.202 0.112 0.082
18799

21 0.3206 1.77 0.182 0.196 0.087 0.088 0.220 0.217 0.121 0.091
18430

22 0.3362 1.72 0.211 0.229 0.090 0.091 0.256 0.253 0.142 0.106
19010

23 0.3519 1.69 0.249 0.273 0.094 0.095 0.303 0.301 0.169 0.124
20580

24 0.3675 1.65 0.281 0.310 0.097 0.098 0.341 0.341 0.190 0.139
21426

25 0.3831 1.62 0.324 0.357 0.101 0.102 0.394 0.392 0.218 0.159
22399

26 0.3988 1.58 0.376 0.421 0.105 0.106 0.456 0.463 0.252 0.187
22809

27 0.4144 1.55 0.434 0.482 0.109 0.110 0.526 0.529 0.291 0.213
23657

28 0.4301 1.52 0.488 0.547 0.114 0.115 0.592 0.599 0.328 0.241
24248

29	0.4457	1.50	0.546	0.608	0.118	0.119	0.662	0.666	0.367	0.267
24777										
30	0.4613	1.47	0.667	0.742	0.123	0.124	0.809	0.812	0.447	0.325
25334										

$$

Overall:			0.123	0.124	0.123	0.124	0.151	0.139	0.085	0.061
431952										

N	1/d^2	Dmid	Rmrg	RmrgOv	Rcum	RcumOv	Rmeas	RmeasOv	Rpim	RpimOv
Nmeas										

By intensity bins

==========

All statistics in this table are relative to the overall mean I+/- (anomalous off)

$TABLE: Analysis against intensity, New:

$GRAPHS:Rmerge v Intensity:N:1,2,4,5:

$$

Imax	Rmrg	Rcum	Rmeas	Rpim	Nmeas	AvI	RMSdev	sd	I/RMS	Mn(I/sd)
FrcBias	$$	$$								
11	0.544	0.544	0.597	0.240	236141	11	10	9	1.2	3.6
-0.037										
44	0.176	0.336	0.193	0.078	76305	45	10	10	4.3	11.3
-0.019										
79	0.119	0.259	0.130	0.053	40693	80	13	13	6.3	15.4
-0.016										
119	0.096	0.216	0.105	0.043	27099	120	16	17	7.7	17.4
-0.017										
166	0.084	0.191	0.094	0.039	17783	166	19	22	8.6	18.3
-0.020										
223	0.074	0.173	0.083	0.037	12166	222	23	28	9.7	18.1
-0.022										

```
        293  0.068  0.161  0.079  0.038     7971       291     28     34   10.3     17.8
-0.034
        388  0.063  0.152  0.075  0.039     5536       385     34     41   11.2     17.6
-0.030
        536  0.053  0.145  0.065  0.037     3359       531     39     50   13.5     17.3
-0.031
       1389  0.047  0.124  0.060  0.038     4899      1358    111     99   12.2     18.2
-0.035
$$
Overall:    0.124  0.124  0.139  0.061   431952        79     18     14    4.4      9.7
-0.025

      Imax   Rmrg   Rcum  Rmeas   Rpim    Nmeas      AvI  RMSdev    sd  I/RMS Mn(I/sd)
FrcBias

Rmeas by resolution for each run
--------------------------------


$TABLE:  Analysis against resolution for each run in dataset, New:
$GRAPHS:Rmeas v. resolution for each run:0|0.469156x0|0.887629:2,4,5:
 $$
  N  1/d^2    Dmid   Run1   Run2   $$ $$
  1  0.0078  11.31  0.125  0.129
  2  0.0235   6.53  0.087  0.070
  3  0.0391   5.06  0.065  0.062
  4  0.0547   4.27  0.052  0.059
  5  0.0704   3.77  0.055  0.051
  6  0.0860   3.41  0.058  0.056
  7  0.1017   3.14  0.066  0.065
  8  0.1173   2.92  0.075  0.069
  9  0.1329   2.74  0.081  0.079
 10  0.1486   2.59  0.085  0.084
```

11	0.1642	2.47	0.087	0.090
12	0.1798	2.36	0.092	0.094
13	0.1955	2.26	0.090	0.101
14	0.2111	2.18	0.094	0.109
15	0.2268	2.10	0.101	0.120
16	0.2424	2.03	0.109	0.130
17	0.2580	1.97	0.122	0.145
18	0.2737	1.91	0.139	0.161
19	0.2893	1.86	0.163	0.198
20	0.3050	1.81	0.186	0.223
21	0.3206	1.77	0.206	0.233
22	0.3362	1.72	0.237	0.276
23	0.3519	1.69	0.282	0.329
24	0.3675	1.65	0.319	0.372
25	0.3831	1.62	0.362	0.438
26	0.3988	1.58	0.430	0.511
27	0.4144	1.55	0.497	0.574
28	0.4301	1.52	0.557	0.662
29	0.4457	1.50	0.620	0.734
30	0.4613	1.47	0.761	0.888

$$

Overall:			0.139	0.140
N	1/d^2	Dmid	Run1	Run2

Completeness and multiplicity, including reflections measured only once

==========

%poss is completeness in the shell, C%poss in cumulative to that resolution

The anomalous completeness values (AnomCmpl) are the percentage of possible anomalous differences measured

AnomFrc is the % of measured acentric reflections for which an anomalous difference

has been measured

Anomalous multiplicity AnoMlt is calculated for reflections with both I+ and I- measured, and is defined as:

Sum{[Min(n+, n-) + Dn/(Dn+1)]}/NanomMeasured, where n+, n- are the number of measurements of I+, I-, Dn = |n+ - n-|

$TABLE: Completeness & multiplicity v. resolution, New:

$GRAPHS:Completeness v Resolution :N:2,7,8,10,11:

:Multiplicity v Resolution:0|0.469156x0|6.42942:2,9,12:

$$

N	1/d^2	Dmid	Nmeas	Nref	Ncent	%poss	C%poss	Mlplct	AnoCmp	AnoFrc	AnoMlt
1	0.0078	11.31	724	369	79	66.6	66.6	2.0	31.2	44.1	1.4
2	0.0235	6.53	1556	717	89	75.1	72.1	2.2	33.4	42.8	1.6
3	0.0391	5.06	2073	924	101	73.6	72.8	2.2	35.7	47.6	1.6
4	0.0547	4.27	2346	1054	90	73.1	72.9	2.2	34.3	46.1	1.6
5	0.0704	3.77	2822	1213	97	75.3	73.5	2.3	36.1	47.2	1.7
6	0.0860	3.41	3393	1382	101	76.0	74.1	2.5	35.8	46.5	1.9
7	0.1017	3.14	4298	1582	113	80.6	75.5	2.7	47.8	58.7	1.9
8	0.1173	2.92	6159	1850	138	88.3	77.8	3.3	60.5	68.0	2.1
9	0.1329	2.74	8074	2049	140	91.7	80.0	3.9	70.3	76.2	2.3
10	0.1486	2.59	10231	2264	150	96.2	82.4	4.5	80.4	83.0	

2.5

11	0.1642	2.47	12089	2440	156	97.9	84.5	5.0	86.1	87.7
2.7										
12	0.1798	2.36	13359	2552	160	98.4	86.2	5.2	90.4	91.5
2.7										
13	0.1955	2.26	15194	2696	177	99.2	87.7	5.6	94.1	94.7
2.9										
14	0.2111	2.18	16505	2759	170	99.6	88.9	6.0	97.3	97.6
3.0										
15	0.2268	2.10	18107	2932	172	99.8	90.0	6.2	98.6	98.8
3.1										
16	0.2424	2.03	18836	2982	174	99.9	90.9	6.3	99.4	99.4
3.2										
17	0.2580	1.97	19874	3101	179	100.0	91.7	6.4	99.6	99.6
3.2										
18	0.2737	1.91	20452	3181	169	99.9	92.4	6.4	99.8	99.8
3.2										
19	0.2893	1.86	18748	3264	179	99.6	92.9	5.7	98.2	98.4
2.8										
20	0.3050	1.81	18863	3322	164	99.3	93.4	5.7	97.9	98.4
2.8										
21	0.3206	1.77	18496	3417	175	100.0	93.9	5.4	97.4	97.4
2.7										
22	0.3362	1.72	19076	3537	172	99.7	94.3	5.4	97.9	98.0
2.7										
23	0.3519	1.69	20610	3594	173	99.8	94.6	5.7	98.5	98.6
2.8										
24	0.3675	1.65	21437	3668	180	100.0	94.9	5.8	99.6	99.6
2.9										
25	0.3831	1.62	22413	3775	179	100.0	95.2	5.9	99.6	99.6
2.9										
26	0.3988	1.58	22819	3791	180	99.9	95.5	6.0	99.4	99.4
3.0										

27	0.4144	1.55	23668	3914	182	100.0	95.8	6.0	99.5	99.5	3.0
28	0.4301	1.52	24256	3976	180	100.0	96.0	6.1	99.9	99.9	3.0
29	0.4457	1.50	24784	4036	174	100.0	96.2	6.1	99.9	99.9	3.0
30	0.4613	1.47	25344	4113	172	99.8	96.4	6.2	99.8	99.9	3.0

$$

Overall:	436606	80454	4565	96.4	96.4	5.4	89.3	92.3	2.8
	Nmeas	Nref	Ncent	%poss	C%poss	MlplctAnoCmp		AnoFrc	AnoMlt

Analysis of standard deviations

==========

This analyses the distribution of the normalised deviations

Delta = (Ihl - Mn(Iothers))/sqrt[sd(Ihl)**2 + sd(Mn(I))**2]

If the SD is a true estimate of the error, this distribution should have

Mean=0.0 and Sigma=1.0 for all ranges of intensity

The analysis is repeated for ranges of increasing Imean

The Mean is expected to increase with Imean since the latter

is a weighted mean and sd(Ihl) & Ihl are correlated

If the Sigma increases with Imean, increase the value of SdAdd

ISa is the predicted asymptotic value of I/sd(I) for large I, see

K.Diederichs, Acta Cryst. D66,733

SD corrections:- SdFac * Sqrt[sd(I)**2 + SdB I + (SdAdd I)**2]

Fulls Partials

Run		SdFac	SdB	SdAdd	ISa	SdFac	SdB	SdAdd	ISa
AllRuns	Fulls & partials	0.80	0.20	0.1679	7.4	0.80	-0.25	0.0858	14.5

$TABLE: Run 1, standard deviation v. Intensity, New:
$GRAPHS: Sigma(scatter/SD), Mn(Chi^2), within 5 sd:N:2,13,14,17,18:
: Sigma(scatter/SD), Mn(Chi^2), within 5 sd, all and within 5 sd:N:2,5,6,9,10,13,14,17,18:

		Fulls, all				Partials, all				Fulls, < 5 sd		Partials, < 5 sd		
$$														
Range	Mn(I)	NF	MnF	SdF	ChiSqF	NP	MnP	SdP	ChiSqP	NFc	MnFc	SdFc	ChiSqFc	NPc
MnPc	SdPc	ChiSqPc	$$	$$										
1	11	107322	0.04	0.90	0.82	19616	0.08	0.90	0.82	107296	0.04	0.90	0.81	19581
0.08	0.90	0.81												
2	44	36790	0.08	0.98	0.97	6320	0.11	1.07	1.17	36764	0.07	0.97	0.95	6308
0.11	1.07	1.15												
3	79	19492	0.07	0.91	0.84	3438	0.14	1.09	1.20	19486	0.06	0.91	0.83	3430
0.13	1.07	1.17												
4	119	12898	0.05	0.84	0.71	2436	0.16	1.04	1.11	12894	0.05	0.84	0.70	2433
0.15	1.03	1.08												
5	166	8187	0.01	0.81	0.65	1785	0.12	1.03	1.08	8185	0.01	0.80	0.65	1782
0.11	1.02	1.05												
6	223	5399	-0.00	0.76	0.58	1448	0.09	0.97	0.94	5398	-0.01	0.76	0.57	1447
0.09	0.95	0.92												
7	293	3232	-0.04	0.77	0.59	1201	0.09	0.94	0.89	3230	-0.04	0.76	0.59	1198
0.09	0.93	0.87												
8	388	1836	-0.06	0.77	0.60	1094	0.06	0.99	0.99	1835	-0.05	0.76	0.58	1089
0.05	0.95	0.91												
9	536	808	-0.08	0.77	0.59	965	0.04	0.94	0.88	808	-0.08	0.77	0.59	963
0.03	0.92	0.85												
10	1389	270	-0.28	0.88	0.85	1913	-0.06	1.12	1.26	269	-0.27			

0.86 0.82 1903 -0.06 0.98 0.97

$$

Overall: 196234 0.04 0.91 0.82 40216 0.09 0.98 0.97 196165 0.04 0.90 0.81 40134 0.08 0.96 0.94

$TABLE: Run 2, standard deviation v. Intensity, New:

$GRAPHS: Sigma(scatter/SD), Mn(Chi^2), within 5 sd:N:2,13,14,17,18:

: Sigma(scatter/SD), Mn(Chi^2), within 5 sd, all and within 5 sd:N:2,5,6,9,10,13,14,17,18:

	Fulls, all				Partials, all				Fulls, < 5 sd				Partials, < 5 sd				
Range	Mn(I)	NF	MnF	SdF	ChiSqF	NP	MnP	SdP	ChiSqP	NFc	MnFc	SdFc	ChiSqFc	NPc	MnPc	SdPc	ChiSqPc	$$ $$
1	11	85500	0.02	0.93	0.86	23699	0.08	0.92	0.85	85495	0.02	0.93	0.86	23659	0.08	0.91	0.84	
2	44	25531	-0.02	1.11	1.24	7664	0.13	1.11	1.26	25508	-0.02	1.10	1.21	7623	0.13	1.08	1.19	
3	79	13532	-0.06	1.12	1.25	4231	0.11	1.15	1.35	13512	-0.06	1.10	1.21	4211	0.12	1.12	1.27	
4	119	8824	-0.09	1.07	1.15	2941	0.09	1.12	1.26	8810	-0.09	1.05	1.11	2924	0.10	1.07	1.15	
5	166	5620	-0.11	1.04	1.10	2191	0.15	1.12	1.27	5611	-0.11	1.02	1.06	2179	0.16	1.07	1.17	
6	223	3606	-0.13	1.01	1.04	1713	0.14	1.00	1.02	3603	-0.13	1.00	1.02	1705	0.16	0.96	0.96	
7	293	2040	-0.22	1.04	1.12	1498	0.17	1.06	1.15	2035	-0.22	1.02	1.08	1488	0.17	1.01	1.05	
8	388	1189	-0.25	1.09	1.25	1417	0.12	0.99	1.00	1186	-0.24	1.06	1.19	1404	0.12	0.94	0.91	

9	536	477	-0.28	1.03	1.14	1109	0.07	1.00	1.01	476	-0.28	1.02	1.12	1105	0.08	0.96	0.92
10	1389	202	-0.35	1.19	1.54	2502	0.08	1.11	1.24	197	-0.31	1.08	1.26	2486	0.08	0.98	0.96

$$

Overall:		146521	-0.01	1.00	1.00	48965	0.10	1.02	1.04	146433	-0.01	0.99	0.99	48784	0.10	0.99	0.98

$TABLE: All runs, standard deviation v. Intensity, New:

$GRAPHS: Sigma(scatter/SD), Mn(Chi^2), within 5 sd:N:2,13,14,17,18:

: Sigma(scatter/SD), Mn(Chi^2), within 5 sd, all and within 5 sd:N:2,5,6,9,10,13,14,17,18:

		Fulls, all				Partials, all				Fulls, < 5 sd				Partials, < 5 sd			
$$																	
Range	Mn(I)	NF	MnF	SdF	ChiSqF	NP	MnP	SdP	ChiSqP	NFc	MnFc	SdFc	ChiSqFc	NPc	MnPc	SdPc	ChiSqPc
$$																	
1	11	192822	0.03	0.91	0.83	43315	0.08	0.91	0.84	192791	0.03	0.91	0.00	43240	0.08	0.90	0.83
2	44	62321	0.04	1.04	1.07	13984	0.12	1.10	1.08	62272	0.04	1.03	0.00	13931	0.12	1.08	1.06
3	79	33024	0.02	1.00	1.00	7669	0.12	1.13	1.01	32998	0.01	0.99	0.00	7641	0.12	1.10	0.99
4	119	21722	-0.01	0.94	0.88	5377	0.12	1.09	0.89	21704	-0.01	0.93	0.00	5357	0.12	1.05	0.87
5	166	13807	-0.04	0.91	0.83	3976	0.14	1.08	0.84	13796	-0.04	0.90	0.00	3961	0.14	1.05	0.82
6	223	9005	-0.06	0.87	0.76	3161	0.12	0.99	0.76	9001	-0.06	0.86	0.00	3152	0.12	0.96	0.75
7	293	5272	-0.11	0.89	0.79	2699	0.13	1.01	0.80	5265	-0.11						

0.88 0.00 2686 0.13 0.98 0.78
8 388 3025 -0.13 0.91 0.84 2511 0.10 0.99 0.85 3021 -0.12
0.90 0.00 2493 0.09 0.95 0.82
9 536 1285 -0.16 0.88 0.79 2074 0.06 0.97 0.80 1284 -0.15
0.88 0.00 2068 0.05 0.94 0.79
10 1389 472 -0.31 1.03 1.08 4415 0.02 1.12 1.15 466 -0.29
0.96 0.00 4389 0.02 0.98 1.01
$$
Overall: 342755 0.02 0.95 0.89 89181 0.10 1.00 0.90 342598 0.02
0.94 0.00 88918 0.10 0.98 0.89

Effect of allowing for parameter variance in estimation of sig(I)
==========

Corrected sd'(I') = Sqrt[sd(I')^2 + I'^2 (sd(k)/k)^2]; I' = kI

Maximum relative correction relSD = (sd'(I') - sd(I'))/sd'(I') = 0.663

Maximum relative sd(scale), sd(k)/k = 0.0218
for observation:
HKL -52, 39, 9, resolution(A): 1.46, batch: 1180, scale: 7.235, sd(scale): 0.158
I': 20.8, sd(I'): 16.6, corrected sd'(I'): 16.6

Analysis by resolution

$TABLE: Effect of parameter variance on sd(I):
$GRAPHS:Mean sd(k)/k and relative Delta(sd(I)) vs. resolution:0|0.469156x0|0.00993072:2,4,5:
$$
N 1/d^2 Dmid sd(k)/k relSD Number $$ $$
1 0.0084 10.91 0.0060 0.155 3340

2	0.0240	6.45	0.0060	0.081	6387
3	0.0396	5.02	0.0060	0.088	8230
4	0.0553	4.25	0.0061	0.087	9734
5	0.0709	3.76	0.0061	0.070	10554
6	0.0865	3.40	0.0062	0.047	10593
7	0.1021	3.13	0.0062	0.031	10760
8	0.1177	2.91	0.0063	0.021	12325
9	0.1334	2.74	0.0064	0.016	13755
10	0.1490	2.59	0.0065	0.012	14859
11	0.1646	2.46	0.0066	0.010	15916
12	0.1802	2.36	0.0067	0.009	16659
13	0.1958	2.26	0.0068	0.007	17481
14	0.2114	2.17	0.0069	0.006	18134
15	0.2271	2.10	0.0071	0.004	19186
16	0.2427	2.03	0.0072	0.003	19656
17	0.2583	1.97	0.0073	0.002	20350
18	0.2739	1.91	0.0075	0.002	20875
19	0.2895	1.86	0.0076	0.001	19323
20	0.3052	1.81	0.0078	0.001	19531
21	0.3208	1.77	0.0079	0.001	19297
22	0.3364	1.72	0.0081	0.001	19800
23	0.3520	1.69	0.0082	0.000	21335
24	0.3676	1.65	0.0084	0.000	22031
25	0.3833	1.62	0.0086	0.000	23026
26	0.3989	1.58	0.0087	0.000	23405
27	0.4145	1.55	0.0089	0.000	24163
28	0.4301	1.52	0.0091	0.000	24731
29	0.4457	1.50	0.0093	0.000	25269
30	0.4613	1.47	0.0095	0.000	25779

$$

Overall:			0.0077	0.011	516484

Matrix of correlations of E^2 between runs

==========

Weighted correlation coefficients are calculated for each run pair in resolution ranges,
  then averaged over bins

Bins in averages over resolution are weighted by number of reflections

Run 1 maximum resolution   1.460 Dataset: New/New/New
Run 2 maximum resolution   1.460 Dataset: New/New/New

	Run	2
Run	1 CC(E^2)	0.931
	N	56233

$TABLE: ==== Run pair correlations by resolution:
$GRAPHS:Run pair correlations by resolution:N:2,4:
 $$

N	1/d^2	Dmid	CC2-1	$$ $$
1	0.0084	10.91	0.622	
2	0.0240	6.45	0.987	
3	0.0396	5.02	0.989	
4	0.0553	4.25	0.995	
5	0.0709	3.76	0.995	
6	0.0865	3.40	0.993	
7	0.1021	3.13	0.993	
8	0.1177	2.91	0.991	
9	0.1333	2.74	0.991	
10	0.1490	2.59	0.992	
11	0.1646	2.46	0.991	
12	0.1802	2.36	0.990	
13	0.1958	2.26	0.990	
14	0.2114	2.17	0.989	

15	0.2271	2.10	0.988
16	0.2427	2.03	0.987
17	0.2583	1.97	0.984
18	0.2739	1.91	0.981
19	0.2895	1.86	0.972
20	0.3051	1.81	0.967
21	0.3208	1.77	0.956
22	0.3364	1.72	0.947
23	0.3520	1.69	0.939
24	0.3676	1.65	0.932
25	0.3832	1.62	0.913
26	0.3988	1.58	0.893
27	0.4145	1.55	0.868
28	0.4301	1.52	0.842
29	0.4457	1.50	0.818
30	0.4613	1.47	0.748

$$

Overall: 0.941

==========

<!--SUMMARY_BEGIN--> $TEXT:Result: $$ $$

Summary data for Project: New Crystal: New Dataset: New

	Overall	InnerShell	OuterShell
Low resolution limit	41.16	41.16	1.48
High resolution limit	1.46	8.00	1.46
Rmerge (within I+/I-)	0.123	0.101	0.667
Rmerge (all I+ and I-)	0.124	0.094	0.742
Rmeas (within I+/I-)	0.151	0.141	0.809
Rmeas (all I+ & I-)	0.139	0.127	0.812
Rpim (within I+/I-)	0.085	0.098	0.447

Rpim (all I+ & I-)	0.061	0.085	0.325
Rmerge in top intensity bin	0.047	-	-
Total number of observations	436606	724	25344
Total number unique	80454	369	4113
Mean((I)/sd(I))	9.7	19.6	2.5
Mn(I) half-set correlation CC(1/2)	0.989	0.876	0.738
Completeness	96.4	66.6	99.8
Multiplicity	5.4	2.0	6.2
Mean(Chi^2)	0.89	1.38	0.84
Anomalous completeness	89.3	31.2	99.8
Anomalous multiplicity	2.6	1.4	3.0
DelAnom correlation between half-sets	-0.026	0.649	-0.049
Mid-Slope of Anom Normal Probability	0.924	-	-

The anomalous signal appears to be weak so anomalous flag was left OFF

Estimates of resolution limits: overall

from half-dataset correlation CC(1/2) > 0.30: limit = 1.46A == maximum resolution

from Mn(I/sd) > 1.50: limit = 1.46A == maximum resolution

from Mn(I/sd) > 2.00: limit = 1.46A == maximum resolution

Estimates of resolution limits in reciprocal lattice directions:

Along h axis

from half-dataset correlation CC(1/2) > 0.30: limit = 1.46A == maximum resolution

from Mn(I/sd) > 1.50: limit = 1.46A == maximum resolution

Along k axis

from half-dataset correlation CC(1/2) > 0.30: limit = 1.46A == maximum resolution

from Mn(I/sd) > 1.50: limit = 1.46A == maximum resolution

Along l axis

from half-dataset correlation CC(1/2) > 0.30: limit = 1.46A == maximum resolution

from Mn(I/sd) > 1.50: limit = 1.46A == maximum resolution

Anisotropic deltaB (i.e. range of principal components), A^2: 3.78

Average unit cell: 94.07   99.35 103.13   90.00   90.00   90.00
Space group: I 2 2 2
Average mosaicity: 0.04

Minimum and maximum SD correction factors: Fulls   0.74 17.74 Partials   0.25 26.73

$$ <!--SUMMARY_END-->
==

==== Writing merged data for dataset New/New/New to file /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_3_mtz.tmp

Number of reflections written   80454 maximum resolution   1.460

$TEXT:Reference: $$ Please cite $$
P.R.Evans and G.N.Murshudov, 'How good are my data and what is the resolution?' Acta Cryst. D69, 1204-1214 (2013).

PDF
$$

End of aimless job, total time: cpu time: 51.98 secs, elapsed time: 53.0 secs

<B><FONT COLOR='#FF0000'><!--SUMMARY_BEGIN-->
<html> <!-- CCP4 HTML LOGFILE -->
<hr>
<pre>

 ##
 ##
 ##

```
 ### CCP4 7.1.009: ctruncate        version 1.17.29 : 02/01/18##
 ##############################################################
 User: yoshihisasuzuki  Run date: 25/10/2021 Run time: 11:51:58


 Please reference: Collaborative Computational Project, Number 4. 2011.
 "Overview of the CCP4 suite and current developments". Acta Cryst. D67, 235-242.
 as well as any specific reference in the program write-up.

<!--SUMMARY_END--></FONT></B>
<B><FONT COLOR='#FF0000'><!--SUMMARY_BEGIN-->

USER SUPPLIED INPUT:

hklin    /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_3_mtz.tmp
hklout   /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_5_mtz_New.tmp
colin    /*/*/[IMEAN,SIGIMEAN]
colano   /*/*/[I(+),SIGI(+),I(-),SIGI(-)]
colout   New
xmlout
         /Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_G
I_pf_7_New_ctruncate.xml
<!--SUMMARY_END--></FONT></B>
** JQ

Reflection File INFO:

Reflection file name: /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_3_mtz.tmp
Crystal/dataset names: /New/New
Spacegroup: I 2 2 2 (number   23)
Cell parameters:    94.0711    99.3468   103.1345    90.0000    90.0000    90.0000

Reflection Data INFO:
```

Reflection data type: I_sigI

Number of observations (including Freidal mates): 80452

Number of unique reflections (excluding Freidal): 80452 (Acentric: 75888, Centric: 4564)

Resolution range of data: 41.156 - 1.460 A

Maximum index h (a*): 64 (1.470 A) - by symm. - 64 (1.470 A)

Maximum index k (b*): 68 (1.461 A) - by symm. - 68 (1.461 A)

Maximum index l (c*): 70 (1.473 A) - by symm. - 70 (1.473 A)

<B><FONT COLOR='#FF0000'><!--SUMMARY_BEGIN-->

Estimated Optical Resolution: 1.293

<!--SUMMARY_END--></FONT></B>

COMPLETENESS ANALYSIS (using intensities):

The following uses I/sigI Completeness levels, in particular targeting completeness above 85%. The Completeness with I/sigma above 3 indicates a strong signal (A better estimate is available using CC1/2 in aimless).

I/sigI>N	range(A)	%refln	
15.0	NaN - NaN	0.0	
10.0	NaN - NaN	0.0	
5.0	2.94 - 1.96	29.3	
3.0	2.96 - 1.88	35.3	***
2.0	2.98 - 1.76	45.5	
1.5	2.98 - 1.67	55.7	
1.0	2.99 - 1.59	66.5	
N/A	3.03 - 1.46		

The resolution range with I/sigI > 3 with completeness above 0.85, the estimated strong

data resolution range of this data, is 2.96A to 1.88A.

  This corresponds to approximately 35% of the reflections in the file.

$TABLE: Intensity Completeness analysis:

$GRAPHS: Completeness & (I/sigI)>N v resolution:N:1,2,3,4,5,6,7,8:

: Completeness & Rstandard v resolution:N:1,2,9:

$$ 1/resol^2 Completeness (I/s>15) (I/s>10) (I/s>5) (I/s>3) (I/s>2) (I/s>1) Rstandard$$

$$

0.0084	0.666	0.609	0.636	0.641	0.645	0.651	0.652	0.001
0.0185	0.738	0.677	0.730	0.733	0.734	0.735	0.735	0.001
0.0266	0.743	0.650	0.728	0.736	0.736	0.740	0.740	0.002
0.0337	0.755	0.681	0.747	0.752	0.752	0.752	0.752	0.001
0.0401	0.722	0.663	0.710	0.712	0.715	0.716	0.716	0.001
0.0460	0.744	0.674	0.733	0.735	0.737	0.739	0.740	0.001
0.0516	0.731	0.677	0.725	0.725	0.730	0.730	0.730	0.001
0.0570	0.729	0.657	0.721	0.727	0.727	0.729	0.729	0.001
0.0620	0.738	0.681	0.728	0.730	0.731	0.731	0.734	0.001
0.0670	0.749	0.698	0.742	0.744	0.745	0.747	0.747	0.001
0.0718	0.758	0.695	0.751	0.754	0.755	0.755	0.756	0.001
0.0763	0.750	0.668	0.728	0.734	0.737	0.739	0.747	0.001
0.0808	0.720	0.645	0.701	0.707	0.714	0.714	0.716	0.002
0.0852	0.766	0.669	0.753	0.761	0.763	0.765	0.765	0.001
0.0895	0.784	0.647	0.764	0.772	0.774	0.776	0.778	0.002
0.0937	0.788	0.675	0.769	0.777	0.784	0.784	0.786	0.002
0.0977	0.804	0.646	0.776	0.788	0.793	0.795	0.799	0.002
0.1017	0.773	0.628	0.749	0.762	0.767	0.769	0.773	0.002
0.1057	0.830	0.668	0.796	0.801	0.815	0.817	0.822	0.002
0.1095	0.854	0.668	0.827	0.839	0.840	0.840	0.844	0.002
0.1133	0.861	0.707	0.832	0.846	0.852	0.853	0.855	0.003
0.1171	0.895	0.737	0.863	0.871	0.881	0.883	0.883	0.003
0.1207	0.880	0.745	0.848	0.863	0.867	0.873	0.878	0.002
0.1244	0.910	0.748	0.883	0.897	0.900	0.902	0.903	0.002

0.1279	0.909	0.740	0.877	0.899	0.901	0.903	0.904	0.003
0.1315	0.918	0.783	0.875	0.884	0.891	0.900	0.900	0.003
0.1349	0.918	0.735	0.879	0.896	0.910	0.912	0.915	0.003
0.1385	0.916	0.760	0.882	0.901	0.907	0.909	0.911	0.003
0.1418	0.962	0.781	0.917	0.947	0.949	0.952	0.955	0.003
0.1451	0.949	0.749	0.895	0.912	0.923	0.932	0.939	0.003
0.1486	0.957	0.777	0.924	0.935	0.938	0.947	0.954	0.003
0.1518	0.963	0.767	0.915	0.931	0.939	0.943	0.953	0.003
0.1551	0.981	0.791	0.917	0.938	0.958	0.961	0.961	0.004
0.1583	0.980	0.793	0.935	0.957	0.964	0.970	0.971	0.003
0.1615	0.969	0.793	0.906	0.931	0.945	0.949	0.955	0.003
0.1646	0.983	0.803	0.926	0.940	0.953	0.966	0.970	0.004
0.1678	0.987	0.801	0.936	0.949	0.955	0.970	0.974	0.003
0.1709	0.978	0.801	0.935	0.950	0.963	0.965	0.967	0.003
0.1740	0.983	0.789	0.931	0.957	0.967	0.971	0.976	0.003
0.1771	0.992	0.802	0.934	0.959	0.969	0.973	0.980	0.003
0.1801	0.979	0.784	0.917	0.938	0.951	0.953	0.961	0.004
0.1830	0.975	0.782	0.908	0.930	0.951	0.966	0.970	0.003
0.1861	0.993	0.780	0.909	0.946	0.962	0.973	0.980	0.004
0.1890	0.998	0.814	0.924	0.949	0.969	0.975	0.979	0.004
0.1919	0.984	0.786	0.924	0.947	0.962	0.962	0.968	0.003
0.1948	0.990	0.790	0.924	0.954	0.966	0.969	0.974	0.004
0.1978	0.993	0.791	0.914	0.964	0.967	0.974	0.983	0.003
0.2006	0.995	0.792	0.925	0.956	0.967	0.970	0.986	0.004
0.2034	0.998	0.796	0.923	0.952	0.963	0.974	0.977	0.004
0.2064	0.999	0.816	0.939	0.970	0.978	0.982	0.987	0.004
0.2091	0.994	0.811	0.925	0.959	0.963	0.973	0.981	0.004
0.2119	0.993	0.771	0.900	0.925	0.949	0.967	0.977	0.004
0.2147	0.999	0.782	0.908	0.951	0.970	0.983	0.992	0.004
0.2176	0.994	0.786	0.907	0.939	0.959	0.973	0.983	0.004
0.2202	0.999	0.755	0.912	0.949	0.969	0.975	0.983	0.004
0.2229	0.996	0.739	0.907	0.956	0.964	0.976	0.984	0.004
0.2257	0.998	0.723	0.892	0.942	0.960	0.979	0.984	0.005

0.2284	0.996	0.740	0.868	0.933	0.957	0.972	0.983	0.004
0.2311	0.999	0.705	0.878	0.931	0.948	0.964	0.971	0.005
0.2337	0.997	0.731	0.895	0.926	0.951	0.965	0.976	0.005
0.2363	0.998	0.707	0.868	0.920	0.947	0.964	0.977	0.005
0.2390	0.999	0.670	0.857	0.917	0.942	0.948	0.960	0.006
0.2416	1.000	0.728	0.865	0.908	0.942	0.964	0.978	0.005
0.2441	1.000	0.694	0.866	0.918	0.949	0.958	0.973	0.006
0.2468	1.000	0.685	0.864	0.918	0.952	0.963	0.973	0.005
0.2494	1.000	0.697	0.866	0.914	0.945	0.963	0.972	0.006
0.2520	0.998	0.629	0.830	0.906	0.928	0.953	0.967	0.006
0.2545	1.000	0.665	0.849	0.908	0.934	0.944	0.959	0.006
0.2570	0.999	0.675	0.823	0.902	0.934	0.961	0.970	0.006
0.2596	1.000	0.668	0.867	0.924	0.949	0.957	0.969	0.007
0.2622	1.000	0.622	0.816	0.877	0.909	0.934	0.964	0.007
0.2647	1.000	0.621	0.803	0.893	0.936	0.953	0.963	0.007
0.2671	0.998	0.614	0.798	0.877	0.914	0.939	0.957	0.008
0.2695	0.999	0.638	0.835	0.928	0.954	0.962	0.972	0.007
0.2721	0.999	0.577	0.788	0.859	0.904	0.931	0.955	0.008
0.2746	1.000	0.562	0.798	0.878	0.914	0.942	0.962	0.008
0.2770	1.000	0.567	0.811	0.893	0.943	0.964	0.969	0.008
0.2794	1.000	0.552	0.813	0.897	0.932	0.943	0.962	0.009
0.2819	0.997	0.527	0.783	0.862	0.900	0.932	0.948	0.010
0.2843	0.998	0.443	0.727	0.830	0.877	0.916	0.947	0.013
0.2867	0.996	0.422	0.723	0.826	0.903	0.924	0.950	0.011
0.2892	1.000	0.424	0.689	0.833	0.878	0.899	0.925	0.018
0.2915	0.997	0.401	0.728	0.828	0.878	0.923	0.947	0.013
0.2939	0.991	0.414	0.714	0.819	0.872	0.915	0.937	0.014
0.2963	0.992	0.420	0.690	0.816	0.883	0.905	0.933	0.013
0.2986	0.990	0.340	0.637	0.780	0.860	0.889	0.926	0.016
0.3010	0.995	0.387	0.672	0.779	0.856	0.894	0.915	0.015
0.3034	0.997	0.365	0.664	0.801	0.864	0.881	0.905	0.014
0.3057	0.985	0.361	0.665	0.788	0.849	0.885	0.902	0.015
0.3080	0.991	0.363	0.663	0.782	0.839	0.870	0.900	0.016

0.3103	0.997	0.374	0.678	0.784	0.853	0.881	0.932	0.014
0.3127	0.998	0.354	0.652	0.756	0.837	0.880	0.915	0.017
0.3150	1.000	0.391	0.682	0.810	0.879	0.898	0.930	0.014
0.3173	1.000	0.331	0.633	0.765	0.840	0.867	0.893	0.018
0.3195	1.000	0.324	0.650	0.795	0.861	0.894	0.925	0.018
0.3218	1.000	0.299	0.599	0.779	0.849	0.885	0.921	0.019
0.3241	1.000	0.316	0.641	0.778	0.837	0.867	0.926	0.018
0.3264	1.000	0.259	0.595	0.769	0.840	0.877	0.928	0.020
0.3287	0.998	0.274	0.569	0.736	0.825	0.864	0.910	0.022
0.3308	1.000	0.259	0.588	0.736	0.827	0.878	0.910	0.021
0.3331	1.000	0.230	0.570	0.740	0.815	0.854	0.900	0.024
0.3353	0.999	0.287	0.598	0.727	0.808	0.851	0.899	0.021
0.3376	1.000	0.284	0.606	0.767	0.834	0.886	0.926	0.020
0.3399	1.000	0.271	0.569	0.731	0.828	0.871	0.914	0.022
0.3421	0.988	0.267	0.553	0.709	0.787	0.828	0.885	0.023
0.3442	0.987	0.239	0.541	0.705	0.781	0.821	0.872	0.024
0.3463	0.997	0.223	0.534	0.680	0.784	0.842	0.890	0.027
0.3486	1.000	0.180	0.477	0.665	0.753	0.813	0.881	0.029
0.3508	1.000	0.217	0.536	0.679	0.791	0.855	0.903	0.026
0.3531	1.000	0.199	0.511	0.692	0.790	0.839	0.888	0.028
0.3552	0.999	0.177	0.453	0.631	0.734	0.803	0.870	0.169
0.3573	0.999	0.191	0.512	0.692	0.778	0.832	0.869	0.030
0.3594	1.000	0.185	0.481	0.662	0.775	0.851	0.901	0.033
0.3616	0.998	0.165	0.470	0.668	0.777	0.830	0.887	0.032
0.3637	1.000	0.168	0.445	0.630	0.731	0.808	0.873	0.035
0.3659	1.000	0.183	0.472	0.637	0.764	0.811	0.872	0.034
0.3681	1.000	0.188	0.502	0.685	0.777	0.818	0.880	0.045
0.3702	1.000	0.181	0.456	0.633	0.739	0.786	0.847	0.034
0.3723	1.000	0.132	0.484	0.664	0.742	0.814	0.873	0.035
0.3743	1.000	0.151	0.436	0.637	0.747	0.801	0.855	0.038
0.3766	1.000	0.135	0.443	0.614	0.716	0.783	0.847	0.035
0.3787	0.999	0.130	0.447	0.637	0.742	0.804	0.867	0.038
0.3807	0.999	0.146	0.434	0.611	0.719	0.798	0.845	0.296

0.3829	1.000	0.113	0.388	0.601	0.729	0.796	0.857	0.047
0.3850	1.000	0.124	0.413	0.647	0.757	0.824	0.875	0.038
0.3870	1.000	0.129	0.376	0.569	0.675	0.746	0.809	0.044
0.3890	1.000	0.106	0.345	0.549	0.706	0.768	0.853	0.048
0.3911	1.000	0.096	0.391	0.582	0.717	0.782	0.856	0.045
0.3932	1.000	0.099	0.361	0.577	0.703	0.771	0.835	0.048
0.3953	1.000	0.095	0.361	0.568	0.693	0.757	0.810	0.052
0.3974	0.997	0.098	0.358	0.560	0.707	0.776	0.856	0.046
0.3994	1.000	0.082	0.365	0.526	0.698	0.753	0.825	0.052
0.4014	1.000	0.083	0.346	0.552	0.704	0.783	0.843	0.052
0.4034	1.000	0.079	0.303	0.522	0.705	0.765	0.841	0.052
0.4055	0.999	0.074	0.276	0.511	0.680	0.757	0.845	0.061
0.4076	1.000	0.071	0.331	0.530	0.683	0.777	0.838	0.054
0.4096	1.000	0.058	0.271	0.489	0.656	0.740	0.805	2.252
0.4116	1.000	0.061	0.311	0.523	0.630	0.710	0.817	0.057
0.4137	1.000	0.036	0.247	0.474	0.636	0.713	0.801	0.070
0.4156	0.998	0.063	0.300	0.535	0.690	0.778	0.847	0.053
0.4176	1.000	0.046	0.291	0.516	0.651	0.738	0.814	0.057
0.4196	1.000	0.060	0.298	0.479	0.636	0.714	0.795	3.211
0.4216	0.999	0.048	0.244	0.471	0.585	0.671	0.789	0.073
0.4237	1.000	0.082	0.304	0.483	0.637	0.722	0.824	0.064
0.4256	1.000	0.044	0.279	0.460	0.599	0.715	0.795	0.065
0.4276	1.000	0.040	0.249	0.446	0.594	0.685	0.789	0.075
0.4296	1.000	0.034	0.238	0.453	0.602	0.679	0.763	0.068
0.4316	1.000	0.042	0.218	0.428	0.592	0.686	0.782	0.087
0.4335	0.999	0.033	0.227	0.461	0.602	0.694	0.782	0.076
0.4354	0.999	0.026	0.212	0.429	0.580	0.668	0.781	0.085
0.4374	1.000	0.041	0.226	0.458	0.626	0.713	0.800	0.068
0.4394	1.000	0.030	0.239	0.450	0.612	0.695	0.797	0.081
0.4414	1.000	0.047	0.198	0.415	0.578	0.652	0.762	0.085
0.4433	1.000	0.020	0.189	0.394	0.541	0.638	0.746	0.093
0.4453	1.000	0.035	0.204	0.420	0.600	0.680	0.774	0.081
0.4472	1.000	0.034	0.195	0.385	0.569	0.654	0.752	0.086

0.4491	0.998	0.039	0.210	0.382	0.552	0.653	0.757	0.098
0.4511	1.000	0.018	0.183	0.380	0.569	0.660	0.751	0.100
0.4530	0.998	0.014	0.152	0.355	0.534	0.624	0.736	0.099
0.4550	1.000	0.027	0.170	0.385	0.501	0.611	0.742	0.107
0.4569	1.000	0.014	0.139	0.336	0.514	0.601	0.722	0.199
0.4588	1.000	0.006	0.127	0.324	0.488	0.588	0.696	0.118
0.4607	1.000	0.019	0.151	0.321	0.497	0.620	0.709	0.104
0.4626	1.000	0.006	0.150	0.357	0.495	0.608	0.729	0.120
0.4645	1.000	0.008	0.119	0.296	0.488	0.602	0.699	0.123
0.4663	1.000	0.004	0.149	0.328	0.459	0.572	0.682	0.121
0.4682	0.962	0.008	0.132	0.316	0.501	0.573	0.685	0.120

$$

The completeness at various resolution limit plots gives the completeness after applying a I/sigI cutoff. The profiles give an indication of the quality of the data. The Rstandard plot (<sigF>/<F>) gives an alternative indicator. Strongly recorded resolution bins would typically have values below 0.1.

Low Resolution Intensity Completeness analysis:

1/resol^2	Range	Completeness
0.0026	0.000-0.004	0.629 [22.8:36.2]
0.0059	0.004-0.007	0.665 [28.0:42.1]
0.0085	0.007-0.010	0.638 [27.5:43.1]
0.0109	0.010-0.012	0.691 [29.4:42.5]
0.0129	0.012-0.014	0.699 [30.5:43.6]
0.0149	0.014-0.016	0.703 [32.2:45.9]
0.0169	0.016-0.018	0.742 [32.8:44.1]
0.0186	0.018-0.020	0.752 [33.8:44.9]
0.0203	0.020-0.021	0.770 [35.5:46.1]
0.0219	0.021-0.023	0.966 [42.6:44.1]

Low completeness at low resolution can lead to map distortions and other difficulties.

This often arises through experimental effects such as incorrectly alligned crystal, poorly positioned backstop, or over exposure.

ICE RING SUMMARY:

reso	ice_ring	mean_I	mean_Sigma	Estimated_I	Ratio	Zscore	Completeness	Ave_Completeness
3.90	no	978.65	55.64	918.99	1.06	1.07	0.74	0.73
3.67	no	862.37	50.66	784.67	1.10	1.53	0.74	0.73
3.44	no	677.74	40.72	598.68	1.13	1.94	0.74	0.73
2.67	no	230.22	15.53	235.77	0.98	-0.36	0.94	0.94
2.25	no	163.39	10.51	159.38	1.03	0.38	0.99	0.99
2.08	no	109.43	6.96	122.75	0.89	-1.91	1.00	1.00
1.95	no	73.52	5.34	74.81	0.98	-0.24	1.00	1.00
1.92	no	67.17	4.98	70.49	0.95	-0.67	1.00	1.00
1.89	no	60.39	4.90	60.55	1.00	-0.03	1.00	1.00
1.73	no	32.47	4.44	32.44	1.00	0.01	1.00	1.00

The ice rings table shows data Z-scores and completeness for ice ring sensitive resolutions in comparison with neighbouring ice-ring insensitive resolutions. Large z-scores and low completeness at give a strong hint to the presence of ice rings. It may be required to exclude these resolution ranges.

WILSON SCALING:

Estimated number of residues = 349

Results Wilson B-factor:

Estimate of Wilson B factor: 11.586 A^(-2), with sigma 0.474

Estimate of scale factor on intensity = 1982.3726 (intercept -7.592, sigma 0.052)

The isotropic Wilson temperature estimate (B-value) is an approximation to the fall-off of scattering with resolution. This should be correlated with the refined atomic B-values. This averages out any anisotropy in the experimental observations. This approximation will be misleading for strongly anisotropic data.

$TABLE: Wilson plot:
$GRAPHS: Wilson plot - estimated B factor = 11.6 :A:1,2,3:
$$ 1/resol^2 ln(I/I_th) Reference_prot $$
$$

0.02166	-8.00722	-8.18965
0.04685	-7.50540	-7.45367
0.06627	-7.44663	-7.45442
0.08303	-7.69621	-7.62101
0.09767	-8.04866	-7.88480
0.11062	-8.28493	-8.09230
0.12200	-8.33333	-8.26309
0.13257	-8.44431	-8.38936
0.14253	-8.49096	-8.45610
0.15185	-8.53921	-8.51494
0.16074	-8.55679	-8.56205
0.16934	-8.51572	-8.59192
0.17772	-8.52940	-8.60559
0.18592	-8.61024	-8.61945
0.19385	-8.57865	-8.62870
0.20161	-8.58028	-8.65241
0.20925	-8.66261	-8.68496
0.21672	-8.71641	-8.73029
0.22402	-8.78098	-8.75381
0.23128	-8.84603	-8.80083
0.23838	-8.97100	-8.87236

0.24534	-8.93536	-8.92963
0.25229	-9.02804	-9.00279
0.25903	-9.11531	-9.08104
0.26579	-9.13396	-9.16276
0.27242	-9.25593	-9.24934
0.27897	-9.28369	-9.32367
0.28550	-9.40396	-9.39266
0.29190	-9.47645	-9.47176
0.29831	-9.53929	-9.54070
0.30468	-9.56963	-9.61264
0.31093	-9.58158	-9.66932
0.31712	-9.61171	-9.72026
0.32317	-9.70405	-9.77123
0.32928	-9.78355	-9.80869
0.33520	-9.78440	-9.84274
0.34125	-9.81320	-9.88985
0.34708	-9.89546	-9.93279
0.35302	-9.96617	-9.98264
0.35875	-9.97845	-10.00988
0.36449	-10.03800	-10.02878
0.37026	-10.01220	-10.05962
0.37587	-10.09203	-10.08518
0.38152	-10.12210	-10.12396
0.38707	-10.16276	-10.15444
0.39262	-10.19416	-10.18257
0.39816	-10.24997	-10.21973
0.40356	-10.31630	-10.24841
0.40906	-10.32740	-10.27098
0.41447	-10.39992	-10.29696
0.41974	-10.41622	-10.33613
0.42516	-10.38159	-10.37264
0.43045	-10.52482	-10.39737
0.43563	-10.47294	-10.42193

```
   0.44093  -10.51582  -10.44619
   0.44612  -10.51888  -10.48574
   0.45125  -10.57763  -10.52837
   0.45646  -10.66382  -10.56387
   0.46155  -10.72869  -10.59328
   0.46657  -10.73044  -10.62582
$$
```

Computed using Popov & Bourenkov, Acta D (2003) D59, 1145

The wilson plot shows the fall off of the mean intensity with resolution. This is then used calculate an absolute scale and temperature factor for a set of observed intensities, using the theory of A C Wilson. The reference_plot is based upon an analysis of high resolution datasets in the PDB (BEST), which takes into account the none random distribution of atoms within the crystal. Some deviation from the reference plot is to be expected, however, significant deviation may indicate problems, such as ice rings, detector issues, or missprocessed.

OUTLIER RING SUMMARY:

Outliers total 1.0% of the bins.

reso	mean_I	mean_Sigma	Estimated_I	Ratio	Zscore	Completeness	Ave_Completeness
3.20	349.14	23.22	493.11	0.71	-6.20	0.76	0.80
3.05	291.12	17.48	410.78	0.71	-6.85	0.85	0.82
2.97	262.30	15.50	360.66	0.73	-6.34	0.85	0.86
2.91	213.97	14.46	338.39	0.63	-8.61	0.86	0.88

The outlier rings table shows data Z-scores and completeness for problem resolution bins in comparison with the Wilson B-factor fit. Large z-scores and low completeness at give a strong hint to the presence of problems. It may be required to exclude these resolution ranges.

Estimated limits of anomalous signal:

Bijvoet ratio (<deltaI>/<I>) > 1.0%	: 9.24 - 1.46 A
Anomalous signal to noise (<deltaI/sigdI>) > 1.3	: NaN - NaN
Measurability limit (Nanon/Nov) > 5%	: NaN - NaN

Warning: NO anomalous signal.

These calculations are performed using scaled and merged data. More accurate estimates of the limit of the anomalous signal
can be obtained using scaled and unmerged data in the half dataset correlation calculation of aimless.

The measurability is defined as the fraction of the anomalous differences for which the signal to noise for deltaI,
I(+) and I(-) are all > 3. The resolution limits are derived from I/sigI of 1.2 for the signal to noise, and measurability above 5%.
For well processed data having more than 5% of the measured data satisfying this criteria is a good
indicator, particularly when combined with a significate mean signal to noise of the anomalous difference in a
resolution shell.

$TABLE: Intensity anomalous analysis:
$GRAPHS: Mn(dI/sigdI) v resolution:N:1,2:
: Mn(dI/I) v resolution:N:1,3:
: Mesurability v resolution:N:1,4:
$$ 1/resol^2 Mn(dI/sigdI)) Mn(dI/I) measurability$$
$$

0.011716	1.3533e+00	4.5517e-02	1.9640e-02
0.024529	3.6426e-01	2.5031e-02	8.5470e-03
0.034265	3.7123e-01	2.8597e-02	4.2150e-03

0.043020	3.8968e-01	3.2182e-02	4.2083e-03
0.050940	3.7062e-01	2.6770e-02	4.1754e-03
0.058366	3.2412e-01	2.3568e-02	6.2112e-03
0.065334	3.6274e-01	2.5257e-02	0.0000e+00
0.071759	3.5911e-01	2.6235e-02	8.3770e-03
0.077995	3.0229e-01	2.0217e-02	0.0000e+00
0.084148	3.6179e-01	2.3504e-02	4.1537e-03
0.089747	3.3980e-01	2.2447e-02	0.0000e+00
0.095073	4.0449e-01	2.6305e-02	0.0000e+00
0.100229	3.9482e-01	2.8423e-02	2.0640e-03
0.105312	4.2908e-01	3.3235e-02	6.1038e-03
0.109932	3.7114e-01	2.9421e-02	0.0000e+00
0.114403	4.7419e-01	3.4466e-02	4.1863e-03
0.118521	4.9111e-01	3.5760e-02	4.1026e-03
0.122789	4.9268e-01	4.1190e-02	2.0587e-03
0.126724	4.8065e-01	3.7527e-02	2.0346e-03
0.130744	5.5131e-01	4.5511e-02	6.2016e-03
0.134482	5.2192e-01	4.6076e-02	0.0000e+00
0.138352	5.6705e-01	5.0241e-02	2.0429e-03
0.141929	6.0054e-01	5.5876e-02	8.3507e-03
0.145480	5.7338e-01	5.7881e-02	2.0502e-03
0.149032	5.7339e-01	5.2760e-02	4.1005e-03
0.152404	5.5906e-01	5.3638e-02	0.0000e+00
0.155795	5.9134e-01	6.0329e-02	0.0000e+00
0.159115	6.0228e-01	6.0148e-02	4.0692e-03
0.162387	5.8070e-01	5.5251e-02	2.0790e-03
0.165680	6.1710e-01	6.2153e-02	2.0419e-03
0.168836	5.7351e-01	5.4478e-02	4.1152e-03
0.171983	6.3491e-01	6.3281e-02	2.0768e-03
0.175166	5.9507e-01	5.9993e-02	4.0984e-03
0.178221	6.3042e-01	6.9328e-02	2.0715e-03
0.181290	6.2739e-01	6.7906e-02	0.0000e+00
0.184418	6.4512e-01	7.2833e-02	0.0000e+00

0.187459	6.2747e-01	6.5209e-02	2.0877e-03
0.190375	6.5153e-01	6.3622e-02	2.0367e-03
0.193310	6.4490e-01	6.8788e-02	2.0597e-03
0.196369	6.5776e-01	7.0862e-02	6.1381e-03
0.199240	6.1299e-01	6.6955e-02	2.0429e-03
0.202069	6.2883e-01	6.6160e-02	0.0000e+00
0.204951	6.2901e-01	7.3183e-02	0.0000e+00
0.207884	7.0715e-01	7.8241e-02	6.1665e-03
0.210570	6.7971e-01	7.3237e-02	0.0000e+00
0.213399	6.6481e-01	8.3205e-02	2.0587e-03
0.216227	6.7355e-01	7.4856e-02	2.0233e-03
0.219107	7.4702e-01	8.9327e-02	4.1068e-03
0.221656	6.9198e-01	8.1064e-02	4.1110e-03
0.224502	7.4760e-01	8.6146e-02	4.1068e-03
0.227199	7.4216e-01	8.7823e-02	4.1195e-03
0.229964	7.0744e-01	8.4718e-02	2.0408e-03
0.232565	7.0660e-01	8.8545e-02	4.1089e-03
0.235217	7.1075e-01	8.6249e-02	2.0460e-03
0.237903	6.8548e-01	8.7518e-02	4.1558e-03
0.240596	6.7926e-01	8.8230e-02	0.0000e+00
0.243178	6.9265e-01	8.6186e-02	8.2988e-03
0.245737	7.0988e-01	9.0940e-02	0.0000e+00
0.248345	6.8445e-01	8.6081e-02	4.1110e-03
0.250992	7.3501e-01	9.6093e-02	4.0942e-03
0.253587	7.2370e-01	9.6786e-02	2.0597e-03
0.256035	7.5008e-01	1.0147e-01	2.0305e-03
0.258585	6.9456e-01	9.0097e-02	2.0387e-03
0.261199	7.4842e-01	1.0614e-01	2.0566e-03
0.263742	7.0212e-01	9.8721e-02	0.0000e+00
0.266206	6.7056e-01	1.0047e-01	2.0263e-03
0.268637	7.7295e-01	1.1178e-01	2.0555e-03
0.271135	8.1445e-01	1.1721e-01	6.1538e-03
0.273701	7.7526e-01	1.1920e-01	6.1412e-03

0.276181	7.5760e-01	1.2002e-01	0.0000e+00
0.278550	7.4957e-01	1.1861e-01	2.0263e-03
0.281026	7.4480e-01	1.2501e-01	2.0305e-03
0.283464	7.4962e-01	1.3231e-01	2.0801e-03
0.285875	7.4387e-01	1.3870e-01	4.0858e-03
0.288368	6.9388e-01	1.3788e-01	2.0812e-03
0.290659	7.4828e-01	1.5101e-01	2.0141e-03
0.293113	7.3506e-01	1.4332e-01	3.9565e-03
0.295566	6.7598e-01	1.3451e-01	4.1951e-03
0.297885	7.4795e-01	1.6310e-01	6.1856e-03
0.300302	6.9483e-01	1.6163e-01	6.0976e-03
0.302712	7.7745e-01	1.6958e-01	2.0534e-03
0.305021	7.1150e-01	1.4696e-01	7.9562e-03
0.307420	7.7210e-01	1.6407e-01	6.1100e-03
0.309742	7.7325e-01	1.5805e-01	6.1350e-03
0.312138	7.6335e-01	1.7461e-01	4.1068e-03
0.314478	7.5809e-01	1.5972e-01	6.0852e-03
0.316779	7.4352e-01	1.7106e-01	1.6495e-02
0.318982	7.1059e-01	1.7280e-01	6.1038e-03
0.321263	7.4598e-01	1.8801e-01	6.1100e-03
0.323550	7.3333e-01	1.8557e-01	4.0984e-03
0.325882	7.0289e-01	1.8761e-01	4.0858e-03
0.328235	7.1822e-01	1.9827e-01	8.1301e-03
0.330356	7.3213e-01	2.0879e-01	4.1258e-03
0.332581	7.2343e-01	2.0149e-01	8.1466e-03
0.334786	6.9786e-01	1.9865e-01	2.0284e-03
0.337118	8.0654e-01	2.2383e-01	4.0568e-03
0.339374	7.3576e-01	2.0500e-01	2.0715e-03
0.341613	7.7117e-01	2.2300e-01	2.0233e-03
0.343810	7.4144e-01	2.0279e-01	2.0367e-03
0.345959	7.2009e-01	2.1271e-01	0.0000e+00
0.348164	7.1688e-01	2.2871e-01	2.0408e-03
0.350385	7.8650e-01	2.4243e-01	0.0000e+00

0.352688	7.4583e-01	2.3411e-01	0.0000e+00
0.354878	7.7051e-01	2.5656e-01	4.1195e-03
0.356934	7.7975e-01	2.6633e-01	6.1350e-03
0.359066	7.6828e-01	2.5775e-01	0.0000e+00
0.361316	7.8845e-01	2.5780e-01	1.0096e-02
0.363403	8.1141e-01	2.8817e-01	2.0555e-03
0.365607	7.7002e-01	2.7162e-01	4.0424e-03
0.367826	7.1970e-01	2.5185e-01	0.0000e+00
0.369919	7.9283e-01	2.6681e-01	4.1068e-03
0.371982	7.7392e-01	2.7637e-01	2.0243e-03
0.374005	7.6477e-01	2.8357e-01	4.0942e-03
0.376260	7.8045e-01	2.8972e-01	2.0040e-03
0.378373	7.6699e-01	3.0203e-01	4.1152e-03
0.380422	7.7835e-01	3.0910e-01	2.0608e-03
0.382627	7.1863e-01	2.7850e-01	4.0201e-03
0.384691	7.1747e-01	2.8424e-01	6.1507e-03
0.386730	7.6282e-01	3.1200e-01	4.0692e-03
0.388763	7.4343e-01	3.2796e-01	4.0465e-03
0.390844	7.4578e-01	3.1485e-01	4.1365e-03
0.392982	7.8584e-01	3.4374e-01	0.0000e+00
0.395060	7.6770e-01	3.4231e-01	6.1162e-03
0.397168	8.0916e-01	3.6279e-01	1.0395e-02
0.399182	7.7082e-01	3.6260e-01	4.0323e-03
0.401204	8.1108e-01	3.6057e-01	2.0243e-03
0.403199	7.3924e-01	3.7400e-01	0.0000e+00
0.405281	8.0199e-01	4.0598e-01	1.0163e-02
0.407407	7.4141e-01	3.4935e-01	4.0506e-03
0.409376	7.6441e-01	4.1445e-01	2.0502e-03
0.411424	7.4558e-01	3.8212e-01	0.0000e+00
0.413516	7.3090e-01	4.3729e-01	4.0900e-03
0.415447	7.6019e-01	3.9135e-01	4.1005e-03
0.417402	7.3124e-01	3.9552e-01	0.0000e+00
0.419376	7.8581e-01	4.1987e-01	4.1026e-03

0.421408	7.4084e-01	4.4330e-01	4.0201e-03
0.423537	7.4163e-01	3.8467e-01	2.0747e-03
0.425436	7.5109e-01	4.1724e-01	2.0243e-03
0.427434	7.3566e-01	4.3205e-01	2.0060e-03
0.429476	7.5031e-01	4.6245e-01	0.0000e+00
0.431426	7.3570e-01	4.8279e-01	0.0000e+00
0.433404	8.1517e-01	5.0347e-01	2.0222e-03
0.435321	7.3811e-01	4.8486e-01	2.0942e-03
0.437228	7.3941e-01	4.4775e-01	0.0000e+00
0.439271	7.8275e-01	4.7005e-01	0.0000e+00
0.441292	7.9475e-01	5.1904e-01	2.0192e-03
0.443198	7.2693e-01	5.1414e-01	2.0576e-03
0.445155	7.8379e-01	5.0966e-01	2.0040e-03
0.447100	7.0492e-01	4.6421e-01	0.0000e+00
0.449004	6.9673e-01	4.5590e-01	6.0852e-03
0.450964	7.4461e-01	5.2162e-01	2.0141e-03
0.452858	7.1299e-01	5.3856e-01	2.0534e-03
0.454868	6.9210e-01	5.2129e-01	4.0816e-03
0.456782	7.1817e-01	5.6059e-01	4.1152e-03
0.458708	6.7125e-01	5.9437e-01	0.0000e+00
0.460640	7.3364e-01	5.8099e-01	0.0000e+00
0.462511	6.8042e-01	5.5581e-01	0.0000e+00
0.464387	6.6243e-01	5.7414e-01	2.0367e-03
0.466263	7.3296e-01	6.1236e-01	0.0000e+00
0.468142	7.1335e-01	6.3585e-01	2.0212e-03

$$

<B><FONT COLOR='#FF0000'><!--SUMMARY_BEGIN-->

TRANSLATIONAL NCS:

No translational NCS detected (with resolution limited to 4.00 A)

The analysis uses the peak heights in the patterson map that are further than 14 A (approx. 4 Ca-Ca) from the origin. The presence of a large off origin peak (above 20%) and/or a very low Q-score, below 1.0, is a string indicator of the presence of tNCS. An intermidiate Q-score, between 5.0 and 1.0, may indicate weak tNCS or be the result of cross vector of a large scatterer such as a cluster or heavy metal.

Reference: P. Zwarts CCP4 Newsletter 42

<!--SUMMARY_END--></FONT></B>

ANISOTROPY ANALYSIS:

Analysis using data from   2.96A to   1.88A.

Eigenvalues: 12.3025 10.4218 11.2434
Eigenvalue ratios: 1.0000   0.9535   0.9735

Little or no anisotropy detected.
The presence of anisotropy may indicate that the crystal is poorly ordered along one of the axes.

Anisotropic B scaling (orthogonal coords):

| 11.243387   0.000000   0.000000 |
| 0.000000 12.302508   0.000000 |
| 0.000000   0.000000 10.421767 |

Anisotropic U (orthogonal coords):

| 0.284798   0.000000   0.000000 |
| 0.000000   0.311626   0.000000 |

| 0.000000   0.000000   0.263986 |

Eigenvector breakdown:

Eigenvalue Eigenvector(a*,b*,c*)
  0.311626 (0.000000   1.000000   0.000000)
  0.263986 (0.000000   0.000000   1.000000)
  0.284798 (1.000000   0.000000   0.000000)

Anisotropic correction (orthogonal coords):

| -0.000924 -0.000000   0.000000 |
| -0.000000   0.012095 -0.000000 |
| 0.000000 -0.000000 -0.011171 |

$TABLE: Intensity statistics:
$GRAPHS: Mn(I) v resolution:N:1,2,3,4,5:
: Mn(I/sd) v resolution:N:1,6,7,8,9:
: No. reflections v resolution:N:1,10,11,12,13:
$$ 1/resol^2 Mn(I(1)) Mn(I(2)) Mn(I(3)) Mn(I) Mn(I/s(1)) Mn(I/s(2)) Mn(I/s(3)) Mn(I/s)
N(1)   N(2)   N(3)   N$$
$$
   0.0138   413.50   388.46   381.22   385.87   22.00   16.04   13.38
19.27   928.0   504.0   536.0   5424.0
   0.0303   328.55   340.12   220.62   292.98   21.89   14.65   12.70
18.03   952.0   640.0   576.0   5888.0
   0.0432   520.93   436.53   447.81   486.26   20.09   14.83   12.11
17.90   1024.0   560.0   608.0   5824.0
   0.0546   417.03   550.43   377.00   506.26   20.81   15.24   13.12
18.00   960.0   648.0   520.0   5824.0
   0.0648   491.78   479.46   366.18   483.37   19.92   16.75   13.78
18.21   984.0   584.0   536.0   5896.0
   0.0744   377.48   440.40   281.07   414.47   19.32   15.32   12.97

17.15 1008.0 624.0 624.0 5992.0

0.0834 240.15 403.63 245.34 331.82 17.79 14.72 11.49

16.52 984.0 528.0 576.0 5920.0

0.0920 300.04 169.98 160.68 263.28 18.93 14.15 11.57

16.25 976.0 712.0 608.0 6296.0

0.1002 191.31 173.64 110.21 194.06 18.10 13.89 9.86

15.72 1000.0 680.0 768.0 6256.0

0.1081 132.48 181.07 138.68 169.81 16.73 14.13 9.69

15.18 1072.0 848.0 808.0 6800.0

0.1157 141.00 135.35 117.09 146.28 19.86 13.29 11.12

15.89 1088.0 864.0 888.0 7032.0

0.1231 136.51 169.05 114.39 148.92 19.76 14.64 10.84

16.04 1104.0 968.0 936.0 7240.0

0.1303 121.21 136.59 101.69 128.08 20.06 13.69 11.71

15.92 1104.0 936.0 928.0 7352.0

0.1373 112.73 125.78 111.40 120.08 20.81 14.15 10.85

16.00 1056.0 1000.0 1016.0 7344.0

0.1441 99.21 111.22 102.95 109.62 19.86 13.05 11.46

15.79 1120.0 984.0 1048.0 7704.0

0.1508 111.07 110.52 106.10 107.60 20.74 14.85 11.85

15.89 1064.0 1056.0 1024.0 7672.0

0.1573 79.19 92.72 107.86 95.19 19.29 13.34 11.28

15.48 1056.0 1064.0 1040.0 7976.0

0.1637 91.46 107.06 102.88 97.77 20.07 13.59 12.01

15.79 1184.0 1056.0 1064.0 7792.0

0.1700 91.94 116.38 88.84 97.47 19.30 13.89 11.27

15.67 1128.0 1096.0 1040.0 7936.0

0.1762 95.00 117.33 86.79 99.47 18.99 13.84 11.10

15.63 1024.0 1112.0 1016.0 7984.0

0.1823 92.87 88.66 80.27 88.04 18.90 13.80 11.62

15.51 1128.0 992.0 1160.0 7848.0

0.1883 60.15 93.48 83.94 80.07 18.51 13.53 10.62

15.36 1048.0 1088.0 1056.0 8008.0

0.1942 72.84 94.13 79.27 84.25 19.07 13.41 10.79
15.58 1168.0 1136.0 1072.0 8000.0
0.2000 55.13 108.96 83.11 81.51 17.88 13.86 11.24
15.41 1048.0 1048.0 1120.0 8024.0
0.2058 52.95 96.77 81.40 77.99 18.88 14.35 12.01
16.08 1184.0 1128.0 1040.0 8064.0
0.2114 50.85 80.08 73.64 70.39 18.32 12.92 11.67
14.97 1040.0 1072.0 1136.0 8000.0
0.2170 56.68 76.34 65.48 68.36 16.47 14.04 11.60
15.17 1136.0 1144.0 1088.0 8048.0
0.2224 44.83 78.34 62.27 62.83 16.95 12.84 11.20
14.59 1136.0 1048.0 1048.0 8024.0
0.2279 37.88 77.38 59.45 58.65 16.50 12.86 10.91
14.35 1072.0 1104.0 1144.0 8056.0
0.2333 38.92 59.73 47.51 54.73 15.17 12.91 10.09
13.99 1120.0 1056.0 1072.0 8064.0
0.2386 38.24 50.41 57.15 48.13 15.46 12.12 10.42
13.57 1096.0 1144.0 1160.0 8008.0
0.2439 32.42 55.00 53.73 47.87 15.21 12.96 9.97
13.60 1088.0 1064.0 1088.0 8120.0
0.2491 32.64 54.09 49.88 47.08 14.18 12.86 10.25
13.20 1160.0 1136.0 1120.0 8040.0
0.2543 27.16 41.95 40.82 42.11 13.61 11.46 8.96
12.81 1056.0 1056.0 1032.0 8080.0
0.2593 31.39 44.61 38.04 39.31 14.81 11.46 9.22
12.53 1152.0 1176.0 1064.0 8096.0
0.2645 32.79 41.29 33.56 36.77 14.62 11.27 8.44
12.11 1016.0 1096.0 1192.0 8032.0
0.2694 30.77 45.94 31.59 35.86 14.00 11.92 8.80
12.25 1144.0 1064.0 1040.0 8088.0
0.2745 26.48 42.18 30.28 32.54 12.99 11.42 8.35
11.30 1104.0 1136.0 1184.0 8032.0
0.2793 25.72 39.95 24.00 30.34 12.51 10.54 7.46

10.82 1080.0 1104.0 1000.0 8032.0

0.2842 20.40 36.85 23.08 27.38 10.31 9.46 6.68

9.69 1112.0 1088.0 1192.0 8160.0

0.2891 14.10 32.03 23.68 25.10 8.09 8.31 6.75

8.98 1088.0 1096.0 1136.0 7992.0

0.2939 16.89 30.03 23.99 25.58 8.67 8.42 6.68

9.38 1144.0 976.0 1040.0 8024.0

0.2987 12.85 24.00 22.23 21.88 7.55 7.39 6.32

8.43 1136.0 1160.0 1128.0 8048.0

0.3034 13.38 23.75 22.73 22.14 7.63 7.98 6.18

8.42 968.0 1016.0 1096.0 7960.0

0.3080 14.32 21.96 20.63 21.04 8.68 8.51 5.98

8.57 1224.0 952.0 1128.0 7976.0

0.3128 14.20 23.24 22.10 21.38 8.21 8.14 6.17

8.37 1080.0 1104.0 1064.0 8064.0

0.3174 14.14 18.12 19.87 19.53 8.01 7.66 5.42

7.94 1016.0 1120.0 1168.0 8056.0

0.3219 13.16 19.44 17.12 17.69 7.75 7.67 4.64

7.48 1240.0 1104.0 1024.0 8096.0

0.3266 14.72 17.92 20.82 17.65 7.71 6.57 5.01

7.20 1040.0 1048.0 1080.0 8064.0

0.3310 10.65 17.57 14.43 15.91 6.83 7.42 3.98

6.81 1040.0 1128.0 1232.0 8064.0

0.3355 12.44 21.02 14.71 16.14 7.29 8.01 3.75

7.06 1208.0 1096.0 984.0 8024.0

0.3401 9.88 14.79 16.10 15.65 6.38 6.84 4.86

6.88 1064.0 1072.0 1112.0 8128.0

0.3445 9.68 16.33 15.14 14.61 6.45 6.62 4.62

6.55 1056.0 1088.0 1024.0 7928.0

0.3488 8.10 15.67 15.18 12.95 5.26 6.84 4.77

5.92 1224.0 1128.0 1080.0 8112.0

0.3533 9.35 13.67 13.36 12.98 6.36 6.28 4.42

6.10 1024.0 1088.0 1088.0 8072.0

0.3576 8.17 16.30 12.31 12.70 5.64 7.20 3.84
5.87 1152.0 1048.0 1096.0 8144.0
0.3620 7.44 13.99 11.43 11.86 5.06 6.69 3.83
5.66 1056.0 1128.0 1136.0 7952.0
0.3663 7.30 12.91 10.31 11.36 5.69 6.21 3.62
5.74 1120.0 1160.0 1048.0 8128.0
0.3706 7.29 12.11 11.37 11.77 5.22 5.87 3.90
5.69 1152.0 1024.0 1120.0 8064.0
0.3748 6.14 13.58 11.19 10.96 4.36 6.09 3.84
5.17 968.0 1200.0 1104.0 8120.0
0.3791 6.93 12.53 11.22 10.04 5.07 6.01 3.85
4.98 1176.0 1072.0 1040.0 7984.0
0.3833 7.04 14.16 11.85 10.40 4.92 6.59 4.06
5.04 1024.0 1008.0 1152.0 8088.0
0.3875 5.67 13.47 8.99 9.40 4.03 6.12 3.07
4.69 1104.0 1216.0 1024.0 8096.0
0.3916 6.17 11.56 8.31 9.21 4.81 5.59 3.03
4.61 1168.0 1088.0 1152.0 8064.0
0.3958 5.01 11.31 7.62 8.82 3.85 5.35 2.92
4.54 1080.0 1064.0 1040.0 8040.0
0.4000 6.12 10.88 8.34 8.46 3.94 5.50 3.15
4.33 1024.0 1112.0 1144.0 8104.0
0.4040 4.80 11.77 8.31 7.82 3.77 5.63 3.08
4.08 1160.0 1064.0 1064.0 7992.0
0.4081 4.98 9.14 9.13 7.71 3.48 4.63 3.29
3.94 1136.0 1144.0 1104.0 8144.0
0.4123 5.07 9.22 7.92 7.13 3.79 4.40 2.94
3.68 984.0 1120.0 1096.0 8128.0
0.4163 5.39 9.23 7.81 7.42 4.02 4.77 2.92
3.92 1144.0 1104.0 1064.0 8024.0
0.4202 4.57 9.76 5.87 6.83 3.27 4.77 2.29
3.60 1128.0 1080.0 1144.0 8056.0
0.4243 4.98 9.23 6.52 7.18 3.33 4.63 2.60

3.72 1088.0 1136.0 1072.0 8104.0
0.4283 3.84 9.95 7.28 6.49 3.12 4.99 2.74
3.45 1048.0 1056.0 1056.0 8048.0
0.4323 4.66 8.02 6.18 6.04 3.37 4.15 2.43
3.28 1160.0 1128.0 1032.0 8056.0
0.4361 4.59 9.05 6.75 6.24 3.19 4.23 2.53
3.26 1072.0 1048.0 1168.0 8040.0
0.4402 4.25 8.58 6.46 6.24 2.81 4.34 2.42
3.27 1120.0 1192.0 1184.0 8144.0
0.4441 3.67 6.51 6.05 5.63 2.84 3.55 2.26
2.99 1088.0 968.0 1000.0 8056.0
0.4480 4.08 8.73 5.56 6.01 3.01 4.21 2.19
3.10 1104.0 1192.0 1040.0 8080.0
0.4518 3.62 8.52 5.17 5.37 2.51 4.08 2.00
2.78 1120.0 1032.0 1224.0 8072.0
0.4558 3.12 6.86 4.77 5.10 2.29 3.49 1.87
2.68 1152.0 1144.0 1040.0 8032.0
0.4596 3.00 6.18 4.11 4.67 2.25 3.23 1.69
2.53 1048.0 1048.0 1064.0 8104.0
0.4634 2.89 5.84 3.83 4.64 2.12 2.99 1.57
2.45 1040.0 1232.0 1072.0 8080.0
0.4672 3.17 6.07 4.94 4.60 2.18 3.12 1.90
2.44 1120.0 968.0 1200.0 8088.0
$$

The directional plots are along the directions of the moments of the anisotropy temperature matrix. These are ordered such that direction 1 has maximum alignment with a*, directions 2 with b*, etc.

TWINNING ANALYSIS:

Global twinning statistics.

These tests rely on the fact that it is highly improbably that very weak or very strong reflections will coincide, therefore, the tails for the distribution of twinned datasets will be less pronounced

Data truncated to 2.96 - 1.88 A resolution
$TABLE: Cumulative intensity distribution:
$GRAPHS: Cumulative intensity distribution (Acentric and centric):N:1,2,3,4,5,6:
$$ Z Acent_theor Acent_twin Acent_obser Cent_theor Cent_obser $$
$$

0.00000	0.00000	0.00000	0.02637	0.00000	0.08274
0.04000	0.03921	0.00303	0.05218	0.15852	0.17199
0.08000	0.07688	0.01151	0.08410	0.22270	0.23425
0.12000	0.11308	0.02458	0.11525	0.27097	0.28451
0.16000	0.14786	0.04148	0.14752	0.31084	0.32466
0.20000	0.18127	0.06155	0.17962	0.34528	0.36248
0.24000	0.21337	0.08420	0.21016	0.37579	0.39293
0.28000	0.24422	0.10891	0.24035	0.40330	0.42159
0.32000	0.27385	0.13524	0.26990	0.42839	0.44896
0.36000	0.30232	0.16279	0.29855	0.45149	0.47498
0.40000	0.32968	0.19121	0.32508	0.47291	0.49980
0.44000	0.35596	0.22021	0.35160	0.49288	0.51599
0.48000	0.38122	0.24953	0.37682	0.51158	0.53314
0.52000	0.40548	0.27895	0.40203	0.52916	0.55042
0.56000	0.42879	0.30829	0.42576	0.54574	0.56503
0.60000	0.45119	0.33737	0.44837	0.56142	0.57890
0.64000	0.47271	0.36607	0.47095	0.57629	0.59228
0.68000	0.49338	0.39428	0.49184	0.59041	0.60601
0.72000	0.51325	0.42190	0.51194	0.60386	0.62254
0.76000	0.53233	0.44885	0.53131	0.61667	0.63654
0.80000	0.55067	0.47507	0.54988	0.62891	0.65003
0.84000	0.56829	0.50052	0.56758	0.64060	0.66103
0.88000	0.58522	0.52516	0.58520	0.65180	0.67222

0.92000	0.60148	0.54896	0.60204	0.66253	0.68024
0.96000	0.61711	0.57191	0.61716	0.67281	0.68869
1.00000	0.63212	0.59399	0.63204	0.68269	0.69894
1.04000	0.64655	0.61521	0.64681	0.69218	0.71372
1.08000	0.66040	0.63557	0.66017	0.70130	0.72441
1.12000	0.67372	0.65507	0.67372	0.71008	0.73631
1.16000	0.68651	0.67373	0.68650	0.71853	0.74319
1.20000	0.69881	0.69156	0.69924	0.72668	0.74900
1.24000	0.71062	0.70857	0.71141	0.73453	0.75509
1.28000	0.72196	0.72480	0.72232	0.74210	0.76375
1.32000	0.73286	0.74025	0.73269	0.74941	0.77008
1.36000	0.74334	0.75495	0.74343	0.75646	0.77400
1.40000	0.75340	0.76892	0.75365	0.76328	0.78020
1.44000	0.76307	0.78220	0.76302	0.76986	0.78788
1.48000	0.77236	0.79480	0.77210	0.77623	0.79417
1.52000	0.78129	0.80675	0.78086	0.78238	0.79951
1.56000	0.78986	0.81807	0.78962	0.78833	0.80486
1.60000	0.79810	0.82880	0.79789	0.79410	0.80896
1.64000	0.80602	0.83895	0.80557	0.79967	0.81418
1.68000	0.81363	0.84855	0.81291	0.80508	0.81995
1.72000	0.82093	0.85763	0.81972	0.81031	0.82588
1.76000	0.82796	0.86621	0.82674	0.81538	0.82944
1.80000	0.83470	0.87431	0.83355	0.82029	0.83526
1.84000	0.84118	0.88196	0.83990	0.82505	0.83947
1.88000	0.84741	0.88917	0.84606	0.82967	0.84436
1.92000	0.85339	0.89597	0.85205	0.83414	0.84814
1.96000	0.85914	0.90238	0.85749	0.83849	0.85169
2.00000	0.86466	0.90842	0.86287	0.84270	0.85569

$$

The culmulative intensity, N(Z), plot is diagnostic for both twinning and tNCS. For twinned data there are fewer weak reflections, therefore, N(Z) is sigmoidal for twinned

data. However, if both twinning and tNCS are present, the effects may cancel each out. Therefore the results of the L-test and patterson test should be consulted

L test for twinning: (Padilla and Yeates Acta Cryst. D59 1124 (2003))
L statistic = 0.481 (untwinned 0.5 perfect twin 0.375)
Data has used to   2.96 -   1.88 A resolution
   Relation between L statistics and twinning fraction:
      Twinning fraction = 0.000 L statistics = 0.500:
      Twinning fraction = 0.100 L statistics = 0.440:
      Twinning fraction = 0.500 L statistics = 0.375:

$TABLE: L test for twinning:
$GRAPHS: cumulative distribution function for |L|, twin fraction of 0.05:0|1x0|1:1,2,3,4:
$$ |L| N(L) Untwinned Twinned $$
$$
0.0000 0.0000 0.0000   0.0000
0.0500 0.0533 0.0500   0.0749
0.1000 0.1061 0.1000   0.1495
0.1500 0.1592 0.1500   0.2233
0.2000 0.2128 0.2000   0.2960
0.2500 0.2659 0.2500   0.3672
0.3000 0.3199 0.3000   0.4365
0.3500 0.3718 0.3500   0.5036
0.4000 0.4237 0.4000   0.5680
0.4500 0.4756 0.4500   0.6294
0.5000 0.5260 0.5000   0.6875
0.5500 0.5769 0.5500   0.7418
0.6000 0.6274 0.6000   0.7920
0.6500 0.6769 0.6500   0.8377

0.7000 0.7265 0.7000 0.8785
0.7500 0.7758 0.7500 0.9141
0.8000 0.8236 0.8000 0.9440
0.8500 0.8710 0.8500 0.9679
0.9000 0.9169 0.9000 0.9855
0.9500 0.9612 0.9500 0.9963
1.0000 1.0000 1.0000 1.0000
$$

The Cumulative |L| plot for acentric data, where L = (I1-I2)/(I1+I2). This depends on the local difference in intensities. The difference operators used link to the neighbouring reflections taking into account possible tNCS operators.
Note that this estimate is not as reliable as obtained via the H-test or ML Britton test if twin laws are available. However, it is less prone to the effects of anisotropy than the H-test

Reference: Padilla, Yeates. A statistic for local intensity differences: robustness to anisotropy and pseudo-centering and utility for detecting twinning. Acta Cryst. D59, 1124-30, 2003.

Mean acentric moments I from input data:

  <I^2>/<I>^2 = 1.988 (Expected = 2.000, Perfect Twin = 1.500)
  <I^3>/<I>^3 = 5.981 (Expected value = 6.000, Perfect Twin = 3.000)
  <I^4>/<I>^4 = 24.431 (Expected value = 24.000, Perfect Twin = 7.500)

$TABLE: Acentric Moments of I:
$GRAPHS: 2nd moment of I 1.988 (Expected value = 2, Perfect Twin = 1.5):0|0.468x0|5:1,2:
: 3rd & 4th Moments of I (Expected values = 6, 24, Perfect twin = 3, 7.5):0|0.468x0|36:1,3,4:
$$ 1/resol^2   <I**2>   <I**3>   <I**4> $$

$$

0.013489	2.155	6.847	27.657
0.027445	2.072	5.982	20.454
0.038027	2.067	6.213	23.558
0.047352	2.007	6.371	27.626
0.055737	1.886	5.014	16.996
0.063445	2.031	6.032	22.744
0.070485	2.030	5.964	21.955
0.077273	2.128	6.637	25.866
0.083937	2.144	7.329	34.919
0.090028	2.083	6.281	23.684
0.095814	2.097	6.408	24.545
0.101358	2.237	7.782	35.467
0.106696	2.034	5.998	22.089
0.111534	2.146	7.191	32.948
0.116296	2.188	8.311	47.050
0.120786	2.166	7.372	33.477
0.125154	1.991	5.952	23.198
0.129395	2.160	8.424	53.377
0.133514	1.991	5.744	20.608
0.137630	2.023	6.500	28.401
0.141548	1.805	4.557	14.381
0.145367	2.075	6.830	30.565
0.149124	1.980	5.809	21.536
0.152748	1.929	5.480	20.110
0.156417	1.875	5.102	18.359
0.159836	2.148	7.287	33.254
0.163346	1.952	5.418	18.488
0.166880	1.837	4.602	13.821
0.170214	1.947	5.565	20.280
0.173630	1.859	4.741	14.642
0.177005	1.982	5.800	21.766
0.180233	2.019	5.975	22.641

0.183497	1.927	5.737	24.354
0.186813	1.984	6.015	24.070
0.189918	2.175	7.257	32.325
0.193045	1.967	5.518	19.148
0.196289	1.871	5.019	16.882
0.199368	1.977	5.979	25.277
0.202408	1.994	5.886	22.470
0.205515	1.854	5.251	21.119
0.208552	1.974	5.728	21.339
0.211490	1.992	6.117	25.404
0.214469	2.026	6.104	23.475
0.217572	2.160	8.883	61.263
0.220413	1.992	5.975	23.543
0.223269	1.966	5.629	20.581
0.226221	1.995	6.097	25.942
0.229194	1.971	5.741	22.183
0.231961	2.095	7.457	42.153
0.234729	1.984	5.750	21.142
0.237621	2.120	7.382	36.815
0.240483	1.844	4.760	15.153
0.243193	1.967	5.703	21.270
0.245907	1.966	5.654	20.360
0.248671	1.942	5.369	18.327
0.251531	2.129	6.889	29.601
0.254241	1.903	5.161	17.838
0.256836	1.973	5.783	22.217
0.259561	1.867	4.939	16.191
0.262268	1.994	5.845	21.791
0.264962	2.089	6.495	25.469
0.267585	1.902	5.057	16.426
0.270213	1.894	5.240	18.659
0.272849	1.946	5.369	18.457
0.275521	1.966	5.603	20.287

0.278027	2.030	6.159	24.199
0.280591	1.910	5.435	20.375
0.283176	2.025	6.378	26.361
0.285788	2.231	8.402	46.683
0.288410	2.137	7.203	33.267
0.290837	1.986	5.841	22.095
0.293376	1.986	5.712	20.745
0.295945	1.964	5.552	19.657
0.298455	2.049	6.209	24.341
0.301022	2.177	7.538	35.961
0.303500	2.205	7.429	32.250
0.305960	2.040	6.364	27.785
0.308440	2.115	6.941	30.620
0.310909	2.045	6.311	27.196
0.313412	2.003	6.112	24.879
0.315848	1.949	5.569	20.852
0.318213	1.964	5.637	21.430
0.320599	1.824	4.666	15.142
0.322987	1.961	5.363	18.019
0.325411	1.939	5.615	21.401
0.327893	2.156	8.230	50.501
0.330179	1.966	5.686	21.707
0.332534	1.911	5.301	18.639
0.334845	1.915	4.972	15.484
0.337270	1.928	5.661	22.298
0.339637	1.886	4.990	16.878
0.341976	1.911	5.002	15.921
0.344277	2.130	6.832	28.292
0.346556	2.028	6.077	23.712
0.348922	2.139	7.100	30.630
0.351247	2.141	7.201	31.907
0.353648	2.081	6.230	22.947
0.355909	2.071	6.524	27.140

0.358028	2.039	6.233	24.312
0.360344	2.099	6.610	26.673
0.362588	2.151	7.106	29.971
0.364892	2.155	7.055	29.755
0.367219	1.877	4.979	16.847
0.369484	1.880	4.883	15.878
0.371638	2.033	5.962	21.433
0.373752	2.058	6.352	26.185
0.376095	2.142	6.966	29.513
0.378315	2.021	6.160	24.306
0.380489	2.062	6.155	22.961
0.382796	2.143	6.696	25.502
0.384980	1.987	6.143	25.767
0.387094	2.109	6.366	23.967
0.389217	2.137	7.231	32.883
0.391425	2.175	7.821	40.323
0.393624	2.038	6.161	23.924
0.395837	1.969	5.395	18.127
0.398046	2.053	6.237	23.808
0.400114	1.982	5.581	19.592
0.402244	1.958	5.670	21.125
0.404347	1.983	5.673	19.951
0.406582	1.978	5.625	20.018
0.408657	2.379	10.049	63.771
0.410802	2.017	5.828	21.063
0.412984	2.046	6.279	24.735
0.415096	1.930	5.330	18.965
0.417101	1.958	5.451	18.906
0.419170	2.021	5.892	21.306
0.421290	2.056	6.071	22.790
0.423510	2.045	6.258	24.680
0.425506	2.075	6.304	24.103
0.427606	1.977	5.490	19.420

```
  0.429712       2.014       5.766      21.429
  0.431733       2.052       6.314      26.007
  0.433797       1.772       4.177      12.004
  0.435823       1.999       6.008      25.313
  0.437908       2.131       7.561      39.863
  0.440026       1.979       6.102      27.584
  0.442076       2.136       6.625      25.181
  0.444084       1.889       5.188      19.119
  0.446135       2.045       6.099      23.442
  0.448082       2.168       7.317      32.467
  0.450130       2.182       6.756      25.184
  0.452088       2.114       6.565      26.060
  0.454222       2.236       8.227      41.891
  0.456262       2.077       6.389      26.692
  0.458274       2.012       5.763      21.517
  0.460287       2.113       6.881      29.931
  0.462257       2.014       5.880      22.726
  0.464226       2.078       6.004      21.359
  0.466172       2.160       6.968      29.566
  0.468103       1.886       4.628      13.630
$$

$TABLE: Centric Moments of I:
$GRAPHS: 2nd moment of I 3.494 (Expected = 3, Perfect Twin = 2):0|0.460x0|5:1,2:
: 3rd & 4th Moments of I (Expected = 15, 105, Perfect Twin = 6, 24):0|0.460x0|150:1,3,4:
$$ 1/resol^2   <I**2>     <I**3>     <I**4> $$
$$
  0.019665       3.707      19.855     125.019
  0.054334       3.346      16.121      93.634
  0.087620       4.420      32.226     288.130
  0.115776       6.122      94.369    2019.725
  0.139341       3.255      20.090     167.206
  0.160959       3.048      16.449     119.193
```

0.181104	3.641	27.465	306.830
0.200452	2.376	8.248	35.464
0.219245	3.307	20.638	191.013
0.237970	3.455	18.195	116.486
0.256476	2.852	11.802	57.642
0.274807	2.726	10.648	49.365
0.293279	2.620	9.755	44.206
0.312741	3.139	16.243	110.385
0.331194	2.412	8.170	33.106
0.349876	3.566	22.428	188.963
0.368338	3.013	15.545	112.350
0.386544	3.039	14.342	84.368
0.404845	2.639	9.590	43.938
0.423169	2.924	11.498	53.384
0.441506	3.156	16.483	126.210
0.459674	3.114	13.230	71.367

$$

First principles calculation has found 5 potential twinning operators

#	twinning operator	score	type
0	-h,l,k	2.14	pm
1	-k,-h,-l	3.13	pm
2	k,l,h	4.49	pm
3	-l,-h,k	4.69	pm
4	-l,-k,-h	5.27	pm

m merohedral

pm pseudo-merohedral

The score gives an indication of the closure of the twinning operation. The lower the values

the more higher the overlap.

The appearance of twinning operators only indicates that the crystal symmetry and lattice symmetry permit twinning. It does not mean that there is twinning present. Only the

presence of statistics consistent with twinning gives a strong indicator.

Twinning operator based tests:

H-test: Cumulative plot of H=|I-T(I)|/(I-T(I)) for twin related reflections. This should be linear with slope 1/(1-2a).

$TABLE: H test for twinning
$GRAPHS: cumulative distribution function for |H| (operator -h, l, k) alpha = 0.01:0|1x0|1:1,2,3,4,5,6,7:
: cumulative distribution function for |H| (operator -k, -h, -l) alpha = 0.02:0|1x0|1:1,2,3,4,5,6,8:
: cumulative distribution function for |H| (operator k, l, h) alpha = 0.00:0|1x0|1:1,2,3,4,5,6,9:
: cumulative distribution function for |H| (operator -l, -h, k) alpha = 0.00:0|1x0|1:1,2,3,4,5,6,10:
: cumulative distribution function for |H| (operator -l, -k, -h) alpha = 0.01:0|1x0|1:1,2,3,4,5,6,11:
$$ |H| 0.4 0.3 0.2 0.1 0.0 -h,l,k -k,-h,-l k,l,h -l,-h,k -l,-k,-h$$
$$
0.00 0.0 0.0 0.0 0.0 0.0 0.00 0.00 0.00 0.00 0.00
0.05 - - - - - 0.07 0.07 0.05 0.05 0.07
0.10 - - - - - 0.12 0.12 0.10 0.10 0.12
0.15 - - - - - 0.16 0.17 0.15 0.15 0.17
0.20 - - - - - 0.21 0.22 0.20 0.20 0.21
0.25 - - - - - 0.26 0.27 0.25 0.25 0.27
0.30 - - - - - 0.32 0.32 0.30 0.30 0.32
0.35 - - - - - 0.37 0.37 0.36 0.36 0.36
0.40 - - - - - 0.42 0.42 0.40 0.40 0.41
0.45 - - - - - 0.47 0.47 0.45 0.45 0.46
0.50 - - - - - 0.52 0.52 0.51 0.51 0.51
0.55 - - - - - 0.57 0.57 0.56 0.56 0.56

0.60 - - - - - 0.62 0.62 0.61 0.61 0.61

0.65 - - - - - 0.67 0.67 0.65 0.65 0.66

0.70 - - - - - 0.72 0.73 0.71 0.71 0.71

0.75 - - - - - 0.77 0.78 0.76 0.76 0.76

0.80 - - - - - 0.81 0.82 0.81 0.81 0.81

0.85 - - - - - 0.86 0.87 0.86 0.86 0.86

0.90 - - - - - 0.91 0.92 0.91 0.91 0.91

0.95 - - - - - 0.96 0.96 0.96 0.96 0.96

1.00 5.0 2.5 1.67 1.25 1.0 1.00 1.00 1.00 1.00 1.00

$$

Britton plot: Plot of number of negative detwinned intensities.

$TABLE: Britton plot for twinning

$GRAPHS: aI1+(1-a)I2 > 0 (operator -h, l, k) alpha = 0.00:A:1,2:

: aI1+(1-a)I2 > 0 (operator -k, -h, -l) alpha = 0.00:A:1,3:

: aI1+(1-a)I2 > 0 (operator k, l, h) alpha = 0.00:A:1,4:

: aI1+(1-a)I2 > 0 (operator -l, -h, k) alpha = 0.00:A:1,5:

: aI1+(1-a)I2 > 0 (operator -l, -k, -h) alpha = 0.00:A:1,6:

$$ alpha -h,l,k -k,-h,-l k,l,h -l,-h,k -l,-k,-h$$

$$

0.00 0.00 0.00 0.00 0.00 0.00

0.03 0.02 0.02 0.02 0.02 0.02

0.05 0.05 0.05 0.04 0.05 0.04

0.07 0.07 0.07 0.07 0.07 0.07

0.10 0.09 0.09 0.09 0.10 0.09

0.12 0.12 0.11 0.12 0.12 0.12

0.15 0.14 0.14 0.14 0.15 0.14

0.17 0.17 0.16 0.17 0.17 0.17

0.20 0.19 0.19 0.19 0.20 0.19

0.23 0.21 0.22 0.22 0.22 0.21

0.25 0.24 0.24 0.24 0.24 0.24

0.28	0.26	0.26	0.27	0.27	0.26
0.30	0.29	0.29	0.29	0.29	0.29
0.33	0.31	0.31	0.31	0.32	0.31
0.35	0.34	0.34	0.34	0.34	0.33
0.38	0.36	0.36	0.36	0.37	0.36
0.40	0.39	0.39	0.39	0.40	0.39
0.42	0.41	0.41	0.41	0.42	0.41
0.45	0.44	0.44	0.44	0.45	0.43
0.47	0.46	0.46	0.46	0.47	0.46

$$

ML-Britton: Plot of number of negative detwinned intensities. The ML element corrects for the sigma in the observed intensity and for the effects of a single tNCS operator, if it is present.

$TABLE: ML-Britton test for twinning
$GRAPHS: aI1+(1-a)I2 > 0 (operator -h, l, k) alpha = 0.00:A:1,2:
: aI1+(1-a)I2 > 0 (operator -k, -h, -l) alpha = 0.00:A:1,3:
: aI1+(1-a)I2 > 0 (operator k, l, h) alpha = 0.00:A:1,4:
: aI1+(1-a)I2 > 0 (operator -l, -h, k) alpha = 0.00:A:1,5:
: aI1+(1-a)I2 > 0 (operator -l, -k, -h) alpha = 0.00:A:1,6:
$$ alpha -h,l,k -k,-h,-l k,l,h -l,-h,k -l,-k,-h$$
$$

0.00	0.18	0.18	0.18	0.18	0.18
0.03	5037.90	3816.69	5169.02	4382.12	4055.91
0.05	21427.26	18669.27	21913.15	20873.90	19977.19
0.07	46123.49	40792.34	48021.23	45932.19	46279.47
0.10	78882.31	69646.13	80285.70	76422.73	77175.56
0.12	112539.51	102350.75	117933.61	111211.84	113345.33
0.15	150881.01	138780.31	161503.38	149165.13	152585.69
0.17	191646.74	178571.44	206832.87	190733.90	196201.73
0.20	232824.72	219253.65	251640.85	233495.81	241992.61

0.23 278168.04 264728.95 300940.68 279630.13 289211.80
0.25 324734.15 311951.29 350303.29 328037.93 338837.65
0.28 373092.84 360312.54 402088.83 379271.93 390155.22
0.30 423850.94 411762.16 456049.39 430692.67 441350.34
0.33 475256.14 465233.30 510888.51 482852.33 496461.22
0.35 527806.72 518781.05 567956.57 538413.49 552720.40
0.38 583513.03 576299.23 626152.69 595243.67 610898.55
0.40 640938.82 630711.05 687545.41 651173.52 669412.79
0.42 698795.28 690066.82 749185.07 710920.46 730461.33
0.45 757797.62 749543.21 810848.85 770775.67 791230.90
0.47 812614.53 805379.20 869131.00 826124.30 848722.35
$$

Twin fraction estimates based on global statistics:
  Twin fraction estimate from L-test: 0.05
  Twin fraction estimate from moments: 0.01

Twin fraction estimates by twinning operator

The following operator based twinning estimates analyse data with each of the possible twin operators. If twinning is present the most likely operator will have a low RTwin score (<I-T(I)>/<I+T(I)>) and estimates of the twin fraction above 0.

| operator | L-test | |Rtwin| | H-test | Britton | ML Britton |

| -h, l, k | No | 0.48 | 0.01 | 0.00 | 0.00 (N/A) |
| -k, -h, -l | No | 0.48 | 0.02 | 0.00 | 0.00 (N/A) |

k, l, h	No	0.50	0.00	0.00	0.00 (N/A)
-l, -h, k	No	0.50	0.00	0.00	0.00 (N/A)
-l, -k, -h	No	0.49	0.01	0.00	0.00 (N/A)

TWINNING SUMMARY

Twinning fraction from H-test: 0.02
Twinning fraction from L-Test: 0.05

No twinning or very low twinning fraction.

Twinning, if any, can be safely be ignored. However, twin refinement may be attempted, but not before the
model is completely build.

Analysis of mean intensity by parity for reflection classes

For each class, Mn(I/sig(I)) is given for even and odd parity with respect to the condition,
eg group 1: h even & odd; group 7 h+k+l even & odd; group 8 h+k=2n & h+l=2n & k+l=2n or not

Range	Min_S	Dmax	Nref	1	2	3	4	5	6	7	8
				h	k	l	h+k	h+l	k+l	h+k+l	h+k,h+l,k+l
1	0.00236	20.60	116	18.0 21.6	19.0 20.5	19.6 19.9	19.6 19.9	19.0 20.5	18.0 21.6	19.7 0.0	17.4 20.7

2 0.00707 11.89 128 19.0 20.6 18.3 21.6 20.0 19.7 20.0 19.7 18.3 21.6 19.0 20.6 19.8 0.0 17.7 20.6

3 0.01178 9.21 160 18.4 19.7 18.0 20.1 20.6 17.9 20.6 17.9 18.0 20.1 18.4 19.7 19.1 0.0 18.7 19.2

4 0.01649 7.79 197 17.8 19.8 18.2 19.4 18.2 19.3 18.2 19.3 18.2 19.4 17.8 19.8 18.7 0.0 16.9 19.5

5 0.02121 6.87 219 17.0 19.2 17.9 18.1 17.5 18.4 17.5 18.4 17.9 18.1 17.0 19.2 18.0 0.0 16.6 18.5

6 0.02592 6.21 229 17.4 18.4 17.9 17.9 18.6 17.3 18.6 17.3 17.9 17.9 17.4 18.4 17.9 0.0 18.1 17.9

7 0.03063 5.71 270 18.7 17.8 18.2 18.4 18.2 18.4 18.2 18.4 18.2 18.4 18.7 17.8 18.3 0.0 18.5 18.2

8 0.03535 5.32 260 17.4 18.7 18.1 18.0 17.2 19.0 17.2 19.0 18.1 18.0 17.4 18.7 18.0 0.0 16.6 18.5

9 0.04006 5.00 289 17.6 18.3 17.5 18.5 17.8 18.1 17.8 18.1 17.5 18.5 17.6 18.3 17.9 0.0 17.0 18.3

10 0.04477 4.73 292 18.0 18.1 17.6 18.4 18.2 17.8 18.2 17.8 17.6 18.4 18.0 18.1 18.0 0.0 17.8 18.1

11 0.04948 4.50 307 18.5 18.7 19.0 18.2 18.0 19.2 18.0 19.2 19.0 18.2 18.5 18.7 18.6 0.0 18.3 18.7

12 0.05420 4.30 330 17.2 17.7 17.1 17.8 17.8 17.1 17.8 17.1 17.1 17.8 17.2 17.7 17.5 0.0 17.2 17.5

13 0.05891 4.12 343 18.2 18.6 17.8 19.0 18.0 18.8 18.0 18.8 17.8 19.0 18.2 18.6 18.4 0.0 17.3 18.8

14 0.06362 3.96 361 18.2 18.1 18.0 18.4 17.8 18.6 17.8 18.6 18.0 18.4 18.2 18.1 18.2 0.0 17.6 18.4

15 0.06833 3.83 376 17.2 17.7 17.5 17.3 17.0 17.9 17.0 17.9 17.5 17.3 17.2 17.7 17.4 0.0 16.9 17.6

16 0.07305 3.70 365 16.8 17.7 17.1 17.3 17.3 17.2 17.3 17.2 17.1 17.3 16.8 17.7 17.2 0.0 16.7 17.4

17 0.07776 3.59 391 16.5 16.6 16.5 16.6 16.4 16.7 16.4 16.7 16.5 16.6 16.5 16.6 16.5 0.0 16.4 16.6

18 0.08247 3.48 413 16.4 16.6 16.2 16.8 16.6 16.4 16.6 16.4 16.2

16.8 16.4 16.6 16.5 0.0 16.2 16.6

19 0.08718 3.39 430 16.1 16.0 15.7 16.4 15.8 16.3 15.8 16.3 15.7 16.4 16.1 16.0 16.0 0.0 15.4 16.3

20 0.09190 3.30 453 16.0 16.7 16.4 16.3 15.9 16.8 15.9 16.8 16.4 16.3 16.0 16.7 16.3 0.0 15.7 16.6

21 0.09661 3.22 467 15.7 15.2 15.4 15.5 15.6 15.3 15.6 15.3 15.4 15.5 15.7 15.2 15.5 0.0 15.8 15.3

22 0.10132 3.14 470 15.6 16.1 15.9 15.8 15.6 16.1 15.6 16.1 15.9 15.8 15.6 16.1 15.8 0.0 15.4 16.0

23 0.10604 3.07 526 15.1 15.0 15.1 15.0 15.1 14.9 15.1 14.9 15.1 15.0 15.1 15.0 15.0 0.0 15.2 15.0

24 0.11075 3.00 525 16.4 15.2 15.5 16.1 15.3 16.3 15.3 16.3 15.5 16.1 16.4 15.2 15.8 0.0 15.6 15.8

25 0.11546 2.94 578 16.0 16.1 15.7 16.4 15.7 16.4 15.7 16.4 15.7 16.4 16.0 16.1 16.0 0.0 15.3 16.3

26 0.12017 2.88 566 15.7 16.1 16.0 15.9 15.9 16.0 15.9 16.0 16.0 15.9 15.7 16.1 15.9 0.0 15.7 16.0

27 0.12489 2.83 607 16.3 15.4 15.4 16.3 15.5 16.3 15.5 16.3 15.4 16.3 16.3 15.4 15.9 0.0 15.4 16.0

28 0.12960 2.78 624 15.6 16.1 15.7 16.0 15.2 16.4 15.2 16.4 15.7 16.0 15.6 16.1 15.8 0.0 14.9 16.2

29 0.13431 2.73 591 16.0 15.9 15.9 15.9 16.1 15.8 16.1 15.8 15.9 15.9 16.0 15.9 15.9 0.0 16.1 15.9

30 0.13902 2.68 683 16.2 16.1 15.9 16.3 16.0 16.2 16.0 16.2 15.9 16.3 16.2 16.1 16.1 0.0 15.9 16.2

31 0.14374 2.64 662 15.9 15.9 15.9 16.0 15.7 16.2 15.7 16.2 15.9 16.0 15.9 15.9 15.9 0.0 15.6 16.0

32 0.14845 2.60 696 15.1 16.1 15.7 15.4 15.6 15.6 15.6 15.6 15.7 15.4 15.1 16.1 15.6 0.0 15.2 15.7

33 0.15316 2.56 701 15.6 15.6 15.3 15.9 15.7 15.4 15.7 15.4 15.3 15.9 15.6 15.6 15.6 0.0 15.4 15.6

34 0.15787 2.52 741 15.3 15.9 15.5 15.7 15.5 15.7 15.5 15.7 15.5 15.7 15.3 15.9 15.6 0.0 15.1 15.7

35 0.16259 2.48 715 15.1 16.7 15.9 15.9 15.7 16.1 15.7 16.1 15.9 15.9 15.1 16.7 15.9 0.0 15.0 16.2

36 0.16730 2.44 760 15.7 15.9 15.9 15.7 16.1 15.5 16.1 15.5 15.9 15.7 15.7 15.9 15.8 0.0 16.1 15.7

37 0.17201 2.41 747 15.1 15.8 15.2 15.7 15.5 15.4 15.5 15.4 15.2 15.7 15.1 15.8 15.4 0.0 14.9 15.6

38 0.17673 2.38 798 15.3 15.9 15.4 15.8 15.7 15.5 15.7 15.5 15.4 15.8 15.3 15.9 15.6 0.0 15.2 15.7

39 0.18144 2.35 728 15.4 15.5 15.3 15.6 15.2 15.7 15.2 15.7 15.3 15.6 15.4 15.5 15.4 0.0 15.0 15.6

40 0.18615 2.32 821 15.5 15.6 15.0 16.1 15.4 15.7 15.4 15.7 15.0 16.1 15.5 15.6 15.5 0.0 14.8 15.8

41 0.19086 2.29 795 15.1 15.9 15.5 15.6 15.5 15.6 15.5 15.6 15.5 15.6 15.1 15.9 15.5 0.0 15.0 15.7

42 0.19558 2.26 831 15.6 15.7 15.9 15.3 15.7 15.6 15.7 15.6 15.9 15.3 15.6 15.7 15.6 0.0 15.9 15.5

43 0.20029 2.23 816 15.3 16.1 15.7 15.6 15.5 15.8 15.5 15.8 15.7 15.6 15.3 16.1 15.6 0.0 15.1 15.8

44 0.20500 2.21 842 15.2 16.4 15.8 15.8 15.7 15.9 15.7 15.9 15.8 15.8 15.2 16.4 15.8 0.0 15.1 16.0

45 0.20971 2.18 847 15.3 14.6 14.8 15.1 14.7 15.1 14.7 15.1 14.8 15.1 15.3 14.6 14.9 0.0 14.9 14.9

46 0.21443 2.16 824 15.0 15.4 14.9 15.5 15.2 15.2 15.2 15.2 14.9 15.5 15.0 15.4 15.2 0.0 14.7 15.4

47 0.21914 2.14 875 14.6 14.9 14.9 14.6 14.8 14.7 14.8 14.7 14.9 14.6 14.6 14.9 14.7 0.0 14.8 14.7

48 0.22385 2.11 879 14.0 14.7 14.3 14.5 13.9 14.8 13.9 14.8 14.3 14.5 14.0 14.7 14.4 0.0 13.5 14.7

49 0.22857 2.09 890 13.7 14.4 14.0 14.2 14.2 14.0 14.2 14.0 14.0 14.2 13.7 14.4 14.1 0.0 13.7 14.2

50 0.23328 2.07 886 13.9 13.8 13.7 14.1 13.8 14.0 13.8 14.0 13.7 14.1 13.9 13.8 13.9 0.0 13.6 14.0

51 0.23799 2.05 889 13.5 13.6 13.1 14.1 13.4 13.8 13.4 13.8 13.1

14.1 13.5 13.6 13.6 0.0 12.9 13.8

52 0.24270 2.03 930 13.6 13.4 13.5 13.5 13.5 13.5 13.5 13.5 13.5 13.5 13.6 13.4 13.5 0.0 13.6 13.5

53 0.24742 2.01 894 12.7 13.3 12.6 13.5 12.8 13.3 12.8 13.3 12.6 13.5 12.7 13.3 13.0 0.0 12.0 13.4

54 0.25213 1.99 948 13.1 12.6 12.7 13.0 12.8 12.9 12.8 12.9 12.7 13.0 13.1 12.6 12.9 0.0 12.9 12.9

55 0.25684 1.97 916 12.4 12.8 12.5 12.6 12.3 12.9 12.3 12.9 12.5 12.6 12.4 12.8 12.6 0.0 12.1 12.8

56 0.26155 1.96 949 12.3 12.0 11.8 12.5 12.0 12.3 12.0 12.3 11.8 12.5 12.3 12.0 12.2 0.0 11.8 12.3

57 0.26627 1.94 954 12.4 12.0 12.3 12.0 11.9 12.5 11.9 12.5 12.3 12.0 12.4 12.0 12.2 0.0 12.2 12.2

58 0.27098 1.92 938 11.2 11.6 11.4 11.4 11.4 11.4 11.4 11.4 11.4 11.4 11.2 11.6 11.4 0.0 11.2 11.5

59 0.27569 1.90 988 11.0 11.2 11.1 11.2 11.3 11.0 11.3 11.0 11.1 11.2 11.0 11.2 11.1 0.0 11.1 11.1

60 0.28040 1.89 961 10.0 10.1 10.0 10.1 9.9 10.2 9.9 10.2 10.0 10.1 10.0 10.1 10.0 0.0 9.8 10.1

Totals: 36787 14.8 15.1 14.8 15.1 14.9 15.1 14.9 15.1 14.8 15.1 14.8 15.1 15.0 0.0 14.6 15.1

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INTENSITY TO AMPLITUDE CONVERSION:

Norm calculation summary:

Calculation using Wilson prior.

Anisotropy correction applied to norm.

Number of outliers and ice ring reflections not used in norm calculation (Read (1999)): 0

During the truncate procedure 2 intensities have been flagged as unphysical (too small).

Number of outliers detected in final norm (Read (1999)): 0

<!--SUMMARY_END--></FONT></B>

$TABLE: Phil plot:
$GRAPHS: Phil plot - normalised values:A:1,2,3,4:
: Phil plot - vs sigma:A:1,5,6,7:
$$ Value Io/Sigma I/Sigma F/Sigma**0.5 Io/sigIo I/sigI F/sigF$$
$$

-5.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-4.92500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-4.85000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-4.77500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-4.70000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-4.62500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-4.55000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-4.47500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-4.40000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-4.32500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-4.25000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-4.17500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-4.10000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-4.02500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-3.95000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-3.87500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-3.80000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-3.72500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-3.65000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-3.57500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-3.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

-3.42500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-3.35000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-3.27500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-3.20000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-3.12500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-3.05000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-2.97500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-2.90000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-2.82500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-2.75000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-2.67500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-2.60000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-2.52500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-2.45000	0.50000	0.00000	0.00000	0.00000	0.00000	0.00000
-2.37500	0.50000	0.00000	0.00000	0.50000	0.00000	0.00000
-2.30000	0.00000	0.00000	0.00000	1.00000	0.00000	0.00000
-2.22500	0.50000	0.00000	0.00000	0.50000	0.00000	0.00000
-2.15000	0.50000	0.00000	0.00000	1.99999	0.00000	0.00000
-2.07500	0.00000	0.00000	0.00000	2.00000	0.00000	0.00000
-2.00000	0.50000	0.00000	0.00000	2.50000	0.00000	0.00000
-1.92500	1.50000	0.00000	0.00000	3.00000	0.00000	0.00000
-1.85000	1.00000	0.00000	0.00000	1.50000	0.00000	0.00000
-1.77500	0.50000	0.00000	0.00000	3.50000	0.00000	0.00000
-1.70000	2.00000	0.00000	0.00000	8.50000	0.00000	0.00000
-1.62500	3.00000	0.00000	0.00000	12.50000	0.00000	0.00000
-1.55000	4.00000	0.00000	0.00000	14.00000	0.00000	0.00000
-1.47500	4.00000	0.00000	0.00000	15.50000	0.00000	0.00000
-1.40000	4.00000	0.00000	0.00000	14.50000	0.00000	0.00000
-1.32500	5.00000	0.00000	0.00000	18.99999	0.00000	0.00000
-1.25000	5.00000	0.00000	0.00000	26.00000	0.00000	0.00000
-1.17500	5.50000	0.00000	0.00000	30.00000	0.00000	0.00000
-1.10000	8.50000	0.00000	0.00000	44.49999	0.00000	0.00000
-1.02500	14.00000	0.00000	0.00000	54.50000	0.00000	0.00000

-0.95000	15.00000	0.00000	0.00000	70.50001	0.00000	0.00000
-0.87500	13.50000	0.00000	0.00000	79.00000	0.00000	0.00000
-0.80000	19.50000	0.00000	0.00000	84.50000	0.00000	0.00000
-0.72500	31.50000	0.00000	0.00000	96.50000	0.00000	0.00000
-0.65000	41.50000	0.00000	0.00000	102.00001	0.00000	0.00000
-0.57500	41.50000	0.00000	0.00000	121.00000	0.00000	0.00000
-0.50000	58.50000	0.00000	0.00000	142.00000	0.00000	0.00000
-0.42500	93.00000	0.00000	0.00000	160.50000	0.00000	0.00000
-0.35000	135.00000	0.00000	0.00000	187.00000	0.00000	0.00000
-0.27500	183.50000	0.00000	0.00000	213.00000	0.00000	0.00000
-0.20000	269.49999	0.00000	0.00000	232.00000	0.00000	0.00000
-0.12500	445.50000	0.00000	0.00000	250.50000	0.00000	0.00000
-0.05000	968.49999	212.50000	7.00000	265.00000	0.00000	0.00000
0.02500	1945.00001	1243.00001	84.00000	304.50000	0.00000	0.00000
0.10000	2546.00000	2295.00001	307.50001	329.00000	0.00000	0.00000
0.17500	2593.50000	2746.49998	686.99998	347.50000	0.00000	0.00000
0.25000	2601.50000	3047.00000	1190.50000	374.00000	0.00000	0.00000
0.32500	2538.00002	3093.00001	1781.99990	372.50000	0.00000	0.00000
0.40000	2470.00000	3056.00000	2441.50005	374.50000	0.00000	0.00000
0.47500	2439.50000	2976.00001	3082.49995	386.00000	0.00000	0.00000
0.55000	2335.49997	2757.99996	3577.50006	407.50000	0.00000	0.00000
0.62500	2210.50000	2583.50000	3876.50000	443.00000	0.00000	0.00000
0.70000	2178.50000	2462.00003	3968.50000	463.50000	4.00000	0.00000
0.77500	2128.00004	2294.50005	3978.99999	452.50001	95.49994	0.00000
0.85000	1966.99994	2131.99995	3924.99995	446.00000	211.00002	0.00000
0.92500	1893.00001	2021.99999	3805.49998	483.50001	251.50000	0.00000
1.00000	1885.50000	1966.00000	3720.00000	512.50000	219.50000	0.00000
1.07500	1798.49993	1843.49988	3643.49995	479.99997	239.50008	0.00000
1.15000	1692.50003	1713.00002	3555.00003	475.49999	600.99981	0.00000
1.22500	1615.99998	1672.50000	3418.99995	497.00000	1183.00018	0.00000
1.30000	1560.50004	1622.00006	3224.00014	495.00000	1507.99995	1.50000
1.37500	1523.00000	1539.00000	3023.00000	499.50000	1446.50000	65.00000
1.45000	1495.99998	1486.49998	2822.99986	486.49998	1343.50000	162.50005

1.52500	1445.00002	1412.50004	2668.00003	496.49998	1295.00003	201.50000
1.60000	1372.99997	1327.49998	2475.49991	503.99999	1174.99995	196.49999
1.67500	1268.00008	1265.00005	2257.00009	472.50001	1058.50006	157.50004
1.75000	1212.50000	1210.50000	2083.00000	477.00000	961.50000	117.50000
1.82500	1173.99994	1160.49996	1883.99988	468.99997	863.49994	93.49998
1.90000	1111.50001	1103.50001	1719.00004	481.99998	804.50001	75.00000
1.97500	1085.99999	1067.49999	1578.49995	485.49998	758.49998	78.00000
2.05000	1052.50003	1025.00004	1373.50017	456.00000	704.00003	188.99987
2.12500	1012.50000	1005.00000	1202.00000	468.00000	651.50000	472.00000
2.20000	983.49999	968.99994	1081.99990	475.50000	614.99999	793.00018
2.27500	926.99989	869.99987	893.49972	458.49996	592.49996	961.50007
2.35000	878.00001	846.99992	751.00009	444.50000	554.50006	990.99999
2.42500	857.50002	854.50003	698.50002	442.00001	543.99998	918.50010
2.50000	842.50000	816.00000	627.50000	437.00000	518.50000	836.00000
2.57500	790.49993	776.49997	506.49991	425.99999	488.50001	832.00000
2.65000	738.50000	732.99995	432.99999	413.49999	474.99995	800.49991
2.72500	704.00009	701.00003	376.00013	417.49998	453.50000	740.00007
2.80000	689.49997	698.49999	303.00003	425.50000	441.00002	690.00003
2.87500	707.50000	671.00000	255.00000	421.50000	434.00000	640.50000
2.95000	667.99995	624.49999	210.49998	405.49999	435.50000	599.49998
3.02500	610.49995	604.99997	187.49999	416.50005	409.99994	547.99991
3.10000	592.99999	584.00003	162.00005	423.50004	400.99997	506.50001
3.17500	589.00001	572.00000	129.00002	397.50001	395.00002	485.50002
3.25000	562.50000	553.50000	101.00000	385.50000	369.00000	463.00000
3.32500	534.99999	516.99998	73.49998	371.49998	360.00000	445.49999
3.40000	510.99996	486.49997	61.50000	357.00000	343.49996	414.49995
3.47500	488.00002	483.49998	53.00002	371.49996	350.49995	382.50003
3.55000	480.50000	470.50003	40.50000	387.50000	370.50000	375.99999
3.62500	463.00000	466.00000	38.00000	373.00000	359.50000	374.00000
3.70000	436.49999	445.99995	24.99998	346.49999	352.00000	354.99998
3.77500	409.49995	399.99998	11.50000	336.50000	343.49997	327.49996
3.85000	394.49999	401.99997	13.00000	340.99999	333.00000	322.99997
3.92500	397.00000	413.50000	13.50000	346.50000	320.00002	313.50003

4.00000	407.50000	400.50000	9.50000	333.50000	316.00000	297.00000
4.07500	406.00007	373.50007	7.49999	324.99996	312.50006	301.00000
4.15000	378.99996	349.49997	5.99999	331.50000	308.50002	293.49998
4.22500	337.00007	330.00002	3.50000	326.50001	320.99999	274.50003
4.30000	311.00001	313.99996	3.50000	323.50001	314.99995	256.99997
4.37500	314.50000	296.50000	2.00000	309.50000	307.50000	250.00000
4.45000	294.50011	273.50006	1.00000	316.99988	307.50001	269.49990
4.52500	290.00004	270.00002	1.00000	318.49995	306.00000	262.99993
4.60000	288.50005	286.99998	0.50000	306.99997	293.00004	233.00001
4.67500	277.00004	273.49989	0.50000	306.49995	277.49999	239.00005
4.75000	273.00000	252.50000	1.50000	292.00000	289.00000	241.50000
4.82500	263.99999	250.50001	2.00000	299.49994	302.50000	229.50003
4.90000	249.99996	230.99996	2.00000	302.99998	304.50000	214.99998
4.97500	220.00004	223.49998	1.50000	301.99998	294.50003	217.99997
5.05000	203.49999	222.99995	0.50000	310.50001	290.50004	218.99994
5.12500	217.50000	216.00000	0.00000	299.50000	284.00000	207.50000
5.20000	222.00006	199.50010	0.00000	281.00003	276.99996	202.00003
5.27500	205.99999	184.00001	0.00000	276.00000	266.49996	200.50001
5.35000	188.50003	179.50002	0.00000	271.50001	248.50000	204.00000
5.42500	166.99996	159.99994	0.00000	256.49995	262.50007	212.50004
5.50000	165.00000	151.00000	0.00000	261.50000	289.00000	205.50000
5.57500	160.50005	161.49996	0.00000	283.49996	271.50015	190.00000
5.65000	148.50000	165.99999	0.00000	289.50000	238.99999	190.00000
5.72500	160.99996	145.50004	0.00000	279.50002	260.49994	201.99997
5.80000	153.99989	131.50001	0.00000	275.50002	277.99996	192.49989
5.87500	135.50000	150.50000	0.00000	272.00000	271.50000	180.00000
5.95000	142.49998	144.50011	0.00000	252.00006	264.50004	181.00004
6.02500	137.99998	134.00003	0.00000	254.50004	244.99997	172.50000
6.10000	136.99998	142.50001	0.00000	262.00002	243.99997	171.00000
6.17500	138.99997	130.49996	0.00000	249.49997	266.00006	171.00001
6.25000	128.50000	122.50000	0.00000	258.50000	258.50000	171.00000
6.32500	124.00000	122.50000	0.00000	250.00012	253.99993	169.00001
6.40000	125.00000	116.49999	0.00000	247.50005	242.99994	158.99998

6.47500	114.00003	112.50000	0.00000	258.00003	244.99993	155.99998
6.55000	114.00006	106.99996	0.00000	252.00002	260.99994	165.00002
6.62500	116.00000	96.50000	0.00000	250.50000	275.50000	172.50000
6.70000	100.00003	92.50000	0.00000	274.49985	322.99989	178.49999
6.77500	89.99999	91.00000	0.50000	272.99992	357.00003	175.99999
6.85000	93.99998	86.00001	0.50000	282.99990	400.49992	167.50001
6.92500	96.49997	76.49997	0.00000	308.49992	437.50003	165.50001
7.00000	81.50000	71.50000	0.00000	320.50000	389.00000	164.50000
7.07500	70.50001	78.49997	0.00000	387.49980	313.50011	166.49997
7.15000	74.50001	82.49999	0.00000	433.50002	282.49998	162.49998
7.22500	79.50000	76.50001	0.00000	437.50001	258.50004	158.99998
7.30000	86.00004	79.50003	0.00000	366.49965	242.99999	155.49995
7.37500	85.50000	83.00000	0.00000	268.50000	223.50000	152.00000
7.45000	68.50005	72.00004	0.00000	229.00005	204.50000	160.49999
7.52500	68.50002	62.50000	0.00000	221.00001	216.00003	150.49997
7.60000	70.00002	62.99999	0.00000	218.50001	226.50000	148.99997
7.67500	64.00001	61.99998	0.00000	212.49999	217.49996	161.00001
7.75000	61.00000	54.00000	0.00000	225.00000	219.00000	154.00000
7.82500	55.00001	50.49999	0.00000	230.00005	219.50004	140.00003
7.90000	51.49999	57.00001	0.00000	213.49998	207.49999	140.00002
7.97500	55.49998	57.00001	0.00000	206.50000	200.00001	152.49998
8.05000	57.99998	47.49998	0.00000	201.49997	194.99999	148.99995
8.12500	56.50000	42.00000	0.00000	209.00000	193.50000	155.50000
8.20000	52.00004	42.49999	0.00000	205.50008	195.99998	163.00005
8.27500	38.00007	44.99999	0.00000	189.49999	203.49995	143.50011
8.35000	42.50012	41.99996	0.00000	200.50011	198.99991	144.00011
8.42500	46.49996	43.50003	0.00000	208.99999	197.00004	144.99995
8.50000	46.50000	44.00000	0.00000	210.00000	211.50000	147.00000
8.57500	50.00002	35.50002	0.00000	204.50004	214.00003	151.50004
8.65000	42.50004	32.00000	0.00000	200.99995	205.00004	140.50004
8.72500	33.49994	29.49997	0.00000	215.50010	199.49998	153.00016
8.80000	27.50000	29.00001	0.00000	211.99993	196.99999	156.49994
8.87500	30.00000	34.50000	0.00000	202.00000	197.00000	137.50000

```
   8.95000    34.99999    36.50001     0.00000   201.00002   197.50000   133.49999
   9.02500    37.99999    31.50004     0.00000   198.99998   194.50003   145.99990
   9.10000    33.49994    29.00001     0.00000   192.99992   185.99994   142.99987
   9.17500    31.50002    31.00001     0.00000   191.00003   184.00002   125.49998
   9.25000    28.50000    30.50000     0.00000   194.50000   194.50000   135.00000
   9.32500    22.99999    29.99999     0.00000   199.49996   210.99995   148.50000
   9.40000    27.99996    31.99999     0.00000   206.50001   213.50008   144.00004
   9.47500    29.49997    30.49997     0.00000   210.50005   219.50014   147.50008
   9.55000    29.50001    26.99999     0.00000   213.49999   231.99999   159.50002
   9.62500    29.00000    26.00000     0.00000   212.00000   233.50000   146.50000
   9.70000    25.00001    26.00000     0.00000   236.49988   240.49998   137.99995
   9.77500    25.49998    25.50001     0.00000   246.50015   258.49986   141.00006
   9.85000    25.49998    22.49997     0.00000   234.00002   279.00007   140.00005
   9.92500    22.99999    21.50001     0.00000   232.99998   284.49999   145.50000
$$


<B><FONT COLOR='#FF0000'><!--SUMMARY_BEGIN-->
ctruncate: Normal termination
Times: User:      18.6s System:    0.2s Elapsed:     0:19
</pre>
</html>
<!--SUMMARY_END--></FONT></B>
<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->
<html> <!-- CCP4 HTML LOGFILE -->
<hr>
<!--SUMMARY_END--></FONT></B>
<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->
<pre>

 ################################################################
 ################################################################
 ################################################################
```

```
 ### CCP4 7.1.009: MTZDUMP              version 1.1 :         ##
 ##############################################################
 User: yoshihisasuzuki  Run date: 25/10/2021 Run time: 11:52:17


 Please reference: Collaborative Computational Project, Number 4. 2011.
 "Overview of the CCP4 suite and current developments". Acta Cryst. D67, 235-242.
 as well as any specific reference in the program write-up.

<!--SUMMARY_END--></FONT></B>
  List  reflection:    0
  Symmetry to be listed

 OPENED INPUT MTZ FILE
 Logical            Name:            HKLIN                                    Filename:
/tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_5_mtz_New.tmp

 * Title:

 From Clipper CCP4MTZfile

 * Base dataset:

        0 HKL_base
          HKL_base
          HKL_base

 * Number of Datasets = 1

 * Dataset ID, project/crystal/dataset names, cell dimensions, wavelength:

        1 New
          New
```

New

94.0711 99.3468 103.1345 90.0000 90.0000 90.0000

0.89999

* Number of Columns = 18

* Number of Reflections = 80452

* Missing value set to NaN in input mtz file

* Column Labels :

H K L F_New SIGF_New DANO_New SIGDANO_New F_New(+) SIGF_New(+) F_New(-) SIGF_New(-) ISYM_New IMEAN_New SIGIMEAN_New I_New(+) SIGI_New(+) I_New(-) SIGI_New(-)

* Column Types :

H H H F Q D Q G L G L Y J Q K M K M

* Associated datasets :

0 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

* Cell Dimensions : (obsolete - refer to dataset cell dimensions above)

94.0711 99.3468 103.1345 90.0000 90.0000 90.0000

* Resolution Range :

0.00059 0.46913 (41.156 - 1.460 A)

* Sort Order :

```
     0     0     0     0     0

* Number of Symmetry Operations = 8
* Number of Primitive Operations = 4
* Space Group = 23 'I 2 2 2'
* Lattice Type = I
* Point Group Name = PG222

* Symmetry Operations :

Symmetry 1 X,  Y,  Z
 1.00  0.00  0.00  0.00
 0.00  1.00  0.00  0.00
 0.00  0.00  1.00  0.00
 0.00  0.00  0.00  1.00
Symmetry 2 X,  -Y,  -Z
 1.00  0.00  0.00  0.00
 0.00 -1.00  0.00  0.00
 0.00  0.00 -1.00  0.00
 0.00  0.00  0.00  1.00
Symmetry 3 -X,  Y,  -Z
-1.00  0.00  0.00  0.00
 0.00  1.00  0.00  0.00
 0.00  0.00 -1.00  0.00
 0.00  0.00  0.00  1.00
Symmetry 4 -X,  -Y,  Z
-1.00  0.00  0.00  0.00
 0.00 -1.00  0.00  0.00
 0.00  0.00  1.00  0.00
 0.00  0.00  0.00  1.00
Symmetry 5 X+1/2,  Y+1/2,  Z+1/2
 1.00  0.00  0.00  0.50
 0.00  1.00  0.00  0.50
```

```
 0.00  0.00  1.00  0.50
 0.00  0.00  0.00  1.00
Symmetry 6 X+1/2,  -Y+1/2,  -Z+1/2
 1.00  0.00  0.00  0.50
 0.00 -1.00  0.00  0.50
 0.00  0.00 -1.00  0.50
 0.00  0.00  0.00  1.00
Symmetry 7 -X+1/2,  Y+1/2,  -Z+1/2
-1.00  0.00  0.00  0.50
 0.00  1.00  0.00  0.50
 0.00  0.00 -1.00  0.50
 0.00  0.00  0.00  1.00
Symmetry 8 -X+1/2,  -Y+1/2,  Z+1/2
-1.00  0.00  0.00  0.50
 0.00 -1.00  0.00  0.50
 0.00  0.00  1.00  0.50
 0.00  0.00  0.00  1.00

 (only pointgroup is fixed so far)


 ******   EPSILON ZONES -  Reflection Classes and their multiplicity ******

 EPSILON Zone   1
 Reflections of type  h00
 Multiplicity   4

 EPSILON Zone   2
 Reflections of type  0k0
 Multiplicity   4

 EPSILON Zone   3
 Reflections of type  00l
```

Multiplicity 4

EPSILON Zone 4
Reflections of type hkl
Multiplicity 2

****** CENTRIC ZONES ******

CENTRIC Zone 1
Reflections of type 0kl

CENTRIC Zone 2
Reflections of type h0l

CENTRIC Zone 3
Reflections of type hk0

OVERALL FILE STATISTICS for resolution range 0.001 - 0.469
==========

Col num	Sort order	Min	Max	Num Missing	% complete	Mean	Mean abs.	Resolution Low	Resolution High	Type	Column label
1	ASC	0	64	0	100.00	24.4	24.4	41.16	1.46	H	H
2	NONE	0	68	0	100.00	26.0	26.0	41.16	1.46	H	K
3	NONE	0	70	0	100.00	26.7	26.7	41.16	1.46	H	L
4	NONE	3.1	3923.7	1	100.00	367.60	367.60	41.16	1.46	F	F_New
5	NONE	0.7	151.3	1	100.00	22.48	22.48	41.16	1.46	Q	SIGF_New
6	NONE	-1861.3	1532.6	5837	92.74	-2.26	25.65	41.16	1.46	D	DANO_New
7	NONE	0.0	174.9	5837	92.74	38.13	38.13	41.16	1.46	Q	

SIGDANO_New

8 NONE 3.1 3923.7 3294 95.91 335.97 335.97 41.16 1.46 G F_New(+)

9 NONE 0.9 151.3 3294 95.91 30.35 30.35 41.16 1.46 L SIGF_New(+)

10 NONE 3.1 3923.7 2543 96.84 346.35 346.35 41.16 1.46 G F_New(-)

11 NONE 0.7 144.6 2543 96.84 27.77 27.77 41.16 1.46 L SIGF_New(-)

12 NONE 0 2 0 100.00 0.1 0.1 41.16 1.46 Y ISYM_New

13 NONE -18.4 7982.3 0 100.00 137.17 137.27 41.16 1.46 J IMEAN_New

14 NONE 0.0 551.0 0 100.00 10.11 10.11 41.16 1.46 Q SIGIMEAN_New

15 NONE -19.1 7925.9 0 100.00 107.81 108.06 41.16 1.46 K I_New(+)

16 NONE 0.0 548.7 0 100.00 11.14 11.14 41.16 1.46 M SIGI_New(+)

17 NONE -20.8 7982.3 0 100.00 115.93 116.13 41.16 1.46 K I_New(-)

18 NONE 0.0 551.0 0 100.00 10.96 10.96 41.16 1.46 M SIGI_New(-)

No. of reflections used in FILE STATISTICS 80452

<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->

MTZDUMP: NO REFLECTIONS LISTED

Times: User: 0.1s System: 0.0s Elapsed: 0:01

</pre>

</html>

<!--SUMMARY_END--></FONT></B>

<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->

<html> <!-- CCP4 HTML LOGFILE -->

<hr>

<!--SUMMARY_END--></FONT></B>

<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->
<pre>

 ##
 ##
 ##
 ### CCP4 7.1.009: UNIQUE   version 7.1.009 :   ##
 ##
 User: yoshihisasuzuki Run date: 25/10/2021 Run time: 11:52:18

 Please reference: Collaborative Computational Project, Number 4. 2011.
 "Overview of the CCP4 suite and current developments". Acta Cryst. D67, 235-242.
 as well as any specific reference in the program write-up.

<!--SUMMARY_END--></FONT></B>
 Data line--- CELL 94.0711 99.3468 103.1345 90.0000 90.0000 90.0000
 Data line--- SYMMETRY 'I 2 2 2'
 Data line--- LABOUT F=FUNI SIGF=SIGFUNI
 Data line--- RESOLUTION 1.460
 Comment line--- ## This script run with the command   ##########
 Comment   line---   #   /Applications/ccp4-7.1/bin/unique   HKLOUT
"/tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_7_mtz.tmp"
 Comment line--- ##
Reciprocal space symmetry:
Space group: "I 2 2 2" Point group: "PG222" Laue group: "mmm"
Reference asymmetric unit: "h>=0 and k>=0 and l>=0"
  (change of basis may be applied)

 Spacegroup 23 "I 2 2 2"
 Original indices for reflection hkl with symmetry number ISYM

                                Bijvoet positive

	ISYM		ISYM		ISYM		ISYM	
ISYM	1	+h,+k,+l	3	-h,-k,+l	5	+h,-k,-l	7	-h,+k,-l

Bijvoet negative

	ISYM		ISYM		ISYM		ISYM	
ISYM	2	-h,-k,-l	4	+h,+k,-l	6	-h,+k,+l	8	+h,-k,+l

Maximum and minimum Bragg spacings 1.460 10000.000 Angstroms

Limits on H,K,L.. 0 to 64 0 to 68 0 to 70

WRITTEN OUTPUT MTZ FILE
Logical Name: HKLOUT Filename: /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_7_mtz.tmp

* Title:

* Base dataset:

0 HKL_base
HKL_base
HKL_base

* Number of Datasets = 0

* Dataset ID, project/crystal/dataset names, cell dimensions, wavelength:

* Number of Columns = 5

* Number of Reflections = 83816

* Missing value set to NaN in input mtz file

* Column Labels :

H K L FUNI SIGFUNI

* Column Types :

H H H F Q

* Associated datasets :

0 0 0 0 0

* Cell Dimensions : (obsolete - refer to dataset cell dimensions above)

  94.0711   99.3468 103.1345   90.0000   90.0000   90.0000

* Resolution Range :

   0.00020   0.46913   (71.550 -   1.460 A)

* Sort Order :

     1   2   3   0   0

* Space group = 'I 2 2 2' (number   23)

    318435 reflections tested

83816 reflections within resolution limits written to output file

<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->

UNIQUE: Normal Termination

Times: User: 0.1s System: 0.0s Elapsed: 0:00

</pre>

</html>

<!--SUMMARY_END--></FONT></B>

<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->

<html> <!-- CCP4 HTML LOGFILE -->

<hr>

<!--SUMMARY_END--></FONT></B>

<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->

<pre>

 ##

 ##

 ##

 ### CCP4 7.1.009: FREERFLAG   version 2.2 : 26/03/20##

 ##

 User: yoshihisasuzuki Run date: 25/10/2021 Run time: 11:52:18

 Please reference: Collaborative Computational Project, Number 4. 2011.

 "Overview of the CCP4 suite and current developments". Acta Cryst. D67, 235-242.

 as well as any specific reference in the program write-up.

<!--SUMMARY_END--></FONT></B>

 Data line--- FREERFRAC 0.05

 Data line--- END

 OPENED INPUT MTZ FILE

 Logical Name: HKLIN   Filename: /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_7_mtz.tmp

* Title:

* Base dataset:

0 HKL_base
HKL_base
HKL_base

* Number of Datasets = 0

* Dataset ID, project/crystal/dataset names, cell dimensions, wavelength:

* Number of Columns = 5

* Number of Reflections = 83816

* Missing value set to NaN in input mtz file

* Column Labels :

H K L FUNI SIGFUNI

* Column Types :

H H H F Q

* Associated datasets :

0 0 0 0 0

* Cell Dimensions : (obsolete - refer to dataset cell dimensions above)

  94.0711   99.3468 103.1345   90.0000   90.0000   90.0000

* Resolution Range :

   0.00020   0.46913   (71.550 -   1.460 A)

* Sort Order :

     1   2   3   0   0

* Space group = 'I 2 2 2' (number   23)

 ******   EPSILON ZONES - Reflection Classes and their multiplicity ******

 EPSILON Zone   1
 Reflections of type h00
 Multiplicity   4

 EPSILON Zone   2
 Reflections of type 0k0
 Multiplicity   4

 EPSILON Zone   3
 Reflections of type 00l
 Multiplicity   4

 EPSILON Zone   4
 Reflections of type hkl
 Multiplicity   2

```
 Grid of reflections initialized:
 H K L min   -66 -70 -72
 H K L max    66  70  72
 H K L inc   133 141 145
 ngrid      2719185

 lookup =           -1          -1          -1           0
 lsprgi = H                              K
 L                             FREE
***** COMPLETE keyword was not used.
*****   All Reflections binned into  20 segments
 *** labelled 0 through to  19 *****

 Number of symmetry operations in the composition point group: 24


 WRITTEN OUTPUT MTZ FILE
 Logical Name: HKLOUT   Filename: /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_8_mtz.tmp

 * Title:




 * Base dataset:

       0 HKL_base
         HKL_base
         HKL_base

 * Number of Datasets = 0

 * Dataset ID, project/crystal/dataset names, cell dimensions, wavelength:
```

* Number of Columns = 6

* Number of Reflections = 83816

* Missing value set to NaN in input mtz file

* Column Labels :

H K L FUNI SIGFUNI FreeR_flag

* Column Types :

H H H F Q I

* Associated datasets :

0 0 0 0 0 0

* Cell Dimensions : (obsolete - refer to dataset cell dimensions above)

  94.0711   99.3468 103.1345   90.0000   90.0000   90.0000

* Resolution Range :

   0.00020   0.46913   (71.550 -   1.460 A)

* Sort Order :

     1   2   3   0   0

* Space group = 'I 2 2 2' (number   23)

Number of reflections: 83816

Number for flagged reflections for each bin:

Reflection flag =	Number:		
0	4161	0	
1	4051	0	
2	4361	0	
3	4205	0	
4	4303	0	
5	4130	0	
6	4256	0	
7	4341	0	
8	4136	0	
9	4255	0	
10	4058	0	
11	4033	0	
12	4197	0	
13	4013	0	
14	4112	0	
15	4386	0	
16	4337	0	
17	4138	0	
18	4295	0	
19	4048	0	
Averages:	9.489	4190	0

<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->

FREERFLAG: Normal termination

Times: User: 0.4s System: 0.0s Elapsed: 0:00

</pre>

</html>

<!--SUMMARY_END--></FONT></B>

<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->

<html> <!-- CCP4 HTML LOGFILE -->

<hr>

<!--SUMMARY_END--></FONT></B>
<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->
<pre>

 ##
 ##
 ##
 ### CCP4 7.1.009: CAD   version 7.1.009 :   ##
 ##
 User: yoshihisasuzuki Run date: 25/10/2021 Run time: 11:52:18

 Please reference: Collaborative Computational Project, Number 4. 2011.
 "Overview of the CCP4 suite and current developments". Acta Cryst. D67, 235-242.
 as well as any specific reference in the program write-up.

<!--SUMMARY_END--></FONT></B>
 Data line--- LABI FILE 2 E1=FreeR_flag
 Data line--- LABI FILE 1 ALLIN
 Data line--- END
 No CTYP lines input for file: 1
 No CTYP lines input for file: 2
    Indices output even if all data items flagged "missing"
 Warning, NOT all LABOUT data lines given
 Warning, NOT all LABOUT data lines given

 OPENED INPUT MTZ FILE
 Logical   Name: HKLIN1   Filename:
/tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_5_mtz_New.tmp

 * Title:

 From Clipper CCP4MTZfile

* Base dataset:

0 HKL_base
HKL_base
HKL_base

* Number of Datasets = 1

* Dataset ID, project/crystal/dataset names, cell dimensions, wavelength:

1 New
New
New
94.0711 99.3468 103.1345 90.0000 90.0000 90.0000
0.89999

* Number of Columns = 18

* Number of Reflections = 80452

* Missing value set to NaN in input mtz file

* Column Labels :

H K L F_New SIGF_New DANO_New SIGDANO_New F_New(+) SIGF_New(+) F_New(-) SIGF_New(-)
ISYM_New IMEAN_New SIGIMEAN_New I_New(+) SIGI_New(+) I_New(-) SIGI_New(-)

* Column Types :

H H H F Q D Q G L G L Y J Q K M K M

* Associated datasets :

0 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

* Cell Dimensions : (obsolete - refer to dataset cell dimensions above)

94.0711 99.3468 103.1345 90.0000 90.0000 90.0000

* Resolution Range :

0.00059 0.46913 (41.156 - 1.460 A)

* Sort Order :

0 0 0 0 0

* Space group = 'I 2 2 2' (number 23)

(only pointgroup is fixed so far)

Reciprocal space symmetry:
Space group: "I 2 2 2" Point group: "PG222" Laue group: "mmm"
Reference asymmetric unit: "h>=0 and k>=0 and l>=0"
(change of basis may be applied)

Spacegroup 23 "I 2 2 2"
Original indices for reflection hkl with symmetry number ISYM

Bijvoet positive

ISYM	ISYM	ISYM	ISYM
ISYM 1 +h,+k,+l	3 +h,-k,-l	5 -h,+k,-l	7 -h,-k,+l

Bijvoet negative

ISYM	ISYM	ISYM	ISYM

```
 ISYM   2  -h,-k,-l        4  -h,+k,+l        6  +h,-k,+l        8  +h,+k,-l


 Chosen Asymmetric unit of reciprocal space:
 [mmm] hkl:h>=0, k>=0, l>=0


 ** "Missing" flag set in HKLIN1 to Nan:


 ** "Missing" entries LISTED as            -999.000
 Data line--- LABIN  E1=F_New  E2=SIGF_New  E3=DANO_New  E4=SIGDANO_New  E5=F_New(+)
E6=SIGF_New(+)      E7=F_New(-)      E8=SIGF_New(-)      E9=ISYM_New      E10=IMEAN_New
E11=SIGIMEAN_New  E12=I_New(+)  E13=SIGI_New(+)  E14=I_New(-)  E15=SIGI_New(-)


 After Processing File_Number:  1
 Number of columns so far    :  18
 Accumulated Out_Put_MTZ_labels are:
  E11=F_New  E21=SIGF_New  E31=DANO_New  E41=SIGDANO_New
  E51=F_New(+)  E61=SIGF_New(+)  E71=F_New(-)  E81=SIGF_New(-)
  E91=ISYM_New  E101=IMEAN_New  E111=SIGIMEAN_New  E121=I_New(+)
  E131=SIGI_New(+)  E141=I_New(-)  E151=SIGI_New(-)


 MTZOUT_LABELS are H K L and -
  F_New  SIGF_New  DANO_New  SIGDANO_New
  F_New(+)  SIGF_New(+)  F_New(-)  SIGF_New(-)
  ISYM_New  IMEAN_New  SIGIMEAN_New  I_New(+)
  SIGI_New(+)  I_New(-)  SIGI_New(-)

 OPENED INPUT MTZ FILE
 Logical Name: HKLIN2   Filename: /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_8_mtz.tmp
```

* Title:

* Base dataset:

0 HKL_base
HKL_base
HKL_base

* Number of Datasets = 0

* Dataset ID, project/crystal/dataset names, cell dimensions, wavelength:

* Number of Columns = 6

* Number of Reflections = 83816

* Missing value set to NaN in input mtz file

* Column Labels :

H K L FUNI SIGFUNI FreeR_flag

* Column Types :

H H H F Q I

* Associated datasets :

0 0 0 0 0 0

```
* Cell Dimensions : (obsolete - refer to dataset cell dimensions above)

  94.0711   99.3468  103.1345   90.0000   90.0000   90.0000

*  Resolution Range :

   0.00020    0.46913     (     71.550 -      1.460 A )

* Sort Order :

     1     2     3     0     0

* Space group = 'I 2 2 2' (number     23)

Data line--- LABIN  E1=FreeR_flag


After Processing File_Number:  2
Number of columns so far    :  19
Accumulated Out_Put_MTZ_labels are:
 E11=F_New  E21=SIGF_New  E31=DANO_New  E41=SIGDANO_New
 E51=F_New(+)  E61=SIGF_New(+)  E71=F_New(-)  E81=SIGF_New(-)
 E91=ISYM_New  E101=IMEAN_New  E111=SIGIMEAN_New  E121=I_New(+)
 E131=SIGI_New(+)  E141=I_New(-)  E151=SIGI_New(-)  E12=FreeR_flag



MTZOUT_LABELS are H K L and -
 F_New  SIGF_New  DANO_New  SIGDANO_New
 F_New(+)  SIGF_New(+)  F_New(-)  SIGF_New(-)
 ISYM_New  IMEAN_New  SIGIMEAN_New  I_New(+)
 SIGI_New(+)  I_New(-)  SIGI_New(-)  FreeR_flag
```

```
        3 sort keys, in columns    1   2   3


 Data line--- LABIN  E1=F_New  E2=SIGF_New  E3=DANO_New  E4=SIGDANO_New  E5=F_New(+)
E6=SIGF_New(+)      E7=F_New(-)      E8=SIGF_New(-)      E9=ISYM_New      E10=IMEAN_New
E11=SIGIMEAN_New  E12=I_New(+)  E13=SIGI_New(+)  E14=I_New(-)  E15=SIGI_New(-)

 OPENED INPUT MTZ FILE
 Logical            Name:            HKLIN1                                    Filename:
/tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_5_mtz_New.tmp

 * Title:

 From Clipper CCP4MTZfile

 * Base dataset:

        0 HKL_base
          HKL_base
          HKL_base

 * Number of Datasets = 1

 * Dataset ID, project/crystal/dataset names, cell dimensions, wavelength:

        1 New
          New
          New
             94.0711   99.3468  103.1345   90.0000   90.0000   90.0000
             0.89999
```

* Number of Columns = 18

* Number of Reflections = 80452

* Missing value set to NaN in input mtz file

* Column Labels :

H K L F_New SIGF_New DANO_New SIGDANO_New F_New(+) SIGF_New(+) F_New(-) SIGF_New(-) ISYM_New IMEAN_New SIGIMEAN_New I_New(+) SIGI_New(+) I_New(-) SIGI_New(-)

* Column Types :

H H H F Q D Q G L G L Y J Q K M K M

* Associated datasets :

0 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

* Cell Dimensions : (obsolete - refer to dataset cell dimensions above)

  94.0711   99.3468 103.1345   90.0000   90.0000   90.0000

* Resolution Range :

   0.00059   0.46913   (41.156 -   1.460 A)

* Sort Order :

     0   0   0   0   0

* Space group = 'I 2 2 2' (number   23)

(only pointgroup is fixed so far)

Column pairs- F+ F-: 8   10

Column pairs- F+ F-: 10   8

Column pairs - SIGs: 9   11

Column pairs - SIGs: 11   9

Column pairs - SIGs: 16   18

Column pairs - SIGs: 18   16

Column pairs - I+ I-: 15   17

Column pairs - I+ I-: 17   15

Reading from HKLIN mtz file_Number = :1
This file written with MTZLIB Version Number : MTZ:V1.1
File HKLIN1 contains a total of   18 Columns
and a total of   80452 Reflections

****** EPSILON ZONES - Reflection Classes and their multiplicity ******

EPSILON Zone 1
Reflections of type hOO
Multiplicity 4

EPSILON Zone 2
Reflections of type 0k0
Multiplicity 4

EPSILON Zone 3
Reflections of type 00l
Multiplicity 4

EPSILON Zone 4
Reflections of type hkl
Multiplicity 2

****** CENTRIC ZONES ******

CENTRIC Zone 1
Reflections of type 0kl

CENTRIC Zone 2
Reflections of type h0l

CENTRIC Zone 3
Reflections of type hk0

For file HKLIN1
Total Number of HKL read = 80452

```
Total Number of HKL systematic absent            =          0
Total Number of HKL reject for resolution limits =          0
Total Number of HKL passed to sort for this file =      85122
Data line--- LABIN  E1=FreeR_flag

OPENED INPUT MTZ FILE
Logical Name: HKLIN2   Filename: /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_8_mtz.tmp

* Title:



* Base dataset:

       0 HKL_base
         HKL_base
         HKL_base

* Number of Datasets = 0

* Dataset ID, project/crystal/dataset names, cell dimensions, wavelength:


* Number of Columns = 6

* Number of Reflections = 83816

* Missing value set to NaN in input mtz file

* Column Labels :

H K L FUNI SIGFUNI FreeR_flag
```

* Column Types :

H H H F Q I

* Associated datasets :

0 0 0 0 0 0

* Cell Dimensions : (obsolete - refer to dataset cell dimensions above)

  94.0711   99.3468 103.1345   90.0000   90.0000   90.0000

* Resolution Range :

   0.00020   0.46913   (71.550 -   1.460 A)

* Sort Order :

     1   2   3   0   0

* Space group = 'I 2 2 2' (number   23)

Reading from HKLIN mtz file_Number = :2
This file written with MTZLIB Version Number : MTZ:V1.1
File HKLIN2 contains a total of   6 Columns
and a total of   83816 Reflections

For file HKLIN2
Total Number of HKL read   =   83816
Total Number of HKL systematic absent   =   0
Total Number of HKL reject for resolution limits =   0

```
 Total Number of HKL passed to sort for this file =      89409


 Total number read for all files    =     164268
 Total passed to sort for all files =     174531
 Total number systematic absent     =          0
 Total number rejected outside resol=          0


 Number of columns per file:
 File_Number =    1 Number_Columns_Selected =    15

 File_Number =    2 Number_Columns_Selected =     1

 Data line--- LABOUT E11=F_New E21=SIGF_New E31=DANO_New E41=SIGDANO_New E51=F_New(+)
E61=SIGF_New(+)     E71=F_New(-)     E81=SIGF_New(-)     E91=ISYM_New     E101=IMEAN_New
E111=SIGIMEAN_New   E121=I_New(+)    E131=SIGI_New(+)    E141=I_New(-)    E151=SIGI_New(-)
E12=FreeR_flag

 WRITTEN OUTPUT MTZ FILE
 Logical Name: HKLOUT   Filename: /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_9_mtz.tmp

 * Title:

 From Clipper CCP4MTZfile

 * Base dataset:

        0 HKL_base
          HKL_base
          HKL_base

 * Number of Datasets = 1
```

* Dataset ID, project/crystal/dataset names, cell dimensions, wavelength:

1 New
New
New
94.0711 99.3468 103.1345 90.0000 90.0000 90.0000
0.89999

* Number of Columns = 19

* Number of Reflections = 83816

* Missing value set to NaN in input mtz file

* Column Labels :

H K L FreeR_flag F_New SIGF_New DANO_New SIGDANO_New F_New(+) SIGF_New(+) F_New(-) SIGF_New(-) ISYM_New IMEAN_New SIGIMEAN_New I_New(+) SIGI_New(+) I_New(-) SIGI_New(-)

* Column Types :

H H H I F Q D Q G L G L Y J Q K M K M

* Associated datasets :

0 0 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

* Cell Dimensions : (obsolete - refer to dataset cell dimensions above)

94.0711 99.3468 103.1345 90.0000 90.0000 90.0000

* Resolution Range :

```
   0.00020    0.46913     (     71.550 -      1.460 A )

 * Sort Order :

      1     2     3     0     0

 * Space group = 'I 2 2 2' (number     23)

  (only pointgroup is fixed so far)



 Total number from Sorting Routine =     174531
 Final Total of Unique records to HKLOUT =      83816
 Final Total of Missing records to HKLOUT =          0
<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->
 CAD:   *** Normal Termination of CAD ***
Times: User:       0.6s System:    0.1s Elapsed:     0:01
</pre>
</html>
<!--SUMMARY_END--></FONT></B>
<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->
<html> <!-- CCP4 HTML LOGFILE -->
<hr>
<!--SUMMARY_END--></FONT></B>
<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->
<pre>

 ################################################################
 ################################################################
 ################################################################
 ### CCP4 7.1.009: FREERFLAG            version 2.2 : 26/03/20##
```

```
 ##################################################################
 User: yoshihisasuzuki  Run date: 25/10/2021 Run time: 11:52:19


 Please reference: Collaborative Computational Project, Number 4. 2011.
 "Overview of the CCP4 suite and current developments". Acta Cryst. D67, 235-242.
 as well as any specific reference in the program write-up.

<!--SUMMARY_END--></FONT></B>
 Data line--- COMPLETE FREE=FreeR_flag
 Data line--- END

 OPENED INPUT MTZ FILE
 Logical Name: HKLIN   Filename: /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_9_mtz.tmp

 * Title:

 From Clipper CCP4MTZfile

 * Base dataset:

        0 HKL_base
          HKL_base
          HKL_base

 * Number of Datasets = 1

 * Dataset ID, project/crystal/dataset names, cell dimensions, wavelength:

        1 New
          New
          New
             94.0711   99.3468  103.1345   90.0000   90.0000   90.0000
```

0.89999

* Number of Columns = 19

* Number of Reflections = 83816

* Missing value set to NaN in input mtz file

* Column Labels :

H K L FreeR_flag F_New SIGF_New DANO_New SIGDANO_New F_New(+) SIGF_New(+) F_New(-) SIGF_New(-) ISYM_New IMEAN_New SIGIMEAN_New I_New(+) SIGI_New(+) I_New(-) SIGI_New(-)

* Column Types :

H H H I F Q D Q G L G L Y J Q K M K M

* Associated datasets :

0 0 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

* Cell Dimensions : (obsolete - refer to dataset cell dimensions above)

94.0711 99.3468 103.1345 90.0000 90.0000 90.0000

* Resolution Range :

0.00020 0.46913 (71.550 - 1.460 A)

* Sort Order :

1 2 3 0 0

```
 * Space group = 'I 2 2 2' (number     23)

  (only pointgroup is fixed so far)


  ******   EPSILON ZONES -  Reflection Classes and their multiplicity ******

  EPSILON Zone   1
  Reflections of type  hOO
  Multiplicity   4

  EPSILON Zone   2
  Reflections of type  0k0
  Multiplicity   4

  EPSILON Zone   3
  Reflections of type  00l
  Multiplicity   4

  EPSILON Zone   4
  Reflections of type  hkl
  Multiplicity   2

 Grid of reflections initialized:
 H K L min   -66 -70 -72
 H K L max    66  70  72
 H K L inc   133 141 145
 ngrid      2719185

***** Twin laws are not used but reflections that are symmetry equivalent in the crystal
point group acquire the same flag.
 lookup =            1           2           3           4
 lsprgi = H                              K
```

```
 L                              FREE
***** COMPLETE keyword was used.
The number of missing flags =          0
*****   All Reflections binned into  20 segments
 *** labelled 0 through to  19 *****

 Number of symmetry operations in the composition point group:  4


 WRITTEN OUTPUT MTZ FILE
 Logical            Name:            HKLOUT                                    Filename:
/Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/collection_pointless1_sca
led1.mtz

 * Title:

 From Clipper CCP4MTZfile

 * Base dataset:

        0 HKL_base
          HKL_base
          HKL_base

 * Number of Datasets = 1

 * Dataset ID, project/crystal/dataset names, cell dimensions, wavelength:

        1 New
          New
          New
             94.0711   99.3468  103.1345   90.0000   90.0000   90.0000
             0.89999
```

* Number of Columns = 19

* Number of Reflections = 83816

* Missing value set to NaN in input mtz file

* Column Labels :

H K L FreeR_flag F_New SIGF_New DANO_New SIGDANO_New F_New(+) SIGF_New(+) F_New(-) SIGF_New(-) ISYM_New IMEAN_New SIGIMEAN_New I_New(+) SIGI_New(+) I_New(-) SIGI_New(-)

* Column Types :

H H H I F Q D Q G L G L Y J Q K M K M

* Associated datasets :

0 0 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

* Cell Dimensions : (obsolete - refer to dataset cell dimensions above)

94.0711 99.3468 103.1345 90.0000 90.0000 90.0000

* Resolution Range :

0.00020 0.46913 (71.550 - 1.460 A)

* Sort Order :

1 2 3 0 0

* Space group = 'I 2 2 2' (number 23)

(only pointgroup is fixed so far)

Number of reflections: 83816

Number for flagged reflections for each bin:

Reflection flag =	Number:		
	0	4159	4159
	1	4074	4074
	2	4199	4199
	3	4113	4113
	4	4199	4199
	5	4215	4215
	6	4240	4240
	7	4184	4184
	8	4141	4141
	9	4174	4174
	10	4219	4219
	11	4235	4235
	12	4132	4132
	13	4141	4141
	14	4179	4179
	15	4244	4244
	16	4375	4375
	17	4243	4243
	18	4169	4169
	19	4181	4181
Averages:	9.534	4190	4190

<B><FONT COLOR="#FF0000"><!--SUMMARY_BEGIN-->

FREERFLAG: Normal termination

Times: User: 0.5s System: 0.1s Elapsed: 0:01

</pre>

</html>

<!--SUMMARY_END--></FONT></B>

#CCP4I TERMINATION STATUS 1

#CCP4I TERMINATION TIME 25 Oct 2021 11:52:23

#CCP4I TERMINATION OUTPUT_FILES /tmp/yoshihisasuzuki/merge_roomtemp_GI_pf_7_2_mtz.tmp merge_roomtemp_GI_pf /Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7.scales merge_roomtemp_GI_pf /Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_rogues.log merge_roomtemp_GI_pf /Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_normplot.xmgr merge_roomtemp_GI_pf /Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_anomplot.xmgr merge_roomtemp_GI_pf /Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_rogueplot.xmgr merge_roomtemp_GI_pf /Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_correlplot.xmgr merge_roomtemp_GI_pf /Users/yoshihisasuzuki/Documents/JCCG50/merge_roomtemp_GI_pf/merge_roomtemp_GI_pf_7_aimless_pipe.xml merge_roomtemp_GI_pf

#CCP4I MESSAGE Task completed successfully