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

INPUT PARAMETER VALUES
----------------------
NAME_TEMPLATE_OF_DATA_FRAMES=../img/prefix_1_?????.img
STARTING_ANGLE=        0.0000     STARTING_FRAME=       1
NX=  3072  NY=  3072    QX=  0.102592  QY=  0.102592
DIRECTION_OF_DETECTOR_X-AXIS=   1.00000   0.00000   0.00000
DIRECTION_OF_DETECTOR_Y-AXIS=   0.00000   1.00000   0.00000
DETECTOR_DISTANCE=   141.025
ORGX=   1539.81  ORGY=   1534.30
NUMBER OF DETECTOR SEGMENTS   1
SEGMENT=    1 3072    1 3072  ! x1,x2,y1,y2 (pixel units)
   SEGMENT_ORGX=      0.00   SEGMENT_ORGY=      0.00
   SEGMENT_DISTANCE=     0.00
   DIRECTION_OF_SEGMENT_X-AXIS=  1.000000  0.000000  0.000000
   DIRECTION_OF_SEGMENT_Y-AXIS=  0.000000  1.000000  0.000000
X-RAY_WAVELENGTH=       0.979263
INCIDENT_BEAM_DIRECTION=  0.000000  0.000000  1.000000
ROTATION_AXIS= -1.000000  0.000000  0.000000
OSCILLATION_RANGE=    1.0000
INDEX_MAGNITUDE=   8    INDEX_ERROR=   0.050    INDEX_QUALITY=  0.80
SEPMIN=  6.00    CLUSTER_RADIUS=     3
MAXIMUM_ERROR_OF_SPOT_POSITION=   3.0
MAXIMUM_ERROR_OF_SPINDLE_POSITION=   2.0
MINIMUM_FRACTION_OF_INDEXED_SPOTS=  0.50
TRUSTED_REGION=  0.00  1.41
INCLUDE_RESOLUTION_RANGE=     50.000     0.000
SPACE GROUP AND CELL PARAMETERS ARE UNKNOWN


AUTOINDEXING IS BASED ON  36949 OUT OF   36949 SPOTS
WITHIN THE ALLOWED RESOLUTION RANGES OF THE FOLLOWING DATA IMAGES:
SPOT_RANGE=       1      10
T_RANGE=       91     100

***** DETERMINATION OF THE RECIPROCAL LATTICE BASIS ******
NUMBER OF DIFFERENCE VECTOR CLUSTERS USED                      205
MAXIMUM RADIUS OF DIFFERENCE VECTOR CLUSTERS (pixels)   3
MINIMUM DISTANCE BETWEEN DIFFRACTION SPOTS (pixel)    6.0
MINIMUM ALLOWED DISTANCE BETWEEN REC. LATTICE POINTS   0.4457E-02
OBSERVED BASIS CELL VOLUME                             0.2345E+06
DIMENSION OF SPACE SPANNED BY DIFFERENCE VECTOR CLUSTERS   3

  #  COORDINATES OF REC. BASIS VECTOR    LENGTH   1/LENGTH

   1  -0.0060535 0.0029941 0.0106114  0.0125782      79.50
   2   0.0103576-0.0026329 0.0066553  0.0125899      79.43
   3   0.0081757 0.0255312-0.0025772  0.0269319      37.13

CLUSTER COORDINATES AND INDICES WITH RESPECT TO REC. LATTICE BASIS VECTORS

  #  COORDINATES OF VECTOR CLUSTER   FREQUENCY       CLUSTER INDICES
   1  0.0164096-0.0055717-0.0038264     1491.      -0.99      1.00      0.00
   2  0.0103101-0.0025191 0.0066429     1452.       0.00      0.99      0.00
   3  0.0267572-0.0081505 0.0026948     1311.      -1.00      2.00      0.00
   4  0.0060412-0.0028957-0.0104856     1300.      -0.99      0.00      0.00
   5  0.0206791-0.0051483 0.0131957     1128.      -0.00      1.99      0.00
   6 -0.0043108-0.0002740-0.0170907     1124.      -0.99     -0.99      0.00
   7 -0.0617249-0.0089453-0.0028257     1068.       2.00     -4.00     -1.00
   8  0.0328498-0.0111800-0.0077914     1059.      -1.99      2.01      0.00
   9 -0.0513763-0.0115198 0.0037868     1055.       2.00     -3.01     -1.00
  10 -0.0947002 0.0019970 0.0049600     1048.       3.99     -6.01     -1.01
  11  0.0431621-0.0138263-0.0012921     1032.      -2.00      3.00      0.00
  12 -0.0677747-0.0059707 0.0077851     1028.       3.00     -4.00     -1.00
  13  0.0781104 0.0033508-0.0012474     1005.      -3.01      4.99      1.00
  14 -0.0349389-0.0171510-0.0001329      987.       1.00     -2.00     -1.00
  15  0.0720762 0.0063719 0.0094054      964.      -2.01      5.00      1.00
  16  0.0371447-0.0107698 0.0092589      962.      -1.00      3.00      0.00
  17 -0.0453072-0.0145662-0.0067014      944.       1.01     -3.00     -1.00
  18 -0.0884807-0.0007752-0.0054801      932.       3.00     -6.00     -1.00
  19  0.0534149-0.0164762 0.0051452      926.      -2.01      3.98      0.00
  20 -0.0841609-0.0004081 0.0116037      911.       3.99     -5.00     -1.00
  21 -0.0146220 0.0022420-0.0238297      902.      -1.00     -1.99     -0.00
  22 -0.0185128-0.0228442-0.0039960      894.       0.01     -1.00     -1.00
  23 -0.0224970 0.0085508 0.0144619      879.       1.99     -1.01     -0.00
  24 -0.0574582-0.0085623 0.0144022      852.       3.00     -3.01     -1.00
  25 -0.0410754-0.0140936 0.0103127      846.       1.99     -2.02     -0.99
  26  0.1048934-0.0048649 0.0015530      837.      -4.00      7.00      1.00
```

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  27 -0.0736351-0.0031476 0.0184373      832.      3.99     -3.98     -1.00
  28  0.0310510-0.0077250 0.0199366      816.      0.00      2.99      0.01
  29 -0.0557168-0.0119177-0.0132875      807.      1.01     -4.00     -1.00
  30 -0.0081816-0.0254058 0.0023566      806.     -0.01     -0.01     -0.99
  31  0.0988368-0.0018407 0.0120907      799.     -3.00      7.00      1.00
  32  0.0246107 0.0197779-0.0063981      787.     -0.99      1.01      1.00
  33 -0.0595736 0.0194623 0.0051480      782.      2.99     -4.00     -0.00
  34 -0.0121204 0.0058288 0.0211365      780.      1.99     -0.00     -0.01
  35 -0.0824745-0.0037582-0.0160198      765.      2.01     -6.00     -1.00
  36 -0.0082209 0.0311374 0.0014773      763.      1.01     -0.99      1.00
  37  0.0017739-0.0032275-0.0278287      740.     -2.00     -1.00      0.00
  38 -0.0492783 0.0168860 0.0116526      736.      2.99     -3.01      0.00
  39 -0.1109378 0.0078651 0.0089833      734.      5.00     -7.00     -1.00
  40 -0.1005864 0.0052431 0.0155875      719.      4.99     -6.00     -1.00
  41  0.1152766-0.0074195 0.0081866      717.     -4.00      8.00      1.00
  42  0.0289093 0.0201832 0.0106097      714.     -0.01      2.00      1.00
  43  0.1212979-0.0104601-0.0023440      712.     -5.00      8.00      1.00
  44  0.0475049-0.0132910 0.0159217      700.     -1.00      3.99      0.01
  45 -0.0249825 0.0049113-0.0305263      698.     -1.00     -3.00      0.00
  46  0.0021086 0.0285278 0.0078908      696.      0.99     -0.01      1.00
  47 -0.0699514 0.0221016-0.0014693      677.      3.00     -5.00     -0.00
  48 -0.0471158-0.0110986 0.0211044      675.      3.01     -2.01     -0.99
  49 -0.0634810-0.0056652 0.0250924      666.      4.00     -3.00     -1.00
  50  0.0660822 0.0093547 0.0199294      664.     -1.01      5.00      1.00
  51 -0.0086614-0.0005403-0.0345891      657.     -2.00     -2.01      0.01
  52 -0.0246014 0.0368679 0.0053151      640.      2.00     -2.00      1.00
  53  0.1092208-0.0043825 0.0187280      639.     -3.01      8.00      1.01
  54 -0.0902356 0.0025273 0.0222715      626.      4.99     -5.00     -1.00
  55  0.1316727-0.0130681 0.0042857      618.     -5.00      9.00      1.00
  56 -0.0928241-0.0011984-0.0227014      613.      2.01     -7.00     -1.00
  57  0.0639490-0.0189829 0.0118974      611.     -2.01      4.99      0.01
  58  0.0414242-0.0103425 0.0266129      609.      0.00      4.00      0.01
  59 -0.1398567-0.0123285-0.0016713      608.      5.00     -9.00     -2.00
  60 -0.1294898-0.0149223 0.0050069      607.      5.00     -8.00     -2.00

 PARAMETERS OF THE REDUCED CELL (ANGSTROEM & DEGREES)
     37.13     79.43     79.50     89.99     89.93     89.95

   #  COORDINATES OF REC. BASIS VECTOR    REDUCED CELL INDICES

    1  -0.0060535 0.0029941 0.0106114    -0.00    0.00    1.00
    2   0.0103576-0.0026329 0.0066553     0.00   -1.00    0.00
    3   0.0081757 0.0255312-0.0025772     1.00   -0.00   -0.00

 ***** RESULTS FROM LOCAL INDEXING OF   3000 OBSERVED SPOTS *****

 MAXIMUM MAGNITUDE OF INDEX DIFFERENCES ALLOWED    8
 MAXIMUM ALLOWED DEVIATION FROM INTEGERAL INDICES     0.050
 MIMINUM QUALITY OF INDICES FOR EACH SPOT IN A SUBTREE    0.80
 QUALITY OF INDICES REQUIRED TO INCLUDE SECOND SUBTREE    0.00
 NUMBER OF SUBTREES    788

 SUBTREE    POPULATION

      1         1056
      2         1003
      3           23
      4           16
      5            6
      6            5
      7            4
      8            4
      9            4
     10            3

 NUMBER OF ACCEPTED SPOTS FROM LARGEST SUBTREE  1056

 ***** SELECTION OF THE INDEX ORIGIN OF THE REFLECTIONS *****
 The origin of the reflection indices determined so far is
 0,0,0 by default which is usually correct. In certain critical
 cases it may happen that this automatic choice is wrong which
 leads to misindexing of the reflections by a constant offset.
 You may replace the default by specifying INDEX_ORIGIN= h k l
 in the input file "XDS.INP" and rerun the IDXREF step.
 Below you find a list of possible alternatives together with a
 measure of their likelihood.
 QUALITY  small values mean a high likelihood for this offset
 DELTA    is the angle between given and refined beam direction
 XD,YD    computed direct beam position (pixels) on detector
          given beam position (pixel):  1539.81  1534.30
```

```
X,Y,Z    computed coordinates of the direct beam wave vector
DH,DK,DL mean absolute difference between observed and
         fitted indices

 INDEX_   QUALITY  DELTA    XD       YD       X       Y       Z       DH      DK      DL
 ORIGIN

  0  0  0      2.2    0.3   1536.5   1540.8 -0.0025  0.0048  1.0212    0.01    0.04    0.05
     1  1     15.4    0.8   1558.6   1532.8  0.0140 -0.0011  1.0211    0.02    0.15    0.21

SELECTED:     INDEX_ORIGIN=  0  0  0


***** REFINED SOLUTION BASED ON INDEXED REFLECTIONS IN SUBTREE # 1 *****

REFINED VALUES OF DIFFRACTION PARAMETERS DERIVED FROM   1054 INDEXED SPOTS
REFINED PARAMETERS:   DISTANCE AXIS BEAM CELL ORIENTATION
STANDARD DEVIATION OF SPOT    POSITION (PIXELS)     1.01
STANDARD DEVIATION OF SPINDLE POSITION (DEGREES)    2.00
SPACE GROUP NUMBER      1
UNIT CELL PARAMETERS     36.318    77.847    78.372  90.265  90.125  89.970
REC. CELL PARAMETERS   0.027535  0.012846  0.012760  89.735  89.875  90.030
COORDINATES OF UNIT CELL A-AXIS    11.074    34.432    -3.280
COORDINATES OF UNIT CELL B-AXIS   -63.824    16.631   -41.352
COORDINATES OF UNIT CELL C-AXIS   -37.713    18.257    66.232
CRYSTAL MOSAICITY (DEGREES)     0.200
LAB COORDINATES OF ROTATION AXIS -0.999580  0.024833  0.014907
DIRECT BEAM COORDINATES (REC. ANGSTROEM)  -0.000106 -0.004401  1.021167
DETECTOR COORDINATES (PIXELS) OF DIRECT BEAM    1536.47   1541.15
DETECTOR ORIGIN (PIXELS) AT                     1536.61   1546.94
CRYSTAL TO DETECTOR DISTANCE (mm)       137.90
LAB COORDINATES OF DETECTOR X-AXIS  1.000000  0.000000  0.000000
LAB COORDINATES OF DETECTOR Y-AXIS  0.000000  1.000000  0.000000


***** INDEXING OF OBSERVED SPOTS IN SPACE GROUP #   1 *****
  30830 OUT OF   36949 SPOTS INDEXED.
      0 REJECTED REFLECTIONS (REASON: OVERLAP)
   6119 REJECTED REFLECTIONS (REASON: TOO FAR FROM IDEAL POSITION)
EXPECTED ERROR IN SPINDLE  POSITION     0.195 DEGREES
EXPECTED ERROR IN DETECTOR POSITION      0.46 PIXELS


***** DIFFRACTION PARAMETERS USED AT START OF INTEGRATION *****

REFINED VALUES OF DIFFRACTION PARAMETERS DERIVED FROM  30830 INDEXED SPOTS
REFINED PARAMETERS:   DISTANCE AXIS BEAM CELL ORIENTATION
STANDARD DEVIATION OF SPOT    POSITION (PIXELS)     0.44
STANDARD DEVIATION OF SPINDLE POSITION (DEGREES)    0.19
SPACE GROUP NUMBER      1
UNIT CELL PARAMETERS     36.908    78.959    78.947  89.976  89.958  90.002
REC. CELL PARAMETERS   0.027094  0.012665  0.012667  90.024  90.042  89.998
COORDINATES OF UNIT CELL A-AXIS    11.199    35.011    -3.316
COORDINATES OF UNIT CELL B-AXIS   -64.914    16.814   -41.689
COORDINATES OF UNIT CELL C-AXIS   -38.039    18.541    66.647
CRYSTAL MOSAICITY (DEGREES)     0.200
LAB COORDINATES OF ROTATION AXIS -0.999999  0.000942  0.000546
DIRECT BEAM COORDINATES (REC. ANGSTROEM)  -0.002920 -0.003140  1.021167
DETECTOR COORDINATES (PIXELS) OF DIRECT BEAM    1536.02   1541.02
DETECTOR ORIGIN (PIXELS) AT                     1539.93   1545.23
CRYSTAL TO DETECTOR DISTANCE (mm)       140.31
LAB COORDINATES OF DETECTOR X-AXIS  1.000000  0.000000  0.000000
LAB COORDINATES OF DETECTOR Y-AXIS  0.000000  1.000000  0.000000


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

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

A lattice character is marked "*" to indicate a lattice consistent with the
observed locations of the diffraction spots. These marked lattices must have
low values for the QUALITY OF FIT and their implicated UNIT CELL CONSTANTS
should not violate the ideal values by more than
MAXIMUM_ALLOWED_CELL_AXIS_RELATIVE_ERROR=  0.03
MAXIMUM_ALLOWED_CELL_ANGLE_ERROR=           3.0 (Degrees)

 LATTICE-  BRAVAIS-   QUALITY  UNIT CELL CONSTANTS (ANGSTROEM & DEGREES)
```

	CHARACTER	LATTICE	OF FIT	a	b	c	alpha	beta	gamma
*	44	aP	0.0	36.9	78.9	79.0	90.0	90.0	90.0
*	31	aP	0.0	36.9	78.9	79.0	90.0	90.0	90.0
*	35	mP	0.8	78.9	36.9	79.0	90.0	90.0	90.0
*	34	mP	1.0	36.9	79.0	78.9	90.0	90.0	90.0
*	25	mC	1.5	111.6	111.7	36.9	90.0	90.0	90.0
*	23	oC	1.5	111.6	111.7	36.9	90.0	90.0	90.0
*	20	mC	1.5	111.7	111.6	36.9	90.0	90.0	90.0
*	33	mP	1.7	36.9	79.0	78.9	90.0	90.0	90.0
*	32	oP	1.8	36.9	78.9	79.0	90.0	90.0	90.0
*	21	tP	2.5	78.9	79.0	36.9	90.0	90.0	90.0
	39	mC	249.2	162.1	36.9	79.0	90.0	90.0	76.9
	37	mC	249.9	162.1	36.9	79.0	90.0	90.0	76.9
	38	oC	250.2	36.9	162.1	79.0	90.0	90.0	103.1
	29	mC	250.2	36.9	162.1	79.0	90.0	90.0	76.9
	28	mC	250.6	36.9	162.2	78.9	90.0	90.0	76.8
	36	oC	250.9	36.9	162.1	79.0	90.0	90.0	103.1
	27	mC	499.3	162.1	36.9	111.6	90.0	133.5	76.9
	19	oI	500.0	36.9	111.6	117.6	90.0	71.7	90.0
	26	oF	623.3	36.9	162.1	162.2	87.0	103.2	103.1
	18	tI	624.0	111.6	117.6	36.9	71.7	90.0	90.0
	1	cF	999.0	117.6	117.6	117.6	95.7	95.6	143.4
	2	hR	999.0	87.1	87.2	117.6	118.4	61.6	100.3
	3	cP	999.0	36.9	78.9	79.0	90.0	90.0	90.0
	5	cI	999.0	87.2	87.1	111.6	50.2	50.2	79.7
	4	hR	999.0	87.2	87.2	117.6	118.4	61.6	100.3
	6	tI	999.0	111.6	87.2	87.1	79.7	50.2	50.2
	7	tI	999.0	87.2	87.1	111.6	50.2	50.2	79.7
	8	oI	999.0	87.1	87.2	111.6	50.2	50.2	79.7
	9	hR	999.0	36.9	87.1	252.4	102.8	98.4	115.0
	10	mC	999.0	87.2	87.1	79.0	90.0	90.0	129.9
	11	tP	999.0	36.9	78.9	79.0	90.0	90.0	90.0
	12	hP	999.0	36.9	78.9	79.0	90.0	90.0	90.0
	13	oC	999.0	87.1	87.2	79.0	90.0	90.0	50.1
	15	tI	999.0	36.9	79.0	180.3	64.1	78.2	90.0
	16	oF	999.0	87.2	87.2	180.3	108.1	118.9	50.1
	14	mC	999.0	87.1	87.2	79.0	90.0	90.0	50.1
	17	mC	999.0	87.2	87.1	87.2	79.7	100.4	50.1
	22	hP	999.0	78.9	79.0	36.9	90.0	90.0	90.0
	24	hR	999.0	180.3	111.7	36.9	90.0	78.2	108.0
	30	mC	999.0	78.9	176.5	36.9	90.0	90.0	63.5
	40	oC	999.0	78.9	176.5	36.9	90.0	90.0	116.5
	42	oI	999.0	36.9	79.0	180.3	115.9	101.8	90.0
	41	mC	999.0	176.5	78.9	36.9	90.0	90.0	63.5
	43	mI	999.0	87.1	180.3	78.9	115.9	154.9	61.1

For protein crystals the possible space group numbers corresponding to each Bravais-type are given below for your convenience. Note, that reflection integration is based only on orientation and metric of the lattice. It does not require knowledge of the correct space group! Thus, if no such information is provided by the user in XDS.INP, reflections are integrated assuming a triclinic reduced cell lattice; the space group is assigned automatically or by the user in the last step (CORRECT) when integrated intensities are available.

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

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

[197,I23] [199,I2(1)3] [211,I432] [214,I4(1)32]

Maximum oscillation range to prevent angular overlap at high resolution limit
assuming zero (!) mosaicity.

Maximum oscillation range (degrees)	High resolution limit (Angstrom)
3.31	4.00
2.49	3.00
1.66	2.00
0.83	1.00

cpu time used 15.5 sec
elapsed wall-clock time 3.4 sec