PLATON ckf file

```
PLATON/checkCIF FCF Validation Document
================================================================================
================================================================================
PLATON/ASYM-(Version   60124)-[Mode=2] FCF-File Validation for:i
================================================================================
For Documentation: http://http://www.platonsoft.nl/FCF-VALIDATION.pdf

Section 1
================================================================================
General Data
================================================================================
Crystal Data From: platon.cif
Fo/Fc   Data From: platon.fcf FCF-TYPE=LIST4
Space Group      : P-1
Wavelength (Ang) :   0.71073
Unit Cell (CIF)  :    5.6690  12.3300  14.1339   91.644   96.314   92.400
SHELX WGHT Pars. :    0.0456   2.2153   0.0000   0.0000   0.0000   0.3333

Section 2
================================================================================
Reflections with abs((I(obs) - I(calc)) / SigW(I)) > 3.0     [I(calc) from FCF]
================================================================================
   Nr   H   K   L  Theta     I(obs)    I(calc) Sigma(I)   Ratio  SigW(I) RatioW
--------------------------------------------------------------------------------
    1   3   3   0  12.23    4771.16    3973.00    71.05   11.23   227.61   3.51
    2  -1   7   0  12.06     592.72     453.35    21.86    6.38    45.88   3.04
    3  -1  10   0  17.02    4735.62    3777.57   156.22    6.13   261.50   3.66
    4  -2  12   0  21.30     196.10      97.94    24.57    4.00    30.47   3.22
    5   2  -9   1  16.57     541.27     261.90    24.18   11.55    40.41   6.91
    6   0  -6   1  10.03    7074.75    5950.28   186.00    6.05   363.04   3.10
    7   2  -1   1   7.66    3575.69    4836.84   106.52  -11.84   248.37  -5.08
    8   2   0   1   7.56     106.88     326.42    10.82  -20.29    28.49  -7.71
    9  -4   2   1  14.78      50.34       9.20    10.55    3.90    12.77   3.22
   10  -1   5   1   9.01    8513.52    6883.85   148.19   11.00   391.30   4.16
   11   3   6   1  15.44    3553.57    2809.96   101.16    7.35   190.92   3.89
   12   2  -6   2  12.57    3075.56    2494.62    58.28    9.97   156.14   3.72
   13   2   2   2   8.93     132.40     285.24    13.10  -11.67    28.37  -5.39
   14   0   6   2  10.49     186.54     115.35     9.36    7.61    20.88   3.41
   15   3 -13   3  24.90     194.47      95.28    26.49    3.74    31.94   3.11
   16   2 -11   3  20.21    2603.85    2020.27   126.46    4.61   176.35   3.31
   17  -1  -6   3  11.36    9834.11    8307.27   153.04    9.98   452.30   3.38
   18   0  -6   3  10.76      72.32      28.21    10.45    4.22    14.43   3.06
   19   4  -6   3  18.33     191.07     402.34    24.05   -8.78    39.28  -5.38
   20  -2  -4   3  10.57    6666.73    5597.60    82.89   12.90   306.22   3.49
   21   3  -2   4  13.23    1022.33    1724.13    45.41  -15.45    99.90  -7.02
   22   3  -1   4  12.99      17.47     214.80    20.74   -9.51    28.40  -6.95
   23   1   2   4   8.07   10016.64    8311.85   195.35    8.73   470.96   3.62
   24   0   4   4   8.98    8709.94    7325.21    87.37   15.85   388.54   3.56
   25   4   5   4  18.89    2239.30    1624.43    67.54    9.10   124.79   4.93
   26  -1   1   5   7.95     662.72    1258.09    17.94  -33.19    70.74  -8.42
   27   3   1   5  14.03      84.30     240.93    11.71  -13.38    25.08  -6.24
   28   3 -12   6  24.79    1148.75     773.86    62.22    6.03    86.85   4.32
   29   2 -11   6  21.74     518.69     872.92    42.93   -8.25    68.56  -5.17
   30   1  -7   6  14.98     112.80      27.76    18.21    4.67    21.50   3.95
   31   3  -2   6  15.01      76.06      29.12    10.76    4.36    14.80   3.17
   32  -6  -6   7  26.12      26.05      97.88    16.52   -4.35    21.17  -3.39
   33   5  -4   7  22.96     101.55     200.02    23.23   -4.24    31.12  -3.16
   34   4  -2   7  19.04      -6.08     100.62     9.91  -10.77    16.01  -6.67
   35   2   1   7  13.41    3849.96    3192.61   115.82    5.68   212.55   3.09
   36   0   0   8  11.68     225.66     683.82    15.10  -30.34    44.62 -10.27
   37   4   0   8  19.93      22.17     124.44    11.31   -9.04    18.58  -5.51
   38   3 -12   9  27.00      38.54     211.15    22.29   -7.74    29.77  -5.80
   39   4  -5   9  22.28     538.44     371.57    40.97    4.07    54.81   3.04
   40  -1  -4   9  14.76     497.28     264.36    23.52    9.90    39.42   5.91
   41   3  -3   9  18.63   12667.89   10009.13   332.99    7.98   617.95   4.30
   42   4   3   9  21.91     168.79     321.39    23.14   -6.59    35.87  -4.25
   43  -1  -1  10  14.77      91.67      35.68    12.57    4.45    16.87   3.32
   44   1  -1  11  17.01     611.21     806.90    25.81   -7.58    58.76  -3.33
   45   5  -1  11  26.29     -16.47      44.04    17.44   -3.47    19.26  -3.14
   46  -5   0  11  23.39    3462.13    2836.86   105.98    5.90   193.03   3.24
   47  -6   2  11  26.56    1197.97     912.75    64.56    4.42    92.26   3.09
   48  -1   2  11  16.61    2265.61    1788.87    49.15    9.70   120.91   3.94
   49   4  -4  12  25.21    2843.95    2012.91    96.16    8.64   158.82   5.23
   50  -1  -3  12  18.26    1191.80     934.18    38.43    6.70    76.81   3.35
   51  -2  -2  12  18.67     482.45     713.28    35.92   -6.43    59.51  -3.88
   52  -3  -2  14  22.74    4424.91    3675.71   102.03    7.34   226.16   3.31
   53   0   1  14  20.88     900.80     630.34    36.53    7.40    63.32   4.27
   54  -1  -3  15  22.67     168.11     388.96    64.83   -3.41    71.47  -3.09
   55   0   4  15  23.61     627.52     398.76    47.43    4.82    61.41   3.73
   56   1   0  17  26.22     291.62      36.82    53.66    4.75    56.39   4.52
                                                 --------         --------
                                        Average =     0.62             0.47

Note: SigW(I) is the SHELXL optimized weight
```

For I(calc) < 2 Sigma(I): = 13.21 and = 13.53

Section 3

Missing Reflections (Asym. Refl. Unit) below sin(th)/lambda = 0.600

Nr	H	K	L	sin(th)/lambda	Theta	I(calc)	I(calc)/I(max)
1	0	1	0	0.041	1.65*	4296.53	0.16688
2	0	4	0	0.162	6.63	29240.04	1.13571
3	0	-2	1	0.088	3.57	25620.82	0.99513
4	-1	-1	1	0.102	4.14	31693.94	1.23102
5	0	0	1	0.036	1.45*	262.36	0.01019
6	1	1	1	0.109	4.45	33913.13	1.31721
7	0	3	1	0.128	5.22	13882.72	0.53922
8	-1	4	1	0.184	7.52	34522.66	1.34089
9	0	-2	2	0.106	4.33	31094.47	1.20773
10	1	1	2	0.129	5.24	46021.09	1.78750
11	0	2	2	0.110	4.48	12198.89	0.47381
12	-2	3	2	0.217	8.89	38239.66	1.48526
13	-1	-2	3	0.154	6.30	32762.61	1.27253
14	1	-1	3	0.150	6.11	181815.84	7.06187
15	0	-2	4	0.162	6.59	31610.19	1.22777
16	-1	0	4	0.159	6.50	21460.98	0.83356
17	-2	1	4	0.218	8.92	27975.17	1.08658
18	0	3	4	0.191	7.78	29378.74	1.14109
19	-1	2	5	0.207	8.47	38326.84	1.48865
20	2	-2	6	0.300	12.30	44942.54	1.74560
21	6	-2	6	0.597	25.11	263.34	0.01023
22	3	3	13	0.578	24.27	549.90	0.02136
23	2	3	15	0.599	25.21	617.56	0.02399

** Note: I(max) is the maximum I(obs) encountered in the fcf-file **

Starred Reflections have a Theta below Theta(Min) = 2.16

From CIF: Theta(Min) = 2.16

Section 4

Resolution & Completeness Statistics (Cumulative and Friedel Pairs Averaged)

Theta	sin(th)/Lambda	Complete	Expected	Measured	Total	Missing	
20.82	0.500	0.990	2059	2039	20		
23.01	0.550	0.993	2735	2715	20		
25.24	0.600	0.994	3543	3520	23		
							ACTA Min. Res. ---
27.48	0.649	0.987	4499	4439	60		

Note: The Reported Completeness refers to the Actual H,K,L Index Range

Section 5

R-Value Statistics as a Function of Resolution (in Resolution Shell)

Theta	sin(Th)/L	#	R1	wR2	S	Rs	av(I/SigW)	av(I)	av(SigW)
12.38	0.302	438	0.026	0.088	1.354	0.015	14.17	3974.30	209.50
15.68	0.380	444	0.025	0.082	1.150	0.020	12.54	2458.73	140.31
18.02	0.435	440	0.023	0.070	0.888	0.029	11.20	1785.35	112.74
19.90	0.479	465	0.028	0.086	0.982	0.037	9.73	1270.06	89.27
21.51	0.516	447	0.032	0.090	0.944	0.047	8.85	1043.60	81.18
22.94	0.548	460	0.037	0.102	0.937	0.061	7.52	737.45	67.11
24.22	0.577	447	0.044	0.115	0.901	0.077	6.25	546.17	58.33
25.40	0.603	436	0.043	0.124	0.926	0.087	5.78	532.83	61.08
26.49	0.628	436	0.062	0.163	0.997	0.118	4.71	352.41	51.59
27.48	0.649	426	0.060	0.169	0.949	0.133	4.20	320.04	51.21

R(sig) = sum(sig(I)) / sum(I) = 0.0362

From FCF: R1 = 0.0333(3662), wR2 = 0.0960(4439), S = 1.043
From CIF: R1 = 0.0333(3662), wR2 = 0.0960(4439), S = 1.043, Npar = 263

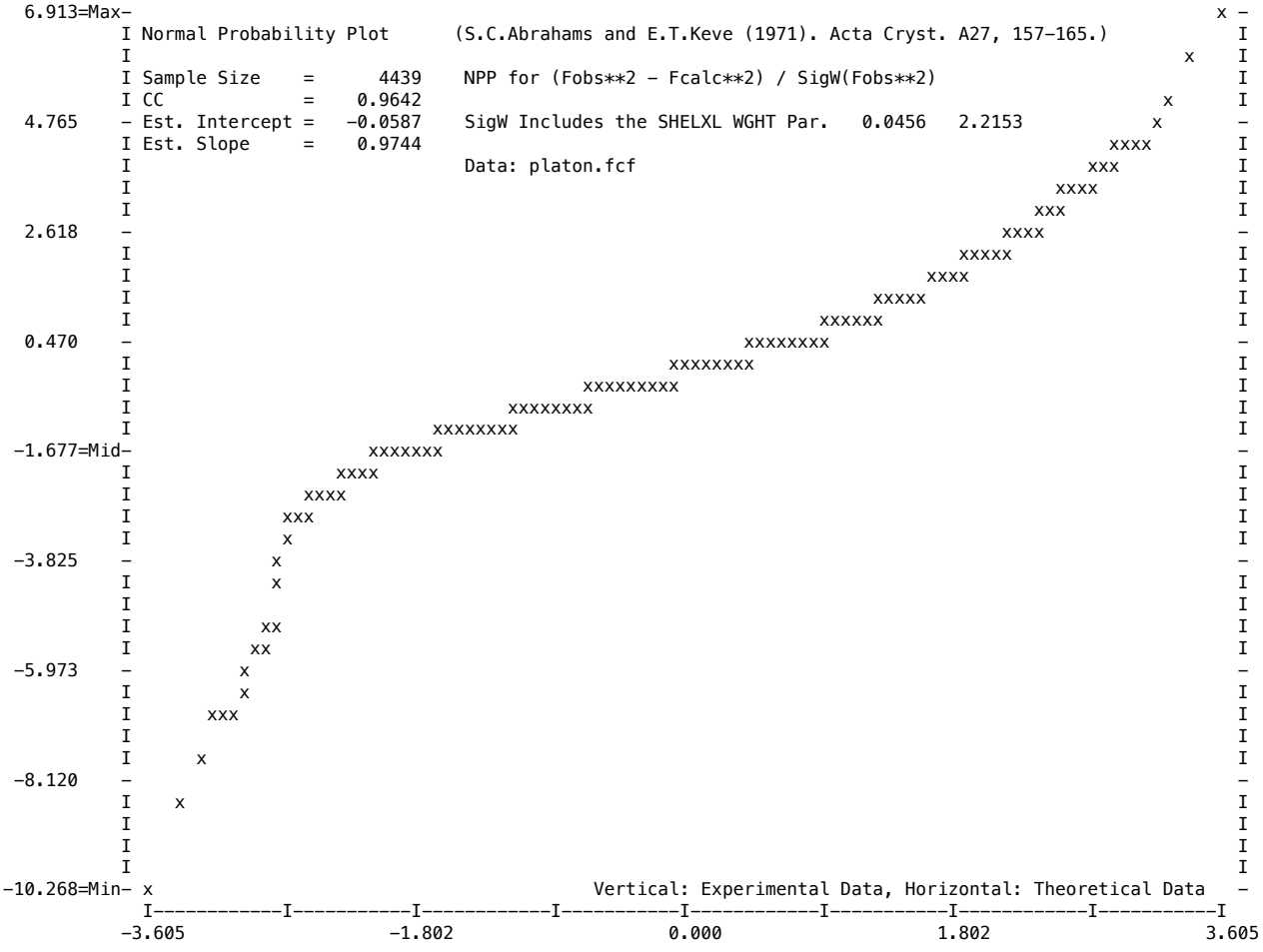
No (SHELXL) Optimized Weights: wR2 = 0.0667 , S = 2.08

Section 6

Summary of Reflection Data in FCF - Note: Friedel Pairs Averaged

Total # of Reflections in FCF. 4439 (Hmax = 7, Kmax = 15, Lmax = 18) Obs
Number above Rep. Theta(Max) . 0
Actual Theta(Max) (Deg.) ... 27.484 (Hmax = 7, Kmax = 15, Lmax = 18) Exp

```
Reported Theta(Max) (Deg.) ... 27.484  (Hmax =  7, Kmax = 15, Lmax = 18) Rep
Actual   Theta(Min) (Deg.) ...  2.163
Reported Theta(Min) (Deg.) ...  2.163

Unique (Expected) .............   4499
Unique (in FCF) ...............   4439
Observed [I .gt. 2 Sig(I)] ...    3662
Less-Thans ....................    777
Negative Intensities .........    249
Negative Intensities < - 2 SIG      0

Missing (Total) ..............     60
Missing Below Th(Min) ........      2
Missing Th(Min) to STh/L=0.600     21
Missing STh/L=0.600 to Th(Max)     37
Missing Very Strong Refl. ....     14
Beamstop Effected Reflections       0

Space Group Absences .........      0


Intensity Distribution [Decay of I/Sigma(I) versus sin(theta)/lambda]
================================================================================
sh  st/l   Ang     #  0.25   1.0   2.0  Percent  Distr. for I .gt. 2.0 * sig(I)
================================================================================
 1 0.301 1.661   434  98.8  97.9  97.0 ***************************************.
 2 0.379 1.318   442  98.6  96.8  94.6 **************************************...
 3 0.434 1.152   432  95.1  93.5  92.1 *************************************.....
 4 0.478 1.046   468  94.9  91.2  87.8 ***********************************.......
 5 0.515 0.971   440  95.0  90.5  85.0 *********************************.........
 6 0.547 0.914   453  92.3  88.1  80.1 *******************************...........
 7 0.576 0.868   448  91.1  83.7  78.3 ******************************............
 8 0.602 0.830   434  88.5  80.4  73.5 ****************************..............
 9 0.626 0.798   432  87.7  80.1  72.7 ****************************..............
10 0.649 0.771   437  87.4  76.2  64.5 ************************................
11 0.670 0.747    19  84.2  63.2  57.9 ************************................
                                    I                  I                  I
                      Percent Observed:   0                 50                100


Maximum Percentage of Reflections with I .gt. 2*s(I) in any Resolution Shell 97

Section 7
================================================================================
Analysis of Variance (F(obs) and F(calc) from FCF)
================================================================================

:: Hmax =    7, Kmax =   15, Lmax =   18

:: SigW(I) Includes the SHELXL WGHT a & b Parameter Values   0.0456   2.2153

:: K = Mean[Fo^2]/Mean[Fc^2] for Group - (Fo^2, Fc^2 from FCF)

Fc/Fc(max)     0.000 0.021 0.043 0.067 0.095 0.128 0.163 0.206 0.267 0.372 1.000
Number in Group    445   445   443   444   443   444   444   444   444   443
           GooF  0.902 1.069 1.049 1.078 1.209 0.874 1.076 1.092 0.986 1.055
              K  0.842 0.925 0.952 0.972 0.975 0.990 0.995 1.014 1.013 1.015

Resolution(A)   0.77  0.80  0.83  0.87  0.91  0.97  1.05  1.15  1.31  1.65  9.41
Number in Group    445   444   444   444   443   443   445   444   444   442
           GooF  0.969 1.036 0.934 0.952 0.962 0.969 1.017 0.924 1.182 1.395
              K  0.990 1.008 1.011 1.016 1.021 1.022 1.015 1.006 1.002 1.011

Resolution Dependence for Fc/Fc(max) .LT.  0.043
Resolution(A)   0.77  0.80  0.83  0.87  0.91  0.97  1.05  1.15  1.31  1.65  9.41
Number in Group    149   116   120    98   101    78    65    66    56    41
           GooF  0.931 1.058 0.893 0.936 0.815 0.934 0.898 0.905 1.404 1.134
              K  1.074 0.825 0.739 0.757 0.866 0.791 0.840 0.954 1.236 1.127

Abs(H)         0    1    2    3    4    5    6    7
Number       446  885  845  757  645  485  289   87
PerObs Fo2    83   81   81   78   77   74   65   61
PerObs Fc2    81   81   82   80   77   75   68   60

Abs(K)         0    1    2    3    4    5    6    7    8    9   10   11   12   13
Number       208  416  404  397  389  377  355  341  316  287  253  221  183  143
PerObs Fo2    83   80   82   80   79   81   79   79   78   78   74   72   69   69
PerObs Fc2    82   80   82   81   80   82   81   80   79   79   75   71   68   68

Abs(L)         0    1    2    3    4    5    6    7    8    9   10   11   12   13
Number       181  360  358  353  345  333  324  311  294  275  257  237  207  181
PerObs Fo2    85   84   83   83   79   83   77   80   77   77   79   73   72   72
PerObs Fc2    84   83   84   85   80   83   79   79   78   78   79   75   71   73


                    I-----------I-----------I-----------I-----------I-----------I-----------I-----------I-----------I
```



Section 8

```
================================================================================
Check for Unaccounted Twinning with the TwinRotMat Algorithm - N(selec) =    50
================================================================================
Note: This Analysis is Based on Fc calculated from Coordinates in the CIF.
================================================================================

2-axis (   1  -1   3 ) [   5  -1   2 ], Angle () [] =  6.96 Deg, Freq =    28
       *************

(-0.217   -0.119    0.366)   (h1)   (h2)                  Nr Overlap =   242
(-0.783   -0.881   -0.366) * (k1) = (k2)                        BASF =  0.25
( 2.348   -0.358    0.098)   (l1)   (l2)                      DEL-R =-0.010

No Applicable Twin Law(s) Detected from Fo/Fc Analysis-or Already Accounted for


Section 8
================================================================================
Check for Unaccounted Twinning with the TwinRotMat Algorithm - N(selec) =    50
================================================================================
Note: This Analysis is Based on Fc Taken from Fo/Fc File (FCF)
================================================================================

No Applicable Twin Law(s) Detected from Fo/Fc Analysis-or Already Accounted for

# R= 0.0333(  3662), wR2= 0.0960(  4439), S = 1.043     (From FCF data only)
# R= 0.0333(  3662), wR2= 0.0960(  4439), S = 1.043, Npar=  263

Section 12: ASYM Reflection Averaging Listing (Embedded hkl Data)
================================================================================

================================================================================================================================================
PLATON(V- 60124)-Run for: ep-91_a.res in P-1                                                                    TIME: Feb 15 10:16:45 2024
================================================================================================================================================
                                                                                                                (C) 1980-2024 A.L.Spek
                                                  ============
================================================= Crystal Data ==================================================================================
                                                  ============
                      Input Cell  (Lattice Type: P)   -   Temp =   0K            Reduced Cell     (Acta Cryst.(1976),A32,297-298)
------------------------------------------------------------------------------  ------------------------------------------------
a =     5.6690(4)  Angstrom               alpha =     91.644(6) Degree          a  =    5.669     alpha  =   91.64  V  =   980.5
b =    12.3300(9)                          beta =     96.314(6)                 b  =   12.330     beta   =   96.31
```

```
c =    14.1339(9)                        gamma =     92.400(6)                  c  =   14.134     gamma  =   92.40

V =       980.537 Cubic-Angstrom         d(100) =      5.6288   Angstrom                    Niggli Values
                                         d(010) =     12.3123                            32.138   152.029   199.767
Lambda(MoKa) =   0.71073 Angstrom        d(001) =     14.0403                            -4.999    -8.812    -2.927

                                                 =========================
================================================ Orthogonalization Matrices ================================================
                                                 =========================

(See e.g. J.D.Dunitz, Xray Analysis and Structure Determination of Organic Molecules, Cornell Univ. Press, 1979, P236)

(XO)   (   5.66900  -0.51633  -1.55441 ) (X)   ,   (X)   (   0.17640   0.00739   0.01978 ) (XO)      Orthogonal Axes AO, BO and CO
(YO) = (         0  12.31918  -0.47100 )*(Y)   ,   (Y) = (         0   0.08117   0.00272 )*(YO)            are defined as:
(ZO)   (         0         0  14.04027 ) (Z)   ,   (Z)   (         0         0   0.07122 ) (ZO)     AO // A, CO // C*, BO // CO X AO

                                                 ====================
================================================ Space Group Symmetry ======================================================
                                                 ====================

(See e.g. G. Burns & A.M. Glazer, Space Groups for Solid State Scientists, Academic Press, 1990 or Int. Tables A)

Space Group  H-M:  P-1                                      Laue:   -1
Space Group Hall: -P 1                                [Schoenflies: Ci^1  ]
Lattice Type: aP,  Centric,    Triclinic, Multiplicity:   2( 1), No:   2

Non-Sohnke - No Absolute Structure

  Nr            ***** Symmetry Operation(s) *****

   1               X ,              Y ,              Z
   2             - X ,            - Y ,            - Z

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

:: Reflection Data are READ from File : lasym.hkl - ( OBS-Data)

:: Reflection Data are READ from File : lasym.hkl - ( OBS-Data)

:: Hmax =  0 Kmax =  0 Lmax=  0 ,  Sorting Order : Fast H,  Medium K, Slow L

:: No Recognizable Reflections Encountered for ep-91_a.re


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


                                                       ===========
****************************************************** N O T I C E **************************************************
                                                       ===========

- PLATON Reference : Spek, A.L. (2003). J. Appl. Cryst. 36, 7-13.
                     Spek, A.L. (2009). Acta Cryst. D65, 148-155.
                     Spek, A.L. (2015). Acta Cryst. C71, 9-18.

- Output Values (Esd) may have  been set to 99, 999 or 9999 to Avoid Format Overflow

- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken
  into Account (e.g. Those Involving Atoms That were Refined with Constraints)

- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters.
  However, differences should be within the associated esd-range.

- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced
  Features are Experimental and may Contain Loose Ends.

- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@uu.nl

- Recent versions of PLATON may be obtained from http://www.platonsoft.nl/xraysoft

- More INFO can be found on http://http://www.platonsoft.nl/


================================================================================================================================
Page - Index
================================================================================

Page   1 --- ASYM
Page   3 --- SUMMARY


================================================================================
Summary and Remarks : N = NOTE, W = WARNING, E = ERROR
================================================================================
N: No S.U.'s (esd) on observed/calculated parameters.
```

```
==============================================================================

:: Input Xtal Data from File lasym.ins - Data Type RES

:: NORMAL END of PLATON :     4 Pages on FILE lasym.lis
```