checkCIF (basic structural check) running

checkCIF/PLATON (basic structural check)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found.   CIF dictionary
Please wait while processing ....   Interpreting this report

Datablock: BaLiGaSb

Bond precision: Sb-Sb = 0.0013 A   Wavelength=0.71073

Cell: a=18.105(6)   b=4.9319(15)   c=13.023(4)
             alpha=90   beta=126.676(4)   gamma=90

Temperature: 200 K

	Calculated	Reported
Volume	932.6(5)	932.6(5)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	Sb2, 4(Ba), 4(Sb), 0.334(Ga), 6.666(Li)	?
Sum formula	Ba4 Ga0.33 Li6.67 Sb6	Ba4 Ga0.35 Li6.65 Sb6
Mr	1349.43	1350.41
Dx,g cm-3	4.806	4.809
Z	2	2
Mu (mm-1)	17.272	17.294
F000	1120.7	1122.0
F000'	1111.74	
h,k,lmax	23,6,16	23,6,16
Nref	1161	1162
Tmin,Tmax	0.459,0.527	0.321,0.467
Tmin'	0.236	

Correction method= # Reported T Limits: Tmin=0.321 Tmax=0.467
AbsCorr = MULTI-SCAN

Data completeness= 1.001   Theta(max)= 27.232

R(reflections)= 0.0263(1042)   wR2(reflections)= 0.0592(1162)

S = 1.071   Npar= 41

The following ALERTS were generated. Each ALERT has the format
    test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

🔘 Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
        a literature citation. This should be contained in the
        _exptl_absorpt_process_details field.
        Absorption correction given as multi-scan
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..   Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   2.32 Report
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ....   4 Check

🔘 Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
        _chemical_formula_sum and the formula from the _atom_site* data.
        Atom count from _chemical_formula_sum:Ba4 Ga0.35 Li6.65 Sb6
        Atom count from the _atom_site data: Ba4 Ga0.334 Li6.666 Sb6
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
        From the CIF: _cell_formula_units_Z   2
        From the CIF: _chemical_formula_sum Ba4 Ga0.35 Li6.65 Sb6
        TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Ba	8.00	8.00	0.00
Ga	0.70	0.67	0.03
Li	13.30	13.33	-0.03
Sb	12.00	12.00	0.00

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF   Please Do !
PLAT128_ALERT_4_G Alternate Setting for Input Space Group   C2/m   I2/m Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6)   100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 9)   100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd 1   1.50 Check
And 9 other PLAT304 Alerts
More ...
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters   1 Info

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  0 **ALERT level A** = Most likely a serious problem - resolve or explain
  0 **ALERT level B** = A potentially serious problem, consider carefully
  6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 18 **ALERT level G** = General information/check it is not something unexpected

  5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  2 ALERT type 2 Indicator that the structure model may be wrong or deficient
  1 ALERT type 3 Indicator that the structure quality may be low
 15 ALERT type 4 Improvement, methodology, query or suggestion
  1 ALERT type 5 Informative message, check

Datablock: BaLiInSb

Bond precision: Sb-Sb = 0.0008 A   Wavelength=0.71073

Cell: a=18.146(3)   b=4.9397(9)   c=13.080(2)
              alpha=90   beta=126.680(2)   gamma=90

Temperature: 200 K

	Calculated	Reported
Volume	940.3(3)	940.3(3)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	In1.15 Sb8, 2(Sb2), 8(Ba), 12.848(Li)	?
Sum formula	Ba8 In1.15 Li12.85 Sb12	Ba4 In0.55 Li6.40 Sb6
Mr	2781.20	1387.43
Dx,g cm-3	4.911	4.900
Z	1	2
Mu (mm-1)	17.351	17.321
F000	1155.0	1152.0
F000'	1145.04	
h,k,lmax	23,6,16	23,6,16
Nref	1173	1174
Tmin,Tmax	0.478,0.555	0.372,0.493
Tmin'	0.243	

Correction method= # Reported T Limits: Tmin=0.372 Tmax=0.493
AbsCorr = MULTI-SCAN

Data completeness= 1.001   Theta(max)= 27.249

R(reflections)= 0.0220(1060)   wR2(reflections)= 0.0504(1174)

S = 1.037   Npar= 43

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

⬤ Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
   a literature citation. This should be contained in the
   _exptl_absorpt_process_details field.
   Absorption correction given as multi-scan
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 6.34 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .... 4 Check

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⬤ Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
   _chemical_formula_sum and the formula from the _atom_site* data.
   Atom count from _chemical_formula_sum:Ba4 In0.55 Li6.4 Sb6
   Atom count from the _atom_site data: Ba4 In0.576 Li6.424 Sb6
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
   From the CIF: _cell_formula_units_Z 2
   From the CIF: _chemical_formula_sum Ba4 In0.55 Li6.40 Sb6
   TEST: Compare cell contents of formula and atom_site data

   atom Z*formula cif sites diff
   Ba 8.00 8.00 0.00
   In 1.10 1.15 -0.05
   Li 12.80 12.85 -0.05
   Sb 12.00 12.00 0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/m I2/m Note
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1) 13% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 7) 100% Note

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 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 9 **ALERT level G** = General information/check it is not something unexpected

 7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 1 ALERT type 2 Indicator that the structure model may be wrong or deficient
 2 ALERT type 3 Indicator that the structure quality may be low
 3 ALERT type 4 Improvement, methodology, query or suggestion
 2 ALERT type 5 Informative message, check

Datablock: BaLiInBi

Bond precision: Sb-Sb = 0.0000 A   Wavelength=0.71073

Cell: a=18.4090(13) b=5.0133(4) c=13.2823(10)
   alpha=90 beta=126.2927(11) gamma=90

Temperature: 200 K

	Calculated	Reported
Volume	988.02(13)	988.02(13)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	Bi8 In0.92, 4(Bi), 8(Ba), 13.08(Li)	?
Sum formula	Ba8 Bi12 In0.92 Li13.08	Ba4 Bi6 In0.45 Li6.55
Mr	3802.81	1900.37
Dx,g cm-3	6.391	6.388

```
Z                       1                       2
Mu (mm-1)               61.538                  61.527
F000                    1528.3                  1527.0
F000'                   1482.00
h,k,lmax                23,6,17                 23,6,17
Nref                    1243                    1243
Tmin,Tmax               0.011,0.021             0.014,0.041
Tmin'                   0.000

Correction method= # Reported T Limits: Tmin=0.014 Tmax=0.041
AbsCorr = MULTI-SCAN

Data completeness= 1.000           Theta(max)= 27.250

R(reflections)= 0.0256( 1158)          wR2(reflections)= 0.0623( 1243)

S = 1.039               Npar= 42
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

● Alert level C
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..   Please Check
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ....   4 Check

● Alert level G
FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
        _chemical_formula_sum and the formula from the _atom_site* data.
        Atom count from _chemical_formula_sum:Ba4 Bi6 In0.45 Li6.55
        Atom count from the _atom_site data: Ba4 Bi6 In0.46 Li6.54
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF   Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large   9.25 Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group   C2/m   I2/m Note
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)   10% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 7)   100% Note

   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   0 **ALERT level B** = A potentially serious problem, consider carefully
   4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
   8 **ALERT level G** = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check

Datablock: EuLiInBi

```
Bond precision:          Bi-Eu = 0.0009 A                Wavelength=0.71073
Cell:        a=17.607(3)      b=4.8222(8)     c=12.826(2)
             alpha=90         beta=125.9287(17) gamma=90
Temperature: 200 K
                    Calculated                  Reported
Volume              881.8(3)                    881.8(2)
Space group         C 2/m                       C 2/m
Hall group          -C 2y                       -C 2y
Moiety formula      Bi12 Eu8 In0.79, 13.208(Li)  ?
Sum formula         Bi12 Eu8 In0.79 Li13.21     Bi6 Eu4 In0.40 Li6.60
Mr                  3906.12                     1953.45
```

Dx,g cm-3	7.356	7.357
Z	1	2
Mu (mm-1)	74.086	74.091
F000	1578.4	1579.0
F000'	1534.23	
h,k,lmax	22,6,16	22,6,16
Nref	1113	1113
Tmin,Tmax	0.047,0.081	0.028,0.087
Tmin'	0.002	

Correction method= # Reported T Limits: Tmin=0.028 Tmax=0.087
AbsCorr = MULTI-SCAN

Data completeness= 1.000   Theta(max)= 27.227

R(reflections)= 0.0251(1010)   wR2(reflections)= 0.0609(1113)

S = 1.119   Npar= 43

The following ALERTS were generated. Each ALERT has the format
        test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

⬤ Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
        a literature citation. This should be contained in the
        _exptl_absorpt_process_details field.
        Absorption correction given as multi-scan
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..   Please Check
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ....   4 Check

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⬤ Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF   Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.50 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT128_ALERT_4_G Alternate Setting for Input Space Group   C2/m   I2/m Note
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)   4% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4)   100% Note

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   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   0 **ALERT level B** = A potentially serious problem, consider carefully
   3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
   7 **ALERT level G** = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check

Datablock: BaLiBi

Bond precision: Bi-Eu = 0.0000 A   Wavelength=0.71073

Cell: a=18.407(3)   b=5.0258(9)   c=18.353(3)
             alpha=90   beta=104.426(3) gamma=90

Temperature: 200 K

	Calculated	Reported
Volume	1644.3(5)	1644.3(5)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	10(Bi), 7(Ba), 11(Li)	?
Sum formula	Ba7 Bi10 Li11	Ba7 Bi10 Li11
Mr	3127.45	3127.52

```
Dx,g cm−3              6.317                        6.317
Z                      2                            2
Mu (mm−1)              61.494                       61.493
F000                  2510.0                        2510.0
F000'                 2433.83
h,k,lmax              23,6,23                       23,6,23
Nref                  2063                          2063
Tmin,Tmax            0.098,0.292                    0.097,0.216
Tmin'                0.074

Correction method= # Reported T Limits: Tmin=0.097 Tmax=0.216
AbsCorr = MULTI−SCAN

Data completeness= 1.000          Theta(max)= 27.247

R(reflections)= 0.0298( 1689)          wR2(reflections)= 0.0651( 2063)

S = 1.054              Npar= 68
```

The following ALERTS were generated. Each ALERT has the format
    test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

⬤ Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
          a literature citation. This should be contained in the
          _exptl_absorpt_process_details field.
          Absorption correction given as multi-scan

⬤ Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF   Please Do !
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd 1   0.50 Check
And 14 other PLAT304 Alerts
More ...
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters   2 Info

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   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   0 **ALERT level B** = A potentially serious problem, consider carefully
   1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  17 **ALERT level G** = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
  16 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.
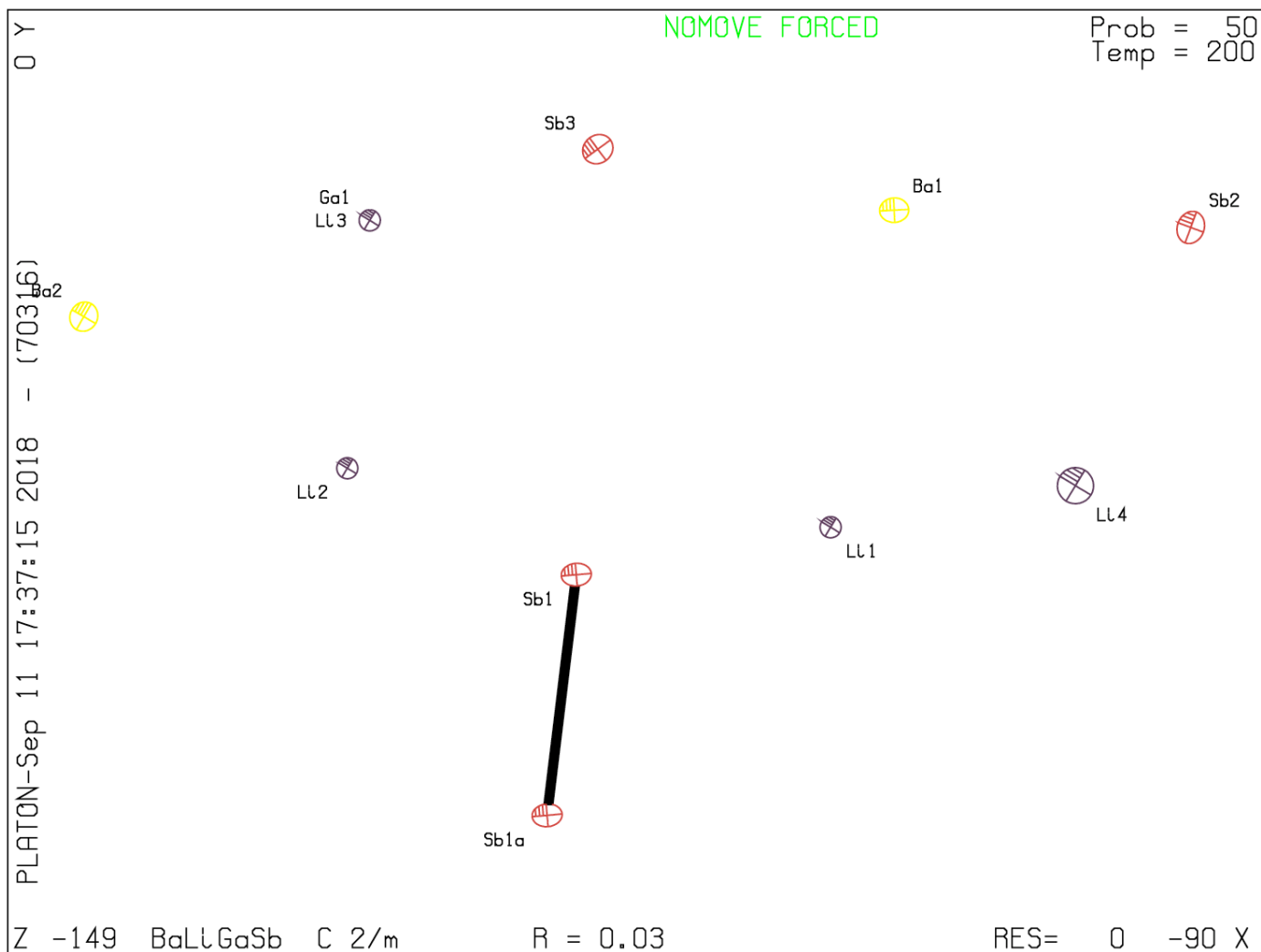
Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.
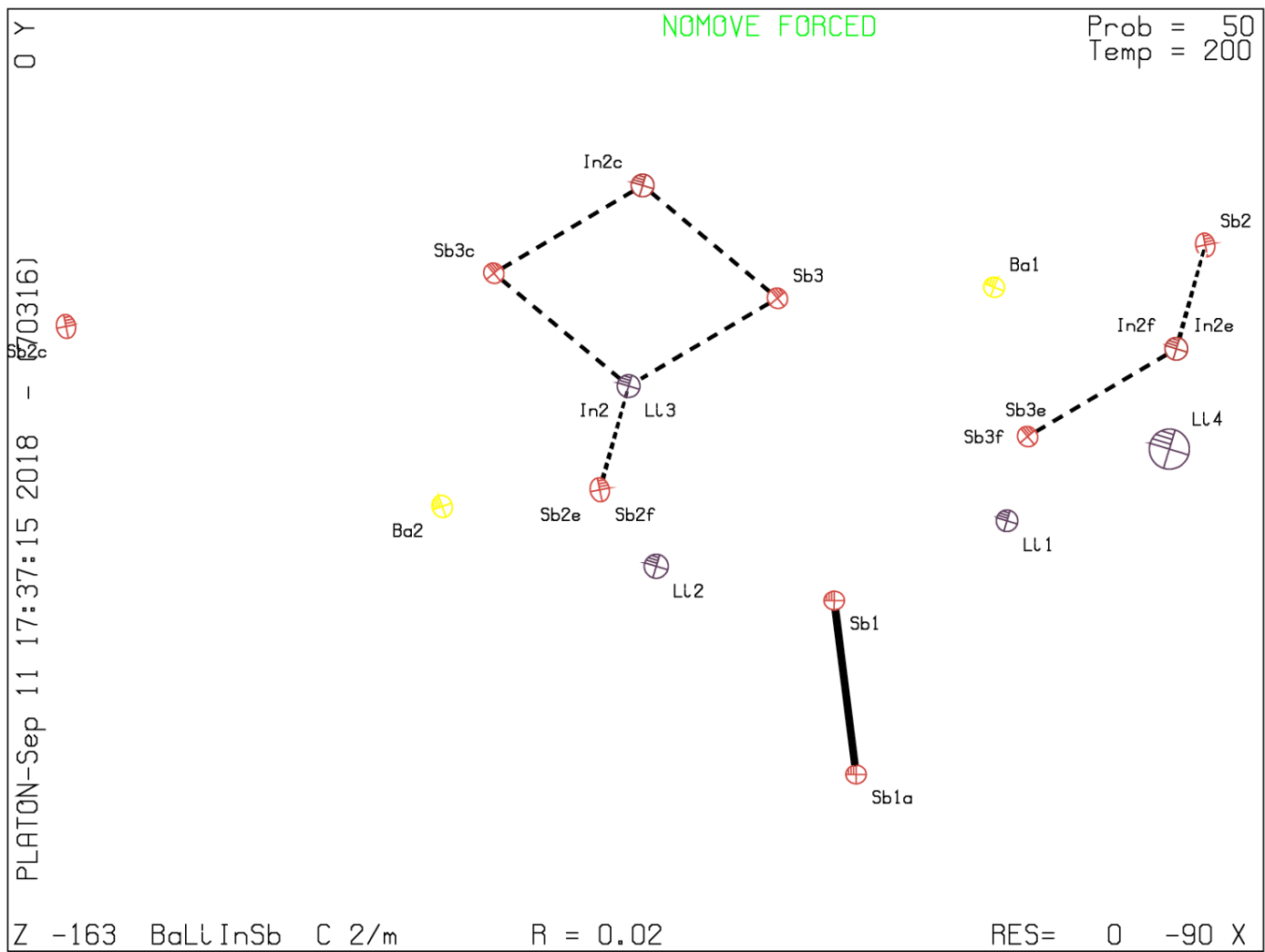
PLATON version of 20/08/2018; check.def file version of 20/08/2018

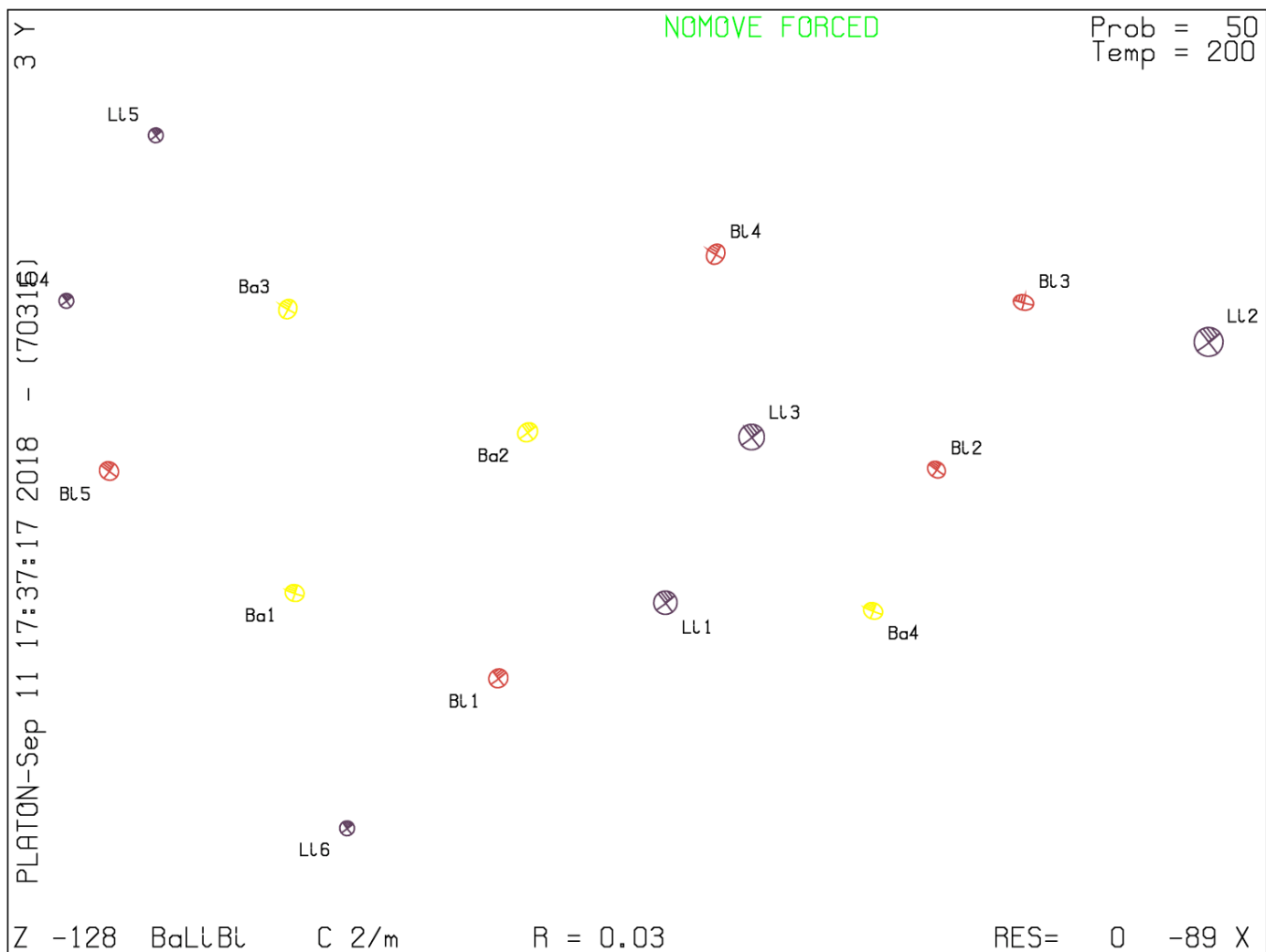## Datablock BaLiGaSb - ellipsoid plot

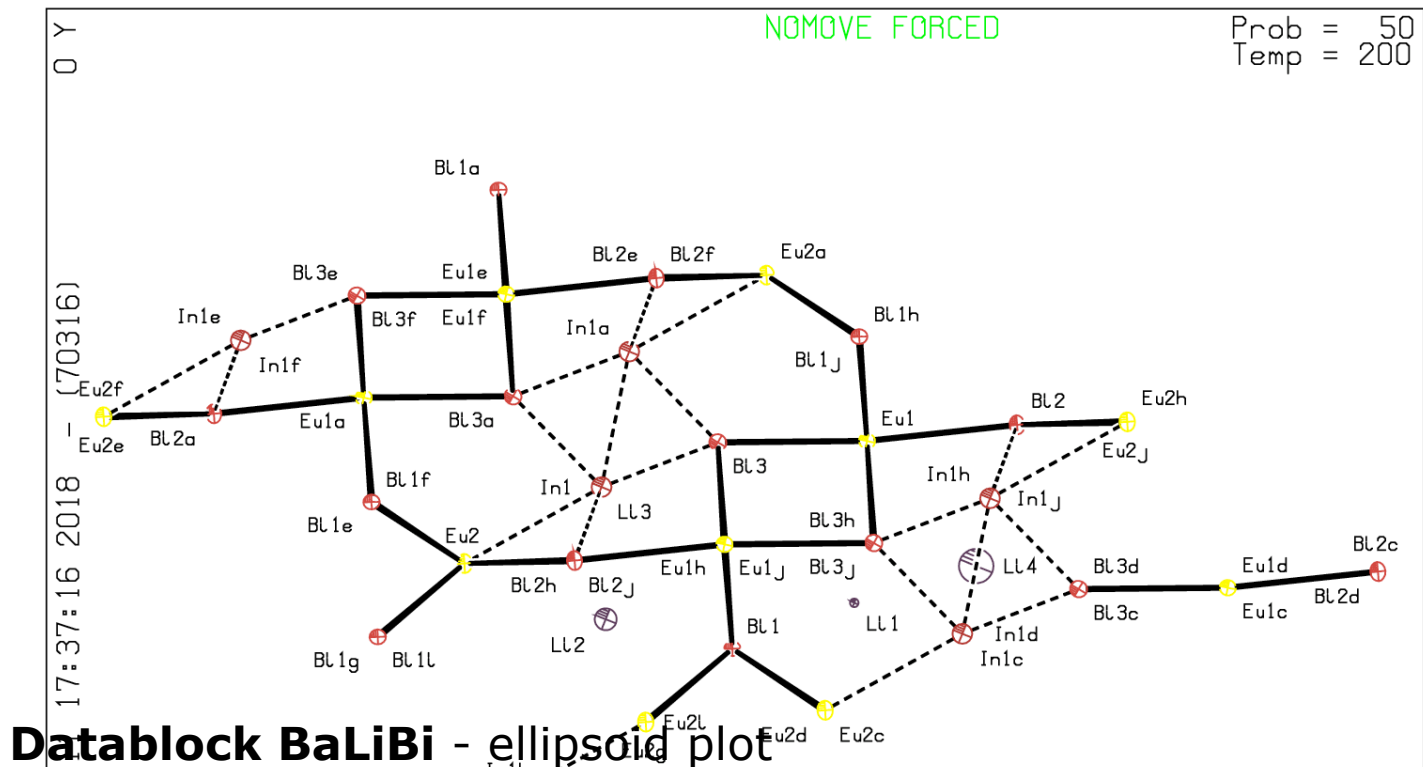## Datablock BaLiInSb - ellipsoid plot

Datablock BaLiInBi - ellipsoid plot

Datablock EuLiInBi - ellipsoid plot

Prob = 50
Temp = 200

O Y

PLATON-Sep 11 17:37:16 2018 - (70316)

Z -162 BaLiInBi C 2/m   R = 0.03   RES=   0   -90 X

In1a

Bi2

Ba1

Bi3a

Bi3

In1d   In1c

In1   Li3

Bi2a

Ba2

Bi3d
Bi3c

Li4

Bi2c   Bi2d

Li1

Li2

Bi1

Datablock BaLiBi - ellipsoid plot

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Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry