checkCIF/PLATON report

Structure factors have been supplied for datablock(s) sad

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sad

```
Bond precision:  C-C = 0.0023 A          Wavelength=0.71073

Cell:          a=9.2087(4)       b=10.5543(4)     c=12.6990(5)
               alpha=71.752(1)   beta=70.245(1)   gamma=73.105(1)
Temperature:   100 K
```

	Calculated	Reported
Volume	1079.35(8)	1079.35(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C22 H26 N O2 P S Si	C22 H26 N O2 P S Si
Sum formula	C22 H26 N O2 P S Si	C22 H26 N O2 P S Si
Mr	427.56	427.56
Dx,g cm-3	1.316	1.316
Z	2	2
Mu (mm-1)	0.298	0.298
F000	452.0	452.0
F000’	452.76	
h,k,lmax	10,12,15	10,12,15
Nref	3796	3796
Tmin,Tmax	0.898,0.917	0.682,0.746
Tmin’	0.888	

```
Correction method= # Reported T Limits: Tmin=0.682 Tmax=0.746
AbsCorr = EMPIRICAL

Data completeness= 1.000          Theta(max)= 25.000

R(reflections)= 0.0290( 3473)     wR2(reflections)= 0.1189( 3796)

S = 1.049                 Npar= 264
```

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 G

```
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.001 Degree
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) Still          86 %
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density          11 Note
```

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

   1 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
   1 ALERT type 3 Indicator that the structure quality may be low
   0 ALERT type 4 Improvement, methodology, query or suggestion
   0 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

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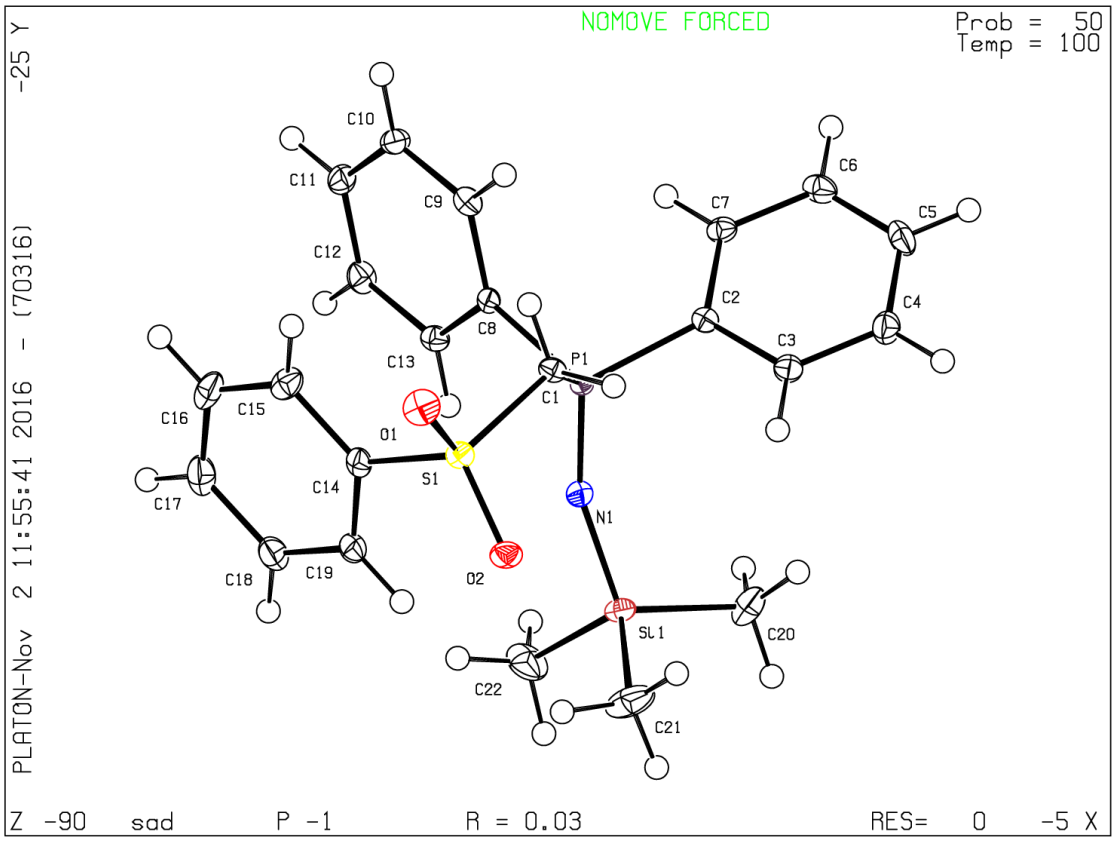
PLATON version of 11/08/2016; check.def file version of 04/08/2016

Datablock sad - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) sad2

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: sad2

Bond precision: C-C = 0.0055 A Wavelength=0.71073

Cell: a=25.265(3) b=18.972(2) c=24.452(3)
alpha=90 beta=116.547(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	10485(2)	10485(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	4(C92 H106 Li8 N4 O9 P4 S4 Si4), 4(C4 H10 O), O2, 4(C2 H5)	C92 H106 Li8 N4 O9 P4 S4 Si4, C4 H10 O,O0.25 C2 H5
Sum formula	C392 H484 Li32 N16 O42 P16 S16 Si16	C98 H121 Li8 N4 O10.50 P4 S4 Si4
Mr	7771.98	1942.98
Dx,g cm-3	1.231	1.231
Z	1	4
Mu (mm-1)	0.254	0.254
F000	4100.0	4100.0
F000’	4106.25	
h,k,lmax	30,22,29	30,22,29
Nref	18469	18468
Tmin,Tmax	0.982,0.985	0.696,0.745
Tmin’	0.963	

Correction method= # Reported T Limits: Tmin=0.696 Tmax=0.745
AbsCorr = EMPIRICAL

Data completeness= 1.000 Theta(max)= 24.997

R(reflections)= 0.0494(11964) wR2(reflections)= 0.1144(18468)

S = 1.012 Npar= 1254

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

```
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range        5.0 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1   H Uiso(max)/Uiso(min) Range        4.6 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C91 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         O9 Check
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00548 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...     -1.293 Report
PLAT977_ALERT_2_C Check the Negative Difference Density on    H91A      -0.34 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density           0 Note
```

Alert level G

```
FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C98 H121 Li8 N4 O10.5 P4 S4
           Atom count from _chemical_formula_moiety:C98 H121 Li8 N4 O10.25 P4 S
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.25 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       9.76 Why ?
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C91    --  C92B    ..        6.9 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of <O1A_1  is Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of <O1B_1  is Constrained at       0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C1A_1  is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C2A_1  is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H1AA_1 is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H1AB_1 is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H1AC_1 is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H2A_1  is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H2B_1  is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C2B_1  is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C1B_1  is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H2C_1  is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H2D_1  is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H1BA_1 is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H1BB_1 is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H1BC_1 is Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..... Percentage =          1 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =         33 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   0.50) in Resd. #          3 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   3.50) in Resd. #          4 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   3.50) in Resd. #          5 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      O1A_1 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      O1B_1 Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for     C1     Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for     C23    Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for     C45    Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for     C67    Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         16 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.16 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         12 Check
             O2   -S1   -LI3     1.555   1.555   1.555            41.67 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         18 Check
             C1   -S1   -LI2     1.555   1.555   1.555            44.46 Deg.
```

```
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         28 Check
             N1   -P1   -LI3     1.555   1.555   1.555             43.23 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         33 Check
             C1   -P1   -LI2     1.555   1.555   1.555             44.51 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         43 Check
             N1   -SI1  -LI3     1.555   1.555   1.555             33.52 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        113 Check
             N2   -P2   -LI5     1.555   1.555   1.555             42.49 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        128 Check
             N2   -SI2  -LI5     1.555   1.555   1.555             34.99 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        180 Check
             O4   -S2   -LI5     1.555   1.555   1.555             41.22 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        195 Check
             O6   -S3   -LI7     1.555   1.555   1.555             41.13 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        206 Check
             N3   -P3   -LI7     1.555   1.555   1.555             43.51 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        308 Check
             O8   -S4   -LI1     1.555   1.555   1.555             44.95 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        318 Check
             N4   -P4   -LI1     1.555   1.555   1.555             43.82 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        328 Check
             N4   -SI4  -LI1     1.555   1.555   1.555             35.59 Deg.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         16 Check
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) Still          45 %
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)           3 Note
PLAT933_ALERT_2_G Number of OMIT records in Embedded RES .........          1 Note
```

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

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

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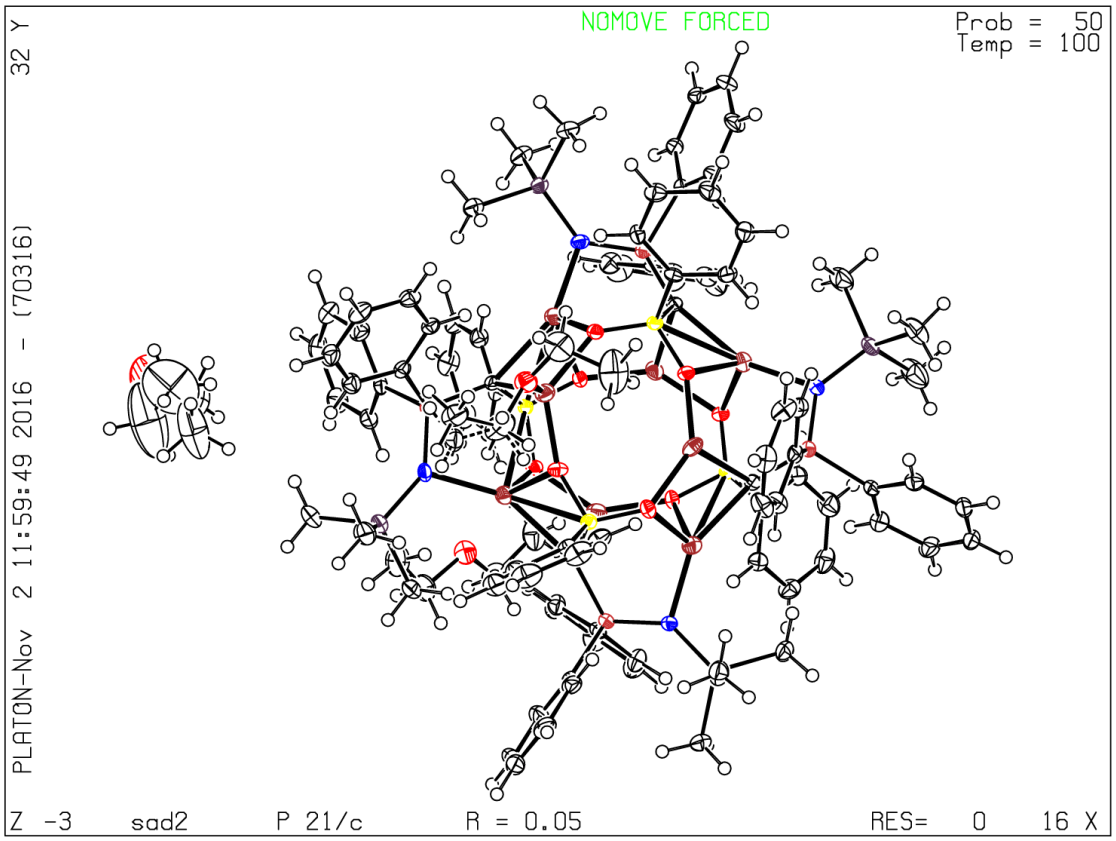
PLATON version of 11/08/2016; check.def file version of 04/08/2016

Datablock sad2 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) platon_pl

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: platon_pl

```
Bond precision:  C-C = 0.0050 A          Wavelength=0.71073

Cell:          a=11.2841(10)      b=15.3705(14)    c=16.8163(15)
               alpha=112.315(3)   beta=90.340(3)   gamma=110.779(3)
Temperature:   100 K
```

	Calculated	Reported
Volume	2489.2(4)	2489.2(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H50 K2 N2 O4 P2 S2 Si2, C4 H8 O	?
Sum formula	C48 H58 K2 N2 O5 P2 S2 Si2	C48 H58 K2 N2 O5 P2 S2 Si2
Mr	1003.40	1003.40
Dx,g cm-3	1.339	1.339
Z	2	2
Mu (mm-1)	0.433	0.433
F000	1056.0	1056.0
F000’	1058.36	
h,k,lmax	13,18,19	13,18,19
Nref	8772	8770
Tmin,Tmax	0.974,0.983	0.653,0.745
Tmin’	0.937	

```
Correction method= # Reported T Limits: Tmin=0.653 Tmax=0.745
AbsCorr = EMPIRICAL

Data completeness= 1.000          Theta(max)= 24.998

R(reflections)= 0.0408( 6524)     wR2(reflections)= 0.1028( 8770)

S = 1.001                 Npar= 605
```

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

```
PLAT222_ALERT_3_C Non-Solvent Resd 1   H Uiso(max)/Uiso(min) Range        4.6 Ratio
PLAT245_ALERT_2_C U(iso) H44A    Smaller than U(eq) C44     by ...      0.017 AngSq
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00503 Ang.
PLAT350_ALERT_3_C Short   C-H (X0.96,N1.08A)  C1     -   H1     ..       0.84 Ang.
PLAT350_ALERT_3_C Short   C-H (X0.96,N1.08A)  C23    -   H23    ..       0.78 Ang.
```

Alert level G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.003 Degree
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.          8 Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         13 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.22 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         99 Check
              N1   -SI1  -K1      1.555   1.555   1.555             39.65 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        123 Check
              O2   -S1   -K1      1.555   1.555   1.555             32.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        127 Check
              O2   -S1   -K2      1.555   1.555   1.555             34.31 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        211 Check
              N2   -P2   -K1      1.555   1.555   1.555             40.54 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        222 Check
              O3   -S2   -K1      1.555   1.555   1.555             42.50 Deg.
PLAT793_ALERT_4_G The Model has Chirality at S1      (Centro SPGR)          S Verify
PLAT793_ALERT_4_G The Model has Chirality at S2      (Centro SPGR)          S Verify
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) Still          59 %
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)          3 Note
PLAT933_ALERT_2_G Number of OMIT records in Embedded RES .........         1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density          1 Note
```

```
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```

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PLATON version of 11/08/2016; check.def file version of 04/08/2016

Datablock platon_pl - ellipsoid plot