checkCIF/PLATON report

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

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: LTP

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Bond precision:   C-C = 0.0200 A          Wavelength=0.71073

Cell:           a=8.1501(3)        b=9.0775(2)       c=15.8322(3)
                alpha=83.869(1)    beta=84.399(2)    gamma=87.646(2)
Temperature:    173 K

                Calculated                Reported
Volume          1158.49(5)                1158.49(5)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  I6 Pb2, 2(C3 H10 N)       I6 Pb2, 2(C3 H10 N)
Sum formula     C6 H20 I6 N2 Pb2          C6 H20 I6 N2 Pb2
Mr              1296.04                   1296.04
Dx,g cm-3       3.715                     3.715
Z               2                         2
Mu (mm-1)       22.495                    22.495
F000            1104.0                    1104.0
F000'           1086.35
h,k,lmax        11,12,22                  11,12,21
Nref            6896                      5972
Tmin,Tmax
Tmin'

Correction method= Not given

Data completeness= 0.866           Theta(max)= 30.229

R(reflections)= 0.0599( 5081)                wR2(reflections)=
                                             0.1678( 5972)
S = 1.186                Npar= 149
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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

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PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...     Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...     Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...     Please Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............       0.02 Ang.
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N1       --H1B      .     Please Check
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Alert level G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          4 Report
PLAT012_ALERT_1_G N.O.K.   _shelx_res_checksum Found in CIF ......     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     124.16 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1      --I5       .       10.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1      --I6_a     .        6.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb2      --I3       .       10.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb2      --I4       .        5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb2      --I1_b     .       13.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb2      --I2_b     .       13.2 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       2.08 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2       (II)      .       2.05 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..........        4.8 Low
```

```
   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
  14 ALERT level G = General information/check it is not something unexpected

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
   0 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check
```

Datablock: ITP

Bond precision: Pb- I = 0.0011 A Wavelength=0.71073

Cell:	a=9.8984(9)	b=15.0923(10)	c=8.0597(5)
	alpha=90	beta=97.887(7)	gamma=90
Temperature:	253 K		

	Calculated	Reported
Volume	1192.65(15)	1192.65(15)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	I3 Pb, C3 H10 N	I3 Pb, C3 H10 N
Sum formula	C3 H10 I3 N Pb	C3 H10 I3 N Pb
Mr	648.01	648.01
Dx,g cm-3	3.609	3.609
Z	4	4
Mu (mm-1)	21.851	21.851
F000	1104.0	1104.0
F000'	1086.32	
h,k,lmax	13,21,11	13,21,10
Nref	1760	1522
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.865 Theta(max)= 30.080

R(reflections)= 0.0516(1133) wR2(reflections)= 0.1591(1522)

S = 1.103 Npar= 40

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

PLAT052_ALERT_1_C	Info on Absorption Correction Method Not Given	Please Do !
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...	Please Check
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.62 Report
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Pb1 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C2 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including C2	0.235 Check

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Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	6 Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1 Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	10.38 Why ?
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	1 Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1 Report

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PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1      --I1       .        5.9 s.u.
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        50% Note
PLAT414_ALERT_2_G Short Intra D-H..H-X       H2B      ..H1A      .       2.05 Ang.
                                               1-x,y,3/2-z  =      2_656 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H2B      ..H1C      .       2.06 Ang.
                                               1-x,y,3/2-z  =      2_656 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H2C      ..H1A      .       1.99 Ang.
                                               1-x,y,3/2-z  =      2_656 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H2C      ..H1C      .       2.00 Ang.
                                               1-x,y,3/2-z  =      2_656 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       2.08 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        37 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.3 Low
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```
   0 ALERT level A = Most likely a serious problem - resolve or explain
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   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  12 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
   7 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
```

Datablock: HTP

Bond precision: Pb- I = 0.0020 A Wavelength=0.71073

Cell:	a=9.2432(5)	b=9.2432(5)	c=8.1797(4)
	alpha=90	beta=90	gamma=120
Temperature:	333 K		

	Calculated	Reported
Volume	605.22(7)	605.22(7)
Space group	P 63/m m c	P 63/m m c
Hall group	-P 6c 2c	-P 6c 2c
Moiety formula	C3 N, 3(I Pb0.33)	C3 H10 N, I3 Pb
Sum formula	C3 I3 N Pb	C3 H10 I3 N Pb
Mr	637.94	648.02
Dx,g cm-3	3.501	3.501
Z	2	2
Mu (mm-1)	21.527	21.527
F000	532.0	532.0
F000'	523.21	
h,k,lmax	13,13,11	13,12,11
Nref	378	357
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.944 Theta(max)= 30.144

R(reflections)= 0.0577(202) wR2(reflections)= 0.1950(357)

S = 1.035 Npar= 16

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 B

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 10.08 Check

Author Response: H atoms on cations did not be added because of highly disordered state of organic cations.

PLAT260_ALERT_2_B Large Average Ueq of Residue Including C2 0.316 Check

Author Response: The large average ueq of residue is caused by highly disordered state. of organic cations.

Alert level C

DENSD01_ALERT_1_C The ratio of the submitted crystal density and that calculated from the formula is outside the range 0.99 <> 1.01

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            Crystal density given    =      3.501
            Calculated crystal density =      3.556
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT046_ALERT_1_C Reported Z, MW and D(calc) are Inconsistent ....      3.556 Check
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...     Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...     Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...     Please Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Pb1      0.161 Check
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Author Response: The large average ueq of residue is caused by highly disordered state. of organic cations.

Alert level G

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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:C3 H10 I3 N1 Pb1
            Atom count from the _atom_site data:  C3. I3 N1.0046 Pb1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
           From the CIF: _cell_formula_units_Z    2
           From the CIF: _chemical_formula_sum  C3 H10 I3 N Pb
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C          6.00      6.00   -0.00
           H         20.00      0.00   20.00
           I          6.00      6.00    0.00
           N          2.00      2.00    0.00
           Pb         2.00      2.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         2 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         2 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         1 Info
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records         1 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records         1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records         1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1      --I1       .      14.5 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of N1         Constrained at    0.1666 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1         Constrained at    0.1667 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )       67% Note
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .      2.06 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        15 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
```

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```
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  6 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
  8 ALERT type 4 Improvement, methodology, query or suggestion
  2 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

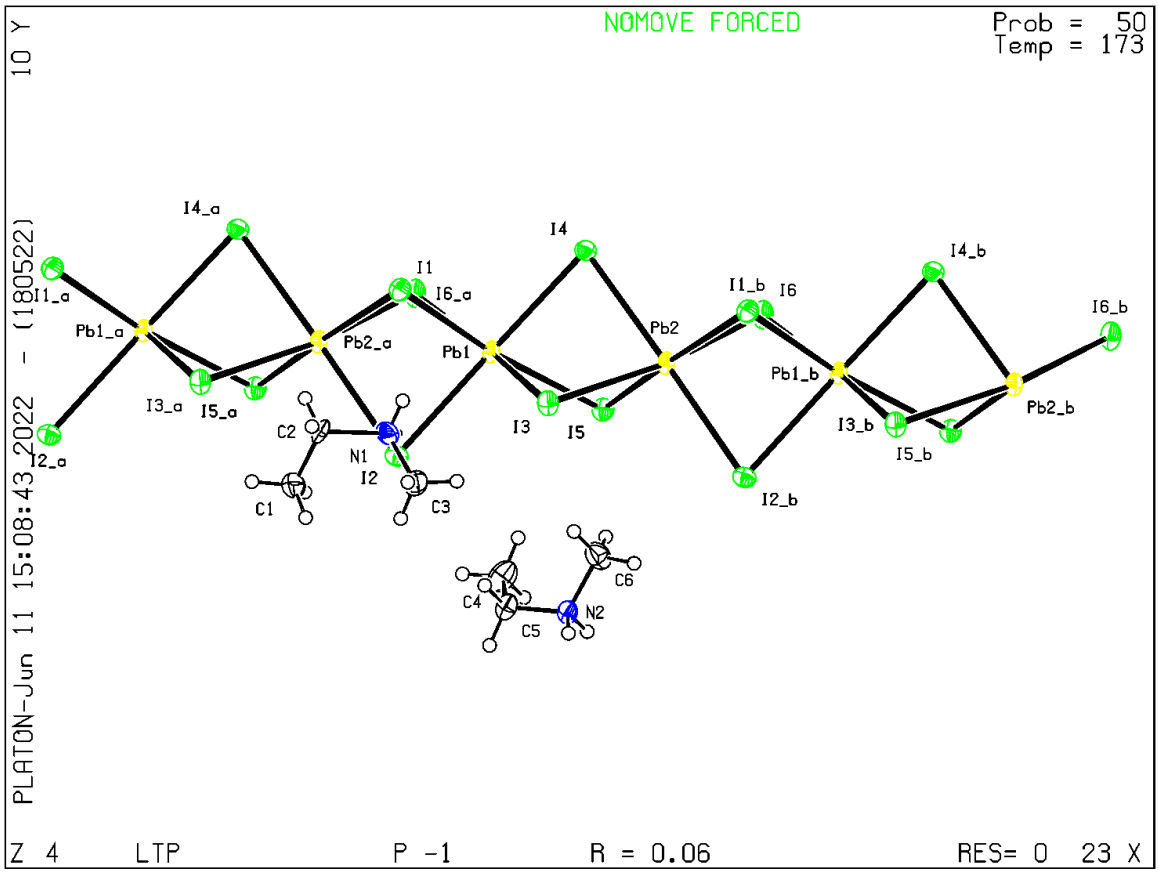
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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.

Publication of your CIF in other journals

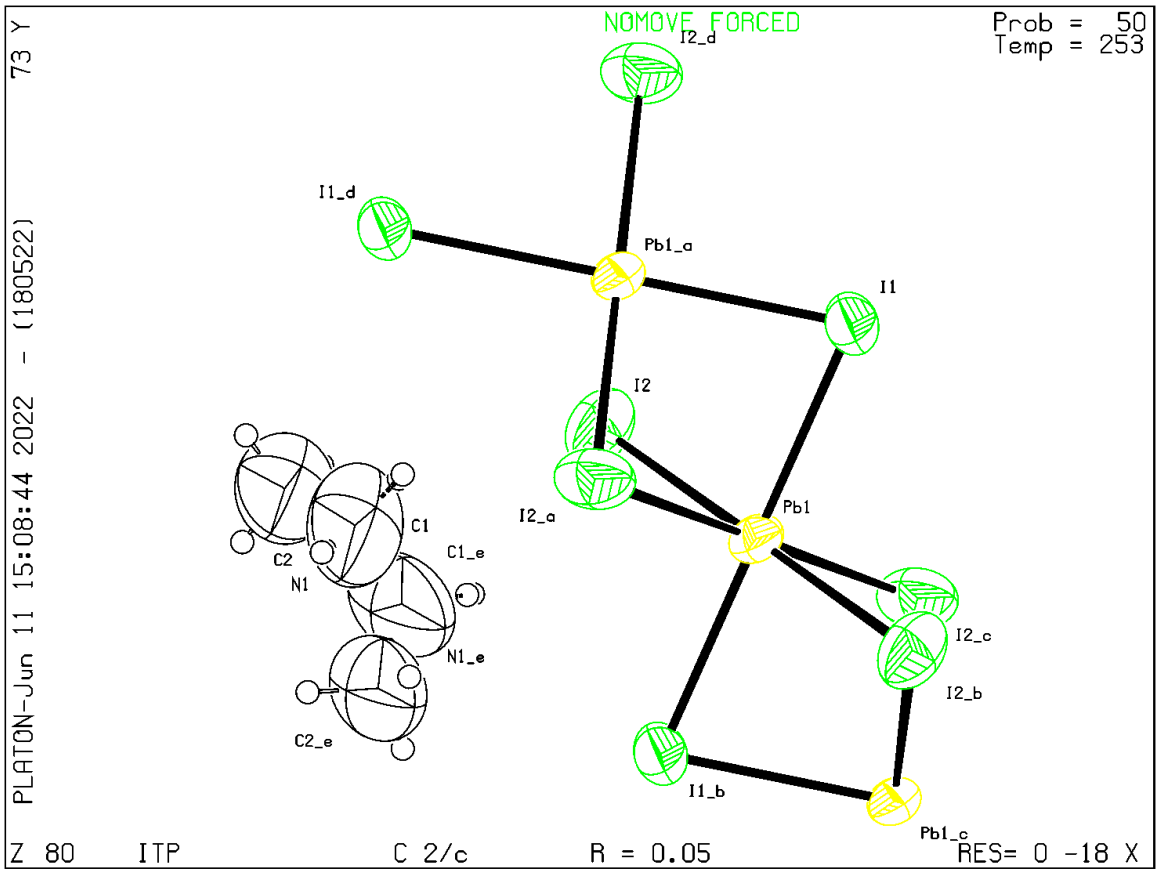
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 18/05/2022; check.def file version of 17/05/2022

Datablock LTP - ellipsoid plot



Datablock ITP - ellipsoid plot



Datablock HTP - ellipsoid plot