checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1208_a

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: 1208_a

Bond precision: C-C = 0.0160 A Wavelength=0.71073

Cell: a=12.094(3) b=12.656(3) c=16.868(4)
alpha=84.788(7) beta=88.519(7) gamma=82.676(7)
Temperature: 289 K

	Calculated	Reported
Volume	2549.9(11)	2549.9(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C47 H35 I4 N7 Ni O5 Pb2	C47 H35 I3 N7 Ni O5 Pb2, I
Sum formula	C47 H35 I4 N7 Ni O5 Pb2	C47 H35 I4 N7 Ni O5 Pb2
Mr	1758.51	1758.51
Dx,g cm-3	2.290	2.290
Z	2	2
Mu (mm-1)	9.424	9.424
F000	1620.0	1620.0
F000'	1604.45	
h,k,lmax	13,14,18	13,14,18
Nref	7382	7348
Tmin,Tmax	0.265,0.243	0.580,0.745
Tmin'	0.223	

Correction method= # Reported T Limits: Tmin=0.580 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 23.317

R(reflections)= 0.0481(5979) wR2(reflections)= 0.1128(7348)

S = 1.037 Npar= 601

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

```
THETM01_ALERT_3_B  The value of sine(theta_max)/wavelength is less than 0.575
           Calculated sin(theta_max)/wavelength =    0.5569
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).         11 Note
               1  0  0,  -1  1  0,   0  1  0,   1  1  0,   0 -1  1,  -1  0  1,
               0  0  1,   1  0  1,   0  1  1,   1  1  1,   0  0  2,
```

Alert level C

```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C47 H35 I4 N7 Ni O5 Pb2
             Rep.: C47 H35 I3 N7 Ni O5 Pb2, I
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.8 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  N   Ueq(max)/Ueq(min) Range        3.5 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        5.5 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         I1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Pb3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N3 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01598 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.557         22 Report
             -10  8  0, -10  8  1,  -7 11  1, -13  1  3, -13  0  4, -12  4  4,
              -5 12  5,   1 -3  6,  12 -2  7, -12 -2  8,  12  5  8,   4 13  8,
               6 12  9,  10  7 11,   0 12 11, -10  1 12,   1 11 13,   2 11 13,
               9  0 14,   0  7 17,   2  7 17,   2  5 18,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.19Ang From I2              1.59 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.70Ang From I3             -2.23 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.68Ang From I3             -2.21 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.80Ang From I2             -2.11 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.65Ang From I3             -2.09 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.57Ang From I2             -1.95 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.61Ang From I2             -1.92 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.63Ang From I2             -1.77 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.58Ang From I3             -1.67 eA-3
```

Alert level G

```
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          66 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      50.00 Why ?
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...          2 Units
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)       0.007 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP 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
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used      0.0100 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1      --I1       .       22.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1      --I2       .       40.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1      --I4_a     .       54.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb3      --I3       .       23.7 s.u.
```

```
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb3      --I2_b     .       27.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb2      --I1       .       28.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb2      --I2       .       48.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb2      --I4_a     .       61.2 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)         2% Note
PLAT794_ALERT_5_G Tentative Bond Valency for Pb3       (II)      .       2.04 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1       (II)      .       2.23 Info
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON          14 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        615 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still         57% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
                1 -3  6,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.809 Note
             Predicted wR2: Based on SigI**2  4.02 or SHELX Weight 10.88
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

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

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

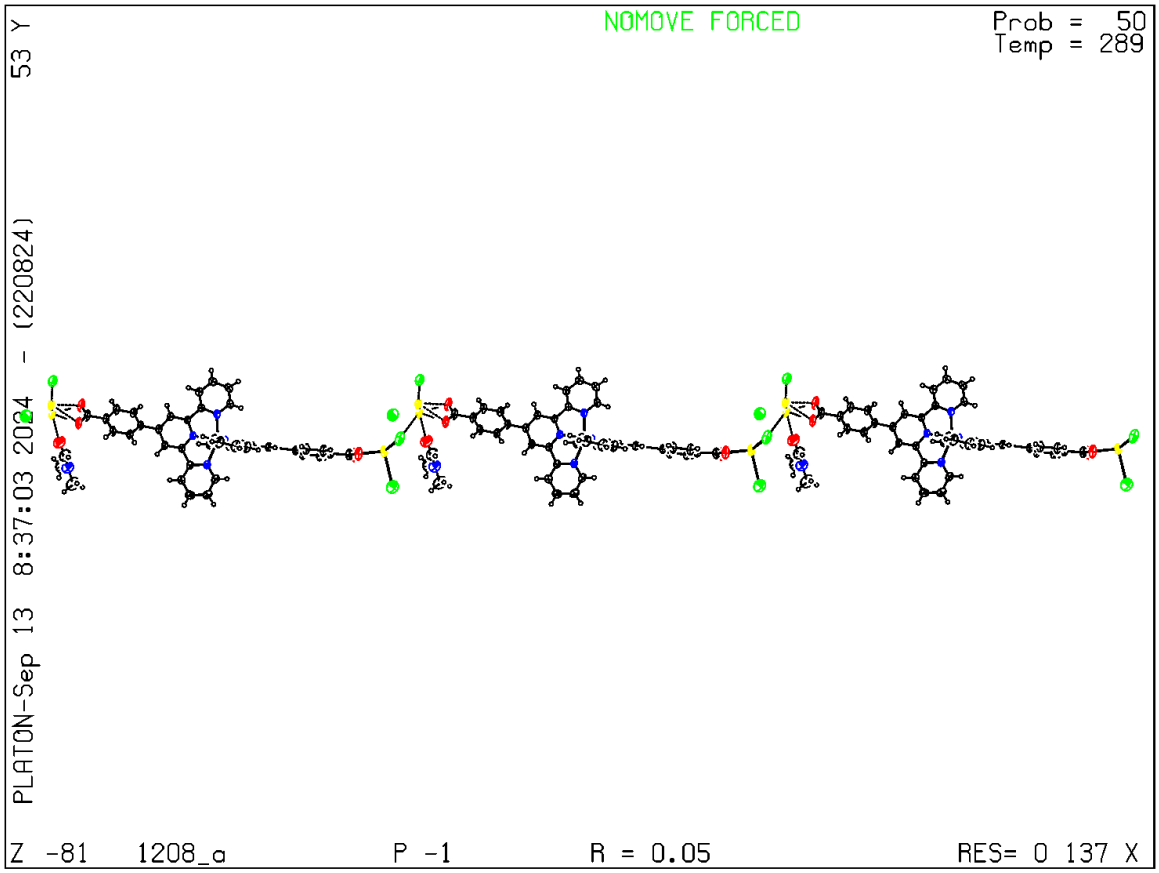
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 22/08/2024; check.def file version of 21/08/2024

Datablock 1208_a - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_231208c_0m

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: mo_231208c_0m

```
Bond precision:   C-C = 0.0101 A           Wavelength=0.71076

Cell:           a=12.0479(12)      b=12.6442(10)     c=16.8631(15)
                alpha=84.801(4)    beta=88.484(2)    gamma=82.612(2)
Temperature:    289 K
```

	Calculated	Reported
Volume	2536.8(4)	2536.8(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C47 H35 Co I4 N7 O5 Pb2	C47 H35 Co I3 N7 O5 Pb2, I
Sum formula	C47 H35 Co I4 N7 O5 Pb2	C47 H35 Co I4 N7 O5 Pb2
Mr	1758.75	1758.73
Dx,g cm-3	2.303	2.302
Z	2	2
Mu (mm-1)	9.429	9.429
F000	1618.0	1618.0
F000'	1602.47	
h,k,lmax	14,14,19	14,14,19
Nref	8676	8656
Tmin,Tmax	0.265,0.243	0.432,0.745
Tmin'	0.223	

```
Correction method= # Reported T Limits: Tmin=0.432 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.998           Theta(max)= 24.738

R(reflections)= 0.0338( 7378)                    wR2(reflections)=
                                                 0.0711( 8656)
S = 1.030                  Npar= 597
```

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

```
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).         11 Note
                1  0  0,  -1  1  0,   0  1  0,   1  1  0,   0 -1  1,  -1  0  1,
                0  0  1,   1  0  1,   0  1  1,   1  1  1,   0  0  2,
```

Alert level C

```
RADNW01_ALERT_1_C  The radiation wavelength lies outside the expected range
           for the supplied radiation type. Expected range 0.71065-0.71075
           Wavelength given =    0.71076
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5888
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C47 H35 Co I4 N7 O5 Pb2
             Rep.: C47 H35 Co I3 N7 O5 Pb2, I
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.8 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        5.6 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O4 Check
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        Pb2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N7 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01007 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.589         10 Report
             -13  4  2, -10  9  3,  -5 13  4,  -4 13  7, -11 -7  9,  -9  0 15,
              -4  9 15,  -6  6 16,  -7  0 17,   6  4 18,
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.73Ang From I4             -2.09 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.61Ang From I4             -1.83 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.53Ang From I4             -1.76 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.79Ang From I2             -1.69 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.55Ang From I2             -1.64 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.78Ang From I2             -1.62 eA-3
```

Alert level G

```
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          65 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      20.00 Why ?
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
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1      --I1       .       17.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1      --I4       .       60.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1      --I3_b     .       91.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb2      --I2       .       26.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb2      --I3       .       11.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb2      --I4_a     .       34.4 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       1.92 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2       (II)      .       2.04 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (III)     .       2.78 Info
```

```
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON          10 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        606 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        65% Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.712 Note
              Predicted wR2: Based on SigI**2  2.62 or SHELX Weight  6.90
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  21 ALERT type 2 Indicator that the structure model may be wrong or deficient
   8 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   6 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

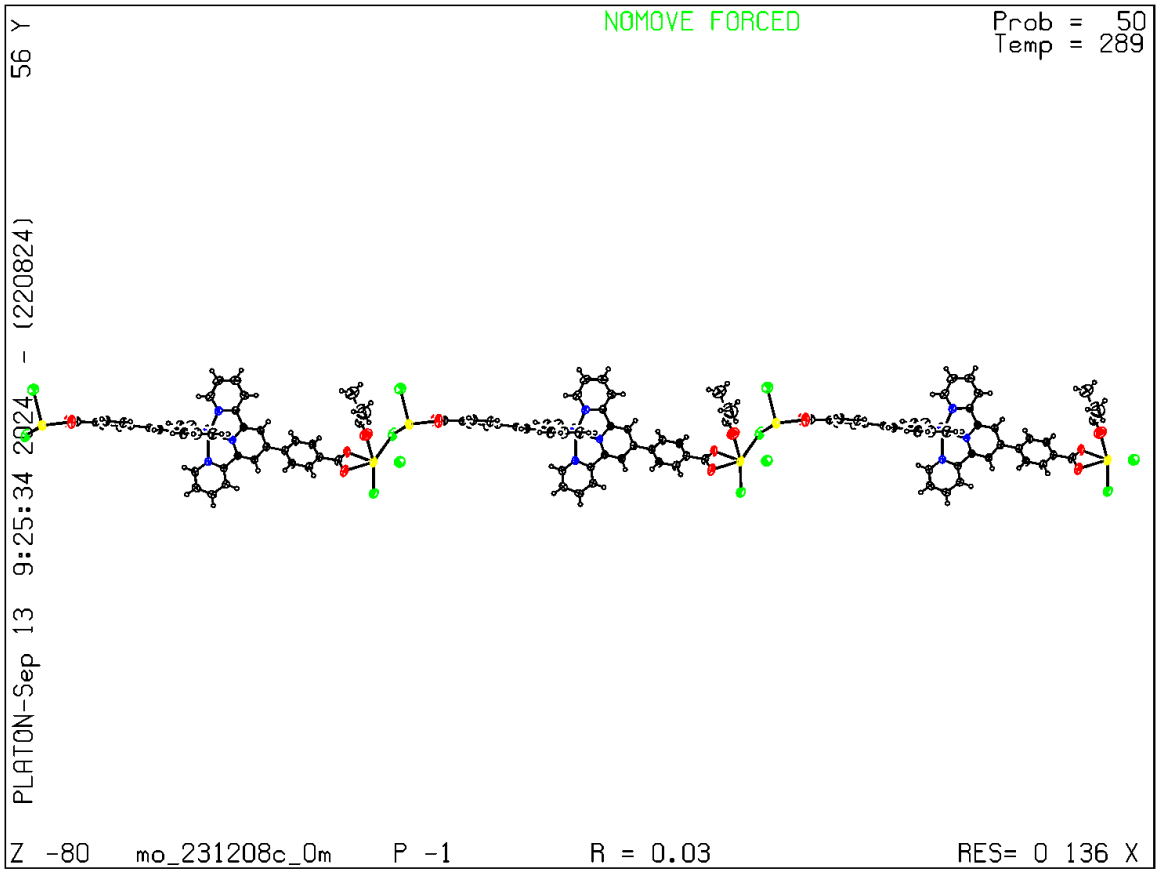
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 22/08/2024; check.def file version of 21/08/2024

Datablock mo_231208c_0m - ellipsoid plot



checkCIF/PLATON report

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

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_231129b_01m_a

Bond precision: C-C = 0.0170 A Wavelength=0.71073

Cell: a=12.295(3) b=12.487(3) c=16.692(4)
alpha=85.561(8) beta=87.022(9) gamma=81.497(9)
Temperature: 278 K

	Calculated	Reported
Volume	2524.8(11)	2524.8(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C47 H35 Fe I4 N7 O5 Pb2	C47 H35 Fe I3 N7 O5 Pb2, I
Sum formula	C47 H35 Fe I4 N7 O5 Pb2	C47 H35 Fe I4 N7 O5 Pb2
Mr	1755.67	1755.65
Dx,g cm-3	2.309	2.309
Z	2	2
Mu (mm-1)	9.432	9.432
F000	1616.0	1616.0
F000'	1600.46	
h,k,lmax	14,14,19	14,14,19
Nref	8614	8602
Tmin,Tmax	0.265,0.243	0.378,0.746
Tmin'	0.223	

Correction method= # Reported T Limits: Tmin=0.378 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 24.707

R(reflections)= 0.0573(5859) wR2(reflections)= 0.1326(8602)

S = 1.071 Npar= 597

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

```
RINTA01_ALERT_3_B  The value of Rint is greater than 0.18
           Rint given   0.230
```

Alert level C

```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
          Calculated sin(theta_max)/wavelength =    0.5881
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C47 H35 Fe I4 N7 O5 Pb2
             Rep.: C47 H35 Fe I3 N7 O5 Pb2, I
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.8 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  N   Ueq(max)/Ueq(min) Range        3.5 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        5.3 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O1 Check
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        Pb2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N1 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............      0.017 Ang.
```

Alert level G

```
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms         65 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........      0.230 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      30.00 Why ?
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
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1      --I05      .       10.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1      --I07      .       51.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1      --I2_b     .       39.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb2      --I0B      .       21.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb2      --I2       .       16.2 s.u.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          3 Note
             I0B     I05     I07
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.96000 Dev...       0.01 Ang.
             C47      -H47C            1_555   1_555 ........     #  113 Check
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.96000 Dev...       0.01 Ang.
             C48      -H48C            1_555   1_555 ........     #  116 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       1.88 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2       (II)      .       2.01 Info
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON          11 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        631 Note
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          2 Note
              -2 -1  3,  -1  1  0,
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain

```
 1 ALERT level B = A potentially serious problem, consider carefully
10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
21 ALERT level G = General information/check it is not something unexpected

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

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Datablock mo_231129b_01m_a - ellipsoid plot