# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) p21c

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: p21c

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```
Bond precision:   C-C = 0.0144 A          Wavelength=0.71073

Cell:             a=12.862(5)     b=17.754(7)          c=19.260(7)
                  alpha=90        beta=94.926(11)      gamma=90
Temperature:      296 K
```

| | Calculated | Reported |
|---|---|---|
| Volume | 4382(3) | 4382(3) |
| Space group | P 21/c | P 1 21/c 1 |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C44 H28 Br4 Co N6 O4 Pb2 [+ solvent] | C44 H28 Br4 Co N6 O4 Pb2 |
| Sum formula | C44 H28 Br4 Co N6 O4 Pb2 [+ solvent] | C44 H28 Br4 Co N6 O4 Pb2 |
| Mr | 1497.66 | 1497.67 |
| Dx,g cm-3 | 2.270 | 2.270 |
| Z | 4 | 4 |
| Mu (mm-1) | 11.737 | 11.738 |
| F000 | 2788.0 | 2788.0 |
| F000' | 2760.46 | |
| h,k,lmax | 14,20,22 | 14,20,22 |
| Nref | 7239 | 7098 |
| Tmin,Tmax | 0.094,0.136 | 0.418,0.745 |
| Tmin' | 0.060 | |

```
Correction method= # Reported T Limits: Tmin=0.418 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.981           Theta(max)= 24.435
```

R(reflections)= 0.0849( 4601)

wR2(reflections)= 0.1767( 7098)

S = 1.062 Npar= 454

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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.

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## Alert level C

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.164
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5820
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .........      0.164 Report
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        Br3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Pb2 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.01441 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      8.778 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.680 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          7 Note
                 1  0  0,   1  1  0,   0  2  0,  -1  1  1,   0  1  1,   1  1  1,
                 0  0  2,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.582        134 Report
                 4  0  0,   3  1  0,   1  2  0,   2  2  0,   1  5  0,   2  5  0,
                 2  7  0,   0  8  0,  -5  1  1,  -2  1  1,   3  1  1,  -1  2  1,
                 0  2  1,   2  2  1,  -5  3  1,  -2  3  1,   1  3  1,   5  3  1,
                -6  4  1,  -1  4  1,   1  4  1,   2  4  1,   3  4  1,   0  5  1,
                -1  6  1,   2  6  1,  -4  7  1,   4 17  1,   0 20  1,   2  0  2,
                 4  0  2,  -3  1  2,   3  1  2,  -1  2  2,   6  2  2,  -2  3  2,
                 3  3  2,  -1  4  2,   0  4  2,   4  4  2,   5  4  2,  -5  5  2,
                -2  5  2,   0  5  2,  -4  6  2,  -2  6  2,   0  7  2,   3  7  2,
                 0  8  2,  -3  9  2,  -6  1  3,  -5  1  3,  -1  1  3,   0  1  3,
                 3  1  3,  -1  2  3,   0  2  3,   4  2  3,  -2  3  3,  -1  4  3,
                 2  4  3,   4  4  3,   0  5  3,  -4  6  3,  -1  6  3,   4  6  3,
                 2  7  3,   2  8  3,  -5  0  4,  -4  0  4,  -2  0  4,  -1  0  4,
                 1  0  4,   4  0  4,  -5  1  4,  -1  1  4,  -5  2  4,  -4  2  4,
                -2  2  4,  -1  2  4,   1  2  4,   4  2  4,   0  3  4,  -4  4  4,
                -2  4  4,  -1  4  4,  -4  5  4,   0  5  4,   3  5  4,  -1  6  4,
                 0  7  4,   1  7  4,  -2  8  4,   3  8  4,   6 16  4,   0  1  5,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.70Ang From Pb1             1.73 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.44Ang From Pb1             1.54 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.10Ang From O3              1.54 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.63Ang From Pb2            -2.06 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.51Ang From Pb2            -2.02 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.57Ang From Pb2            -1.93 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.86Ang From Pb2            -1.73 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H34       .      -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H39       .      -0.43 eA-3
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## Alert level G

```
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms         61 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     200.00 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      --Br3      .        6.7 s.u.
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure         49 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       2.42 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2       (II)      .       2.33 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (III)     .       3.02 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        570 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still         33% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         128 Note
               -6  1  3,  -6  4  1,  -5  0  4,  -5  1  1,  -5  1  3,  -5  1  4,
               -5  2  4,  -5  3  1,  -5  3  5,  -5  5  2,  -4  0  4,  -4  2  4,
               -4  4  4,  -4  5  4,  -4  6  2,  -4  6  3,  -4  7  1,  -3  0  6,
               -3  0  8,  -3  1  2,  -3  2  6,  -3  4  7,  -3  6  5,  -3  9  2,
               -2  0  4,  -2  1  1,  -2  1  7,  -2  2  4,  -2  2  6,  -2  3  1,
               -2  3  2,  -2  3  3,  -2  4  4,  -2  5  2,  -2  6  2,  -2  8  4,
               -1  0  4,  -1  1  3,  -1  1  4,  -1  2  1,  -1  2  2,  -1  2  3,
               -1  2  4,  -1  4  1,  -1  4  2,  -1  4  3,  -1  4  4,  -1  6  1,
               -1  6  3,  -1  6  4,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.804 Note
             Predicted wR2: Based on SigI**2  6.30 or SHELX Weight 16.63
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 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
19 **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

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

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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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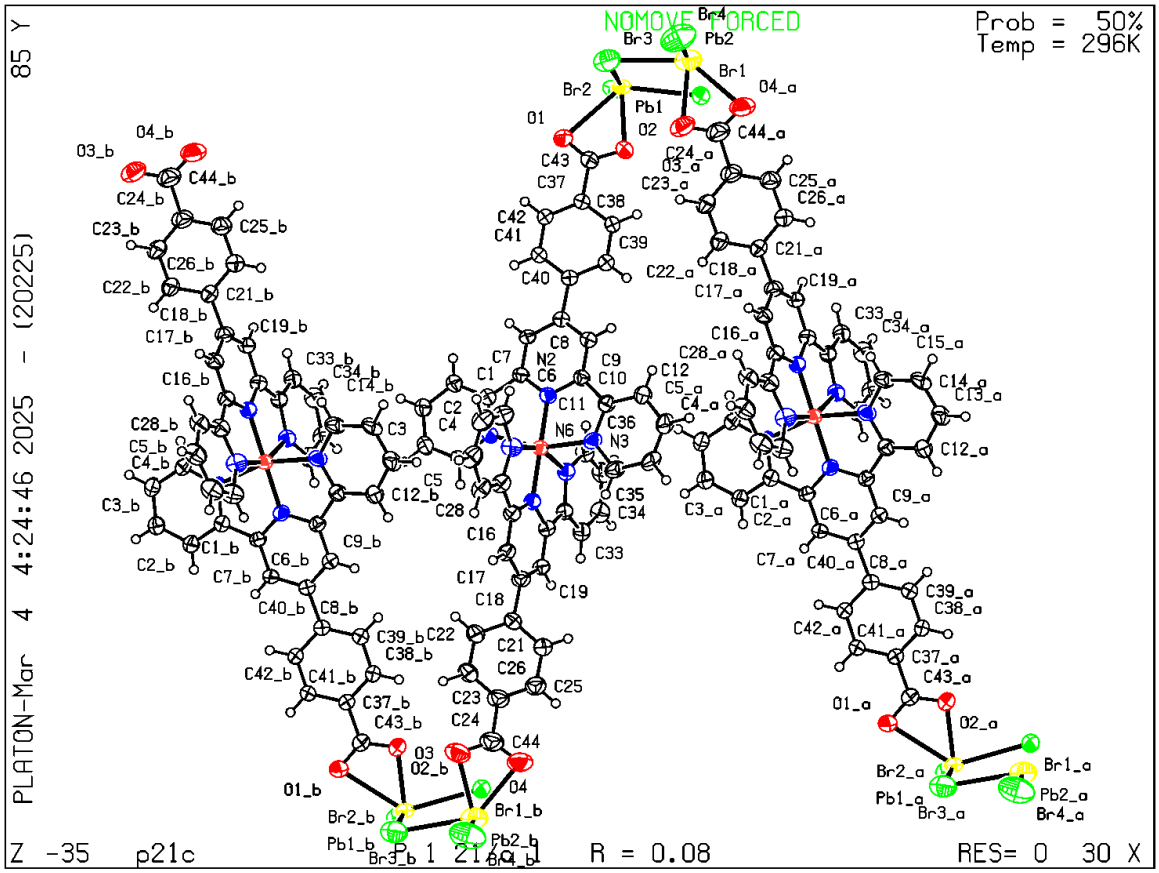
**PLATON version of 02/02/2025; check.def file version of 02/02/2025**

**Datablock p21c** - ellipsoid plot



# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_fe_br_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: mo_fe_br_a

---

```
Bond precision:   C-C = 0.0155 A          Wavelength=0.71073

Cell:             a=12.8594(19)     b=17.715(2)         c=19.123(3)
                  alpha=90          beta=96.048(4)      gamma=90
Temperature:      273 K
```

| | Calculated | Reported |
|---|---|---|
| Volume | 4332.1(11) | 4332.0(10) |
| Space group | P 21/c | P 1 21/c 1 |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C44 H28 Br4 Fe N6 O4 Pb2 [+ solvent] | C44 H28 Br4 Fe N6 O4 Pb2 |
| Sum formula | C44 H28 Br4 Fe N6 O4 Pb2 [+ solvent] | C44 H28 Br4 Fe N6 O4 Pb2 |
| Mr | 1494.58 | 1494.59 |
| Dx,g cm-3 | 2.292 | 2.292 |
| Z | 4 | 4 |
| Mu (mm-1) | 11.824 | 11.825 |
| F000 | 2784.0 | 2784.0 |
| F000' | 2756.44 | |
| h,k,lmax | 15,21,22 | 15,21,22 |
| Nref | 7669 | 7596 |
| Tmin,Tmax | 0.137,0.170 | 0.420,0.745 |
| Tmin' | 0.103 | |

```
Correction method= # Reported T Limits: Tmin=0.420 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.990          Theta(max)= 25.048
```

R(reflections)= 0.0948( 5425)

wR2(reflections)= 0.2003( 7596)

S = 1.017 Npar= 458

---

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

```
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        Br1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        Br2 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0155 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C18      - C21      .       1.53 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C35      - C44      .       1.53 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     12.734 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.108 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          7 Note
                1  0  0,   1  1  0,   0  2  0,  -1  1  1,   0  1  1,   1  1  1,
                0  0  2,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.596         67 Report
                4  0  0,   0  4  0,  -5  1  1,   3  1  1,   0  2  1,   2  2  1,
               -1  4  1,   2  4  1,  -2  9  1,   1  0  2,   2  0  2,   4  0  2,
                1  1  2,   3  1  2,   0  2  2,  -2  3  2,   3  3  2,   0  4  2,
                4  4  2,   0  5  2,   3  5  2,   3  7  2,   0  8  2,   2  8  2,
                5  8  2,  -3  9  2,  -5  1  3,  -1  2  3,   4  2  3,  -2  3  3,
               -1  4  3,   2  4  3,  -1  6  3,  -4  0  4,  -2  0  4,  -5  1  4,
                0  1  4,  -4  2  4,   4  2  4,   0  3  4, -15  4  4,  -4  4  4,
               -1  4  4,   0  5  4,   3  5  4,   0  7  4, -13 11  4,   0  1  5,
                0  3  5,   1  6  5,  -1  7  5,   9 16  5,   0  0  6,  -4  1  6,
                5  1  6,  -3  2  6,  -5  6  6,  -2  1  7,   1  1  7,   5  1  7,
               -1  7  7,   0 20  7,  -1  1 12,   5 16 12, -13  0 14,  -2 14 17,
                4  3 21,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.62Ang From Pb3              1.96 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.01Ang From Br3              1.95 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.42Ang From Pb1              1.65 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.53Ang From Pb2             -2.34 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.70Ang From Pb2             -2.30 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.55Ang From Pb2             -2.20 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  1.00Ang From Pb3             -1.55 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7        .       -0.38 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H14       .       -0.34 eA-3
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## Alert level G

```
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms          62 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      300.00 Why ?
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
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        273 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        273 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1      --Br2      .        14.5 s.u.
```

```
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1      --Br3_a    .       17.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb3      --Br2      .       14.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb3      --Br3_a    .       16.0 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)         2% Note
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure         41 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2       (II)      .       2.36 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        609 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        40% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        58 Note
               -5  1  1,  -5  1  3,  -5  1  4,  -5  6  6,  -4  0  4,  -4  1  6,
               -4  2  4,  -4  4  4,  -3  2  6,  -3  9  2,  -2  0  4,  -2  1  7,
               -2  3  2,  -2  3  3,  -2  9  1,  -1  1 12,  -1  2  3,  -1  4  1,
               -1  4  3,  -1  4  4,  -1  6  3,  -1  7  5,  -1  7  7,   0  0  6,
                0  1  4,   0  1  5,   0  2  1,   0  2  2,   0  3  4,   0  3  5,
                0  4  0,   0  4  2,   0  5  2,   0  5  4,   0  7  4,   0  8  2,
                1  1  2,   1  1  7,   1  6  5,   2  0  2,   2  2  1,   2  4  1,
                2  4  3,   2  8  2,   3  1  1,   3  1  2,   3  3  2,   3  5  2,
                3  5  4,   3  7  2,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      3.092 Note
             Predicted wR2: Based on SigI**2  6.48 or SHELX Weight 19.68
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 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
  18 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  23 ALERT level G = General information/check it is not something unexpected

   3 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
   9 ALERT type 3 Indicator that the structure quality may be low
   5 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
```

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**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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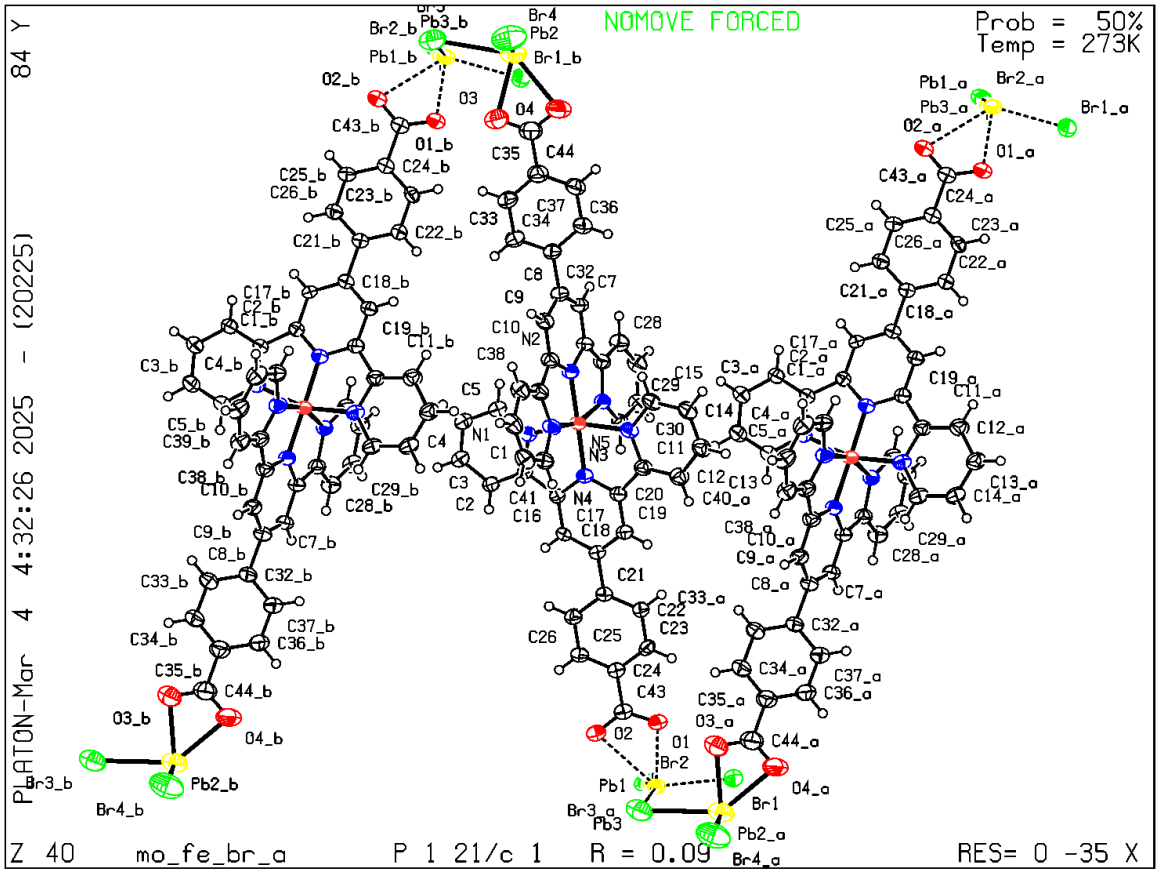
**PLATON version of 02/02/2025; check.def file version of 02/02/2025**

**Datablock mo_fe_br_a** - ellipsoid plot



# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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No syntax errors found. CIF dictionary Interpreting this report

# Datablock: 1

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```
Bond precision:   C-C = 0.0277 A           Wavelength=0.71073

Cell:              a=12.882(8)      b=17.747(12)       c=19.366(11)
                   alpha=90         beta=84.80(3)      gamma=90
Temperature:       296 K

                 Calculated                  Reported
Volume           4409(5)                     4409(5)
Space group      P 21/c                      P 1 21/c 1
Hall group       -P 2ybc                     -P 2ybc
Moiety formula   C44 H28 Br4 N6 Ni O4 Pb2    C44 H28 Br4 N6 Ni O4 Pb2
Sum formula      C44 H28 Br4 N6 Ni O4 Pb2    C44 H28 Br4 N6 Ni O4 Pb2
Mr               1497.42                     1497.45
Dx,g cm-3        2.256                       2.256
Z                4                           4
Mu (mm-1)        11.716                      11.715
F000             2792.0                      2792.0
F000'            2764.44
h,k,lmax         14,19,21                    14,19,21
Nref             6178                        6112
Tmin,Tmax        0.121,0.173                 0.430,0.745
Tmin'            0.084

Correction method= # Reported T Limits: Tmin=0.430 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.989            Theta(max)= 23.059

R(reflections)= 0.1078( 2440)                    wR2(reflections)=
                                                 0.2403( 6112)
S = 1.090                  Npar= 454
```

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 A

RINTA01_ALERT_3_A The value of Rint is greater than 0.25
Rint given 0.311

**Author Response: This is due to the poor diffraction of the crystal.**

PLAT020_ALERT_3_A The Value of Rint is Greater Than 0.12 ..... 0.311 Report

**Author Response: This is due to the poor diffraction of the crystal.**

## Alert level B

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5511

**Author Response: crystal diffracted weakly, the diffraction limit can only reach 0.91.**

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02773 Ang.

**Author Response: Poor data quality in context with large assymetric unit.**

## Alert level C

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 40% Check
PLAT082_ALERT_2_C High R1 Value ..... 0.11 Report
PLAT157_ALERT_4_C Non-standard Monoclinic Beta Angle less 90 Deg 84.80 Degree
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS <= 60 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 15.443 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.989 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 10 Note
1 0 0, 1 1 0, 0 2 0, -1 1 1, 0 1 1, 1 1 1,
0 2 1, 0 0 2, 1 0 2, 0 1 2,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.551 56 Report
14 2 0, -14 1 1, -3 1 1, 2 1 1, 14 3 1, -8 16 1,
7 17 1, -4 0 2, 4 0 2, -3 1 2, 1 2 2, 14 3 2,
0 4 2, 1 4 2, -13 7 2, 0 1 3, 14 3 3, 0 5 3,
9 15 3, 2 0 4, -4 2 4, -1 2 4, 14 2 4, -12 9 4,
0 1 5, 14 1 5, -9 14 5, -13 3 6, 0 1 7, 13 6 7,
13 4 9, -10 10 9, 13 1 10, 13 2 10, 12 7 10, -9 11 10,
8 7 11, -6 14 11, 12 4 12, -10 4 13, -7 10 14, 7 12 14,
10 3 16, 8 3 17, -7 4 17, 9 4 17, -5 0 18, 7 3 18,
6 8 18, 5 9 18, -1 1 19, 1 2 19, 1 0 20, -1 1 21,
1 2 21, 0 3 21,

```
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.31Ang From Pb1            1.99 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.95Ang From Pb2           -2.07 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.72Ang From Pb2           -2.02 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.74Ang From Pb2           -1.93 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.68Ang From Pb2           -1.85 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3       .      -0.40 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H4       .      -0.37 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H7       .      -0.36 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H12      .      -0.45 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H26      .      -0.43 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H40      .      -0.43 eA-3
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## Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         2 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j)  Restrained non-H-Atoms        61 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         1 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    230.00 Why ?
PLAT158_ALERT_4_G The Input Unit Cell is NOT Standard/Reduced .....    Please Check
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
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used    0.0100 Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         1 Note
             Ni03
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       2.46 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2       (II)      .       2.30 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ni03      (II)      .       2.24 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       571 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        13 Note
               -4  0  2,  -4  2  4,  -3  1  1,  -3  1  2,  -1  2  4,   0  1  3,
                0  1  5,   0  1  7,   0  4  2,   0  5  3,   1  2  2,   1  4  2,
                2  1  1,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.4 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     1.689 Note
             Predicted wR2: Based on SigI**2 14.23 or SHELX Weight 22.05
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
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   2 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
  18 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  18 ALERT type 2 Indicator that the structure model may be wrong or deficient
  12 ALERT type 3 Indicator that the structure quality may be low
   6 ALERT type 4 Improvement, methodology, query or suggestion
   5 ALERT type 5 Informative message, check
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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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**PLATON version of 02/02/2025; check.def file version of 02/02/2025**

**Datablock 1** - ellipsoid plot