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: 1025

Bond precision: C-C = 0.0176 A Wavelength=0.71073

Cell: a=12.706(6) b=17.590(8) c=19.196(9)
alpha=90 beta=94.703(18) gamma=90
Temperature: 283 K

	Calculated	Reported
Volume	4276(3)	4276(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C44 H28 Cl4 Co N6 O4 Pb2 [+ solvent]	C44 H28 Cl4 Co N6 O4 Pb2
Sum formula	C44 H28 Cl4 Co N6 O4 Pb2 [+ solvent]	C44 H28 Cl4 Co N6 O4 Pb2
Mr	1319.86	1319.83
Dx,g cm-3	2.050	2.050
Z	4	4
Mu (mm-1)	8.540	8.541
F000	2500.0	2500.0
F000'	2478.34	
h,k,lmax	14,20,22	14,20,22
Nref	7234	7195
Tmin,Tmax	0.343,0.426	0.560,0.745
Tmin'	0.317	

Correction method= # Reported T Limits: Tmin=0.560 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 24.631

R(reflections)= 0.0667(5734)

wR2(reflections)= 0.2173(7195)

S = 1.042 Npar= 550

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

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.157
THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5864
PLAT234_ALERT_4_C Large Hirshfeld Difference O016 --C01P . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C00Q --C01A . 0.16 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O016 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C01P Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.1 Note
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01759 Ang.

Alert level G

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 ..... 0.157 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.14 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 44.46 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pb --Cl06 . 7.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pb01 --Cl06_a . 7.3 s.u.
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 49 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 88 Note

Pb01	Co03	Cl04	Cl05	Cl06	Cl07	O008	N009
O00A	N00B	N00C	N00D	N00E	N00F	C00G	O00H
C00I	C00J	C00K	H00K	C00L	C00M	C00N	H00N
C00O	H00O	C00P	C00Q	H00Q	C00R	C00S	H00S
C00T	C00U	H00U	C00V	H00V	C00W	C00X	H00X
C00Y	H00Y	C00Z	H00Z	C010	C011	H011	C012
H012	C013	H013	C014	C015	O016	C017	H017
C018	H018	C019	C01A	C01B	H01B	C01C	H01C
C01D	H01D	C01E	H01E	C01F	H01F	C01G	H01G
C01H	H01H	C01I	C01J	H01J	C01K	H01K	C01L
H01L	C01M	H01M	C01N	H01N	C01O	H01O	C01P

PLAT794_ALERT_5_G Tentative Bond Valency for Pb (II) . 2.24 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb01 (II) . 2.22 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Co03 (III) . 2.96 Info
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed ! Info

---

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

```
  7 ALERT type 2 Indicator that the structure model may be wrong or deficient
  4 ALERT type 3 Indicator that the structure quality may be low
  5 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

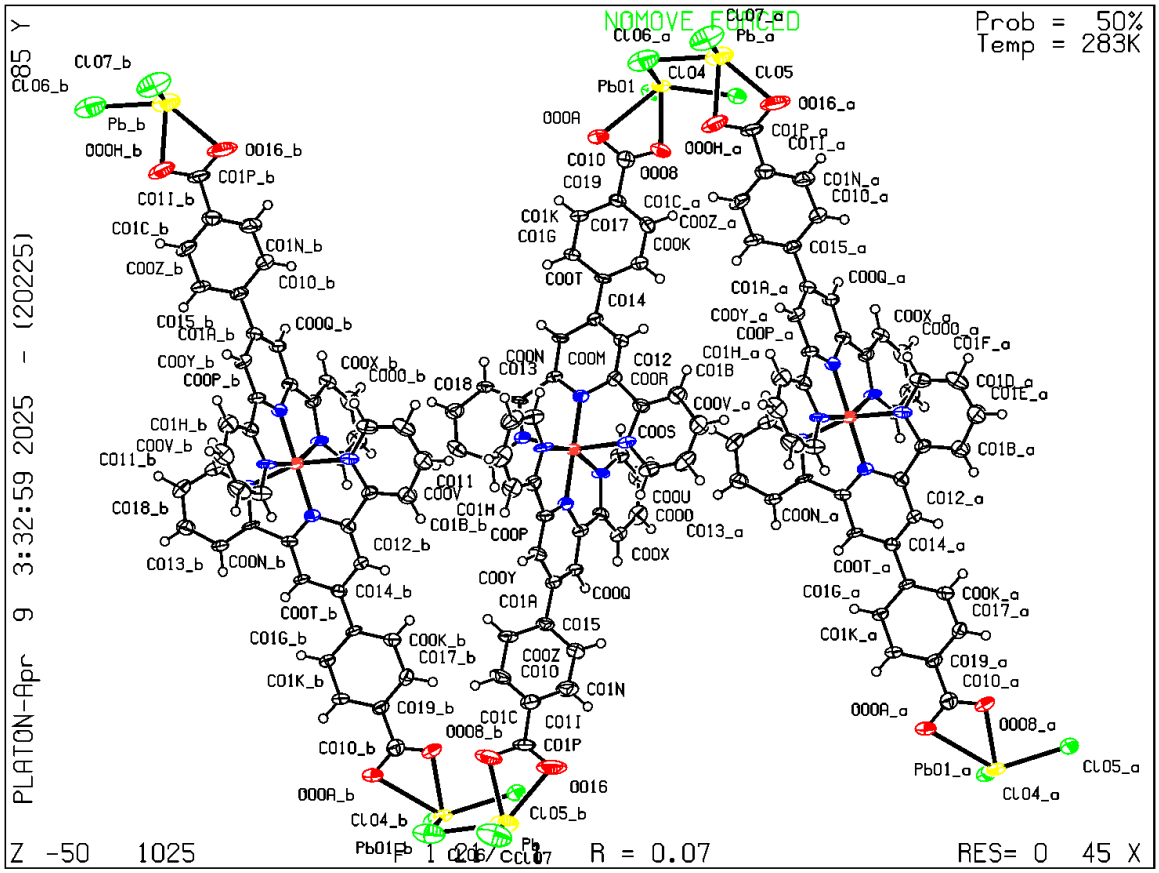
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

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

Datablock 1025 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_240920c_0m_b

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_240920c_0m_b

```
Bond precision:   C-C = 0.0135 A           Wavelength=0.71073

Cell:              a=12.629(3)     b=17.519(4)          c=18.925(4)
                   alpha=90        beta=95.414(8)       gamma=90
Temperature:       286 K
```

	Calculated	Reported
Volume	4168.4(16)	4168.3(16)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C44 H28 Cl4 Fe N6 O4 Pb2 [+ solvent]	C44 H28 Cl4 Fe N6 O4 Pb2, 2[H2O]
Sum formula	C44 H28 Cl4 Fe N6 O4 Pb2 [+ solvent]	C44 H32 Cl4 Fe N6 O6 Pb2
Mr	1316.78	1352.78
Dx,g cm-3	2.098	2.156
Z	4	4
Mu (mm-1)	8.711	8.717
F000	2496.0	2576.0
F000'	2474.32	
h,k,lmax	14,20,22	14,20,22
Nref	6892	6713
Tmin,Tmax	0.295,0.270	0.589,0.745
Tmin'	0.248	

```
Correction method= # Reported T Limits: Tmin=0.589 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.974           Theta(max)= 24.437
```

R(reflections)= 0.0526(5853)

wR2(reflections)= 0.1130(6713)

S = 1.091 Npar= 550

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

```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
           Calculated sin(theta_max)/wavelength =    0.5821
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.974 Why?
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01345 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.469 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         171 Report
                 2  0  0,   3  1  0,   4  1  0,   1  2  0,   2  2  0,   3  2  0,
                 4  2  0,   0  4  0,   1  4  0,   1  5  0,   2  5  0,   5  5  0,
                 0  6  0,   3  6  0,   2  7  0,   5  7  0,   1  9  0,  -5  1  1,
                 2  1  1,   3  1  1,   5  1  1,   2  2  1,  -5  3  1,   0  3  1,
                 1  3  1,   5  3  1,  -6  4  1,  -2  4  1,  -1  4  1,   1  4  1,
                 2  4  1,  -2  5  1,   0  5  1,   1  5  1,   4  5  1,  -1  6  1,
                 1  6  1,   2  6  1,  -3  7  1,  -1  8  1,  -3  9  1,   1  9  1,
                 4  9  1,  -6  0  2,  -2  0  2,  -1  0  2,   1  0  2,   2  0  2,
                 4  0  2,  -3  1  2,  -1  1  2,   1  1  2,   3  1  2,   5  1  2,
                -3  2  2,   0  2  2,   1  2  2,   2  2  2,   6  2  2,  -2  3  2,
                 3  3  2,   6  3  2,  -4  4  2,  -1  4  2,   2  4  2,   4  4  2,
                 0  5  2,   3  5  2,  -2  6  2,   1  6  2,   5  6  2,  -5  7  2,
                -2  7  2,   0  7  2,   2  7  2,   3  7  2,   0  8  2,  -5  1  3,
                -3  1  3,  -2  1  3,   3  1  3,  -1  2  3,   0  2  3,   4  2  3,
                -3  3  3,  -2  3  3,   0  3  3,   3  3  3,  -1  4  3,   2  4  3,
                 0  5  3,   3  5  3,  -4  6  3,  -1  6  3,   0  6  3,   2  7  3,
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.60Ang From Pb2             1.86 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.38Ang From Pb2             1.62 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.48Ang From Pb2             1.56 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.67Ang From Pb2             1.52 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.69Ang From Pb1            -2.43 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.67Ang From Pb1            -2.06 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.45Ang From Pb1            -2.06 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.46Ang From Pb1            -1.84 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H33       .      -0.33 eA-3
```

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:C44 H32 Cl4 Fe1 N6 O6 Pb2
           Atom count from the _atom_site data:  C44 H28 Cl4 Fe1 N6 O4 Pb2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    4
```

```
          From the CIF: _chemical_formula_sum  C44 H32 Cl4 Fe N6 O6 Pb2
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        176.00    176.00    0.00
          H        128.00    112.00   16.00
          Cl        16.00     16.00    0.00
          Fe         4.00      4.00    0.00
          N         24.00     24.00    0.00
          O         24.00     16.00    8.00
          Pb         8.00      8.00    0.00
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
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: C44 H28 Cl4 Fe N6 O4 Pb2
             Rep.: C44 H32 Cl4 Fe N6 O6 Pb2
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C44 H28 Cl4 Fe N6 O4 Pb2
             Rep.: C44 H28 Cl4 Fe N6 O4 Pb2, 2[H2O]
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      80.00 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      --Cl2      .        5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb2      --Cl2_a    .       13.5 s.u.
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure         42 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          9 Note
             C00P    C00X    H00X    C01B    H01B    C014    H014    C015
             H015
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       2.34 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2       (II)      .       2.33 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............        595 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
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         68% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        170 Note
              -6  0  2,  -6  4  1,  -5  1  1,  -5  1  3,  -5  3  1,  -5  5  4,
              -5  7  2,  -4  0  4,  -4  3  8,  -4  4  2,  -4  4  7,  -4  6  3,
              -4  6  5,  -4  7  4,  -3  0  6,  -3  0  8,  -3  1  2,  -3  1  3,
              -3  1  6,  -3  1  8,  -3  2  2,  -3  2  5,  -3  2  6,  -3  3  3,
              -3  4  7,  -3  6  5,  -3  7  1,  -3  8  7,  -3  9  1,  -2  0  2,
              -2  0  4,  -2  1  3,  -2  1  7,  -2  1  9,  -2  2  6,  -2  2  8,
              -2  3  2,  -2  3  3,  -2  3  5,  -2  3  8,  -2  4  1,  -2  4  4,
              -2  5  1,  -2  6  2,  -2  7  2,  -2  8  4,  -1  0  2,  -1  0  4,
              -1  1  2,  -1  1  4,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      3.506 Note
             Predicted wR2: Based on SigI**2  3.22 or SHELX Weight 10.35
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
0 **ALERT level B** = A potentially serious problem, consider carefully
15 **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

```
 16 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
  4 ALERT type 5 Informative message, check
```

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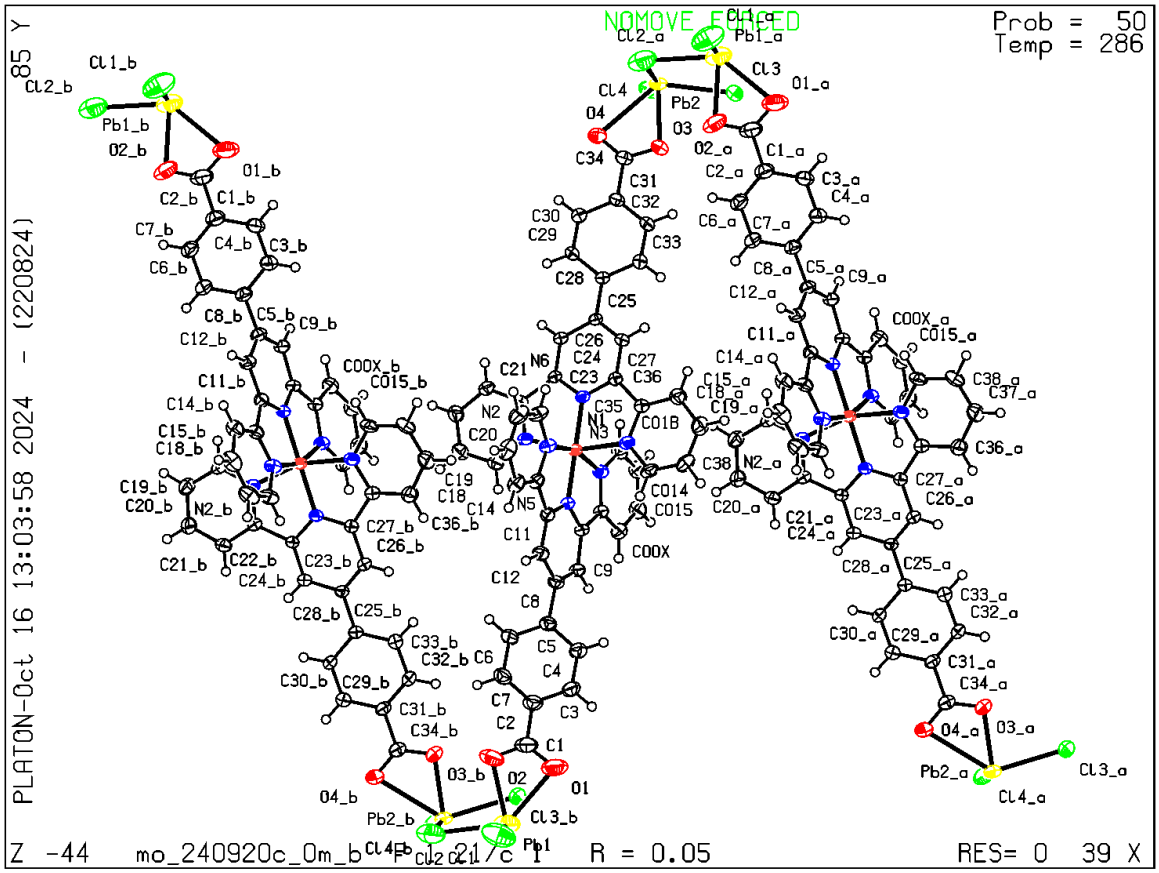
PLATON version of 22/08/2024; check.def file version of 21/08/2024

Datablock mo_240920c_0m_b - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_240906f_a

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: mo_240906f_a

```
Bond precision:   C-C = 0.0140 A           Wavelength=0.71073

Cell:             a=12.4027(10)     b=17.5860(9)       c=19.0115(14)
                  alpha=90          beta=94.761(3)     gamma=90
Temperature:      100 K
```

	Calculated	Reported
Volume	4132.4(5)	4132.4(5)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C44 H28 Cl4 N6 Ni O4 Pb2 [+ solvent]	C44 H28 Cl4 N6 Ni O4 Pb2, 0.75[H2O]
Sum formula	C44 H28 Cl4 N6 Ni O4 Pb2 [+ solvent]	C44 H29.50 Cl4 N6 Ni O4.75 Pb2
Mr	1319.62	1333.12
Dx,g cm-3	2.121	2.143
Z	4	4
Mu (mm-1)	8.891	8.894
F000	2504.0	2534.0
F000'	2482.31	
h,k,lmax	14,20,22	14,20,22
Nref	6835	6689
Tmin,Tmax	0.287,0.263	0.003,0.014
Tmin'	0.242	

```
Correction method= # Reported T Limits: Tmin=0.003 Tmax=0.014
AbsCorr = MULTI-SCAN

Data completeness= 0.979           Theta(max)= 24.437
```

R(reflections)= 0.0516(6193)

wR2(reflections)= 0.1116(6689)

S = 1.089 Npar= 550

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

```
THETM01_ALERT_3_C  The value of sine(theta_max)/wavelength is less than 0.590
          Calculated sin(theta_max)/wavelength =    0.5821
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.979 Why?
PLAT234_ALERT_4_C Large Hirshfeld Difference O2       --C1       .       0.16 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O1 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............      0.014 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.488 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          9 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,   0  1  2,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.582        137 Report
                4  0  0,   3  1  0,   1  2  0,   2  2  0,   1  3  0,   2  3  0,
                3  3  0,   2  5  0,   3  5  0,   0  6  0,   1  6  0,   2  7  0,
                0 10  0,  -5  1  1,  -4  1  1,  -2  1  1,   2  1  1,   3  1  1,
               -2  2  1,   1  2  1,   2  2  1,   3  2  1,  -2  4  1,  -1  4  1,
                0  4  1,   1  4  1,   2  4  1,  -3  5  1,  -1  6  1,   0  6  1,
                1  6  1,  -1  8  1,  -3  9  1,   1  9  1,  -3  0  2,  -2  0  2,
                1  0  2,   2  0  2,  -3  1  2,  -1  1  2,   1  1  2,   2  1  2,
                3  1  2,  -4  2  2,  -1  2  2,   0  2  2,   1  2  2,   3  2  2,
               -4  3  2,  -3  3  2,  -2  3  2,   2  3  2,   3  3  2,  -1  4  2,
                2  4  2,  -4  5  2,  -2  5  2,   0  5  2,   3  5  2,  -2  6  2,
                1  6  2,   3  7  2,   0  8  2,  -5  1  3,  -4  1  3,   0  1  3,
                1  1  3,  -2  2  3,  -1  2  3,   0  2  3,   1  2  3,  -4  3  3,
                0  3  3,   3  3  3,  -1  4  3,   0  4  3,   1  4  3,   2  4  3,
               -1  6  3,   0  6  3,   2  7  3,  -4  0  4,  -3  0  4,  -2  0  4,
               -1  0  4,   0  0  4,  -2  1  4,  -1  1  4,  -6  2  4,  -1  2  4,
                0  2  4,   0  3  4,  -3  4  4,  -1  4  4,   0  4  4,   0  5  4,
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.54Ang From Pb1            -2.49 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.47Ang From Pb1            -2.34 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.48Ang From Pb1            -2.21 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.71Ang From Pb1            -2.13 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.97Ang From O1      .      -0.52 eA-3
```

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:C44 H29.5 Cl4 N6 Ni1 O4.75 Pb2
           Atom count from the _atom_site data:  C44 H28 Cl4 N6 Ni1 O4 Pb2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C44 H29.50 Cl4 N6 Ni O4.75 Pb2
          TEST: Compare cell contents of formula and atom_site data
```

```
          atom    Z*formula  cif sites diff
          C        176.00    176.00    0.00
          H        118.00    112.00    6.00
          Cl        16.00     16.00    0.00
          N         24.00     24.00    0.00
          Ni         4.00      4.00    0.00
          O         19.00     16.00    3.00
          Pb         8.00      8.00    0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: C44 H28 Cl4 N6 Ni O4 Pb2
             Rep.: C44 H29.50 Cl4 N6 Ni O4.75 Pb2
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C44 H28 Cl4 N6 Ni O4 Pb2
             Rep.: C44 H28 Cl4 N6 Ni O4 Pb2, 0.75[H2O]
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      80.00 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb1      --Cl2      .        9.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pb2      --Cl2_b    .        8.5 s.u.
PLAT432_ALERT_2_G Short Inter X...Y Contact  C7       ..C19      .       3.20 Ang.
                                          -1-x,2-y,1-z  =      3_476 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure         42 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1       (II)      .       2.34 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2       (II)      .       2.32 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1       (II)      .       2.24 Info
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
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        85% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          2 Note
              -2  0  2,  -2  0  6,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File        137 Note
              -6  0  6,  -6  2  4,  -5  1  1,  -5  1  3,  -4  0  4,  -4  1  1,
              -4  1  3,  -4  2  2,  -4  3  2,  -4  3  3,  -4  3  5,  -4  5  2,
              -3  0  2,  -3  0  4,  -3  0  6,  -3  0  8,  -3  1  2,  -3  1  6,
              -3  1  8,  -3  2  5,  -3  2  6,  -3  3  2,  -3  4  4,  -3  5  1,
              -3  9  1,  -2  0  2,  -2  0  4,  -2  0  6,  -2  1  1,  -2  1  4,
              -2  1  7,  -2  2  1,  -2  2  3,  -2  2  8,  -2  2  9,  -2  3  2,
              -2  4  1,  -2  5  2,  -2  6  2,  -2  8  4,  -2 10  4,  -1  0  4,
              -1  1  2,  -1  1  4,  -1  1  9,  -1  1 11,  -1  2  2,  -1  2  3,
              -1  2  4,  -1  4  1,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....       3.748 Note
             Predicted wR2: Based on SigI**2  2.98 or SHELX Weight 10.25
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
   0 ALERT level B = A potentially serious problem, consider carefully
  13 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

   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 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
   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 mo_240906f_a - ellipsoid plot