

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) FO5377, FO5454, FO5472, FO5524

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: FO5472

Bond precision: C-C = 0.0041 Å

Wavelength=0.71073

Cell: a=9.3025(3) b=10.1879(4) c=15.2499(6)
 alpha=104.318(2) beta=106.891(2) gamma=95.661(2)
Temperature: 133 K

| | Calculated | Reported |
|----------------|---------------|---------------|
| Volume | 1317.12(9) | 1317.12(8) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C32 H27 Br P2 | C32 H27 Br P2 |
| Sum formula | C32 H27 Br P2 | C32 H27 Br P2 |
| Mr | 553.38 | 553.39 |
| Dx,g cm-3 | 1.395 | 1.395 |
| Z | 2 | 2 |
| Mu (mm-1) | 1.701 | 1.701 |
| F000 | 568.0 | 568.0 |
| F000' | 568.00 | |
| h,k,lmax | 12,13,19 | 12,13,19 |
| Nref | 6129 | 5981 |
| Tmin,Tmax | 0.922,0.937 | 0.632,0.746 |
| Tmin' | 0.922 | |

Correction method= # Reported T Limits: Tmin=0.632 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.976

Theta(max)= 27.650

R(reflections)= 0.0380(5142)

wR2(reflections)= 0.0863(5981)

S = 1.064

Npar= 424

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

| | | | | |
|-------------------|---|------------------------|--------|-------------|
| PLAT029_ALERT_3_C | _diffn_measured_fraction_theta_full | value Low | 0.976 | Note |
| PLAT245_ALERT_2_C | U(iso) H23 | Smaller than U(eq) C23 | by ... | 0.011 AngSq |
| PLAT350_ALERT_3_C | Short C-H (X0.96,N1.08A) | C11 - H11 | .. | 0.83 Ang. |
| PLAT911_ALERT_3_C | Missing # FCF Refl Between THmin & STh/L= | 0.600 | | 37 Report |



Alert level G

| | | | | |
|-------------------|--|---------------------------------------|-------------|--------|
| PLAT005_ALERT_5_G | No Embedded Refinement Details found | in the CIF | Please Do ! | |
| PLAT154_ALERT_1_G | The s.u.'s on the Cell Angles are Equal | ..(Note) | 0.002 | Degree |
| PLAT164_ALERT_4_G | Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. | | 27 | Note |
| PLAT899_ALERT_4_G | SHELXL97 | is Deprecated and Succeeded by SHELXL | 2014 | Note |
| PLAT910_ALERT_3_G | Missing # of FCF Reflection(s) Below Theta(Min) | | 3 | Note |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= | 0.600 | 109 | Note |
| PLAT913_ALERT_3_G | Missing # of Very Strong Reflections in FCF | | 2 | Note |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density | | 14 | Note |

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

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

Datablock: FO5377

Bond precision: C-C = 0.0043 A

Wavelength=0.71073

Cell: a=12.4695(2) b=20.0948(3) c=20.8722(3)

alpha=90 beta=90.828(1) gamma=90

Temperature: 133 K

| | Calculated | Reported |
|----------------|---------------|---------------|
| Volume | 5229.45(14) | 5229.44(14) |
| Space group | P 21/c | P 21/c |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C64 H54 Mg P4 | C64 H54 Mg P4 |
| Sum formula | C64 H54 Mg P4 | C64 H54 Mg P4 |
| Mr | 971.26 | 971.26 |
| Dx,g cm-3 | 1.234 | 1.234 |
| Z | 4 | 4 |
| Mu (mm-1) | 0.197 | 0.197 |
| F000 | 2040.0 | 2040.0 |
| F000' | 2042.40 | |
| h,k,lmax | 16,26,27 | 16,26,27 |
| Nref | 11999 | 11953 |
| Tmin,Tmax | 0.989,0.992 | 0.638,0.746 |
| Tmin' | 0.989 | |

Correction method= # Reported T Limits: Tmin=0.638 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 27.492

R(reflections)= 0.0576(10279) wR2(reflections)= 0.1342(11953)

S = 1.128 Npar= 839

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 | 7.1 | Ratio |
| PLAT245_ALERT_2_C | U(iso) H12 | Smaller than U(eq) C12 by ... | 0.016 | AngSq |
| PLAT245_ALERT_2_C | U(iso) H24 | Smaller than U(eq) C24 by ... | 0.035 | AngSq |
| PLAT340_ALERT_3_C | Low Bond Precision on | C-C Bonds | 0.0043 | Ang. |
| PLAT350_ALERT_3_C | Short C-H (X0.96,N1.08A) | C25 - H25 .. | 0.81 | Ang. |
| PLAT350_ALERT_3_C | Short C-H (X0.96,N1.08A) | C50 - H50 .. | 0.84 | Ang. |
| PLAT350_ALERT_3_C | Short C-H (X0.96,N1.08A) | C63 - H63 .. | 0.84 | Ang. |
| PLAT906_ALERT_3_C | Large K value in the Analysis of Variance | | 2.895 | Check |
| PLAT911_ALERT_3_C | Missing # FCF Refl Between THmin & STh/L= | 0.600 | 24 | Report |



Alert level G

| | | | | |
|-------------------|--|-----------------|------|-------|
| PLAT083_ALERT_2_G | SHELXL Second Parameter in WGHT | Unusually Large | 6.51 | Why ? |
| PLAT870_ALERT_4_G | ALERTS Related to Twinning Effects Suppressed .. | | ! | Info |
| PLAT910_ALERT_3_G | Missing # of FCF Reflection(s) Below Theta(Min) | | 2 | Note |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= | 0.600 | 21 | Note |
| PLAT913_ALERT_3_G | Missing # of Very Strong Reflections in FCF | | 2 | Note |
| PLAT933_ALERT_2_G | Number of OMIT records in Embedded RES | | 4 | Note |

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

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
 6 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: FO5524

Bond precision: C-C = 0.0156 A Wavelength=0.71073

Cell: a=12.3778(3) b=17.8753(4) c=14.3016(3)
 alpha=90 beta=103.851(1) gamma=90
 Temperature: 133 K

| | Calculated | Reported |
|----------------|---------------------------------------|---------------------------------------|
| Volume | 3072.31(12) | 3072.31(12) |
| Space group | P 21/n | P 21/n |
| Hall group | -P 2yn | -P 2yn |
| Moiety formula | C48 H68 Ca2 I2 O10 P2, 2(C4 H10 O) | C48 H68 Ca2 I2 O10 P2, 2(C4 H10 O) |
| Sum formula | C56 H88 Ca2 I2 O12 P2 | C56 H88 Ca2 I2 O12 P2 |
| Mr | 1349.16 | 1349.16 |
| Dx,g cm-3 | 1.458 | 1.458 |
| Z | 2 | 2 |
| Mu (mm-1) | 1.299 | 1.299 |
| F000 | 1392.0 | 1392.0 |
| F000' | 1391.96 | |
| h,k,lmax | 16,23,18 | 16,23,18 |
| Nref | 7057 | 6997 |
| Tmin,Tmax | 0.948,0.959 | 0.675,0.746 |
| Tmin' | 0.943 | |

Correction method= # Reported T Limits: Tmin=0.675 Tmax=0.746
 AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 27.500

R(reflections)= 0.0701(6320) wR2(reflections)= 0.1914(6997)

S = 1.062 Npar= 275

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

| | | | |
|-------------------|--|------|--------------|
| PLAT201_ALERT_2_B | Isotropic non-H Atoms in Main Residue(s) | 7 | Report |
| PLAT220_ALERT_2_B | Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range | 6.5 | Ratio |
| PLAT241_ALERT_2_B | High 'MainMol' Ueq as Compared to Neighbors of | C18 | Check |
| PLAT241_ALERT_2_B | High 'MainMol' Ueq as Compared to Neighbors of | C22 | Check |
| PLAT360_ALERT_2_B | Short C(sp3)-C(sp3) Bond C2T - C3T .. | 1.24 | Ang. |
| PLAT411_ALERT_2_B | Short Inter H...H Contact H3TA .. H9A .. | 1.99 | Ang. |
| PLAT420_ALERT_2_B | D-H Without Acceptor O1T -- H1TA ... | | Please Check |
| PLAT420_ALERT_2_B | D-H Without Acceptor O1T -- H1TB ... | | Please Check |

Alert level C

| | | | |
|-------------------|--|---------|--------|
| PLAT202_ALERT_3_C | Isotropic non-H Atoms in Anion/Solvent | 5 | Check |
| PLAT222_ALERT_3_C | Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range | 5.3 | Ratio |
| PLAT241_ALERT_2_C | High 'MainMol' Ueq as Compared to Neighbors of | C21 | Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | Ca1 | Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | 05 | Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | C17 | Check |
| PLAT242_ALERT_2_C | Low 'MainMol' Ueq as Compared to Neighbors of | C19 | Check |
| PLAT243_ALERT_4_C | High 'Solvent' Ueq as Compared to Neighbors of | O1T | Check |
| PLAT243_ALERT_4_C | High 'Solvent' Ueq as Compared to Neighbors of | C2T | Check |
| PLAT244_ALERT_4_C | Low 'Solvent' Ueq as Compared to Neighbors of | C1T | Check |
| PLAT244_ALERT_4_C | Low 'Solvent' Ueq as Compared to Neighbors of | C3T | Check |
| PLAT342_ALERT_3_C | Low Bond Precision on C-C Bonds | 0.01563 | Ang. |
| PLAT360_ALERT_2_C | Short C(sp3)-C(sp3) Bond C17 - C18 .. | 1.34 | Ang. |
| PLAT360_ALERT_2_C | Short C(sp3)-C(sp3) Bond C23 - C24 .. | 1.39 | Ang. |
| PLAT360_ALERT_2_C | Short C(sp3)-C(sp3) Bond C3T - C4T .. | 1.37 | Ang. |
| PLAT906_ALERT_3_C | Large K value in the Analysis of Variance | 4.287 | Check |
| PLAT910_ALERT_3_C | Missing # of FCF Reflection(s) Below Theta(Min) | 5 | Note |
| PLAT911_ALERT_3_C | Missing # FCF Refl Between THmin & STh/L= 0.600 | 27 | Report |
| PLAT913_ALERT_3_C | Missing # of Very Strong Reflections in FCF | 7 | Note |
| PLAT918_ALERT_3_C | Reflection(s) with I(obs) much Smaller I(calc) . | 3 | Check |
| PLAT971_ALERT_2_C | Check Calcd Residual Density 1.15A From C23 | 2.03 | eA-3 |
| PLAT971_ALERT_2_C | Check Calcd Residual Density 0.95A From C18 | 1.90 | eA-3 |
| PLAT971_ALERT_2_C | Check Calcd Residual Density 0.80A From C22 | 1.66 | eA-3 |
| PLAT971_ALERT_2_C | Check Calcd Residual Density 1.20A From C21 | 1.59 | eA-3 |
| PLAT977_ALERT_2_C | Check the Negative Difference Density on H1TB | -0.32 | eA-3 |
| PLAT977_ALERT_2_C | Check the Negative Difference Density on H3TA | -0.35 | eA-3 |
| PLAT977_ALERT_2_C | Check the Negative Difference Density on H17B | -0.36 | eA-3 |
| PLAT978_ALERT_2_C | Number C-C Bonds with Positive Residual Density | 0 | Note |

Alert level G

| | | | |
|-------------------|---|-------|-------------|
| PLAT005_ALERT_5_G | No Embedded Refinement Details found in the CIF | | Please Do ! |
| PLAT007_ALERT_5_G | Number of Unrefined Donor-H Atoms | 2 | Report |
| PLAT083_ALERT_2_G | SHELXL Second Parameter in WGHT Unusually Large | 17.98 | Why ? |
| PLAT720_ALERT_4_G | Number of Unusual/Non-Standard Labels | 10 | Note |
| PLAT899_ALERT_4_G | SHELXL97 is Deprecated and Succeeded by SHELXL | 2014 | Note |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= 0.600 | 29 | Note |

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

8 **ALERT level B** = A potentially serious problem, consider carefully

28 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

6 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
25 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
7 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

Datablock: FO5454

Bond precision: C-C = 0.0020 A Wavelength=0.71073

Cell: a=11.4609(3) b=11.5457(3) c=14.2003(3)
alpha=90 beta=90 gamma=90
Temperature: 133 K

| | Calculated | Reported |
|----------------|-------------------|-------------------|
| Volume | 1879.04(8) | 1879.04(8) |
| Space group | P b c n | P b c n |
| Hall group | -P 2n 2ab | -P 2n 2ab |
| Moiety formula | C12 H28 Br2 Ca O5 | C12 H28 Br2 Ca O5 |
| Sum formula | C12 H28 Br2 Ca O5 | C12 H28 Br2 Ca O5 |
| Mr | 452.22 | 452.24 |
| Dx,g cm-3 | 1.599 | 1.599 |
| Z | 4 | 4 |
| Mu (mm-1) | 4.600 | 4.600 |
| F000 | 920.0 | 920.0 |
| F000' | 919.09 | |
| h,k,lmax | 14,14,18 | 14,14,18 |
| Nref | 2156 | 2138 |
| Tmin,Tmax | 0.802,0.847 | |
| Tmin' | 0.802 | |

Correction method= Not given

Data completeness= 0.992 Theta(max)= 27.490

R(reflections)= 0.0185(1974) wR2(reflections)= 0.0452(2138)

S = 1.099 Npar= 94

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

| | |
|--|-----------|
| PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 | 11 Report |
| PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF | 9 Note |

● Alert level G

| | | |
|-------------------|---|-------------|
| PLAT005_ALERT_5_G | No Embedded Refinement Details found in the CIF | Please Do ! |
| PLAT910_ALERT_3_G | Missing # of FCF Reflection(s) Below Theta(Min) | 4 Note |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= 0.600 | 3 Note |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density | 2 Note |

-
- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected
- 0 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
3 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
-

checkCIF publication errors

● Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.

-
- 0 **ALERT level A** = Data missing that is essential or data in wrong format
1 **ALERT level G** = General alerts. Data that may be required is missing
-

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.







