

R(reflections)= 0.0147(651)	wR2(reflections)= 0.0327(689)
S = 1.228	Npar= 29

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

PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight Differ by ..	3.97	Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.85Ang From Pb1	-1.65	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.64Ang From Pb1	-1.56	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: H4 O8 Pb6
Atom count from the _atom_site data: O8 Pb6

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 H4 O8 Pb6
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
H	8.00	0.00	8.00
O	16.00	16.00	0.00
Pb	12.00	12.00	0.00

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 6.19 Why ?
PLAT300_ALERT_4_G Atom Site Occupancy of O1 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2 Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 54% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 1) 12.25 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 70.0 Degree

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

- 4 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
1 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

