

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: I

Bond precision:	Pb- O = 0.0042 A	Wavelength=0.71069
Cell:	a=5.9131 (5)	b=7.8478 (6) c=16.8158 (15)
	alpha=90	beta=90.007 (6) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	780.33 (11)	780.33 (11)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yabc
Moiety formula	As Cu2 H7 O9 Pb	?
Sum formula	As Cu2 H7 O9 Pb	As Cu2 H7 O9 Pb
Mr	560.28	560.30
Dx, g cm ⁻³	4.769	4.769
Z	4	4
Mu (mm ⁻¹)	31.154	31.154
F000	1008.0	1008.0
F000'	998.89	
h, k, lmax	8, 11, 23	8, 11, 23
Nref	2268	2269
Tmin, Tmax	0.292, 0.688	0.035, 0.692
Tmin'	0.000	

Correction method= # Reported T Limits: Tmin=0.035 Tmax=0.692
AbsCorr = NUMERICAL

Data completeness= 1.000 Theta(max)= 29.990

R(reflections)= 0.0275 (1869)	wR2(reflections)= 0.0784 (2269)
S = 1.110	Npar= 140

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

PLAT417_ALERT_2_A	Short Inter D-H..H-D	H2OX1	..H2OX1	.	1.68 Ang.
		-x,2-y,1-z	=		3_576 Check

Alert level B

PLAT112_ALERT_2_B	ADDSYM Detects New (Pseudo) Symm. Elem	m			100 %Fit
PLAT112_ALERT_2_B	ADDSYM Detects New (Pseudo) Symm. Elem	b			100 %Fit
PLAT113_ALERT_2_B	ADDSYM Suggests Possible Pseudo/New Space Group				Pnma Check
PLAT416_ALERT_2_B	Short Intra D-H..H-D	H2OX1	..H2OX2	.	1.83 Ang.
		-1+x,y,z	=		1_455 Check
PLAT417_ALERT_2_B	Short Inter D-H..H-D	H2OX1	..H7	.	1.99 Ang.
		-x,2-y,1-z	=		3_576 Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O7	--H7	.	Please Check

Alert level C

PLAT127_ALERT_1_C	Implicit Hall Symbol Inconsistent with Explicit	-P	2yabc	Check	
PLAT314_ALERT_2_C	Small Angle for H2O: Metal-Ox2	-H2OX2	.	91.99 Degree	
PLAT481_ALERT_4_C	Long D...A H-Bond Reported	O7	..OX1	.	3.61 Ang.
PLAT481_ALERT_4_C	Long D...A H-Bond Reported	OX1	..O7	.	3.61 Ang.

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension				2 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF				Please Do !
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)			293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)			293 Check
PLAT303_ALERT_2_G	Full Occupancy Atom H6	with # Connections			2.00 Check
PLAT480_ALERT_4_G	Long H...A H-Bond Reported	H7	..OX1	.	2.77 Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported	H2OX1	..O7	.	2.78 Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels			6 Note
PLAT769_ALERT_4_G	CIF Embedded explicitly supplied scattering data				Please Note
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O1	--H7		2.87 Ang.
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O1	--H4		2.74 Ang.
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O2	--H7		2.99 Ang.
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O2	--H4		2.80 Ang.
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O2	--H1OX2		3.29 Ang.
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O3	--H7		3.17 Ang.
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O3	--H7		2.94 Ang.
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O3	--H4		3.22 Ang.
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O3	--H1OX1		3.27 Ang.
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O3	--H2OX1		3.33 Ang.
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O3	--H2OX1		3.10 Ang.
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O3	--H1OX2		2.96 Ang.
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O3	--H2OX2		2.92 Ang.
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O4	--H6		2.94 Ang.
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O4	--H6		3.11 Ang.
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O4	--H6		1.97 Ang.
PLAT778_ALERT_2_G	Check O..H..X Bond in CIF:	O4	--H1OX1		3.48 Ang.

PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	04	--H1OX1	3.00	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	04	--H1OX2	3.48	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	04	--H2OX2	2.63	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	05	--H4	2.08	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	05	--H1OX1	1.77	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	05	--H2OX1	2.90	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	05	--H1OX2	1.89	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	05	--H2OX2	3.24	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	06	--H7	3.18	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	06	--H4	2.97	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	06	--H4	3.10	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	06	--H4	3.21	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	06	--H1OX1	3.40	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	06	--H1OX1	3.27	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	06	--H1OX2	3.47	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	06	--H2OX2	3.05	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	07	--H6	2.98	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	07	--H2OX1	2.78	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	07	--H1OX2	3.20	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	07	--H2OX2	3.46	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox1	--H7	2.93	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox1	--H7	2.77	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox1	--H4	3.19	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox1	--H6	3.00	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox1	--H6	3.31	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox1	--H1OX1	3.19	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox1	--H2OX1	2.03	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox1	--H1OX2	3.07	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox1	--H1OX2	3.10	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox1	--H2OX2	1.80	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox1	--H2OX2	3.49	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox2	--H7	3.04	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox2	--H7	2.88	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox2	--H4	3.13	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox2	--H6	2.90	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox2	--H6	3.25	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox2	--H1OX1	2.80	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox2	--H1OX1	3.31	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox2	--H2OX1	2.57	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox2	--H2OX1	3.32	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox2	--H1OX2	2.88	Ang.
PLAT778_ALERT_2_G	Check	O..H..X	Bond	in	CIF:	Ox2	--H2OX2	3.02	Ang.
PLAT794_ALERT_5_G	Tentative	Bond	Valency	for	Pb1	(II)	.	1.83	Info
PLAT860_ALERT_3_G	Number of	Least-Squares	Restraints				9	Note
PLAT966_ALERT_5_G	Note:	Non-Standard	(i.e. 2.0)	OMIT	Threshold	of		3.0	Sig(I)

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- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
6 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
71 **ALERT level G** = General information/check it is not something unexpected
- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
68 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
6 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.

Datablock 1 - ellipsoid plot

