

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) PS_37_CCM_a8_Ca23Cu7Mg4_0m_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: PS_37_CCM_a8_Ca23Cu7Mg4_0m_a

Bond precision:	= 0.0000 A	Wavelength=0.71073	
Cell:	a=10.236(2)	b=10.236(2)	c=23.413(5)
	alpha=90	beta=90	gamma=120
Temperature:	293 K		
	Calculated	Reported	
Volume	2124.5(9)	2124.4(9)	
Space group	P 63/m m c	P 63/m m c	
Hall group	-P 6c 2c	-P 6c 2c	
Moiety formula	Cu, 3.296(Ca), 0.561(Mg)	Ca23 Cu7 Mg4	
Sum formula	Ca3.30 Cu Mg0.56	Ca23 Cu7 Mg4	
Mr	209.29	1463.86	
Dx, g cm ⁻³	2.290	2.288	
Z	14	2	
Mu (mm ⁻¹)	6.276	6.269	
F000	1423.1	1422.0	
F000'	1438.48		
h,k,lmax	15,15,36	15,15,36	
Nref	1595	1592	
Tmin,Tmax	0.798,0.882	0.661,0.747	
Tmin'	0.778		

Correction method= # Reported T Limits: Tmin=0.661 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 33.223

R(reflections)= 0.0403(1060)	wR2(reflections)= 0.1320(1592)
S = 1.156	Npar= 41

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

PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ... 1 Check



Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check



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:Ca23 Cu7 Mg4
Atom count from the _atom_site data: Ca23.07 Cu7 Mg3.93
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum Ca23 Cu7 Mg4
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Ca	46.00	46.14	-0.14
Cu	14.00	14.00	0.00
Mg	8.00	7.86	0.14

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 7 Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 8) 100% Note
PLAT301_ALERT_3_G Main Residue Disorder(Resd 9) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 1) 0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 2) 0.08 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 3) 0.17 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 4) 0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 5) 0.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 6) 0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 7) 0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 9) 0.08 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 10) 0.25 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 1 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 5 Note
Ca
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 2 Note

0	ALERT level A	= Most likely a serious problem - resolve or explain
1	ALERT level B	= A potentially serious problem, consider carefully
6	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
9	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
6	ALERT type 3	Indicator that the structure quality may be low
14	ALERT type 4	Improvement, methodology, query or suggestion
0	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 10/05/2023; check.def file version of 10/05/2023

