

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: shelx

Bond precision:	P- O = 0.0050 A	Wavelength=0.71080
Cell:	a=5.4262(11) b=5.4274(11) c=16.387(3)	alpha=87.61(3) beta=98.97(3) gamma=110.56(3)
Temperature:	100 K	
	Calculated	Reported
Volume	446.29(18)	446.27(18)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	Mg0.63 Mn4.28 O22 P4, 1.09(Ba)	?
Sum formula	Ba1.09 Mg0.63 Mn4.28 O22 P4	Ba1.09 Mg0.63 Mn4.28 O24 P4
Mr	876.03	910.84
Dx, g cm ⁻³	3.260	3.389
Z	1	1
Mu (mm ⁻¹)	5.804	5.835
F000	411.6	429.0
F000'	413.34	
h, k, lmax	7, 7, 22	7, 7, 22
Nref	2524	2301
Tmin, Tmax	0.869, 0.971	0.273, 0.433
Tmin'	0.815	

Correction method= # Reported T Limits: Tmin=0.273 Tmax=0.433
AbsCorr = MULTI-SCAN

Data completeness= 0.912 Theta(max)= 29.572

R(reflections)= 0.0495(2115) wR2(reflections)=
0.1401(2301)

S = 1.000 Npar= 157

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**

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.930 Why?

Author Response: The crystal was weakly diffracting

PLAT184_ALERT_1_A Missing _cell_measurement_theta_min Value Please Do !


Author Response: Cell measurement theta min and max values were not recorded by the data collection software

PLAT185_ALERT_1_A Missing _cell_measurement_theta_max Value Please Do !

Author Response: Cell measurement theta min and max values were not recorded by the data collection software

PLAT310_ALERT_2_A O999 Deleted (Close to Ba2) Dist ... 0.233 Ang.

Author Response: There is local disorder in the vicinity of M3 and Ba2 and OW11 are partially occupied sites

 **Alert level B**

PLAT005_ALERT_5_B No Embedded Refinement Details Found in the CIF Please Do !

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 34.81 Check
M3 (MG)

 **Alert level C**

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.

Absorption correction given as multi-scan

RADNW01_ALERT_1_C The radiation wavelength lies outside the expected range for the supplied radiation type. Expected range 0.71065-0.71075
Wavelength given = 0.71080

PLAT041_ALERT_1_C Calc. and Reported SumFormula 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

PLAT155_ALERT_4_C The Triclinic Unitcell is NOT Reduced Please Do !

PLAT220_ALERT_2_C NonSolvent Resd 1 Mn Ueq(max)/Ueq(min) Range 3.1 Ratio

PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 4.9 Ratio

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Ow12 Check

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label M3 Check

	BA2	M3				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Ow11 Check
	BA2	OW11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	M3 Check
	M3	O5				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	M3 Check
	M3	O5				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	M3 Check
	M3	OW12				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	M3 Check
	M3	OW12				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	M3 Check
	M3	OW11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	M3 Check
	M3	OW11				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3 Check
	M3	BA2	O5			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3 Check
	M3	BA2	O8			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3 Check
	M3	BA2	O5			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3 Check
	M3	BA2	OW12			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3 Check
	M3	BA2	OW11			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	Ow11 Check
	O5	BA2	OW11			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	Ow11 Check
	O8	BA2	OW11			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	Ow11 Check
	O5	BA2	OW11			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	Ow11 Check
	OW12	BA2	OW11			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3 Check
	M3	BA2	OW12			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	Ow11 Check
	OW11	BA2	OW12			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3 Check
	M3	BA2	O5			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	Ow11 Check
	OW11	BA2	O5			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3 Check
	M3	BA2	O7			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	Ow11 Check
	OW11	BA2	O7			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3 Check
	M3	BA2	BA2			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	Ow11 Check
	OW11	BA2	BA2			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3 Check
	M3	BA2	OW12			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	Ow11 Check
	OW11	BA2	OW12			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3 Check
	BA2	M3	BA2			
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3 Check
	BA2	M3	O5			

PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	BA2	M3	O5				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	BA2	M3	O5				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	BA2	M3	O5				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	O5	M3	O5				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	BA2	M3	OW12				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	BA2	M3	OW12				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	O5	M3	OW12				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	O5	M3	OW12				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	BA2	M3	OW12				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	BA2	M3	OW12				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	O5	M3	OW12				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	O5	M3	OW11				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	BA2	M3	OW11				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	BA2	M3	OW11				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	O5	M3	OW11				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	O5	M3	OW11				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	OW12	M3	OW11				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	BA2	M3	OW11				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	BA2	M3	OW11				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	O5	M3	OW11				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	O5	M3	OW11				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	OW12	M3	OW11				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	OW12	M3	OW11				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	Ow11	Check
	OW11	M3	OW11				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	P2	O5	M3				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check
	M3	O5	BA2				
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent	Label	M3	Check

	M3	O5	BA2		
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent Label	M3	Check
	M3	O5	BA2		
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent Label	M3	Check
	M3	OW11	BA2		
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent Label	M3	Check
	M3	OW12	BA2		
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent Label	M3	Check
	M3	OW12	BA2		
PLAT712_ALERT_1_C	ANGLE	Unknown or	Inconsistent Label	M3	Check
	M3	OW12	BA2		

● Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT017_ALERT_1_G	Check Scattering Type Consistency of M1 as	MN	
PLAT017_ALERT_1_G	Check Scattering Type Consistency of M2 as	MN	
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.03	Degree
PLAT300_ALERT_4_G	Atom Site Occupancy of M3MN Constrained at	0.28	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of M3MG Constrained at	0.63	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ba2 Constrained at	0.045	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	6%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	7	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT964_ALERT_2_G	SHELXL WEIGHT Parameter in CIF & RES Differ ...		Please Check

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- 4 **ALERT level A** = Most likely a serious problem - resolve or explain
 - 2 **ALERT level B** = A potentially serious problem, consider carefully
 - 72 **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

- 74 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 5 ALERT type 2 Indicator that the structure model may be wrong or deficient
 - 2 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
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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.

