

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:	Fe- O = 0.0040 A	Wavelength=1.54184
Cell:	a=5.3585 (2)	b=10.7114 (5) c=7.2301 (3)
	alpha=107.864 (4)	beta=111.561 (4) gamma=71.694 (4)
Temperature:	270 K	
	Calculated	Reported
Volume	357.71 (3)	357.71 (3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	Fe2 Mg0.07 Mn0.93 O16 P2, 2 (O)	?
Sum formula	Fe2 Mg0.07 Mn0.93 O18 P2	Al0 Fe1 H0 Mg0.033 Mn0.467 O9 P1 Zn0
Mr	514.53	257.30
Dx, g cm-3	2.388	2.389
Z	1	2
Mu (mm-1)	25.801	25.807
F000	250.1	250.0
F000'	249.04	
h, k, lmax	6, 13, 9	6, 13, 9
Nref	1551	1252
Tmin, Tmax	0.002, 0.098	0.037, 0.304
Tmin'	0.000	

Correction method= # Reported T Limits: Tmin=0.037 Tmax=0.304
AbsCorr = GAUSSIAN

Data completeness= 0.807 Theta (max)= 79.930

R(reflections)= 0.0654(1128)

wR2(reflections)=

wR= 0.0643(1252)

S = 3.360

Npar= 110

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

PLAT211_ALERT_2_A ADP of Atom Fe1	is N.P.D. or (nearly) 2D .	Please Check
PLAT211_ALERT_2_A ADP of Atom O2	is N.P.D. or (nearly) 2D .	Please Check
PLAT213_ALERT_2_A Atom Fe2	has ADP max/min Ratio	5.3 prolat



Alert level B

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?)	Ow4 Check
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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 Gaussian

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
Goodness of fit given = 3.360

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.149

PLAT041_ALERT_1_C Calc. and Reported SumFormula	Strings Differ	Please Check
Calc: Fe Mg0.03 Mn0.47 O9 P		
Rep.: Al0 Fe1 H0 Mg0.033 Mn0.467 O9 P1 Zn0		

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 !

PLAT213_ALERT_2_C Atom P	has ADP max/min Ratio	3.1 prolat
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of		Ow3 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1)		3.7 Note



Alert level G

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a

symmetry error - see SYMMG tests

From the CIF: _cell_formula_units_Z 2

From the CIF: _chemical_formula_sum Al0 Fe1 H0 Mg0.033 Mn0.467 O9 P1 Z

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Al	2.00	0.00	2.00
Fe	2.00	2.00	0.00
H	2.00	0.00	2.00
Mg	0.07	0.07	-0.00
Mn	0.93	0.93	0.00
O	18.00	18.00	0.00

P	2.00	2.00	0.00	
Zn	2.00	0.00	2.00	
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension				3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF				Please Do !
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12				0.149 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...				0.500 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...				Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)				0.004 Degree
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1)				9% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels				5 Note
Oh	Ow1	Ow2	Ow3	Ow4
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found				Please Check
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .				Please Do !
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of				3.0 Sig(I)

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

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 8 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
 3 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.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_ABSTY02_I
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_GOODF01_I
;
PROBLEM: The least squares goodness of fit parameter lies
RESPONSE: ...
;
_vrf_RINTA01_I
;
PROBLEM: The value of Rint is greater than 0.12
RESPONSE: ...
;
_vrf_PLAT211_I
;
PROBLEM: ADP of Atom Fe1          is N.P.D. or (nearly) 2D .      Please Check
RESPONSE: ...
;
_vrf_PLAT213_I
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;
PROBLEM: Atom Fe2                has ADP max/min Ratio .....      5.3 prolat
RESPONSE: ...
;
_vrf_PLAT306_I
;
PROBLEM: Isolated Oxygen Atom (H-atoms Missing ?) .....      Ow4 Check
RESPONSE: ...
;
_vrf_PLAT041_I
;
PROBLEM: Calc. and Reported SumFormula      Strings      Differ      Please Check
RESPONSE: ...
;
_vrf_PLAT077_I
;
PROBLEM: Unitcell Contains Non-integer Number of Atoms ..      Please Check
RESPONSE: ...
;
_vrf_PLAT155_I
;
PROBLEM: The Triclinic Unitcell is NOT Reduced .....      Please Do !
RESPONSE: ...
;
_vrf_PLAT241_I
;
PROBLEM: High      'MainMol' Ueq as Compared to Neighbors of      Ow3 Check
RESPONSE: ...
;
_vrf_PLAT250_I
;
PROBLEM: Large U3/U1 Ratio for <U(i,j)> Tensor(Resd      1)      3.7 Note
RESPONSE: ...
;
# end Validation Reply Form

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PLATON version of 22/08/2024; check.def file version of 21/08/2024

Datablock 1 - ellipsoid plot

