

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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:	C-C = 0.0080 A	Wavelength=0.71073
Cell:	a=17.6784(10)	b=29.6003(18) c=11.7133(7)
	alpha=90	beta=98.049(4) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	6069.0(6)	6069.0(6)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc1
Moiety formula	C8 H26 Mg2 N O14, C8 H5 N O4, 3(C8 H6 N O4), H12 Mg O6, 10(H2 O	C8 H26 Mg2 N O14, C8 H5 N O4 3(C8 H6 N O4), H12 Mg O6, 10(H2 O)
Sum formula	C40 H81 Mg3 N5 O46	C40 H81 Mg3 N5 O46
Mr	1441.03	1441.03
Dx, g cm-3	1.577	1.577
Z	4	4
Mu (mm-1)	0.171	0.171
F000	3040.0	3040.0
F000'	3042.66	
h,k,lmax	21,36,14	21,36,14
Nref	11532	11485
Tmin,Tmax	0.976,0.986	0.975,0.986
Tmin'	0.975	

Correction method= MULTI-SCAN

Data completeness= 0.996 Theta(max)= 25.680

R(reflections)= 0.0793(6035) wR2(reflections)= 0.2399(11485)

S = 1.022 Npar= Npar =1045

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	H5W	..	H47W	..	1.58	Ang.
PLAT417_ALERT_2_A	Short Inter D-H..H-D	H11W	..	H47W	..	1.48	Ang.
PLAT417_ALERT_2_A	Short Inter D-H..H-D	H12W	..	H42W	..	1.55	Ang.
PLAT417_ALERT_2_A	Short Inter D-H..H-D	H26W	..	H49W	..	1.41	Ang.

Alert level B

DIFMX01_ALERT_2_B The maximum difference density is > 0.1*ZMAX*1.00
 _refine_diff_density_max given = 1.307
 Test value = 1.200

PLAT097_ALERT_2_B	Large Reported Max. (Positive) Residual Density	1.31	eA-3
PLAT213_ALERT_2_B	Atom N3 has ADP max/min Ratio	5.0	oblate
PLAT417_ALERT_2_B	Short Inter D-H..H-D H16W .. H50W ..	2.03	Ang.
PLAT420_ALERT_2_B	D-H Without Acceptor O15W - H29W ...	Please	Check
PLAT910_ALERT_3_B	Missing # of FCF Reflections Below Th(Min)	36	Why ?

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
 The relevant atom site should be identified.

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
 Rint given 0.147

PLAT020_ALERT_3_C	The value of Rint is greater than 0.12	0.147	
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.65	Why ?
PLAT213_ALERT_2_C	Atom C20 has ADP max/min Ratio	3.3	oblate
PLAT213_ALERT_2_C	Atom O15 has ADP max/min Ratio	3.5	prolat
PLAT213_ALERT_2_C	Atom C25 has ADP max/min Ratio	3.6	prolat
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.3	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.6	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.2	Note
PLAT314_ALERT_2_C	Check Small Angle for H2O: Metal-O10W -H19W	55.33	Degree
PLAT314_ALERT_2_C	Check Small Angle for H2O: Metal-O16W -H32W	73.10	Degree
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0080	Ang.
PLAT417_ALERT_2_C	Short Inter D-H..H-D H1W .. H39W ..	2.13	Ang.
PLAT417_ALERT_2_C	Short Inter D-H..H-D H16W .. H52W ..	2.13	Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	8.264	Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	13	Why ?
PLAT975_ALERT_2_C	Check Calcd Residual Density 1.10A From O26W	0.61	eA-3
PLAT975_ALERT_2_C	Check Calcd Residual Density 0.85A From N2	0.55	eA-3
PLAT975_ALERT_2_C	Check Calcd Residual Density 1.07A From O8W	0.54	eA-3
PLAT976_ALERT_2_C	Check Calcd Residual Density 0.93A From O10W	-0.41	eA-3

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
 _chemical_formula_sum and _chemical_formula_moiety. This is
 usually due to the moiety formula being in the wrong format.
 Atom count from _chemical_formula_sum: C40 H81 Mg3 N5 O46
 Atom count from _chemical_formula_moiety: C24 H69 Mg3 N3 O77

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	97	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	3	Why ?
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	Please	Do !
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large.	0.11	Why ?

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	11.07	Why ?
PLAT303_ALERT_2_G	Full Occupancy H-Atom H19W with # Connections	2.00	Check
PLAT303_ALERT_2_G	Full Occupancy H-Atom H32W with # Connections	2.00	Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H2 O	7	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H2 O	8	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # H2 O	9	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	110	Note

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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
30 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
 _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
 _publ_contact_author_phone are all missing.
 At least one of these should be present.
PUBL006_ALERT_1_A _publ_requested_journal is missing
 e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A _publ_section_abstract is missing.
 Abstract of paper in English.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or
 empty.

7 **ALERT level A** = Data missing that is essential or data in wrong format
1 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_PLAT417_I
;
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PROBLEM: Short Inter D-H...H-D H5W .. H47W .. 1.58 Ang.
RESPONSE: ...
;
end Validation Reply Form

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 05/02/2014; check.def file version of 05/02/2014

Datablock I - ellipsoid plot

