

# checkCIF () running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait .....

## checkCIF/PLATON (full publication check)

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 = 0.0123 Å	Wavelength=0.71073
Cell:	a=11.7432(9) b=47.433(3) c=13.9297(9)	
	alpha=90 beta=97.143(4) gamma=90	
Temperature:	180 K	
	Calculated	Reported
Volume	7698.8(9)	7698.9(10)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety	C40 H34 Mg2 N6 O12,	C40 H34 Mg2 N6 O12,
formula	H2 O	H2 O
Sum formula	C40 H36 Mg2 N6 O13	C40 H36 Mg2 N6 O13
Mr	857.37	857.37
Dx, g cm-3	1.479	1.479
Z	8	8
Mu (mm-1)	0.141	0.141
F000	3568.0	3568.0
F000'	3570.42	
h, k, lmax	13, 52, 15	13, 52, 15
Nref	11043	10997
Tmin, Tmax	0.967, 0.996	0.967, 0.996
Tmin'	0.956	
Correction method= # Reported T Limits: Tmin=0.967 Tmax=0.996 AbsCorr = MULTI-SCAN		
Data completeness=	0.996	Theta(max)= 23.256
R(reflections)=	0.1085( 6552)	wR2(reflections)= 0.3209( 10997)
S =	1.044	Npar= 1178

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

<a href="#">THETM01_ALERT_3_B</a>	The value of sine(theta_max)/wavelength is less than 0.575	
	Calculated sin(theta_max)/wavelength =	0.5555
<a href="#">PLAT023_ALERT_3_B</a>	Resolution (too) Low [sin(theta)/Lambda < 0.6]..	23.26 Degree
<a href="#">PLAT213_ALERT_2_B</a>	Atom C7	has ADP max/min Ratio ..... 4.4 prolat
<a href="#">PLAT213_ALERT_2_B</a>	Atom C34	has ADP max/min Ratio ..... 4.5 prolat

PLAT220_ALERT_2_B	Non-Solvent Resd 1	C	Ueq(max)/Ueq(min) Range	6.2	Ratio
PLAT340_ALERT_3_B	Low Bond Precision on	C-C Bonds	.....	0.0123	Ang.
PLAT414_ALERT_2_B	Short Intra D-H..H-X	H12W	.. H52 ..	1.89	Ang.
PLAT417_ALERT_2_B	Short Inter D-H..H-D	H1W	.. H20W ..	2.08	Ang.

#### And 3 other PLAT417 Alerts

PLAT417_ALERT_2_B	Short Inter D-H..H-D	H3A	.. H33A ..	1.98	Ang.
PLAT417_ALERT_2_B	Short Inter D-H..H-D	H16W	.. H17W ..	2.04	Ang.
PLAT417_ALERT_2_B	Short Inter D-H..H-D	H16W	.. H18W ..	2.09	Ang.
PLAT420_ALERT_2_B	D-H Without Acceptor	O6W	-- H12W ...	Please	Check

#### Alert level C

ALERT LEVEL 1				
DIFMN02_ALERT_2_C	The minimum difference density is DIFMN03_ALERT_1_C The minimum difference density is REFNR01_ALERT_3_C Ratio of reflections to parameters is RFACG01_ALERT_3_C The value of the R factor is > 0.10			
	R factor given	0.108		
RFACR01_ALERT_3_C	The value of the weighted R factor is > 0.25			
	Weighted R factor given	0.321		
PLAT082_ALERT_2_C	High R1 Value .....	0.11	Report	
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25) .....	0.32	Report	
PLAT088_ALERT_3_C	Poor Data / Parameter Ratio .....	9.37	Note	
PLAT098_ALERT_2_C	Large Reported Min. (Negative) Residual Density	-1.10	eA-3	
PLAT213_ALERT_2_C	Atom O4W	has ADP max/min Ratio .....	3.2	prolat

#### And 9 other PLAT213 Alerts

PLAT213_ALERT_2_C	Atom O6	has ADP max/min Ratio	.....	3.4	prolat
PLAT213_ALERT_2_C	Atom C5	has ADP max/min Ratio	.....	3.2	prolat
PLAT213_ALERT_2_C	Atom C8	has ADP max/min Ratio	.....	3.1	prolat
PLAT213_ALERT_2_C	Atom C9	has ADP max/min Ratio	.....	3.2	prolat
PLAT213_ALERT_2_C	Atom C10	has ADP max/min Ratio	.....	3.3	prolat
PLAT213_ALERT_2_C	Atom C11	has ADP max/min Ratio	.....	3.3	prolat
PLAT213_ALERT_2_C	Atom C16	has ADP max/min Ratio	.....	3.3	oblate
PLAT213_ALERT_2_C	Atom C35	has ADP max/min Ratio	.....	3.5	prolat
PLAT213_ALERT_2_C	Atom C75	has ADP max/min Ratio	.....	3.4	prolat
PLAT220_ALERT_2_C	Non-Solvent Resd 2	C	Ueq(max)/Ueq(min) Range	4.0	Ratio
PLAT222_ALERT_3_C	Non-Solvent Resd 1	H	Uiso(max)/Uiso(min) Range	5.2	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C75	-- C78	..	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C76	-- C77	..	0.17	Ang.
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	....	2.3	Note	
PLAT420_ALERT_2_C	D-H Without Acceptor	N4	-- H3A ...	Please	Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N9	-- H6A ...	Please	Check

#### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	39	Note	
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	1	Report	
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report	
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check	
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.17	Report	
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	35.63	Why ?	
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	26	Report	
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report	
PLAT333_ALERT_2_G	Check Large Av C6-Ring C-C Dist. C4 -C9	1.42	Ang.	
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2	Note	
	C40 H34 Mg2 N6 O12			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	4	Note	
	H2 O			
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	45	Note	

0 **ALERT level A** = Most likely a serious problem - resolve or explain  
12 **ALERT level B** = A potentially serious problem, consider carefully  
26 **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

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

10 ALERT type 3 Indicator that the structure quality may be low  
6 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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## checkCIF publication errors

### 🔴 Alert level A

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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.

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### 🟡 Alert level G

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PUBL017\_ALERT\_1\_G The \_publ\_section\_references section is missing or  
empty.

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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

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### 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.

### 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_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: ...
;
# end Validation Reply Form

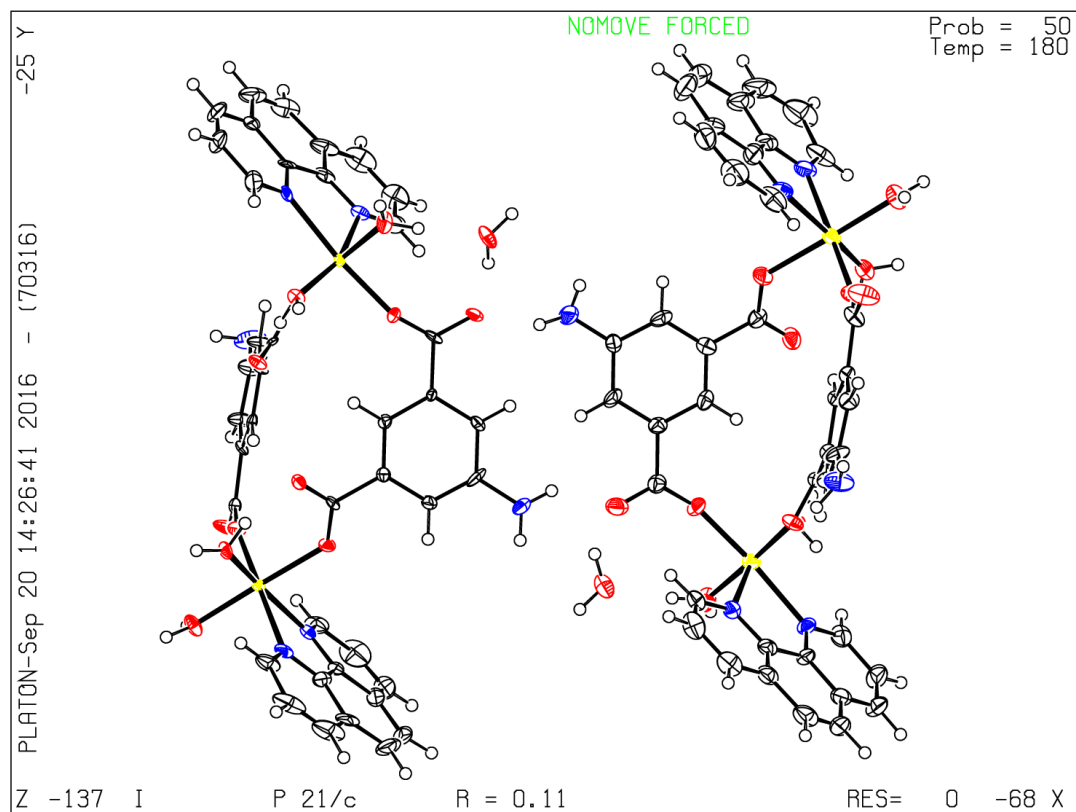
```

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 you wish to submit your CIF for publication in IUCrData 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.

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**PLATON version of 11/08/2016; check.def file version of 04/08/2016**

### Datablock I - ellipsoid plot




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