

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) jm1901

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: jm1901

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Bond precision:	C-C = 0.0027 A	Wavelength=0.71073
Cell:	a=19.0860(8)	b=12.8472(6)      c=20.6882(8)
	alpha=90	beta=111.643(1)      gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	4715.2(3)	4715.1(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C40 H50 Br2 Mg N6, 2(C5 H5 N)	C40 H50 Br2 Mg N6, 2(C5 H5 N)
Sum formula	C50 H60 Br2 Mg N8	C50 H60 Br2 Mg N8
Mr	957.17	957.19
Dx,g cm-3	1.348	1.348
Z	4	4
Mu (mm-1)	1.776	1.776
F000	1992.0	1992.0
F000'	1990.38	
h,k,lmax	26,17,28	26,17,28
Nref	13251	13232
Tmin,Tmax	0.766,0.868	0.699,0.746
Tmin'	0.766	

Correction method= # Reported T Limits: Tmin=0.699 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.999      Theta(max)= 29.604

R(reflections)= 0.0307( 10646)      wR2(reflections)= 0.0680( 13232)

S = 1.038      Npar= 558

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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 C

PLAT220_ALERT_2_C	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	....	3.0	Note



#### Alert level G

PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Br1	--Mg1	.	9.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Br2	--Mg1	.	9.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Mg1	--N6	.	5.2	s.u.
PLAT883_ALERT_1_G	No Info for _atom_sites_solution_primary	.....				Please Do !

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
4 **ALERT level G** = General information/check it is not something unexpected
- 1 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  
0 ALERT type 3 Indicator that the structure quality may be low  
0 ALERT type 4 Improvement, methodology, query or suggestion  
0 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.

PLATON version of 18/02/2019; check.def file version of 18/02/2019

Datablock jm1901 - ellipsoid plot

