

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp\_7294

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: exp\_7294**

Bond precision:	C-C = 0.0189 Å	Wavelength=0.02510	
Cell:	a=6.5943 (16)	b=7.972 (5)	c=18.806 (4)
	alpha=90	beta=93.004 (19)	gamma=90
Temperature:	175 K		

	Calculated	Reported
Volume	987.3(7)	987.3(7)
Space group	I a	I 1 a 1
Hall group	I -2ya	I -2ya
Moiety formula	C9 H7 Al O5	C18 H14 Al2 O10
Sum formula	C9 H7 Al O5	C18 H14 Al2 O10
Mr	222.13	444.26
Dx, g cm <sup>-3</sup>	1.494	1.494
Z	4	2
Mu (mm <sup>-1</sup> )	0.000	0.000
F000	0.0	168.0
F000'	455.93	
h, k, lmax	8, 9, 23	8, 9, 23
Nref	2004[ 1004]	1488
Tmin, Tmax		0.500, 1.000
Tmin'		

```
Correction method= # Reported T Limits: Tmin=0.500 Tmax=1.000
AbsCorr = MULTI-SCAN
```

Data completeness= 1.48/0.74                      Theta(max)= 0.898

```
R(reflections)= 0.1091( 765)      wR2(reflections)=
S = 1.164                        0.3211( 1488)
Npar= 129
```

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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.

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### Alert level A

EXPT005\_ALERT\_1\_A \_exptl\_crystal\_description is missing

Crystal habit description.

The following tests will not be performed.

CRYSR\_01

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low .	0.762 Why?
PLAT250_ALERT_2_A Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1)	10.6 Note
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value .....	Please Do !

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### Alert level B

PLAT213\_ALERT\_2\_B Atom Al00 has ADP max/min Ratio ..... 4.1 prolat

PLAT340\_ALERT\_3\_B Low Bond Precision on C-C Bonds ..... 0.01889 Ang.

PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O008 --H008 . Please Check

PLAT430\_ALERT\_2\_B Short Inter D...A Contact O001 ..O004 . 2.58 Ang.

1/2+x,-y,z = 2\_555 Check

PLAT911\_ALERT\_3\_B Missing FCF Refl Between Thmin & STh/L= 0.600 212 Report

0	2	0,	1	3	0,	0	4	0,	1	5	0,	0	6	0,	2	6	0,
1	7	0,	0	8	0,	2	8	0,	1	9	0,	0	3	1,	-1	4	1,
1	4	1,	-2	5	1,	0	5	1,	-1	6	1,	1	6	1,	-2	7	1,
0	7	1,	2	7	1,	-3	8	1,	-1	8	1,	1	8	1,	-2	9	1,
0	9	1,	2	9	1,	0	2	2,	-1	3	2,	0	4	2,	-1	5	2,
1	5	2,	-2	6	2,	0	6	2,	2	6	2,	-3	7	2,	-1	7	2,
1	7	2,	-2	8	2,	0	8	2,	2	8	2,	-1	9	2,	1	9	2,
0	3	3,	-1	4	3,	1	4	3,	-2	5	3,	0	5	3,	-1	6	3,
1	6	3,	-2	7	3,	0	7	3,	2	7	3,	-3	8	3,	-1	8	3,
1	8	3,	-2	9	3,	0	9	3,	2	9	3,	0	0	4,	0	2	4,
-1	3	4,	0	4	4,	-1	5	4,	1	5	4,	-2	6	4,	0	6	4,
-3	7	4,	-1	7	4,	1	7	4,	-2	8	4,	0	8	4,	2	8	4,
-1	9	4,	1	9	4,	0	3	5,	-1	4	5,	-2	5	5,	0	5	5,
-1	6	5,	1	6	5,	-2	7	5,	0	7	5,	-3	8	5,	-1	8	5,
1	8	5,	-2	9	5,	0	9	5,	0	0	6,	-1	3	6,	0	4	6,
-1	5	6,	1	5	6,	-2	6	6,	0	6	6,	-3	7	6,	-1	7	6,

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### Alert level C

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12

Rint given 0.126

PLAT020\_ALERT\_3\_C The Value of Rint is Greater Than 0.12 ..... 0.126 Report

PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check

Calc: C9 H7 Al O5

Rep.: C18 H14 Al2 O10

PLAT082\_ALERT\_2\_C High R1 Value ..... 0.11 Report

PLAT084\_ALERT\_3\_C High wR2 Value (i.e. > 0.25) ..... 0.32 Report

PLAT089\_ALERT\_3\_C Poor Data / Parameter Ratio (Zmax < 18) ..... 5.86 Note

PLAT213\_ALERT\_2\_C Atom O001 has ADP max/min Ratio ..... 3.1 prolat

PLAT213\_ALERT\_2\_C Atom O004 has ADP max/min Ratio ..... 3.1 prolat

PLAT213\_ALERT\_2\_C Atom O007 has ADP max/min Ratio ..... 3.6 prolat

PLAT213\_ALERT\_2\_C Atom O008 has ADP max/min Ratio ..... 3.8 prolat

PLAT213\_ALERT\_2\_C Atom O00F has ADP max/min Ratio ..... 3.2 prolat

PLAT213_ALERT_2_C Atom C003	has ADP max/min Ratio .....	3.2	prolat
PLAT213_ALERT_2_C Atom C009	has ADP max/min Ratio .....	3.3	prolat
PLAT213_ALERT_2_C Atom C00C	has ADP max/min Ratio .....	3.2	prolat
PLAT213_ALERT_2_C Atom C005	has ADP max/min Ratio .....	3.2	prolat
PLAT213_ALERT_2_C Atom C00D	has ADP max/min Ratio .....	3.2	prolat
PLAT213_ALERT_2_C Atom C00A	has ADP max/min Ratio .....	3.2	prolat
PLAT213_ALERT_2_C Atom C00B	has ADP max/min Ratio .....	3.3	prolat
PLAT213_ALERT_2_C Atom C006	has ADP max/min Ratio .....	3.1	prolat
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of .		64	Ang**3
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4		Please	Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....		3.079	Check

### Alert level G

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
not performed for this radiation type.

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms		15	Report				
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension		3	Info				
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...		2	Check				
PLAT111_ALERT_2_G ADDSYM Detects New (Pseudo) Centre of Symmetry .		93	%Fit				
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space Group		I2/a	Check				
Check Model Parameter Symmetry for Reflection Data Support							
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records		1	Report				
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records		1	Report				
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used		0.0010	Report				
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for First Par		0.0010	Report				
PLAT190_ALERT_3_G A Non-default RIGU Restraint Value for SecondPar		0.0010	Report				
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....		22	Note				
O001	Al00	C003	O004	O007	O008	C009	C00C
H00C	C005	C00D	H00D	C00A	H00A	C00B	C006
C00E	H00B	H00E	H00F	O00F	H008		
PLAT768_ALERT_4_G Embedded RES Explicitly Supplied Scattering Data		Please	Note				
PLAT794_ALERT_5_G Tentative Bond Valency for Al00 (III) .		3.03	Info				
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....		197	Note				
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).		2	Note				
0 1 1, 0 0 2,							
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600		36	Note				
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....		1	Note				
0 1 1,							
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....		3.3	Low				
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....		1.407	Note				
Predicted wR2: Based on SigI**2 22.83 or SHELX Weight 27.58							
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		0	Info				

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

- 5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
23 ALERT type 2 Indicator that the structure model may be wrong or deficient  
15 ALERT type 3 Indicator that the structure quality may be low  
6 ALERT type 4 Improvement, methodology, query or suggestion  
3 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.

### 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_EXPT005_exp_7294
;
PROBLEM: _exptl_crystal_description is missing
RESPONSE: ...
;
_vrf_PLAT029_exp_7294
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low .          0.762 Why?
RESPONSE: ...
;
_vrf_PLAT250_exp_7294
;
PROBLEM: Large U3/U1 Ratio for <U(i,j)> Tensor(Resd      1)          10.6 Note
RESPONSE: ...
;
_vrf_PLAT699_exp_7294
;
PROBLEM: Missing _exptl_crystal_description Value .....      Please Do !
RESPONSE: ...
;
# end Validation Reply Form
```

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

Datablock exp\_7294 - ellipsoid plot

