

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) am\_mnt\_0m

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: am\_mnt\_0m

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Bond precision:      C-C = 0.0017 Å      Wavelength=0.71073

Cell:                      a=36.1508(8)      b=13.6587(3)      c=19.4218(4)  
                                alpha=90      beta=108.956(1)      gamma=90

Temperature:      100 K

	Calculated	Reported
Volume	9069.9(3)	9069.9(3)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C64 Am4 N32 S32, 16(C N0.50), 4(C0.93 N0.50), 4(C1.11 N0.50), 4	Am C28.044 N14 Na5 S8
Sum formula	C112.17 Am4 N56 Na20 S32	C28.04 Am N14 Na5 S8
Mr	4581.71	1147.38
Dx, g cm <sup>-3</sup>	1.678	1.681
Z	2	8
Mu (mm <sup>-1</sup> )	2.146	2.146
F000	4354.1	4354.0
F000'	4300.57	
h, k, lmax	72, 27, 38	72, 27, 38
Nref	38128	38037
Tmin, Tmax	0.504, 0.628	0.626, 0.749
Tmin'	0.403	

Correction method= # Reported T Limits: Tmin=0.626 Tmax=0.749  
AbsCorr = NUMERICAL

Data completeness= 0.998      Theta(max)= 45.346

R(reflections)= 0.0222( 34345)

wR2(reflections)=  
0.0531( 38037)

S = 1.062

Npar= 655

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

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 0.48Ang From Am1 4.36 eA-3

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### Alert level B

PLAT972\_ALERT\_2\_B Check Calcd Resid. Dens. 0.58Ang From S5 -3.28 eA-3

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### Alert level C

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

Calc: C64 Am4 N32 S32, 16(C N0.50), 4(C0.93 N0.50), 4(C1.11 N0.50)

Rep.: Am C28.044 N14 Na5 S8

PLAT043\_ALERT\_1\_C Calculated and Reported Mol. Weight Differ by .. 7.81 Check

PLAT243\_ALERT\_4\_C High 'Solvent' Ueq as Compared to Neighbors of C23 Check

PLAT244\_ALERT\_4\_C Low 'Solvent' Ueq as Compared to Neighbors of C17 Check

PLAT767\_ALERT\_4\_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check

PLAT910\_ALERT\_3\_C Missing # of FCF Reflection(s) Below Theta(Min). 10 Note

1 1 0, 2 0 0, 3 1 0, 4 0 0, -3 1 1, -1 1 1,

1 1 1, -2 0 2, -1 1 2, 0 0 2,

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 14 Report

0 2 0, 3 3 0, -13 1 1, -4 2 1, -10 0 2, -3 1 2,

0 2 2, -8 2 3, 0 2 3, -8 0 4, -3 1 4, 1 1 4,

-9 1 6, -3 1 6,

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.32Ang From S5 2.28 eA-3

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.52Ang From Am1 2.17 eA-3

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.47Ang From S5 2.16 eA-3

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.35Ang From C23 2.04 eA-3

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.59Ang From Am1 1.79 eA-3

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.63Ang From Na3 1.76 eA-3

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.60Ang From Am1 1.62 eA-3

PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 0.10Ang From S5 -1.72 eA-3

PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 0.01Ang From C23 -1.67 eA-3

PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 0.44Ang From Am1 -1.61 eA-3

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### Alert level G

PLAT003\_ALERT\_2\_G Number of Uiso or U(i,j) Restrained non-H Atoms 11 Report

PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT040\_ALERT\_1\_G No H-atoms in this Carbon Containing Compound .. Please Check

PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 0.250 Check

PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 13.67 Why ?

PLAT178\_ALERT\_4\_G The CIF-Embedded .res File Contains SIMU Records 3 Report

PLAT186\_ALERT\_4\_G The CIF-Embedded .res File Contains ISOR Records 3 Report

PLAT188\_ALERT\_3\_G A Non-default SIMU Restraint Value has been used 0.0200 Report

PLAT188\_ALERT\_3\_G A Non-default SIMU Restraint Value has been used 0.0100 Report

PLAT188\_ALERT\_3\_G A Non-default SIMU Restraint Value has been used 0.0100 Report

PLAT299\_ALERT\_4\_G Atom Site Occupancy Constrained at ..... 0.5 Check

C19A	C19B	C20A	C20B	N12	C24	N14A	N14B
C27A	C27B	N11A	C21A	C22A	N13A	N13B	N15A
C29A	C30A	N15B	C29B	C30B	Na2A	Na2B	Na4A
Na4B							

PLAT300\_ALERT\_4\_G Atom Site Occupancy of N11B Constrained at 0.25 Check

PLAT300\_ALERT\_4\_G Atom Site Occupancy of C21B Constrained at 0.25 Check

PLAT300\_ALERT\_4\_G Atom Site Occupancy of C22B Constrained at 0.25 Check

PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 67% Note

PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 67% Note

PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 67% Note

PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 6) 100% Note

PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 7) 100% Note

PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 8) 100% Note

PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 9) 100% Note

PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 10) 100% Note

PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 11) 100% Note

PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 13) 100% Note

PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 14) 100% Note

PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 16) 100% Note

PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 17) 100% Note

PLAT432\_ALERT\_2\_G Short Inter X...Y Contact N13A ..C24 . 2.99 Ang.

1-x,y,3/2-z = 2\_656 Check

PLAT432\_ALERT\_2\_G Short Inter X...Y Contact C24 ..C25A . 3.04 Ang.

1-x,y,3/2-z = 2\_656 Check

PLAT773\_ALERT\_2\_G Check long C-C Bond in CIF: C26B --C25A 2.01 Ang.

PLAT773\_ALERT\_2\_G Check long C-C Bond in CIF: C20B --C19A 1.78 Ang.

PLAT789\_ALERT\_4\_G Atoms with Negative \_atom\_site\_disorder\_group # 15 Check

PLAT811\_ALERT\_5\_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info

PLAT822\_ALERT\_4\_G CIF-embedded .res Contains Negative PART Numbers 12 Check

PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 84 Note

PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 67 Note

PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 20 Note

1	1	1,	-3	1	1,	-2	0	2,	0	0	2,	-1	1	1,	-3	1	4,
-3	1	2,	-9	1	6,	3	3	0,	0	2	3,	-4	2	1,	-13	1	1,
3	1	0,	-8	0	4,	-3	1	6,	1	1	4,	-8	2	3,	0	2	0,
0	2	2,	-10	0	2,												

PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 2.903 Note

Predicted wR2: Based on SigI\*2 1.83 or SHELX Weight 5.00

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- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
- 1 **ALERT level B** = A potentially serious problem, consider carefully
- 17 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
- 38 **ALERT level G** = General information/check it is not something unexpected
- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
- 19 ALERT type 2 Indicator that the structure model may be wrong or deficient
- 6 ALERT type 3 Indicator that the structure quality may be low
- 25 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_PLAT971_am_mnt_0m
;
PROBLEM: Check Calcd Resid. Dens.  0.48Ang From Am1          4.36 eA-3
RESPONSE: ...
;
_vrf_PLAT972_am_mnt_0m
;
PROBLEM: Check Calcd Resid. Dens.  0.58Ang From S5          -3.28 eA-3
RESPONSE: ...
;
# end Validation Reply Form
```

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**PLATON version of 15/07/2024; check.def file version of 15/07/2024**

