

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) smmnt\_030121\_nbb\_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: smmnt\_030121\_nbb\_0m

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Bond precision:	C-C = 0.0038 A	Wavelength=0.71073	
Cell:	a=36.283 (2)	b=13.6371 (9)	c=19.4532 (11)
	alpha=90	beta=108.757 (2)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	9114.2 (9)	9114.2 (10)	
Space group	C 2/c	C 1 2/c 1	
Hall group	-C 2yc	-C 2yc	
Moiety formula	C64 N32 S32 Sm4, 20 (C2 N), 4 (C1.55 N0.55), 1.808 (C N), 20 (Na)	C27 N13.5 Na5 S8 Sm, 0.5 (C2 N)	
Sum formula	C112 N56 Na20 S32 Sm4	C28 N14 Na5 S8 Sm	
Mr	4216.84	1054.20	
Dx, g cm-3	1.537	1.537	
Z	2	8	
Mu (mm-1)	1.741	1.741	
F000	4088.0	4088.0	
F000'	4096.41		
h, k, lmax	51, 19, 27	51, 19, 27	
Nref	13944	13917	
Tmin, Tmax	0.713, 0.840	0.631, 0.746	
Tmin'	0.699		

Correction method= # Reported T Limits: Tmin=0.631 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.998

Theta (max)= 30.534

R(reflections)= 0.0266( 12525)

wR2(reflections)=  
0.0668( 13917)

S = 1.043

Npar= 572

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

PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: C64 N32 S32 Sm4, 20(C2 N), 4(C1.55 N0.55), 1.808(C N), 20(Na  
Rep.: C27 N13.5 Na5 S8 Sm, 0.5(C2 N)

PLAT244\_ALERT\_4\_C Low 'Solvent' Ueq as Compared to Neighbors of C41 Check  
PLAT244\_ALERT\_4\_C Low 'Solvent' Ueq as Compared to Neighbors of C45 Check  
PLAT244\_ALERT\_4\_C Low 'Solvent' Ueq as Compared to Neighbors of C61 Check  
PLAT244\_ALERT\_4\_C Low 'Solvent' Ueq as Compared to Neighbors of C64 Check  
PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including N40 0.112 Check  
PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including N60 0.131 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 5 Report  
-3 1 2, 0 2 2, -3 1 3, -8 0 4, -4 0 6,  
PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 0.93Ang From Na1 -1.64 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.91Ang From C59 . 0.70 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.45Ang From C65 . 0.56 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.79Ang From C65 . 0.51 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 1.01Ang From C56 . 0.48 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.94Ang From C65 . 0.48 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 1.01Ang From C65 . 0.46 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.89Ang From C51 . 0.43 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 1.01Ang From C56 . 0.43 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 1.04Ang From C46 . 0.41 eA-3



### Alert level G

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 23.36 Why ?  
PLAT128\_ALERT\_4\_G Alternate Setting for Input Space Group C2/c I2/a Note  
PLAT299\_ALERT\_4\_G Atom Site Occupancy Constrained at ..... 0.5 Check  
N47 N48 C49 C50 N57 C59 C42 C43  
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) 33% Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 6) 52% Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 9) 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 15) 100% Note  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact C56 ..C54 . 1.77 Ang.  
x,y,z = 1\_555 Check  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact C56 ..N52 . 2.98 Ang.  
x,y,z = 1\_555 Check

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PLAT432_ALERT_2_G Short Inter X...Y Contact C59 ..N52 . 2.96 Ang.
1-x,y,1/2-z = 2_655 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C59 ..C54 . 3.03 Ang.
1-x,y,1/2-z = 2_655 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C56 --C54 1.77 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Sml (III) . 3.18 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 13 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 12 Note
1 1 1, -3 1 1, -2 0 2, 0 0 2, 4 0 0, -1 1 2,
-3 1 2, -8 0 4, -28 2 24, -3 1 3, -4 0 6, 0 2 2,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.291 Note
Predicted wR2: Based on SigI**2 2.91 or SHELX Weight 6.40

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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
19 ALERT level C = Check. Ensure it is not caused by an omission or oversight
22 ALERT level G = General information/check it is not something unexpected

3 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
2 ALERT type 3 Indicator that the structure quality may be low
14 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.

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

Datablock smmnt\_030121\_nbb\_0m - ellipsoid plot

