

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cf\_mnt\_1\_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: cf\_mnt\_1\_0m**

Bond precision:	C-C = 0.0044 Å	Wavelength=0.71073	
Cell:	a=13.6393 (3)	b=18.3172 (4)	c=17.3594 (4)
	alpha=90	beta=92.408 (1)	gamma=90
Temperature:	100 K		

	Calculated	Reported
Volume	4333.14 (17)	4333.13 (17)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C28 H18 Cf N14 Na5 S8	C28 H18 Cf N14 Na5 S8
Sum formula	C28 H18 Cf N14 Na5 S8	C28 H18 Cf N14 Na5 S8
Mr	1174.08	1172.99
Dx, g cm <sup>-3</sup>	1.800	1.798
Z	4	4
Mu (mm <sup>-1</sup> )	2.432	2.432
F000	2260.0	2260.0
F000'	2238.23	
h, k, l <sub>max</sub>	27, 36, 34	27, 36, 34
Nref	36411	36302
Tmin, Tmax	0.747, 0.784	0.611, 0.749
Tmin'	0.615	

```
Correction method= # Reported T Limits: Tmin=0.611 Tmax=0.749
AbsCorr = MULTI-SCAN
```

Data completeness= 0.997                      Theta (max)= 45.346

```
R(reflections)= 0.0420( 29799)      wR2(reflections)=
S = 1.108                          0.0910( 36302)
Npar= 511
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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

PLAT971_ALERT_2_A	Check	Calcd Resid. Dens.	0.53Ang From Cf1	5.52 eA-3
PLAT971_ALERT_2_A	Check	Calcd Resid. Dens.	0.57Ang From Cf1	5.46 eA-3
PLAT971_ALERT_2_A	Check	Calcd Resid. Dens.	0.57Ang From Cf1	5.46 eA-3
PLAT971_ALERT_2_A	Check	Calcd Resid. Dens.	0.51Ang From Cf1	5.35 eA-3
PLAT972_ALERT_2_A	Check	Calcd Resid. Dens.	1.15Ang From C28	-6.19 eA-3
PLAT973_ALERT_2_A	Check	Calcd Positive Resid. Density on	Cf1	4.10 eA-3
PLAT975_ALERT_2_A	Check	Calcd Resid. Dens.	0.98Ang From N11	2.47 eA-3

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#### Alert level B

PLAT220_ALERT_2_B	NonSolvent	Resd 1 C	Ueq(max)/Ueq(min) Range	7.9 Ratio
PLAT971_ALERT_2_B	Check	Calcd Resid. Dens.	0.72Ang From Cf1	3.25 eA-3
PLAT971_ALERT_2_B	Check	Calcd Resid. Dens.	0.63Ang From Cf1	3.23 eA-3
PLAT971_ALERT_2_B	Check	Calcd Resid. Dens.	1.38Ang From C27	2.56 eA-3
PLAT972_ALERT_2_B	Check	Calcd Resid. Dens.	1.15Ang From Na5	-3.38 eA-3

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#### Alert level C

PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N13 Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Na4 Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Na5 Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C19 Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C25 Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C27 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	.....		4.206 Check
PLAT924_ALERT_1_C	The Reported and Calculated Rho(min) Differ by	.		1.41 eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens.	0.98Ang From N11	2.47 eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens.	1.77Ang From N11	2.12 eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens.	0.98Ang From C28	1.82 eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens.	1.23Ang From C28	1.76 eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens.	0.62Ang From Na3	1.51 eA-3
PLAT971_ALERT_2_C	Check	Calcd Resid. Dens.	0.58Ang From Na3	1.51 eA-3

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#### Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		3 Info
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		6.75 Why ?
PLAT432_ALERT_2_G	Short Inter X...Y Contact	S5 ..S7	3.08 Ang.
		5/2-x,1/2+y,3/2-z =	2_756 Check
PLAT780_ALERT_1_G	Coordinates do not Form a Properly Connected Set		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		4 Note
	1 1 0, -1 0 1, 1 0 1, 0 1 1,		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	106 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		1 Note
	1 1 0,		
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	.....	4.2 Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	.....	2.290 Note
	Predicted wr2: Based on SigI**2	3.98 or SHELX Weight	8.22
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0 Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
28 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
2 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_cf_mnt_1_0m
;
PROBLEM: Check Calcd Resid. Dens. 0.53Ang From Cf1 5.52 eA-3
RESPONSE: ...
;
_vrf_PLAT972_cf_mnt_1_0m
;
PROBLEM: Check Calcd Resid. Dens. 1.15Ang From C28 -6.19 eA-3
RESPONSE: ...

```

```

;
_vrf_PLAT973_cf_mnt_1_0m
;
PROBLEM: Check Calcd Positive Resid. Density on          Cf1          4.10 eA-3
RESPONSE: ...
;
_vrf_PLAT975_cf_mnt_1_0m
;
PROBLEM: Check Calcd Resid. Dens.  0.98Ang From N11      .          2.47 eA-3
RESPONSE: ...
;
_vrf_PLAT220_cf_mnt_1_0m
;
PROBLEM: NonSolvent   Resd 1   C   Ueq(max)/Ueq(min) Range          7.9 Ratio
RESPONSE: ...
;
# end Validation Reply Form

```

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

Datablock cf\_mnt\_1\_0m - ellipsoid plot

